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The Free Energy of Dilute Bose Gases at Low Temperature

Eingereicht von
Florian Michael Haberberger
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1. Gutachter: Prof. Dr. Christian Hainzl
2. Gutachter: Prof. Dr. Benjamin Schlein
3. Gutachter: Prof. Søren Fournais

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Abstract (English)

We consider a system of N bosons confined to a box $\Omega \subset \mathbb{R}^3$ interacting via a pair potential V. Solving the interacting case analytically or numerically is infeasible due to the complexity of the Hamiltonian. However, in the dilute limit $\rho\mathfrak{a}^3 \to 0$, a formula for the ground state energy density in the thermodynamic limit $e(\rho)$ has recently been established. Here $\rho = N/|\Omega|$ denotes the particle density and $\mathfrak{a}$ the scattering length of the interaction potential V.

In this thesis, based on the papers [39, 40], we extend this result to positive temperatures up to the order $\rho\mathfrak{a}$, by showing the following formula for the free energy density

$$f(\rho, T) = e(\rho) + \frac{T^{5/2}}{(2\pi)^3} \int_{\mathbb{R}^3} \log\left(1 - e^{-\sqrt{p^4 + \frac{16\pi\rho\mathfrak{a}}{T} p^2}}\right) \mathrm{d}p + o_{\rho\mathfrak{a}^3 \to 0}\big((\rho\mathfrak{a})^{5/2}\big),$$

partially proving a conjecture by Lee, Huang and Yang from 1957. In particular we provide novel proofs for the zero temperature case.

Abstract (Deutsch)

Wir betrachten ein System von N Bosonen, die in einer Box $\Omega \subset \mathbb{R}^3$ gefangen sind und über ein Paarpotential V miteinander wechselwirken. Aufgrund der Komplexität des Hamiltonoperators ist es weder analytisch noch numerisch möglich, den wechselwirkenden Fall zu lösen. Allerdings wurde im verdünnten Grenzfall $\rho\mathfrak{a}^3 \to 0$ kürzlich eine Formel für die Grundzustandsenergiedichte im thermodynamischen Limes $e(\rho)$ hergeleitet. Dabei bezeichnet $\rho = N/|\Omega|$ die Teilchendichte und $\mathfrak{a}$ die Streulänge des Wechselwirkungspotentials V.

In dieser Dissertation erweitern wir dieses Ergebnis, basierend auf den Arbeiten [39, 40], auf positive Temperaturen bis zur Ordnung $\rho\mathfrak{a}$. Wir zeigen die folgende Formel für die freie Energiedichte:

$$f(\rho, T) = e(\rho) + \frac{T^{5/2}}{(2\pi)^3} \int_{\mathbb{R}^3} \log\left(1 - \mathrm{e}^{-\sqrt{p^4 + \frac{16\pi\rho\mathfrak{a}}{T} p^2}}\right) \mathrm{d}p + o_{\rho\mathfrak{a}^3 \to 0}\big((\rho\mathfrak{a})^{5/2}\big)$$

und beweisen dadurch eine Vermutung von Lee, Huang und Yang aus dem Jahr 1957 teilweise. Insbesondere liefern wir neue Beweise für den Fall verschwindender Temperatur.

Contents

1 Summary (English)

In quantum mechanics, a system at equilibrium is described by the stationary Schrödinger equation

$$H\Psi = E\Psi, \tag{1.1}$$

with a given self-adjoint Hamiltonian H acting on a separable Hilbert space and eigenfunctions Ψ with eigenvalues $E \in \mathbb{R}$. A complete characterization of the physical system is equivalent to a spectral resolution of the Hamiltonian.

In this thesis we consider a Hamiltonian of the form

$$H_N = \sum_{i=1}^{N} -\Delta_i + \sum_{1\leqslant i<j\leqslant N} V(x_i - x_j)$$

that describes a system of N particles. We may write $H_N = H_{\mathrm{free}} + H_{\mathrm{int}}$. Here, H_{free} denotes the free Hamiltonian, i.e., it models freely moving particles, while H_{int} represents the interaction part of the Hamiltonian and implements particle interactions via a two-body interaction potential V.

In the free case ($H_{\mathrm{int}} = 0$), the particles do not interact with one another, and instead of facing a complicated N-body problem, equation (1.1) decouples into independent one-body problems, which can be solved explicitly. For instance, it has been known since the groundbreaking works of Satyendra Bose and Albert Einstein [14, 30] that, for bosonic particles at sufficiently low temperatures, a macroscopic fraction of the particles occupies the same quantum state. This phenomenon is known as Bose–Einstein condensation (BEC); see Section 2.2 for the mathematical details and a rederivation of Einstein's original argument. Initially a purely theoretical statement and long believed to be of no physical relevance, Bose–Einstein condensation was experimentally observed in 1995 [27, 2], an achievement that led to the Nobel Prize in 2001 being awarded to Wolfgang Ketterle, Eric Cornell, and Carl Wieman. In these experiments, sodium atoms respectively rubidium-87 atoms were confined in traps and cooled via evaporative cooling to temperatures below 2×10^{-6} K and 1.7×10^{-7} K, respectively. These experiments illustrate that when referring to bosons one does not necessarily mean elementary particles such as photons, although a photon condensate has also been observed [47], but more generally composite bosons, such as particles, atoms, or molecules with integer spin.

In contrast, solving the interacting case explicitly is infeasible due to the complexity of the Hamiltonian. Likewise, numerical approaches quickly become inaccessible because of the curse of dimensionality. Even storing the data required to apply a finite difference method to the Schrödinger equation becomes unmanageable for realistic particle numbers. To illustrate this, consider a spatial grid with M points. The wave function Ψ then depends on $3N$ spatial variables, and each grid value requires 2×8 bytes of storage (8 bytes for double precision and a factor of 2 since Ψ is generally complex-valued). For example, taking $M = 1000$ grid points, corresponding to 10 grid points in each spatial direction, and $N = 8$ particles already requires 1.6×10^{25} bytes of memory. This is hopelessly intractable; for comparison, the total amount of data stored on the internet is estimated to be around 1.75×10^{23} bytes [82]. In the experiments of Ketterle, the condensate contained up to 5×10^5 bosons, highlighting the necessity of effective theoretical descriptions.

One possible strategy is to introduce effective models that are more suitable for numerical analysis while still providing accurate predictions. A prominent and widely used class of such models are density functional theories, where the many-body problem is reformulated in terms of the particle density; see [54] for a mathematical introduction. In a similar spirit, the Gross–Pitaevskii theory is commonly used to model dilute Bose gases.

The approach followed in this thesis is different. We aim to characterize the low-energy spectrum in the dilute regime of small densities ρ or weak interactions, by deriving asymptotic expansions in terms of the diluteness parameter $\rho\mathfrak{a}^3$. Here the scattering length $\mathfrak{a}$ of the potential V, quantifies the effective interaction of two particles, see Section 2.3 for the definition. In particular, we provide explicit formulas for the ground state energy E_0, i.e., the lowest eigenvalue of the Hamiltonian, as well as for the free energy of the system $F_\Omega(N)$. The free energy describes the energy of the system at a given temperature $T > 0$ and particle density $\rho > 0$ and is defined as a thermally weighted average over all admissible energy levels E_i, i.e., the eigenvalues of the Hamiltonian,

$$F_\Omega(N) = -k_B T \log \sum_i e^{-E_i/(k_B T)}. \tag{1.2}$$

Here $k_B = 1.380649 \times 10^{-23}\mathrm{JK}^{-1}$ denotes the Boltzmann constant,[1] which we will set equal to 1 in the following.

We are particularly interested in the free energy density in the thermodynamic limit, where the number of particles tends to infinity while the density is kept fixed. In this limit, microscopic fluctuations become negligible and the macroscopic thermodynamic properties of the system dominate. We denote the free energy density in the thermodynamic limit by $f(\rho, T)$. The main result of this thesis, which was achieved in collaboration with C. Hainzl, P. T. Nam, B. Schlein, R. Seiringer and A. Triay is the following expression for the free energy density in the thermodynamic limit. It is valid in the dilute limit $\rho\mathfrak{a}^3 \to 0$ and at temperatures T up to the order $\rho\mathfrak{a}$:

$$f(\rho,T) = 4\pi\mathfrak{a}\rho^2\left(1+\frac{128}{15\sqrt{\pi}}\sqrt{\rho\mathfrak{a}^3}\right) + \frac{T^{5/2}}{(2\pi)^3}\int_{\mathbb{R}^3}\log\left(1-e^{-\sqrt{p^4+\frac{16\pi\rho\mathfrak{a}}{T}p^2}}\right)\mathrm{d}p + o\big((\rho\mathfrak{a})^{5/2}\big)_{\rho\mathfrak{a}^3\to 0}. \tag{1.3}$$

Remarkably, this formula is universal in the sense that it does not depend on the detailed shape of the interaction potential V, but only on its scattering length $\mathfrak{a}$.

Summary (Deutsch)

In der Quantenmechanik wird ein System im Gleichgewichtszustand durch die stationäre Schrödinger-Gleichung beschrieben.

$$H\Psi = E\Psi. \tag{1.4}$$

Hierbei ist H ein gegebener selbstadjungierter Operator, der auf einem separablen Hilbertraum operiert; Ψ steht für eine Eigenfunktion mit Eigenwert $E \in \mathbb{R}$.

In dieser Thesis beschäftigen wir uns mit Hamiltonoperatoren der Form

$$H_N = \sum_{i=1}^{N} -\Delta_i + \sum_{1\leqslant i<j\leqslant N} V(x_i - x_j),$$

die ein System aus N Teilchen beschreiben. Wir schreiben $H_N = H_{\text{free}} + H_{\text{int}}$, wobei H_{free} für den freien Hamiltonoperator steht und die Teilchenbewegung ohne äußere Einflüsse beschreibt, während H_{int} den Wechselwirkungsteil des Hamiltonoperators repräsentiert. Dieser implementiert die Interaktionen im System über ein Zwei-Teilchen-Wechselwirkungspotential V.

[1]In 2018, the General Conference on Weights and Measures (CGPM) fixed the numerical value of the Boltzmann constant and defined the Kelvin accordingly.

Im freien Fall ($H_{\text{int}} = 0$) interagieren die Teilchen nicht miteinander, und das komplizierte N-Teilchen-Problem (1.4) entkoppelt in unabhängige Einteilchenprobleme. Dieses kann explizit gelöst werden. Zum Beispiel ist bekannt, dass Bosonen bei ausreichend niedrigen Temperaturen kondensieren, d.h., ein makroskopischer Teil der Teilchen besetzt denselben Quantenzustand. Dieses Phänomen ist als Bose–Einstein-Kondensation bekannt (BEC) und wurde in den bahnbrechenden Arbeiten von Satyendra Bose und Albert Einstein [14, 30] entdeckt. Wir zeigen die mathematischen Details sowie Einsteins ursprüngliches Argument in Section 2.2. Ursprünglich wurde dieses Ergebnis als theoretische Besonderheit ohne physikalischen Nutzen angesehen. Allerdings änderte sich diese Einschätzung im Laufe der Zeit, und Bose–Einstein-Kondensation wurde 1995 experimentell beobachtet [27, 2]. Dieses Resultat brachte Wolfgang Ketterle, Eric Cornell und Carl Wieman im Jahr 2001 den Nobelpreis ein. In den Experimenten wurden Natrium- beziehungsweise Rubidium-87-Atome in Fallen gefangen und mittels Verdunstungskühlung auf Temperaturen unter $2\times10^{-6}, \mathrm{K}$ beziehungsweise $1.7\times10^{-7}, \mathrm{K}$ gekühlt. Diese Experimente zeigen auch, dass wir nicht zwingend elementare Teilchen wie Photonen meinen, wenn wir über Bosonen sprechen, auch wenn mittlerweile Photonkondensate beobachtet wurden [47], sondern allgemeiner Kompositbosonen, wie zum Beispiel Teilchen, Atome oder Moleküle mit ganzzahligem Spin.

Im Gegensatz zum freien Fall ist es unmöglich, den wechselwirkenden Fall analytisch exakt zu lösen. Das liegt an der Komplexität des Hamiltonoperators. Numerische Lösungen scheitern am Fluch der Dimensionalität. Allein das Speichern der benötigten Datenmenge für eine Finite-Elemente-Methode für die Schrödinger-Gleichung ist für eine realistische Teilchenzahl nicht machbar. Wir verdeutlichen dies an einer groben Rechnung. Nehmen wir ein Gitter mit M Punkten an. Die Wellenfunktion Ψ hängt von $3N$ Veränderlichen ab, und jeder Gitterpunkt benötigt 2×8 Byte Speicher (8 Byte für eine Double-Precision-Zahl und ein Faktor 2, da Ψ im Allgemeinen komplexwertig ist). Seien beispielhaft in jeder Richtung 10 Gitterpunkte gegeben, dann ist $M = 1000$. Für $N = 8$ Teilchen bräuchten wir also bereits 1.6×10^{25} Byte Speicher. Das ist hoffnungslos. Zum Vergleich: Das gesamte Internet umfasst schätzungsweise 1.75×10^{23} Byte Daten [82]. Im Experiment von Ketterle befinden sich bis zu 5×10^5 Bosonen im Kondensat. Eine effektive theoretische Beschreibung ist daher unumgänglich.

Ein Ansatz besteht darin, effektive Modelle zu betrachten, die numerisch lösbar sind und dennoch gute Vorhersagen liefern. Eine bekannte und häufig verwendete Klasse solcher Modelle sind Dichtefunktionaltheorien. Hier wird das Vielteilchenproblem ausschließlich über die Teilchendichte beschrieben, siehe [54] für eine mathematische Einführung. Eine verwandte Theorie ist die Gross–Pitaevskii-Theorie, die oft zur Analyse verdünnter Bose-Gase verwendet wird.

Der Ansatz, den wir in dieser Thesis verfolgen, ist folgender: Wir wollen das Spektrum niedriger Energien im verdünnten Grenzfall beschreiben. Dies erreichen wir, indem wir die Eigenwerte asymptotisch im Verdünnungsparameter $\rho\mathfrak{a}^3$ entwickeln. Dabei ist ρ die Teilchendichte und $\mathfrak{a}$ die Streulänge des Potentials V, die die effektive Wechselwirkung zwischen zwei Teilchen beschreibt. Die Definition findet sich in Section 2.3. Insbesondere zeigen wir explizite Formeln für die Grundzustandsenergie E_0, d.h. den kleinsten Eigenwert des Hamiltonoperators, sowie für die freie Energie $F_\Omega(N)$ des Systems. Die freie Energie beschreibt die Energie des Systems bei Temperatur $T > 0$ und Teilchendichte $\rho > 0$. Sie ist definiert als thermisch gewichteter Mittelwert aller Energieniveaus E_i, also aller Eigenwerte des Hamiltonoperators,

$$F_\Omega(N) = -k_B T \log \sum_i e^{-E_i/(k_B T)}.$$

Hier ist $k_B = 1.380649 \times 10^{-23}\mathrm{JK}^{-1}$ die Boltzmann-Konstante,[2] die wir im Folgenden gleich 1

[2] Im Jahr 2018 wurde von der General Conference on Weights and Measures (CGPM) die Boltzmann-Konstante auf einen festen Wert festgelegt. Die Einheit Kelvin definiert sich seitdem über die Boltzmann-Konstante.

setzen.

Wir interessieren uns insbesondere für die freie Energiedichte im thermodynamischen Limes, in dem die Teilchenzahl gegen unendlich strebt, während die Dichte fixiert bleibt. In diesem Limes verschwinden mikroskopische Fluktuationen, und die makroskopischen thermodynamischen Eigenschaften dominieren das System. Wir bezeichnen die freie Energiedichte im thermodynamischen Limes mit $f(\rho, T)$. Das Hauptresultat dieser Thesis, das in Zusammenarbeit mit C. Hainzl, P. T. Nam, B. Schlein, R. Seiringer und A. Triay erzielt wurde, ist der folgende Ausdruck für die freie Energiedichte im thermodynamischen Limes. Er gilt im verdünnten Grenzfall $\rho\mathfrak{a}^3 \to 0$ und für Temperaturen T bis zur Ordnung $\rho\mathfrak{a}$:

$$f(\rho, T) = 4\pi\mathfrak{a}\rho^2 \left(1 + \frac{128}{15\sqrt{\pi}}\sqrt{\rho\mathfrak{a}^3}\right) + \frac{T^{5/2}}{(2\pi)^3}\int_{\mathbb{R}^3} \log\left(1 - e^{-\sqrt{p^4 + \frac{16\pi\rho\mathfrak{a}}{T}p^2}}\right) \mathrm{d}p + o\big((\rho\mathfrak{a})^{5/2}\big)_{\rho\mathfrak{a}^3 \to 0}.$$

Bemerkenswerterweise ist diese Formel universell gültig, in dem Sinne, dass sie nicht von der detaillierten Form des Wechselwirkungspotentials V abhängt, sondern nur von dessen Streulänge $\mathfrak{a}$.

2 Mathematical Framework

In this section we thoroughly introduce well known mathematical tools that underlie the proof of (1.3). This includes the formalism of second quantization, a characterization of Bose–Einstein condensation, and the scattering problem on $\mathbb{R}^3$. From now on we adopt the convention that Hamiltonians are self-adjoint and Hilbert spaces are separable.

2.1 Second Quantization

Although we work in the canonical setting, where the total particle number is fixed, it is necessary to allow for states with varying particle numbers. This situation arises, for instance, in the derivation of the lower bound, where the thermodynamic domain is partitioned into smaller boxes. To obtain a lower bound, one must optimize over all particle configurations in these subdomains, and consequently the particle number in each small box is not fixed. Moreover, we factor out the condensate in order to treat only the excited part of the Hamiltonian. Since the number of excited particles is itself not fixed, this again requires a formalism that allows for variable particle numbers. This subsection follows [81] and the lecture notes [89, 70].

Let $\mathfrak{h} = L^2(\Lambda)$ denote the one-particle Hilbert space, equipped with an inner product that is linear in its second argument, where $\Lambda \subset \mathbb{R}^3$ is a given domain. An extension of the following discussion to subspaces of $\Lambda \subset \mathbb{R}^3$ is straightforward, whereas a treatment of more general Hilbert spaces can be found in [89, Chapter 7]. For $n \in \mathbb{N}$, the bosonic n-particle Hilbert space is defined as the n-fold symmetric tensor product of $\mathfrak{h}$. By identifying $\mathfrak{h}^{\otimes n}$ with $L^2(\Lambda^n)$, this space can be characterized as

$$\mathfrak{h}^{\otimes_s n} := \big\{ \Psi^{(n)} \in L^2(\Lambda^n) \,\big|\, \Psi^{(n)}(\dots, x_i, \dots, x_j, \dots) = \Psi^{(n)}(\dots, x_j, \dots, x_i, \dots) \ \forall\, 1 \leqslant i, j \leqslant n \big\},$$

and we shall also write $L^2_s(\Lambda^n)$ for $\mathfrak{h}^{\otimes_s n}$.

Next, we introduce the bosonic creation and annihilation operators $a^*(f)$ and $a(f)$, which create, respectively annihilate, a particle with wave function $f \in \mathfrak{h}$. On the n-particle sector, these operators are defined by

$$\begin{aligned} &a^*(f)\colon \mathfrak{h}^{\otimes_s n} \to \mathfrak{h}^{\otimes_s n+1},\ \big(a^*(f)\Psi^{(n)}\big)(x_1, \dots, x_{n+1}) = \frac{1}{\sqrt{n+1}} \sum_{i=1}^{n+1} f(x_i) \Psi^{(n)}(x_1, \dots, \widehat{x_i}, \dots, x_{n+1}) \\ &a(f)\colon \mathfrak{h}^{\otimes_s n} \to \mathfrak{h}^{\otimes_s n-1},\ \big(a(f)\Psi^{(n)}\big)(x_1, \dots, x_{n-1}) = \sqrt{n} \int_\Lambda \overline{f}(x) \Psi^{(n)}(x_1, \dots, x_{n-1}, x) \mathrm{d}x. \end{aligned} \tag{2.1.1}$$

Here $\widehat{x_i}$ means that we omit this variable. Both definitions are valid for all $n \in \mathbb{N}_0$ by setting $\mathfrak{h}^{\otimes 0} := \mathbb{C}$ and $\mathfrak{h}^{\otimes(-1)} := \{0\}$, with the convention that the empty sums equals zero. Their fundamental property is the canonical commutation relation (CCR),

$$[a(f), a^*(g)] = \langle f, g \rangle_{\mathfrak{h}}, \qquad [a(f), a(g)] = [a^*(f), a^*(g)] = 0, \qquad f, g \in \mathfrak{h},$$

where $[A, B] := AB - BA$ denotes the commutator. Moreover, from the definitions one readily verifies that the map $f \mapsto a^*(f)$ is linear, that $f \mapsto a(f)$ is anti-linear. Additionally, $a(f), a^*(f)$ are bounded and $a^*(f)$ is the adjoint of $a(f)$. More precisely, for $\Psi^{(n)} \in \mathfrak{h}^{\otimes_s n}$ and $\Phi^{(n+1)} \in \mathfrak{h}^{\otimes_s (n+1)}$ one has

$$\begin{aligned} \|a(f)\|_{\mathfrak{h}^{\otimes_s n} \to \mathfrak{h}^{\otimes_s (n-1)}} &= \sqrt{n}\, \|f\|_{\mathfrak{h}}, \\ \|a^*(f)\|_{\mathfrak{h}^{\otimes_s n} \to \mathfrak{h}^{\otimes_s (n+1)}} &\leqslant \sqrt{n+1}\, \|f\|_{\mathfrak{h}}, \\ \langle a(f)\Phi^{(n+1)}, \Psi^{(n)} \rangle_{\mathfrak{h}^{\otimes_s n}} &= \langle \Phi^{(n+1)}, a^*(f)\Psi^{(n)} \rangle_{\mathfrak{h}^{\otimes_s (n+1)}}. \end{aligned} \tag{2.1.2}$$

As discussed in the beginning of this subsection, physically relevant states need not have a fixed particle number but may be superpositions of states with different particle numbers. This motivates the introduction of the bosonic Fock space

$$\mathcal{F} = \mathcal{F}(\mathfrak{h}) := \bigoplus_{n=0}^{\infty} \mathfrak{h}^{\otimes_s n}, \quad \Psi = (\Psi^{(0)}, \Psi^{(1)}, \dots) \in \mathcal{F} :\Leftrightarrow \sum_{n\geqslant 0} \|\Psi^{(n)}\|_{\mathfrak{h}^{\otimes_s n}} < \infty.$$

Equipped with the inner product

$$\langle \Phi, \Psi \rangle_{\mathcal{F}} := \sum_{n\geqslant 0} \langle \Phi^{(n)}, \Psi^{(n)} \rangle_{\mathfrak{h}^{\otimes_s n}} ,$$

$\mathcal{F}$ is a Hilbert space. The vector $\Omega := (1, 0, 0, \dots) \in \mathcal{F}$ is called the vacuum. Moreover, we introduce the number operator

$$\mathcal{N} := \bigoplus_{n\geqslant 0} n\, \mathbb{1}_{\mathfrak{h}^{\otimes_s n}}, \qquad D(\mathcal{N}) = \Big\{ \Psi \in \mathcal{F} : \sum_{n\geqslant 0} n^2 \, \|\Psi^{(n)}\|^2_{\mathfrak{h}^{\otimes_s n}} < \infty \Big\},$$

which measures the expected particle number. Using (2.1.2), one obtains for $\Psi \in D(\sqrt{\mathcal{N}})$ and $f \in \mathfrak{h}$ the bounds

$$\|a(f)\Psi\|_{\mathcal{F}} \leqslant \|f\|_{\mathfrak{h}} \, \|\sqrt{\mathcal{N}}\Psi\|_{\mathcal{F}}, \qquad \|a^*(f)\Psi\|_{\mathcal{F}} \leqslant \|f\|_{\mathfrak{h}} \, \|\sqrt{\mathcal{N}+1}\Psi\|_{\mathcal{F}}.$$

In particular this shows that the, on the Fock space generally unbounded, operators $a(f)$ and $a^*(f)$ are well defined on the dense subset $D(\sqrt{\mathcal{N}}) \subset \mathcal{F}$.

We now recall the second quantization of one- and two-body operators. Let $(u_p)_{p\in\mathbb{N}}$ be an orthonormal basis of $\mathfrak{h}$, which exists since $\mathfrak{h}$ is separable whenever Λ is measurable [61, Lemma 2.17], and define $a_p^* := a^*(u_p)$. Then the vectors

$$\prod_{p=1}^{\infty} (n_p!)^{-1/2} \, (a_p^*)^{n_p} \, \Omega, \tag{2.1.3}$$

with $n_p = 0$ for all but finitely many p, form an orthonormal basis of $\mathcal{F}$. Let h be a self-adjoint operator on $\mathfrak{h}$ and denote by h_i the operator acting as h on the i-th coordinate and as the identity on the remaining coordinates. Then, for an orthonormal basis $\{u_p\}_{p\in\mathbb{N}} \subset D(h)$,

$$\sum_{i=1}^{n} h_i = \sum_{p,q\geqslant 1} \langle u_p, h u_q \rangle \, a_p^* a_q \tag{2.1.4}$$

on $D(\sum_{i=1}^n h_i) \subset \mathfrak{h}^{\otimes_s n}$. This identity extends naturally to the Fock space, at least on the domain $\cup_{M=0}^{\infty} \bigoplus_{n=0}^{M} D(\sum_{i=1}^n h_i) \subset \mathcal{F}$, and we write

$$\mathrm{d}\Gamma(h) := \bigoplus_{n\geqslant 0} \sum_{i=1}^{n} h_i.$$

Analogously, we obtain the second quantization of a two-body operator. Let $W : \mathfrak{h}^{\otimes 2} \to \mathfrak{h}^{\otimes 2}$ be self-adjoint and symmetric under particle exchange, i.e., $W_{ij} = W_{ji}$, where W_{ij} denotes the operator acting as W on the i-th and j-th coordinates. For an orthonormal basis $\{u_p\}_{p\in\mathbb{N}}$ with $u_p \otimes u_q \in D(W)$ we find

$$\bigoplus_{n=0}^{\infty} \sum_{1\leqslant i<j\leqslant n} W_{ij} = \sum_{k,m,p,q\geqslant 1} \langle u_k \otimes u_m, W u_p \otimes u_q \rangle \, a_k^* a_m^* a_p a_q \tag{2.1.5}$$

on $\cup_{M=0}^{\infty}\bigoplus_{n=0}^{M} D(\sum_{1\leqslant i<j\leqslant n} W_{ij}) \subset \mathcal{F}$. Observe that these identities also hold in a form sense on appropriate quadratic form domains.

Equivalently to the momentum-space representation, one may formally introduce the creation and annihilation operators in position-space.

$$a_x = \sum_{p\in\mathbb{N}} u_p(x) a_p, \qquad a_x^* = \sum_{p\in\mathbb{N}} \overline{u_p(x)} a_p^*,$$

for a basis $\{u_p\}_{p\in\mathbb{N}}$ of $\mathfrak{h}$. They formally satisfy the CCR

$$[a_x, a_y^*] = \sum_{p,q\in\mathbb{N}} u_p(x)\overline{u_q(y)}[a_p, a_q^*] = \sum_{p\in\mathbb{N}} u_p(x)\overline{u_p(y)} = \delta(x-y).$$

These expressions can be made rigorous in the sense of quadratic forms; see [81, Theorem X.44], which suffices for the purposes of this thesis.

Finally, we recall the notion of one-particle density matrices. A density matrix on a Hilbert space is a positive, self-adjoint, trace-class operator with unit trace. For a density matrix Γ on $\mathcal{F}$ satisfying $\operatorname{Tr}(\mathcal{N}\Gamma) < \infty$, the associated one-particle density matrix $\gamma_\Gamma : \mathfrak{h} \to \mathfrak{h}$ is defined by

$$\operatorname{Tr}\left(a^*(f)a(g)\Gamma\right) = \langle g, \gamma_\Gamma f\rangle_{\mathfrak{h}}, \qquad \forall f, g \in \mathfrak{h}. \tag{2.1.6}$$

The operator γ_Γ is positive but in general not normalized since $\operatorname{Tr}(\gamma_\Gamma) = \operatorname{Tr}(\mathcal{N}\Gamma)$. For a normalized function $\Psi \in D(\mathcal{N}) \subset \mathcal{F}$, we set $\gamma_\Psi := \gamma_{|\Psi\rangle\langle\Psi|}$. In the special case where $\Psi = \Psi^{(n)} \in \mathfrak{h}^{\otimes_s n}$ has a fixed particle number, $\gamma_{\Psi^{(n)}}$ is given by the integral kernel

$$\gamma_{\Psi^{(n)}}(x,y) = n\int_{\Lambda^{n-1}} \Psi^{(n)}(x, x_2, \ldots, x_n)\,\overline{\Psi^{(n)}(y, x_2, \ldots, x_n)}\,\mathrm{d}x_2 \ldots \mathrm{d}x_n,$$

which follows directly from the definitions (2.1.1). In particular $\operatorname{Tr}\gamma_{\Psi^{(n)}} = n$.

A particularly important class of density matrices are Gibbs states. Let H be a Hamiltonian with finite partition function $Z = \operatorname{Tr}(e^{-H/T}) < \infty$. For temperatures $T > 0$, the associated Gibbs state is given by

$$\Gamma = Z^{-1} e^{-H/T},$$

while in the zero-temperature case it is the orthogonal projection onto the ground state of H. The significance of Gibbs states is, for example, reflected in their direct connection to the free energy; see (1.2).

2.2 Bose–Einstein Condensation

This subsection covers the mathematical characterization of Bose–Einstein condensation (BEC), subsequently also simply denoted condensation. We formulate the notion of condensation on a fixed Hilbert space while allowing the Hamiltonian to vary with the system size. This framework naturally accommodates situations in which the physical volume grows, such as in the thermodynamic limit, by a unitary rescaling of the underlying domain. Equivalently, one could allow the definition to depend explicitly on the Hilbert space; both viewpoints are mathematically equivalent.

Definition 2.1 (BEC). Let $\{\Gamma_n\}_{n\in\mathbb{N}}$ be a sequence of density matrices on $\mathcal{F}(\mathfrak{h})$ with $\operatorname{Tr}(\mathcal{N}\Gamma_n) = n$. We say that the sequence $\{\Gamma_n\}_{n\in\mathbb{N}}$ exhibits *condensation* if their one-particle density matrices γ_n have an eigenvalue of order n, that is, if the largest eigenvalue $\lambda_1^{(n)}$ of γ_n satisfies

$$\liminf_{n\to\infty} \frac{\lambda_1^{(n)}}{n} \geqslant c$$

for some constant $c > 0$. If the limit exists, rather than only the limes inferior, it is called the *condensate fraction*. If the condensate fraction equals 1, we say that $\{\Gamma_n\}_{n\in\mathbb{N}}$ exhibits *complete condensation*.

If there exist normalized eigenfunctions $\phi_1^{(n)}$ corresponding to $\lambda_1^{(n)}$ and a vector $u_0 \in \mathfrak{h}$ such that $\phi_1^{(n)} \to u_0$ as $n \to \infty$, then u_0 is called a *condensate wave function*, and we say that $\{\Gamma_n\}_{n\in\mathbb{N}}$ exhibits condensation in u_0.

Finally, a system described by a sequence of Hamiltonians H_n on $\mathcal{F}(\mathfrak{h})$ is said to exhibit (complete) condensation at temperature $T \geqslant 0$ if the corresponding sequence of Gibbs states exhibits (complete) condensation.

Remark. If a condensate wave function u_0 exists and the eigenspaces corresponding to the largest eigenvalue of γ_n are non-degenerate, then u_0 is unique up to a global phase. Indeed, suppose that there exists another vector $v_0 \in \mathfrak{h}$ and a sequence of eigenfunctions $\psi_1^{(n)}$ of γ_n, also corresponding to $\lambda_1^{(n)}$, such that $\psi_1^{(n)} \to v_0$. By non-degeneracy, there exist $\alpha_n \in [0, 2\pi)$ such that $\psi_1^{(n)} = e^{i\alpha_n}\phi_1^{(n)}$. It follows that

$$|\langle u_0, v_0\rangle| = \lim_{n\to\infty} |\langle u_0, e^{i\alpha_n}\phi_1^{(n)}\rangle| = \lim_{n\to\infty} |\langle u_0, \phi_1^{(n)}\rangle| = 1,$$

and hence u_0 and v_0 coincide up to a phase by the equality case in the Cauchy–Schwarz inequality.

If the expected condensate wave function of a system is known from the setting, one can often give a more direct characterization of complete condensation, as will be done in the following lemma. However, one has to be careful in general. For example, consider $\Gamma_n = |\phi^{\otimes n}\rangle\langle\phi^{\otimes n}|$ with $\phi = \frac{1}{\sqrt{2}}(u_0 + u_1)$, where $u_0, u_1 \in \mathfrak{h}$ are normalized and orthogonal. A direct computation yields

$$\lim_{n\to\infty} \frac{1}{n} \operatorname{Tr}(a^*(u_0)a(u_0)\Gamma_n) = \frac{1}{2},$$

from which one correctly concludes that the sequence exhibits condensation. Nevertheless, it would be wrong to infer the absence of complete condensation. The mistake was the wrong choice of the condensate wave function.

In our applications, the condensate wave function is given by the lowest eigenfunction of the free one-particle Laplacian with periodic or Neumann boundary conditions; in particular, u_0 is constant. Moreover, in some setting, we establish complete condensation. Thus, the pathological example of the type described above is of no relevance to us.

Lemma 2.2 (Characterization of complete BEC)**.** *Let $\{\Gamma_n\}_{n\in\mathbb{N}}$ be a sequence of density matrices on $\mathcal{F}(\mathfrak{h})$ with $\operatorname{Tr}(\mathcal{N}\Gamma_n) = n$. Denote by γ_n the one-particle density matrix of Γ_n and by $\lambda_1^{(n)}$ the largest eigenvalue of γ_n. Let $u_0 \in \mathfrak{h}$ be normalized. Then the following statements are equivalent:*

(i) *$\{\Gamma_n\}_{n\in\mathbb{N}}$ exhibits complete condensation in u_0.*

(ii) $\displaystyle\lim_{n\to\infty} \frac{1}{n} \operatorname{Tr}(a^*(u_0)a(u_0)\Gamma_n) = 1.$

(iii) $\displaystyle\lim_{n\to\infty} \langle u_0, n^{-1}\gamma_n u_0\rangle = 1.$

(iv) *$n^{-1}\gamma_n \to |u_0\rangle\langle u_0|$ strongly in operator norm as $n \to \infty$.*

(v) *$n^{-1}\gamma_n \to |u_0\rangle\langle u_0|$ strongly in trace norm as $n \to \infty$.*

Remark. A corresponding characterization for partial condensation is subtle, as already illustrated by the example discussed in the previous remark.

Historically, the initial notion of BEC was closer to condition (ii), for instance,

$$\liminf_{n\to\infty} \frac{1}{n} \mathrm{Tr}\, (a^*(u_0)a(u_0)\Gamma_n) \geqslant c, \tag{2.2.1}$$

which is particularly natural when the condensate wave function is an eigenstate of the one-body Hamiltonian. In this case, the physical interpretation is immediate: a macroscopic number of particles occupies the lowest-energy mode. By the min-max principle, (2.2.1) readily implies condensation in the sense of Definition 2.1.

For interacting systems, however, this picture is less clear. Definition 2.1 goes back to work of Penrose and Onsager [80] and is now standard in the mathematical physics literature.

If the condensate wave function is close to the constant function, as expected in the regime of very weak interactions or in the ultradilute limit at least for periodic boundary conditions, then Definition 2.1 is equivalent to the condition

$$\frac{1}{n} \int_{\Lambda\times\Lambda} \gamma_n(x,y)\, \mathrm{d}x\, \mathrm{d}y \geqslant c.$$

We finally note that several alternative notions of BEC appear in the literature:

- *Off-diagonal long-range order* (ODLRO), characterized by the absence of decay of the one-particle density matrix $\gamma_n(x,y)$ as $|x-y| \to \infty$. This criterion was introduced by Penrose in his study of the λ-phase transition in liquid helium [79].
- The occurrence of *long permutation cycles* in the Feynman–Kac representation, proposed by Feynman [32] also in the context of liquid helium.
- *Spontaneous symmetry breaking*, where one analyses the response of the system to a perturbation that does not conserve particle number. For a Hamiltonian that commutes with the particle number operator it holds that $\langle a(f)\rangle_G = 0$, where $\langle\cdot\rangle_G$ denotes the expectation value in the Gibbs state. If we perturb the Hamiltonian by $\eta(a^*(f) + a(f))$, we still have $\lim_{\eta\to 0} \langle a(f)\rangle_{G_\eta} = 0$. BEC is then defined as the non-commutativity of the limits $\eta \to 0$ and $N, L \to \infty$, i.e.,
$$\lim_{\eta\to 0} \lim_{N,L\to\infty} \langle a(f)\rangle_{G-\eta} \neq 0.$$

Proof of Lemma 2.2. (ii) and (iii) are equivalent by the definition of the one-particle density matrix, cf. (2.1.6). Furthermore, (v)⇒(iv)⇒(iii) are immediate.

To show (iii)⇒(i), we use the spectral decomposition

$$\gamma_n = \sum_{i\geqslant 1} \lambda_i^{(n)} \,|\phi_i^{(n)}\rangle\,\langle\phi_i^{(n)}|\,, \qquad \lambda_1^{(n)} \geqslant \lambda_2^{(n)} \geqslant \cdots \geqslant 0, \qquad \sum_{i\geqslant 1} \lambda_i^{(n)} = n,$$

with $\{\phi_i^{(n)}\}_{i\geqslant 1}$ an orthonormal system in $\mathfrak{h}$. Assumption (iii) and the min–max principle imply $n^{-1}\lambda_1^{(n)} \to 1$, and hence $n^{-1}\sum_{i\geqslant 2} \lambda_i^{(n)} \to 0$. Since

$$1 \leftarrow \langle u_0,\, n^{-1}\gamma_n u_0\rangle = n^{-1}\lambda_1^{(n)} |\,\langle u_0, \phi_1^{(n)}\rangle\,|^2 + n^{-1} \sum_{i\geqslant 2} \lambda_i^{(n)} |\,\langle u_0, \phi_i^{(n)}\rangle\,|^2,$$

it follows that $|\,\langle u_0, \phi_1^{(n)}\rangle\,| \to 1$. After fixing phases, we obtain a sequence of eigenfunctions converging to u_0, which proves (i).

Finally, (i)⇒(v) follows by writing γ_n in its spectral decomposition and applying the triangle inequality:

$$\left\| n^{-1}\gamma_n - |u_0\rangle\langle u_0| \right\|_1 \leqslant \left|1 - n^{-1}\lambda_1^{(n)}\right| + \left\| |\phi_1^{(n)}\rangle\langle\phi_1^{(n)}| - |u_0\rangle\langle u_0| \right\|_1 + n^{-1}\sum_{i\geqslant 2}\lambda_i^{(n)}.$$

All terms on the right-hand side vanish as $n\to\infty$, using the identity

$$\left\| |\phi_1^{(n)}\rangle\langle\phi_1^{(n)}| - |u_0\rangle\langle u_0| \right\|_1 = 2\sqrt{1 - |\langle u_0, \phi_1^{(n)}\rangle|^2}$$

and the assumption. This establishes (v) and completes the proof. □

2.3 The Scattering Problem

In this subsection, following standard ideas from [58], we define the scattering length of a positive, radial, and compactly supported interaction potential $V : \mathbb{R}^3 \to \mathbb{R}$. These assumptions are satisfied by all potentials considered in this thesis. We briefly remark that the definition extends to more general settings: for sufficiently fast decaying potentials one may define the scattering length as the limit of the scattering length of the truncated potential, while for potentials with a negative part the definition remains meaningful given that no two-body bound states occur; see [58, eq. (C.13)] and [66, Appendix A] for the details.

To motivate the definition, consider the two-body Hamiltonian

$$H_2 = -\Delta_x - \Delta_y + V(x-y)$$

acting on the torus $\Lambda_L\times\Lambda_L$ with $\Lambda_L = [-L/2, L/2]^3$. In the dilute regime, particle collisions are rare and the leading contribution to the ground state energy of an N-body Bose gas is governed by two-body interactions. Heuristically, this suggests[3]

$$\inf\sigma(H_N) \approx \frac{N(N-1)}{2}\inf\sigma(H_2).$$

One readily shows that the ground state wave function of H_2 has to be translation invariant, i.e., it is of the form $\phi(x,y) = L^{-3/2}\Psi(x-y)$ for $\Psi\in L^2(\Lambda_L)$ with $\|\Psi\|_2 = 1$. Then we compute

$$\langle\phi, H_2\phi\rangle = 2\int_{\Lambda_L}|\nabla_r\Psi(r)|^2 + \int_{\Lambda_L}V(r)|\Psi(r)|^2.$$

Ψ is expected to be small in regions where V is large and, since it is normalized, essentially constant outside the support of V, as illustrated in Figure 1. Since V has compact support, taking the limit $L\to\infty$ suggests that the ground state wave function behaves asymptotically like $L^{-3/2}$ at large distances.

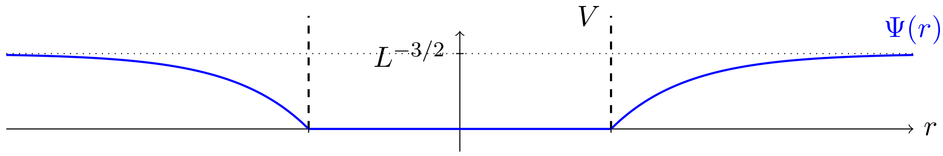

Figure 1: Scat length

[3] This picture is not true in two dimensions since particles see each other over longer distances.

Replacing the normalization condition by the asymptotic behavior allows one to formulate the problem directly on $\mathbb{R}^3$. After rescaling, it is natural to look for a minimizer of the functional

$$\int_{\mathbb{R}^3} |\nabla\Psi|^2 + \frac{1}{2}V|\Psi|^2$$

with $\Psi(x) \to 1$ as $|x| \to \infty$. Writing $\varphi = 1 - \Psi$, this leads to the class

$$D^1(\mathbb{R}^3) := \Big\{\varphi \in L^1_{\mathrm{loc}}(\mathbb{R}^3) \,\Big|\, \int_{\mathbb{R}^3} |\nabla\varphi|^2 < \infty,\ \lim_{|x|\to\infty} \varphi(x) = 0\Big\}, \tag{2.3.1}$$

where the limit at infinity is understood in the sense that

$$\begin{aligned}\lim_{|x|\to\infty} \varphi(x) = 0 &\iff |\{|\varphi| > b\}| < \infty \quad \forall b > 0\\ &\iff \lim_{R\to\infty} |B_R^c \cap \{|\varphi| > b\}| = 0\ \forall b > 0.\end{aligned}$$

The scattering length is defined as the minimum of this variational problem, up to the normalization factor 4π. One can rigorously show that

$$\inf \sigma(H_2) = 8\pi\mathfrak{a}\, L^{-3}\big(1 + o(1)_{L\to\infty}\big),$$

which in turn yields the heuristic relation

$$\lim_{L\to\infty} L^{-3} \inf \sigma(H_N) \approx 4\pi\mathfrak{a}\rho^2, \qquad \rho = \frac{N}{L^3},$$

corresponding to the leading-order term in (1.3). Moreover, taking V to be the hard-core potential of radius R, one finds $\mathfrak{a} = R$, which motivates the interpretation of $\mathfrak{a}$ as an effective interaction range.

Lemma 2.3. *Let $V : \mathbb{R}^3 \to \mathbb{R}$ be positive, radial, and compactly supported with $R > 0$ such that* $\mathrm{supp}(V) \subset B_R(0)$. *The scattering length $\mathfrak{a}$ of V is defined by*

$$4\pi\mathfrak{a} := \inf\left\{\int_{\mathbb{R}^3} |\nabla\varphi|^2 + \frac{1}{2}V|1 - \varphi|^2 :\ \varphi \in D^1(\mathbb{R}^3)\right\}. \tag{2.3.2}$$

This variational problem admits a unique minimizer ω. The function ω is radial, satisfies $0 \leqslant \omega \leqslant 1$, and solves the scattering equation

$$-\Delta\omega = \frac{1}{2}V(1 - \omega) \tag{2.3.3}$$

in the distributional sense, that is,

$$\langle\nabla\varphi, \nabla\omega\rangle = \frac{1}{2}\,\langle\varphi, V(1 - \omega)\rangle \qquad \forall\varphi \in D^1(\mathbb{R}^3).$$

Moreover,

$$\omega(x) = \frac{\mathfrak{a}}{|x|}, \quad |x| > R,$$

and we have the identity

$$\int_{\mathbb{R}^3} V(x)\big(1 - \omega(x)\big)\,\mathrm{d}x = 8\pi\mathfrak{a}. \tag{2.3.4}$$

Proof. We first give an equivalent characterization of the space $D^1(\mathbb{R}^3)$,

$$D^1(\mathbb{R}^3) = \{\varphi \in L^6(\mathbb{R}^3) \,\big|\, \int_{\mathbb{R}^3} |\nabla\varphi|^2 < \infty\}. \tag{2.3.5}$$

The inclusion "$\subset$" follows from the Sobolev inequality $\|\varphi\|_6 \le C\|\nabla\varphi\|_2$ [61, Thm. 8.3]. Here constant functions are excluded by the condition that φ vanishes at infinity. In fact, D^1 is introduced in [61] precisely so that this inequality holds. Conversely, if $\varphi \in L^6(\mathbb{R}^3)$, then for any $b > 0$,

$$|\{|\varphi| > b\}| = \int_{\{|\varphi|>b\}} 1 \leqslant b^{-6} \int |\varphi|^6 < \infty,$$

which implies $\varphi(x) \to 0$ at infinity in the sense of (2.3.1). This shows (2.3.5).

We define the energy functional

$$\mathcal{E}(\varphi) := \int_{\mathbb{R}^3} |\nabla\varphi|^2 + \frac{1}{2}\int_{\mathbb{R}^3} V\,|1-\varphi|^2,$$

and prove existence and uniqueness of a minimizer by the direct method.

Let $\{\varphi_n\}_{n\in\mathbb{N}} \subset D^1(\mathbb{R}^3)$ be a minimizing sequence. Then $\|\nabla\varphi_n\|_2$ is uniformly bounded, and by the Sobolev inequality also $\|\varphi_n\|_6$ is uniformly bounded. By the Banach–Alaoglu theorem, there exists a subsequence, again denoted φ_n, and a function ω such that

$$\varphi_n \rightharpoonup \omega \quad \text{in } L^6(\mathbb{R}^3), \qquad \nabla\varphi_n \rightharpoonup \nabla\omega \quad \text{in } L^2(\mathbb{R}^3).$$

Here, the weak limit of the gradients can be identified with $\nabla\omega$ since for any $\phi \in C_c^\infty(\mathbb{R}^3)$ and $i = 1, 2, 3$,

$$\langle\omega, \partial_i\phi\rangle = \lim_{n\to\infty}\langle\varphi_n, \partial_i\phi\rangle = -\lim_{n\to\infty}\langle\partial_i\varphi_n, \phi\rangle = -\langle(\nabla\omega)_i, \phi\rangle.$$

In particular $\omega \in D^1(\mathbb{R}^3)$. Moreover, up to a subsequence, $\varphi_n \to \omega$ pointwise almost everywhere, see [61, Cor 8.7]. Since $V \ge 0$ and is compactly supported, Fatou's lemma yields

$$\int_{\mathbb{R}^3} V\,|1-\omega|^2 \le \liminf_{n\to\infty}\int_{\mathbb{R}^3} V\,|1-\varphi_n|^2,$$

and weak lower semicontinuity of the L^2-norm gives

$$\int_{\mathbb{R}^3} |\nabla\omega|^2 \le \liminf_{n\to\infty}\int_{\mathbb{R}^3} |\nabla\varphi_n|^2.$$

Combining these inequalities shows that ω is a minimizer,

$$\mathcal{E}(\omega) \le \liminf_{n\to\infty}\mathcal{E}(\varphi_n) = 4\pi\mathfrak{a}.$$

Uniqueness follows from strict convexity of $\mathcal{E}$. Indeed, for $\varphi, \psi \in D^1(\mathbb{R}^3)$ and $\lambda \in (0,1)$,

$$\mathcal{E}(\lambda\varphi + (1-\lambda)\psi) = \lambda\mathcal{E}(\varphi) + (1-\lambda)\mathcal{E}(\psi) - \lambda(1-\lambda)\left(\|\nabla(\varphi-\psi)\|_2^2 + \frac{1}{2}\langle\varphi-\psi, V(\varphi-\psi)\rangle\right).$$

and the last term vanishes if and only if $\varphi = \psi$ almost everywhere by the definiteness of the L^6 norm.

Next, we show the qualitative properties of ω. Radial symmetry follows since V is radial so that the functional is rotationally invariant: for any $R \in SO(3)$, $\varphi \circ R$ is a minimizer whenever φ is. By uniqueness, ω must therefore be radial. Using the diamagnetic inequality

$$|\nabla|\varphi||^2 \le |\nabla\varphi|^2 \quad \text{a.e.},$$

and convexity of the functional, we see that $|\omega|$ and $\min\{1,\omega\} = \frac{1+\omega-|1-\omega|}{2}$ are also minimizers. By uniqueness we find $0 \le \omega \le 1$.

The scattering equation (2.3.3) is obtained by considering $\varepsilon \mapsto \mathcal{E}(\omega + \varepsilon\varphi)$ for $\varphi \in D^1(\mathbb{R}^3)$. Since ω is a minimizer, the derivative at $\varepsilon = 0$ vanishes, yielding

$$\langle \nabla\varphi, \nabla\omega\rangle - \frac{1}{2}\langle \varphi, V(1-\omega)\rangle + \text{h.c.} = 0.$$

Taking $i\varphi$ instead of φ gives (2.3.3).

Testing (2.3.3) with $\varphi = \omega$ yields

$$\int_{\mathbb{R}^3} |\nabla\omega|^2 = \frac{1}{2}\int_{\mathbb{R}^3} V\,\omega(1-\omega),$$

and hence

$$\mathcal{E}(\omega) = \frac{1}{2}\int_{\mathbb{R}^3} V(x)\big(1-\omega(x)\big)\,\mathrm{d}x,$$

which implies (2.3.4).

Finally, since V is supported in $B_R(0)$, the equation $-\Delta\omega = 0$ holds on $\{|x| > R\}$. By Weyl's lemma [61, Thm. 9.3], ω is smooth there. Radiality and the condition $\omega \in D^1(\mathbb{R}^3)$ imply that

$$\omega(x) = \frac{c}{|x|}, \quad |x| > R,$$

with some $c \ge 0$. To identify c, take $\varphi \in C_c^\infty(\mathbb{R}^3)$ with $\varphi \equiv 1$ on $B_R(0)$. Then

$$4\pi\mathfrak{a} = \langle \nabla\varphi, \nabla\omega\rangle = \int_{|x|>R} \overline{\nabla\varphi}\cdot\nabla\omega = \int_{|x|>R} \overline{\varphi}(-\Delta\omega) + \int_{|x|=R} \overline{\varphi}\nabla\omega\cdot\frac{-\vec{x}}{|x|}\mathrm{d}S = 0 + 4\pi c,$$

and hence $c = \mathfrak{a}$, completing the proof. □

We conclude this section by briefly discussing the Born approximation oft the scattering length $\mathfrak{a}$. This is a formal perturbative expansion that is valid for weak potentials; in general, there is no guarantee that the resulting series converges, and the derivation presented here is not rigorous.

Starting from the scattering equation (2.3.3), we introduce a coupling parameter $\lambda > 0$ and regard $V = \lambda W$ as a small perturbation. The scattering equation then becomes

$$-\Delta\omega = \frac{1}{2}\lambda W(1-\omega).$$

We look for a power series solution of the form

$$\omega = \sum_{n=0}^{\infty} \lambda^n\,\omega_n.$$

Inserting this ansatz into the equation and matching powers of λ yields

$$\omega_0 = 0, \qquad \lambda^n\omega_n = (-1)^{n-1}\left(\frac{1}{2(-\Delta)}V\right)^n, \quad n \ge 1.$$

Here we used the boundary condition $\omega(x) \to 0$ as $|x| \to \infty$, which implies $\omega_0 = 0$ and formally inverted $-\Delta$.

Using the identity (2.3.4), we obtain the Born series for the scattering length,

$$8\pi\mathfrak{a} = \int_{\mathbb{R}^3} V(1-\omega) = \int_{\mathbb{R}^3} V - \sum_{n=1}^{\infty} \lambda^n \int_{\mathbb{R}^3} V\omega_n = \int_{\mathbb{R}^3} V + \sum_{n=1}^{\infty} (-1)^n \left\langle V, \left(\frac{1}{2(-\Delta)}V\right)^n \right\rangle. \quad (2.3.6)$$

Writing $\mathfrak{a} = \sum_{n=0}^{\infty} \mathfrak{a}_n$, the first two terms of the expansion are

$$8\pi\mathfrak{a}_0 = \int_{\mathbb{R}^3} V = \widehat{V}(0), \qquad 8\pi\mathfrak{a}_1 = -\left\langle V, \frac{1}{2(-\Delta)}V \right\rangle = -\frac{1}{(2\pi)^3}\left\langle \widehat{V}, \frac{\widehat{V}}{2p^2} \right\rangle.$$

3 Model and Main Result

As presented in Section 1, our goal is to model a Bose gas with two-body interactions in the thermodynamic limit. Accordingly, we consider the usual Hamiltonian for N particles confined to a cubic box $\Omega \subset \mathbb{R}^3$, centered at the origin and equipped with periodic, Dirichlet, or Neumann boundary conditions,

$$H_N = -\sum_{i=1}^{N} \Delta_i + \sum_{1 \leqslant i < j \leqslant N} V(x_i - x_j). \quad (3.1)$$

Here, the kinetic energy term is written in units where the prefactor $\hbar^2/2m$ is set equal to 1.

We initially define H_N on a core domain $C_c^{\infty}(\mathbb{R}^{3N}) \cap L_s^2(\Omega^N)$ and extend it to a self-adjoint operator via the Friedrichs extension. This is justified under the assumption that H_N is bounded from below, which follows immediately from $V \geqslant 0$. The non-negativity of the potential further yields that H_N has compact resolvent and that the associated Gibbs state is well defined; see [81, Chapter XIII].

We define the ground state energy by

$$E_\Omega(N) := \inf \sigma(H_N).$$

For temperatures $T \geqslant 0$, we define the canonical free energy as the variational problem

$$F_\Omega(N) := \inf\left\{ \operatorname{Tr}(H_N\Gamma) - TS(\Gamma) \,\middle|\, 0 \leqslant \Gamma,\ \operatorname{Tr}\Gamma = 1 \right\}, \quad (3.2)$$

where the entropy functional is given by $S(\Gamma) := -\operatorname{Tr}(\Gamma \log \Gamma)$. For convenience, the dependence of $F_\Omega(N)$ on the temperature T is omitted. Note that at zero-temperature the free energy reduces to the ground state energy. Moreover, as the following Lemma shows, the free energy functional admits the Gibbs state as an an explicit minimizer.

Lemma 3.1. *For $T > 0$, the variational problem* (3.2) *admits the Gibbs state*

$$\Gamma_T = Z^{-1} e^{-H_N/T}$$

as its unique minimizer, where

$$Z = \operatorname{Tr}\left(e^{-H_N/T}\right)$$

is the partition function. In particular,

$$F_\Omega(N) = -T \log Z.$$

Proof. Recall $S(x) = -x\log x$ so that $S''(x) = -1/x \leqslant -1$ for $x \in [0,1]$. Hence, for any $x, x_0 \in [0,1]$ there exists ξ between x and x_0 such that

$$S(x) - S(x_0) - S'(x_0)(x - x_0) = \frac{1}{2}S''(\xi)(x-x_0)^2 \leqslant -\frac{1}{2}(x-x_0)^2.$$

Let A and B be self-adjoint trace-class operators with $\mathrm{Tr}\, A = \mathrm{Tr}\, B = 1$. Applying the above inequality to the spectral decompositions of A and B yields

$$\frac{1}{2}\mathrm{Tr}\,|A-B|^2 \leqslant -S(A) + S(B) + \mathrm{Tr}\big((-1-\log B)(A-B)\big) = -S(A) - \mathrm{Tr}\,(A\log B).$$

(This inequality is a special case of Klein's inequality.)

Let now Γ be an arbitrary density matrix with $\mathrm{Tr}\,\Gamma = 1$. We compute

$$\begin{aligned}\mathrm{Tr}\,(H_N\Gamma) - TS(\Gamma) &= -T\log Z + T\big(-S(\Gamma) - \mathrm{Tr}\,(\Gamma\log(Z^{-1}e^{-H_N/T}))\big)\\ &\geqslant -T\log Z + \frac{T}{2}\mathrm{Tr}\left|\Gamma - Z^{-1}e^{-H_N/T}\right|^2.\end{aligned}$$

The last term in the previous line is non-negative if and only if $\Gamma = Z^{-1}e^{-H_N/T}$. This concludes the proof. $\square$

Next, we introduce the relevant thermodynamic quantities; the ground state energy density and the free energy density,

$$e(\rho) := \lim_{\substack{N,|\Omega|\to\infty\\ N/|\Omega|\to\rho}} \frac{E_\Omega(N)}{|\Omega|}, \qquad f(\rho,T) := \lim_{\substack{N,|\Omega|\to\infty\\ N/|\Omega|\to\rho}} \frac{F_\Omega(N)}{|\Omega|}. \tag{3.3}$$

Remark. It is well known that the free energy density $f(\rho,T)$ is well defined and independent of the choice of boundary conditions imposed on Ω; see [83, Section 2.3].

The following two theorems are the main results from [39, 40], which, if combined yield the statement (1.3) from the introduction.

Theorem 3.2 ([39], Lower bound)**.** *Let $V \in L^1(\mathbb{R}^3)$ be non-negative, spherically symmetric, compactly supported and radially decreasing. Let $\nu = 1/5000$ and $0 \le T \le \rho\mathfrak{a}(\rho\mathfrak{a}^3)^{-\nu}$. Then, in the dilute limit $\rho\mathfrak{a}^3 \to 0$, there exists $C > 0$ such that*

$$\begin{aligned}f(\rho,T) \geqslant{}& 4\pi\mathfrak{a}\rho^2\left(1 + \frac{128}{15\sqrt{\pi}}\sqrt{\rho\mathfrak{a}^3}\right) + \frac{T^{5/2}}{(2\pi)^3}\int_{\mathbb{R}^3}\log\left(1 - e^{-\sqrt{p^4 + \frac{16\pi\rho\mathfrak{a}}{T}p^2}}\right)\mathrm{d}p\\ &- C(\rho\mathfrak{a})^{5/2}(\rho\mathfrak{a}^3)^{\nu}.\end{aligned} \tag{3.4}$$

Here the constant $C > 0$ depends only on V.

Theorem 3.3 ([40], Upper Bound)**.** *Let $V \in L^2(\mathbb{R}^3)$ be non-negative, spherically symmetric and compactly supported. Let $0 \leqslant T \leqslant C\rho\mathfrak{a}$ for some $C > 0$. Then, in the dilute limit $\rho\mathfrak{a}^3 \to 0$, there exist $c, \epsilon > 0$ such that*

$$\begin{aligned}f(\rho,T) \leqslant{}& 4\pi\mathfrak{a}\rho^2\left(1 + \frac{128}{15\sqrt{\pi}}\sqrt{\rho\mathfrak{a}^3}\right) + \frac{T^{5/2}}{(2\pi)^3}\int_{\mathbb{R}^3}\log\left(1 - e^{-\sqrt{p^4 + \frac{16\pi\rho\mathfrak{a}}{T}p^2}}\right)\mathrm{d}p.\\ &+ c(\rho\mathfrak{a})^{5/2}(\rho\mathfrak{a}^3)^{\varepsilon}.\end{aligned} \tag{3.5}$$

4 History

This section outlines the physical and mathematical developments that led to the free energy density formula (1.3). We begin with the foundational works of Bose and Einstein and proceed through key advancements in the theory of dilute Bose gases.

The following notations are used throughout this and the following sections:

- "$\sum_{p\neq r}$" denotes the sum over a momentum set, the set being clear from the context, where we exclude the term with $p = r$
- "$\approx$" indicates a heuristic derivation, typically involving a perturbative argument and the omission of subleading contributions
- "$A \prec B$" expresses a heuristic idea that the term A is negligible compared to B, often motivating a particular ansatz or simplification
- "$A \ll B$" for two scalars A, B means precisely that $A/B \to 0$ as $\rho\mathfrak{a}^3 \to 0$
- $A \lesssim B :\Leftrightarrow \exists C > 0 : A \leqslant CB$.

4.1 Heuristic Results

In 1924, Bose sent a letter to Einstein asking him to review a manuscript in which he derived Planck's radiation law by treating photons in phase space. In doing so, Bose implicitly departed from classical Boltzmann statistics, by describing a quantum gas of identical particles by symmetric states under particle permutations; a principle that is nowadays formalized in the bosonic Hilbert space. The full picture only became clear later, when Dirac noticed that many-body wave functions constructed from one-particle states can be either symmetric or antisymmetric. This observation, also known as the spin–statistics theorem, lead to the distinction between two classes of quantum particles: bosons and fermions. Einstein recognized the importance of Bose's work, referred to it as an important advance ("wichtiger Fortschritt"), translated the paper into German, and arranged for its publication in Zeitschrift für Physik [14]. He subsequently extended Bose's ideas and, by applying basic thermodynamic arguments, discovered that an ideal Bose gas at fixed temperature and particle number admits a minimal volume. Since such a constraint is physically impossible as one can compress a gas by applying pressure, Einstein concluded that, beyond a certain density, a macroscopic fraction of the particles must occupy the lowest energy state. This phenomenon is now known as Bose–Einstein condensation. Let us rederive Einstein's argument using the formalism introduced in Section 2.

Einstein's derivation of BEC We consider a free Bose gas confined to the three-dimensional torus $[-L/2, L/2]^3$ in the grand-canonical ensemble. The Hamiltonian is given by

$$H = \sum_{p\in\frac{2\pi}{L}\mathbb{Z}^3} (p^2 - \mu_L)\, a_p^* a_p, \tag{4.1.1}$$

where for temperature $T > 0$ and particle density $\rho > 0$, the chemical potential $\mu_L = \mu_L(\rho, T) < 0$ is defined implicitly by the constraint $\mathrm{Tr}\,(\mathcal{N}\Gamma) = \rho L^3$. Here $\Gamma = Z^{-1}e^{-\beta H}$ denotes the Gibbs state at inverse temperature $\beta = 1/T$.

The eigenstates of H are of the form

$$\prod_{p\in\frac{2\pi}{L}\mathbb{Z}^3} (n_p!)^{-1/2}(a_p^*)^{n_p}\Omega,$$

where $\{n_p\}_p$ is a finite sequence with $n_p \in \mathbb{N}_0$. The corresponding eigenvalue is

$$\sum_{p\in\frac{2\pi}{L}\mathbb{Z}^3} (p^2 - \mu_L)\, n_p.$$

A key advantage of the grand-canonical setting is that the partition function can be computed explicitly:

$$Z = \sum_{\{n_p\}} e^{-\beta\sum_q (q^2-\mu_L)n_q} = \prod_{p\in\frac{2\pi}{L}\mathbb{Z}^3} \sum_{n\geqslant 0} e^{-\beta(p^2-\mu_L)n} = \prod_{p\in\frac{2\pi}{L}\mathbb{Z}^3} \frac{1}{1-e^{-\beta(p^2-\mu_L)}}. \tag{4.1.2}$$

Similarly, one computes the expected particle number,

$$\begin{aligned}
\mathrm{Tr}\,(\mathcal{N}\Gamma) &= Z^{-1}\sum_{\{n_p\}}\sum_{r\in\frac{2\pi}{L}\mathbb{Z}^3} n_r e^{-\beta\sum_{q\in\frac{2\pi}{L}\mathbb{Z}^3}(q^2-\mu_L)n_q} \\
&= Z^{-1}\sum_{r\in\frac{2\pi}{L}\mathbb{Z}^3}\sum_{n\geqslant 0} n e^{-\beta(r^2-\mu_L)n}\prod_{p\neq r}\frac{1}{1-e^{-\beta(p^2-\mu_L)}} \\
&= \sum_{r\in\frac{2\pi}{L}\mathbb{Z}^3}\frac{1}{e^{\beta(r^2-\mu_L)}-1}.
\end{aligned} \tag{4.1.3}$$

This shows that any density $\rho\in(0,\infty)$ can be realized by a suitable choice of $\mu_L\in(-\infty,0)$.

We now analyze the thermodynamic limit. We will show the existence of the limit

$$\rho_0 := \lim_{L\to\infty} L^{-3}\frac{1}{e^{-\beta\mu_L}-1}.$$

Moreover, we will see that the fraction of particles in the zero mode is positive if and only if the density is larger than the critical density, i.e.,

$$\rho_0 = \max\{\rho-\rho_c, 0\} \quad \text{with the critical density} \quad \rho_c = \left(\frac{T}{4\pi}\right)^{3/2}\zeta(3/2).$$

Here $\zeta(s) = \sum_{n\geqslant 1} n^{-s}$ denotes the Riemann zeta function. We find that a state with $\rho_0 > 0$ exhibits BEC in the sense of (2.2.1). Indeed, setting $n = \rho L^3$ yields $\lim_{n\to\infty} n^{-1}\mathrm{Tr}\,(a_0^* a_0\Gamma) = \rho_0/\rho > 0$.

Proof. For fixed $\mu < 0$, the Riemann sum converges

$$\lim_{L\to\infty} L^{-3}\sum_{r\in\frac{2\pi}{L}\mathbb{Z}^3}\frac{1}{e^{\beta(r^2-\mu)}-1} = \frac{1}{(2\pi)^3}\int_{\mathbb{R}^3}\frac{1}{e^{\beta(r^2-\mu)}-1}\,\mathrm{d}r =: G(\mu)$$

and by the same argument and a quick calculation we find that for $\mu = 0$

$$\begin{aligned}
\lim_{L\to\infty} L^{-3}\sum_{r\neq 0}\frac{1}{e^{\beta r^2}-1} &= \frac{1}{(2\pi)^3}\int_{\mathbb{R}^3}\frac{1}{e^{\beta r^2}-1}\mathrm{d}r = \frac{4\pi T^{3/2}}{(2\pi)^3}\int_0^\infty r^2 e^{-r^2}\sum_{n\geqslant 0} e^{-r^2 n}\mathrm{d}r \\
&= \frac{4\pi T^{3/2}}{(2\pi)^3}\sum_{n\geqslant 0}\int_0^\infty \frac{r^2}{n+1}e^{-r^2}\frac{\mathrm{d}r}{\sqrt{n+1}} = \frac{4\pi T^{3/2}}{(2\pi)^3}\zeta(3/2)\int_0^\infty r^2 e^{-r^2}\mathrm{d}r \\
&= \rho_c = G(0).
\end{aligned} \tag{4.1.4}$$

The function $G : (-\infty, 0] \to (0, \rho_c]$ is strictly increasing, and bijective. Let μ_∞ be defined by $G(\mu_\infty) = \rho$.

Case $\rho \leqslant \rho_c$: In this case $\mu_\infty < 0$, and we claim that $\mu_L \to \mu_\infty$ as $L \to \infty$. Suppose, by contradiction, that this is not the case. Then, without loss of generality, there exist $\varepsilon > 0$ and a sequence $L_m \to \infty$ such that $\mu_{L_m} \leqslant \mu_\infty - \varepsilon$ for all m (alternatively reverse all signs in the proof below). Using (4.1.3), we obtain

$$\rho = L_m^{-3} \sum_{r \in \frac{2\pi}{L_m}\mathbb{Z}^3} \frac{1}{e^{\beta(r^2 - \mu_{L_m})} - 1} \leqslant L_m^{-3} \sum_{r \in \frac{2\pi}{L_m}\mathbb{Z}^3} \frac{1}{e^{\beta(r^2 - \mu_\infty + \varepsilon)} - 1}.$$

Taking the limit $m \to \infty$ yields

$$G(\mu_\infty) = \rho \leqslant G(\mu_\infty - \varepsilon),$$

which contradicts the strict monotonicity of G. Hence $\mu_L \to \mu_\infty$ as $L \to \infty$ and we conclude that

$$\rho_0 = \lim_{L\to\infty} L^{-3} \frac{1}{e^{-\beta\mu_L} - 1} = 0.$$

Case $\rho > \rho_c$: Using (4.1.3) and the fact that $\mu_L \leqslant 0$, one finds

$$L^{-3} \frac{1}{e^{-\beta\mu_L} - 1} = \rho - L^{-3} \sum_{r \neq 0} \frac{1}{e^{\beta(r^2 - \mu_L)} - 1} \geqslant \rho - L^{-3} \sum_{r \neq 0} \frac{1}{e^{\beta r^2} - 1}.$$

The right-hand side is positive for L sufficiently large due to (4.1.4) and $\rho > \rho_c$. Thus, there exists a constant $C > 0$ such that $(e^{-\beta\mu_L} - 1) \leqslant CL^{-3}$ for L sufficiently large. Consequently,

$$0 \leqslant L^{-3} \sum_{r \neq 0} \left[\frac{1}{e^{\beta r^2} - 1} - \frac{1}{e^{\beta(r^2 - \mu_L)} - 1} \right] \leqslant (e^{-\beta\mu_L} - 1) L^{-3} \sum_{r \neq 0} \frac{e^{\beta r^2}}{(e^{\beta r^2} - 1)^2} \leqslant CL^{-2}$$

for large L. It follows that

$$\lim_{L\to\infty} L^{-3} \sum_{r \neq 0} \frac{1}{e^{\beta(r^2 - \mu_L)} - 1} = \lim_{L\to\infty} L^{-3} \sum_{r \neq 0} \frac{1}{e^{\beta r^2} - 1} = \rho_c,$$

and hence $\rho_0 = \rho - \rho_c > 0$. □

The physical relevance of Bose–Einstein condensation was initially met with skepticism. As discussed by London [67], this was largely due to the lack of experimental relevance, since known atomic gases were all in a liquid or solid phase at the temperatures required for condensation, as well as to theoretical objections raised by Uhlenbeck [91, Chapter 6]. However, London argued that the λ-transition observed in liquid helium might be related to Einstein's prediction of condensation, and he suggested that the description of a theoretical Bose-metal naturally leads to superconductivity.

Bogoliubov subsequently took up this idea and addressed, in particular, the criticism that London did not rule out interactions between the condensate and the excited particles. He developed a microscopic theory to explain the superfluid behavior of liquid helium in what became arguably the most influential work for the present thesis [13]. In this work, he derived an explicit expansion for the ground state energy of a weakly interacting Bose gas confined to a box Ω of side length L with periodic boundary conditions,

$$E_0 \approx \frac{N}{2} \rho \widehat{V}(0) + \frac{1}{2} \sum_{p \neq 0} \left[\sqrt{p^4 + 2\rho_0 \widehat{V}(p) p^2} - p^2 - \rho_0 \widehat{V}(p) \right], \tag{4.1.5}$$

where V denotes the interaction potential and $\widehat{V}$ its Fourier transform. More importantly, Bogoliubov identified the structure of the low-lying excitations, which are given by

$$E_0 + \sum_{p\neq 0} \sqrt{p^4 + 2\rho_0 \widehat{V}(p) p^2}\, n_p, \tag{4.1.6}$$

where n_p denotes the occupation number of the momentum mode p. In particular, the resulting collective excitations with dispersion relation

$$\epsilon(p) = \sqrt{p^4 + 2\rho_0 \widehat{V}(p) p^2}$$

satisfy Landau's criterion for superfluidity,

$$\min_p \frac{\epsilon(p)}{|p|} \geqslant c_0 > 0,$$

see [49].

Since Bogoliubov's paper is of central importance for the present work, we outline his proof strategy and highlight its key steps. The argument is carried out at the microscopic level by considering an N-body Hamiltonian of the form (3.1) and writing it in the language of second quantization as

$$H_N = \sum_{p\in\frac{2\pi}{L}\mathbb{Z}^3} p^2 a_p^* a_p + \frac{1}{2} \sum_{p,q,k\in\frac{2\pi}{L}\mathbb{Z}^3} \widehat{V}(k) a_p^* a_{q+k}^* a_q a_{p+k}, \tag{4.1.7}$$

where $a_p = a(|\Omega|^{-1/2} e^{ip\cdot})$. Bogoliubov's key assumption is the presence of Bose–Einstein condensation, which, from the ideal gas picture, heuristically implies

$$a_0^* a_0 \succ a_p^* a_p, \qquad p \neq 0.$$

He therefore expanded the interaction term according to the number of creation and annihilation operators acting on the zero-momentum mode.

The leading contribution arises from the term

$$\frac{1}{2}\widehat{V}(0) a_0^* a_0^* a_0 a_0 \approx \frac{1}{2}\widehat{V}(0)\frac{N_0^2}{|\Omega|},$$

where N_0 denotes the number of particles in the condensate. At this stage, Bogoliubov employed the so-called c-number substitution, replacing the operators a_0 and a_0^* by the scalar $\sqrt{N_0}$. This step is heuristically justified by the relation $a_0^* a_0 \succ [a_0, a_0^*] = 1$ and can be made rigorous, for instance, via the excitation map introduced in [56].

A possible linear term vanishes as a consequence of momentum conservation and the cubic and quartic terms are neglected as higher order contributions. The remaining quadratic terms take the form

$$\frac{\widehat{V}(0)}{|\Omega|} \sum_{p\neq 0} a_p^* a_p + \frac{N_0}{|\Omega|} \sum_{p\neq 0} \widehat{V}(p) a_p^* a_p + \frac{N_0}{2|\Omega|} \sum_{p\neq 0} \widehat{V}(p) a_p^* a_{-p}^* + \text{h.c.}$$

Together with the approximation $N_0 \approx N - \sum_{p\neq 0} a_p^* a_p$ and by again omitting quartic terms, one arrives at the effective Hamiltonian

$$H_N \approx \frac{N}{2}\rho\widehat{V}(0) + \sum_{p\neq 0}\big(p^2 + \rho\widehat{V}(p)\big) a_p^* a_p + \frac{1}{2}\sum_{p\neq 0} \rho\widehat{V}(p) a_p^* a_{-p}^* + \text{h.c.}, \tag{4.1.8}$$

where $\rho = N/|\Omega|$ is the particle density. Finally, this quadratic Hamiltonian is diagonalized explicitly by introducing a Bogoliubov transformation. Assuming $\widehat{V}(0) \geqslant 0$ and that V is sufficiently small to ensure positivity of the radicand, one defines

$$\xi_p = \frac{a_p - L_p a_{-p}^*}{\sqrt{1-L_p^2}}, \qquad L_p = \frac{1}{\rho \widehat{V}(p)} \left(\sqrt{p^4 + 2\rho \widehat{V}(p) p^2} - p^2 - \rho \widehat{V}(p) \right),$$

or equivalently

$$\xi_p = \cosh(\varphi_p)\, a_p + \sinh(\varphi_p)\, a_{-p}^*, \qquad \tanh(2\varphi_p) = -\frac{\rho \widehat{V}(p)}{p^2 + \rho \widehat{V}(p)}.$$

Substituting this transformation into (4.1.8) yields

$$H_N \approx \frac{N}{2} \rho \widehat{V}(0) + \frac{1}{2} \sum_{p \neq 0} \left[\sqrt{p^4 + 2\rho \widehat{V}(p) p^2} - p^2 - \rho \widehat{V}(p) \right] + \sum_{p \neq 0} \sqrt{p^4 + 2\rho \widehat{V}(p) p^2}\, \xi_p^* \xi_p. \quad (4.1.9)$$

Since the operators ξ_p and ξ_p^* satisfy the canonical commutation relations, they may be interpreted as creation and annihilation operators of quasiparticles (phonons). This yields the expressions (4.1.5) and (4.1.6).

However, the expression (4.1.9) does not yield the correct ground state energy, as the omission of the cubic and quartic terms in the non-zero modes is too crude. In fact, the correct leading order term was already computed by Lenz [52], who derived the average energy of a single particle in a dilute Bose gas and obtained the expression

$$4\pi \rho \mathfrak{a}.$$

Multiplying this quantity by the total number of particles N leads to the approximation

$$E_0 \approx 4\pi \rho \mathfrak{a} N. \quad (4.1.10)$$

Bogoliubov himself observed, respectively was told by Landau, that, in order to obtain the correct leading-order behavior, the Fourier transform $\widehat{V}$ should be replaced by $\widehat{V(1-\omega)}$, where ω denotes the scattering solution introduced in Lemma 2.3. In particular, this substitution replaces $\widehat{V}(0)$ by $8\pi\mathfrak{a}$. While this yields the correct leading term, the second order term becomes a divergent expression

$$\frac{1}{2(2\pi)^3} \int_{\mathbb{R}^3} \left[\sqrt{p^4 + 16\pi \mathfrak{a} \rho p^2} - p^2 - 8\pi \mathfrak{a} \rho \right] \mathrm{d}p. \quad (4.1.11)$$

Let us follow an argument from [60, Chapter 2] to indicate how the correct formula can be recovered from Bogoliubov's derivation.

By adding and subtracting a suitable counterterm in (4.1.9) and formally taking the thermodynamic limit, one obtains the approximation

$$\begin{aligned} e(\rho) &\approx \frac{\rho^2}{2} \left(\widehat{V}(0) - \frac{1}{(2\pi)^3} \int_{\mathbb{R}^3} \frac{\widehat{V}(p)^2}{2p^2} \mathrm{d}p \right) \\ &\quad + \frac{1}{2(2\pi)^3} \int_{\mathbb{R}^3} \left[\sqrt{p^4 + 2\rho \widehat{V}(p) p^2} - p^2 - \rho \widehat{V}(p) + \frac{\rho^2 \widehat{V}(p)^2}{2p^2} \right] \mathrm{d}p \\ &\approx \frac{\rho^2}{2} 8\pi(\mathfrak{a}_0 + \mathfrak{a}_1) + \frac{\sqrt{8}}{15\pi^2} (\rho 8\pi \mathfrak{a}_0)^{5/2}, \end{aligned} \quad (4.1.12)$$

where, in the second term, we approximated $\widehat{V}(p) \approx \widehat{V}(0) = 8\pi\mathfrak{a}_0$. Here $\mathfrak{a}_0$ and $\mathfrak{a}_1$ are the first two terms in the Born series (2.3.6) of $\mathfrak{a}$. Thus, one is naturally led to the, now correct, expansion

$$e(\rho) = 4\pi\mathfrak{a}\rho^2 + 4\pi\mathfrak{a}\rho^2 \frac{128}{15\sqrt{\pi}} \sqrt{\rho\mathfrak{a}^3} + o\Big((\rho\mathfrak{a})^{5/2}\Big).$$

The correct second-order term was first predicted in 1957 by Lee and Yang[4] [51]. They argued, without detailed proof, that it could be obtained via a binary-collision expansion. In another work, Huang and Yang [44] replaced the interaction with an effective delta-function pseudopotential that model hard-core collisions. This enabled a direct perturbative calculation of the first-order correction to the energy density.

Using this approach, they eventually derived the correct second order term in the seminal paper [50],

$$E_0 \approx 4\pi\mathfrak{a}\rho N + \sum_{p\neq 0} \left[\sqrt{p^4 + 16\pi\mathfrak{a}\rho p^2} - p^2 - 8\pi\mathfrak{a}\rho + \frac{(8\pi\mathfrak{a}\rho)^2}{2p^2} \right]. \tag{4.1.13}$$

In fact, employing a delta interaction alone reproduces the same divergent expression (4.1.11) that Bogoliubov encountered; only after a suitable renormalization of the pseudopotential does the additional counterterm emerge, yielding the correct result.

The pseudopotential method also led to a characterization of the excitation spectrum,

$$E_0 + \sum_{p\neq 0} \sqrt{p^4 + 16\pi\mathfrak{a}\rho p^2}\, n_p, \tag{4.1.14}$$

where, as before, n_p denotes the occupation number of the momentum mode p. From this representation, that resembles the free case except for an energy shift and a different dispersion relation, Lee, Huang and Yang deduced thermodynamic quantities such as the specific heat and the free energy can be computed explicitly. We now carry out this computation, which are similar to the ones we did for the free gas, (4.1.2).

Let

$$H = E_0 + \sum_{p\neq 0} \epsilon(p)\, \xi_p^* \xi_p, \qquad \epsilon(p) = \sqrt{p^4 + 16\pi\mathfrak{a}\rho p^2},$$

acting on the excitation Fock space

$$\mathcal{F}_\perp(L^2(\Omega)) := \mathcal{F}\big(\langle u_0\rangle^\perp\big).$$

The partition function $Z = \mathrm{Tr}\,(e^{-\beta H})$, with $\beta = 1/T$, is obtained by summing over all occupation number configurations of the modes $p \neq 0$. Proceeding as in (4.1.2), we find

$$Z = \sum_{\{n_p\}:n_0=0} e^{-\beta(E_0 + \sum_{q\neq 0} n_q \epsilon(q))} = e^{-\beta E_0} \prod_{p\neq 0} \sum_{n=0}^{\infty} e^{-\beta n \epsilon(p)} = e^{-\beta E_0} \prod_{p\neq 0} \frac{1}{1 - e^{-\beta\epsilon(p)}}. \tag{4.1.15}$$

By Lemma 3.1, the corresponding free energy is given by

$$F_\Omega^{\mathrm{Bog}}(N) = -T\log Z = E_0 - T\sum_{p\neq 0} \log\Big(1 - e^{-\epsilon(p)/T}\Big).$$

Taking a formal thermodynamic limit yields the free energy density

$$f^{\mathrm{Bog}}(\rho, T) = e^{\mathrm{Bog}}(\rho) - \frac{T}{(2\pi)^3} \int_{\mathbb{R}^3} \log\Big(1 - e^{-\sqrt{p^4 + 16\pi\rho\mathfrak{a}p^2}/T}\Big)\, \mathrm{d}p, \tag{4.1.16}$$

[4]Lee and Yang were awarded the Nobel Prize in Physics in 1957 for their prediction of parity violation in weak interactions. In the aftermath, disagreements regarding the extent of their individual contributions arose; see [78, p. 164].

where

$$e^{\mathrm{Bog}}(\rho) = 4\pi\mathfrak{a}\rho^2 \left(1 + \frac{128}{15\sqrt{\pi}}\sqrt{\rho\mathfrak{a}^3}\right). \tag{4.1.17}$$

These expressions are commonly referred to as the Lee–Huang–Yang (LHY) formula.

Finally, they also derived the condensate fraction of the ground state Ψ at zero temperature,

$$\langle \Psi, a_0^* a_0 \Psi \rangle = N \left(1 - \frac{8}{3\sqrt{\pi}}\sqrt{\rho\mathfrak{a}^3}\right). \tag{4.1.18}$$

As mentioned in Section 1, Bose–Einstein condensation was first observed experimentally only in 1995. The LHY coefficient $128/(15\sqrt{\pi}) \approx 4.81$ was measured in [77] to be 4.5(7), corresponding to a one-standard-deviation interval of $[3.8, 5.2]$. Moreover, the condensate depletion formula (4.1.18) was experimentally confirmed in [68].

4.2 Mathematical Results

The rigorous mathematical justification of the formulas Eqs. (4.1.14) and (4.1.16) to (4.1.18) has been a central challenge in the analysis of dilute Bose gases ever since Dyson's pioneering work in 1957 [29]. In 2020, the proof of the ground state energy density expansion (4.1.17) was completed with the derivation of a matching lower bound [36]; see [96] for the corresponding upper bound. A proof of the free energy density formula (4.1.16) was recently obtained in [39, 40] and forms the main result of this thesis. In contrast, a rigorous derivation of the excitation spectrum (4.1.14) and the condensate fraction (4.1.18) in the thermodynamic limit remains open and is one of the major outstanding problems in the field. In particular, a proof of BEC in the thermodynamic limit for general interacting systems is still missing.

In the following, we briefly review the main mathematical developments over the past decades. We distinguish between results at zero temperature and those at positive temperature.

$T = 0$ Dyson proved that for hard-core interactions in a box with periodic boundary conditions,

$$\frac{\sqrt{2}}{5}\pi\mathfrak{a}\rho^2 \;\leqslant\; e(\rho) \;\leqslant\; 4\pi\mathfrak{a}\rho^2\left(1 + C(\rho\mathfrak{a}^3)^{1/3}\right)$$

for some constant $C > 0$. In particular, this established the correct leading-order upper bound in the Lee–Huang–Yang expansion (4.1.17). However, the error term was not optimal, and the lower bound coefficient $\sqrt{2}/5$ differs from the correct value by approximately a factor of 14.

Dyson's upper bound relied on the variational principle, that is any explicit trial state yields an upper bound to the (free) energy. It remains, and this is not trivial, to construct a trial state that yields the correct energy. This strategy underlies all subsequent refinements of upper bounds. His argument was later extended to all positive, spherically symmetric interaction potentials with finite scattering length in [64]. The lower bound is based on what is now known as the Dyson lemma, which allows one to replace the interaction potential by a softer one at the expense of kinetic energy.

This lemma was refined by Lieb and Yngvason [65] and combined with Temple's inequality, a general perturbative estimate relying on a spectral gap, to obtain the asymptotically correct lower bound

$$e(\rho) \;\geqslant\; 4\pi\mathfrak{a}\rho^2\left(1 - C(\rho\mathfrak{a}^3)^{1/17}\right).$$

Since Temple's inequality becomes worse as the volume increases, in the proof the thermodynamic domain is partitioned into smaller boxes. One then establishes lower bounds on each box, and obtains the result on the thermodynamic box by optimizing over all distributions of the N particles among these boxes. A related strategy of going to smaller boxes is also employed in the present thesis, although Temple's inequality is not precise enough to capture the LHY contribution.

The upper bound for the Lee–Huang–Yang formula (4.1.17) was established by Yau and Yin [94], following earlier work for soft potentials [31]. As for the lower bound before, their analysis is restricted to smaller boxes, and a trial state on the full domain is constructed by patching together local states.

These developments motivated a refined analysis of Hamiltonians on intermediate length scales. Specifically, one considers systems where the density vanishes as the box size gets large, compared to the thermodynamic limit, where the density is fixed. We prefer to rescale the box to have volume 1. The Hamiltonian (3.1) on $[-\mathcal{L}/2, \mathcal{L}/2]^3$ is unitarily equivalent to

$$H = -\mathcal{L}^{-2} \sum_{i=1}^{N} \Delta_i + \sum_{1 \leqslant i < j \leqslant N} V\big(\mathcal{L}(x_i - x_j)\big)$$

acting on $L^2_s([-1/2, 1/2]^{3N})$. The unitary map is given by

$$\mathcal{U}_{\mathcal{L}} : L^2_s([-1/2, 1/2]^{3N}) \to L^2_s([-\mathcal{L}/2, \mathcal{L}/2]^{3N}), \qquad (\mathcal{U}_{\mathcal{L}}\psi)(x) = \mathcal{L}^{-3N/2}\psi(x/\mathcal{L}).$$

We set, for $\varkappa \geqslant 0$,

$$\mathcal{L} = \mathfrak{a}(\rho\mathfrak{a}^3)^{-1/2-\varkappa}.$$

The case $\varkappa = 0$ corresponds to the Gross–Pitaevskii (GP) scaling, also known as the healing-length scale. The regime $0 < \varkappa < 2/3$ is referred to as the beyond-GP regime, while, formally, $\varkappa \to \infty$ recovers to the thermodynamic limit. Another regime is the mean-field scaling, for which condensation and energy asymptotics are well understood; see [86, 55, 56, 15].

Using the lower bound of [65] together with the Poincaré inequality, Lieb and Seiringer [63] proved Bose–Einstein condensation in the GP regime, providing the first rigorous proof of condensation for a physically realistic interaction.

A major breakthrough in the GP regime was, after further results on the energy and condensation [64, 62, 75], achieved by Boccato, Brennecke, Cenatiempo, and Schlein in a series of works [8, 10, 9, 7]. They established the Lee–Huang–Yang energy correction (4.1.17) as well as the excitation spectrum (4.1.14) for integrable potentials. Their approach is close to Bogoliubov's original argument, but crucially incorporates an additional cubic transformation that renormalizes the cubic interaction terms.

This idea has since inspired a large body of work, leading to numerous generalizations and simplifications [23, 1, 6, 5, 71, 74, 69, 17, 16, 43, 24, 12, 72, 25, 26]. In particular, the work [6] provides a new proof of the second-order upper bound originally obtained in [94], and some of its techniques will be used in this thesis.

The first proof of a lower bound matching the Lee–Huang–Yang correction was obtained by Fournais and Solovej [36, 37], building on ideas from [18]. Their strategy involves a two-step localization of the Hamiltonian to boxes slightly larger and subsequently slightly smaller than the GP scale, combined with a sliding technique, averaging over possible centers of the smaller boxes, and a completion-of-the-square argument. This approach also led to the strongest available result on Bose–Einstein condensation beyond the GP regime [33], proving condensation for $\varkappa < 1/4$.

A rigorous proof of Bose–Einstein condensation in the thermodynamic limit remains open. In particular, the condensate fraction formula (4.1.18) is completely unresolved and cannot be seen in ultra-dilute limits, where $\rho\mathfrak{a}^3 \to 0$, so that one always obtains complete condensation.

The naive approach to combine the condensate result from smaller boxes fails due to the fact that in each box the ground state wave function can have a different phase.

Recent work in the thermodynamic limit includes extensions to three-body interactions [73, 92, 46], to two-dimensional systems [34], and an upper bound on the third-order correction [20] predicted by Wu [93], Hugenholtz-Pines [45] and Sawada [85]. However, an upper bound for the second-order Lee–Huang–Yang correction for hard-sphere interactions is still missing[5]; the best result to date is [4].

$\boldsymbol{T > 0}$ As we have seen in (4.1.2), (4.1.3), and (4.1.15), many thermodynamic quantities of the ideal Bose gas can be computed explicitly. As another example, consider the grand-canonical pressure of the free Hamiltonian

$$H_0 = \sum_{p \in \frac{2\pi}{L}\mathbb{Z}^3} p^2 a_p^* a_p$$

at temperature $T > 0$ and chemical potential $\mu < 0$. It is given by

$$\begin{aligned} p(\mu, T) &:= \lim_{L\to\infty} L^{-3} T \log \operatorname{Tr} e^{-(H_0 - \mu\mathcal{N})/T} = T \lim_{L\to\infty} L^{-3} \sum_{p\in\frac{2\pi}{L}\mathbb{Z}^3} \log\Big(1 - e^{-(p^2-\mu)/T}\Big) \\ &= \frac{T}{(2\pi)^3} \int_{\mathbb{R}^3} \log\Big(1 - e^{-(p^2-\mu)/T}\Big)\, \mathrm{d}p, \end{aligned}$$

where μ is a fixed parameter, independent of L. By equivalence of ensembles [84, Thm. 3.5.8], the free energy density of the ideal gas is given by the Legendre transform of the pressure,

$$f_0(\rho, T) = \sup_{\mu<0} \left\{ \mu\rho + \frac{T}{(2\pi)^3} \int_{\mathbb{R}^3} \log\Big(1 - e^{-(p^2-\mu)/T}\Big)\, \mathrm{d}p \right\}.$$

Let us analyze this variational problem. From the scaling relation $f_0(\rho, T) = T^{5/2} f_0(\rho T^{-3/2}, 1)$ and a simple maximization of differentiable function we find that if the temperature lies above the critical temperature

$$T_c = 4\pi \left(\frac{\rho}{\zeta(3/2)} \right)^{2/3},$$

or equivalently if the density is below the critical density, the supremum is attained uniquely at $\mu_\infty < 0$, where we recall

$$\frac{1}{(2\pi)^3} \int_{\mathbb{R}^3} \frac{\mathrm{d}p}{e^{(p^2-\mu_\infty)/T} - 1} = \rho.$$

For $T < T_c$ the supremum is attained at $\mu = 0$. In this regime the free energy simplifies to

$$f_0(\rho, T) = \frac{T}{(2\pi)^3} \int_{\mathbb{R}^3} \log\Big(1 - e^{-p^2/T}\Big)\, \mathrm{d}p = -\frac{\zeta(5/2)}{8\pi^{3/2}} T^{5/2},$$

which is independent of ρ. This reflects the fact that the condensate does not contribute to the pressure. Figure 2 illustrates the resulting free energy density for $\rho = 1$ fixed. In particular, we observe a phase transition at $T = T_c$ in the form of non-analytic behavior of the free energy.

As for the ground state energy, the analysis becomes substantially more involved for interacting Bose gases. For instance, it is unclear whether the interaction increases or decreases the critical temperature, although both numerical and theoretical evidence suggest an increase;

[5] A proof was recently announced by Benjamin Schlein at the conference "Emergent phenomena in many-body quantum systems", 8-12 December 2025, CIRM, Marseille

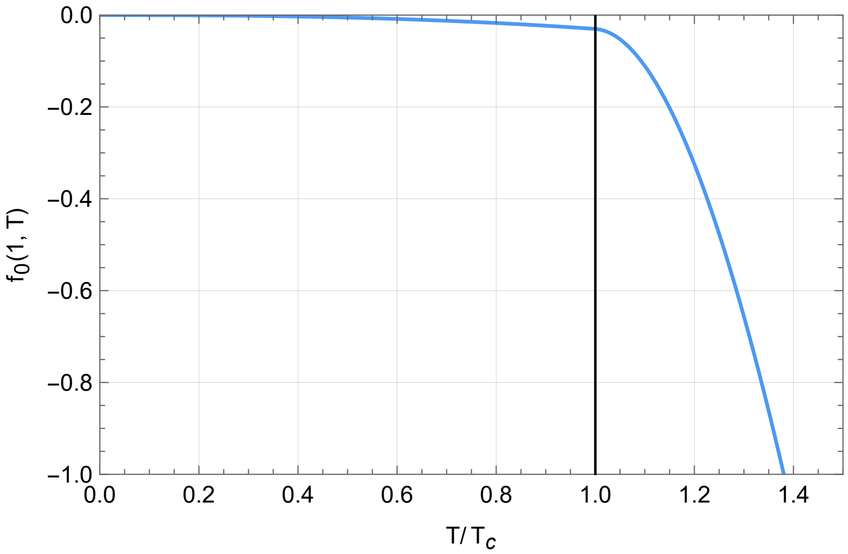

Figure 2: Free energy density of the ideal Bose gas at $\rho = 1$ as a function of T/T_c.

see, for example, [90]. At present, the only rigorous results are an upper bound on the critical temperature [88] and an explicit computation within an effective model [76].

Concerning the free energy density, it is known that, if T/T_c is bounded, then

$$f(\rho, T) = f_0(\rho, T) + 4\pi\mathfrak{a}\rho^2\Big(2 - \big[1 - (T/T_c)^{3/2}\big]_+^2\Big)\big(1 + o(1)_{\rho\mathfrak{a}^3\to 0}\big), \tag{4.2.1}$$

where $[x]_+ := \max\{0, x\}$. The lower bound was proved in [87] for non-negative, compactly supported interaction potentials. The corresponding upper bound was first obtained by Yin [95] and later extended by Basti, Boccato, Cenatiempo, and Deuchert [3] to a larger class of potentials, together with an explicit error estimate.

A formal Taylor expansion of the thermal contribution in our result Theorems 3.2 and 3.3 yields that for $T < T_c$

$$\begin{aligned} &4\pi\mathfrak{a}\rho^2 + \frac{T^{5/2}}{(2\pi)^3}\int_{\mathbb{R}^3} \log\left(1 - e^{-p^2\sqrt{1+\frac{16\pi\rho\mathfrak{a}}{Tp^2}}}\right) \mathrm{d}p \\ &= 4\pi\mathfrak{a}\rho^2 + \frac{T^{5/2}}{(2\pi)^3}\int_{\mathbb{R}^3} \log\left(1 - e^{-p^2}\right) \mathrm{d}p - \frac{T^{5/2}}{(2\pi)^3}\frac{16\pi\rho\mathfrak{a}}{T}\int_{\mathbb{R}^3} p^{-2}\frac{p^2}{2(e^{p^2}-1)}\mathrm{d}p + \ldots \\ &= f_0(\rho, T) + 4\pi\mathfrak{a}\rho^2\left(1 - 2(T/T_c)^{3/2}\right) + \ldots. \end{aligned}$$

Thus, our analysis seems to capture two of the three contributions arising from the expansion of the square in (4.2.1), but does not recover the term of order $\rho^2(T/T_c)^3$. Extracting this contribution would require a quartic transformation. In any case, for the temperature regime considered in this thesis, namely T of the order $\rho\mathfrak{a}$, the missing term $\rho^2(T/T_c)^3$ is of order ρ^3 and is therefore far below the precision accessible with current methods.

Moreover, the Taylor expansion, which can be made rigorous readily for the leading contribution, shows that our result is consistent with (4.2.1). Indeed, in the low-temperature regime $T/T_c = o(1)$, (4.2.1) reduces to

$$f(\rho, T) = \frac{T^{5/2}}{(2\pi)^3}\int_{\mathbb{R}^3} \log\left(1 - e^{-p^2/T}\right) \mathrm{d}p + 4\pi\mathfrak{a}\rho^2 + o(\rho^2\mathfrak{a}),$$

which is precisely the behavior recovered by our formula.

Additionally, it remains an interesting open problem to extend the validity of our result to higher temperatures.

A further question concerns the derivation of subleading corrections to (4.2.1). Assuming $T = \lambda T_c$ for some $\lambda \in (0,1)$, the next-order contribution is expected to be $-\frac{16\sqrt{\pi}}{3}T(\mathfrak{a}\rho_0)^{3/2}$. This term has been derived within an effective model [76] and as an upper bound in the Gross–Pitaevskii regime [11, 22].

The lower bound in our main result was subsequently extended to hard-core interactions in [35] by combining the present approach with the strategy of [34]. By contrast, the corresponding hard-core upper bound remains open, even at zero temperature. Further developments that are beyond the scope of this discussion concern results about the $k-$particle density matrices, trapped Bose gases, high-density regimes, one- or two-dimensional systems, dynamics of BECs and related problems for Fermi gases.

5 Proof Summary

In this section we give a general outline of the proofs of the lower and the upper bound, focusing on the main ideas and strategies while omitting the technical details. We begin by introducing the localization method, which is relevant to both bounds.

5.1 Localization

As discussed in the previous section, a detailed understanding of the low-lying spectrum of the Hamiltonian relies on exploiting the spectral gap of the Laplacian. On a domain of volume $|\Omega|$, this gap is of order $|\Omega|^{-2/3}$ and therefore vanishes in the thermodynamic limit. To overcome this difficulty, the thermodynamic box is partitioned into smaller boxes of fixed side length

$$\mathcal{L} = \mathfrak{a}(\rho\mathfrak{a}^3)^{-1/2-\varkappa},$$

where $\varkappa \geqslant 0$ is a parameter to be chosen appropriately.

The localization technique is inspired by Dirichlet–Neumann bracketing, a standard tool in the spectral analysis of Laplacians. Intuitively, Dirichlet boundary conditions raise the energy since they impose additional constraints on the admissible wave functions. Thus, the basic idea is to partition the domain and to bound the spectrum from below by imposing Neumann boundary conditions on the subdomains, and from above by imposing Dirichlet boundary conditions. In this way we can switch between different boundary conditions. Moreover, both the upper and lower bound proofs use a mechanism that allows to switch between the canonical and grand-canonical ensembles.

While the precise implementation differs between the upper and lower bounds, the overall strategy is similar. In either case, one considers the problem on each small box separately. For the lower bound imposing Neumann boundary conditions on each box yields a lower bound for the kinetic term. By positivity of the potential we may discard interactions between different boxes and we obtain a lower bound on the total energy. For the upper bound, one analyzes the Hamiltonian on a small box with Dirichlet boundary conditions. Then, a trial state on the full domain can be constructed by patching together the local trial states, since Dirichlet boundary conditions ensure that the wave functions vanish on the boundaries of the boxes.

In both cases, the intuition is that

$$\text{Energy in the thermodynamic box} \approx \text{Number of boxes} \times \text{Energy per box.}$$

As mentioned earlier, boundary conditions do not affect the energy density in the thermodynamic limit when the domain grows. Here, however, the boxes remain finite as $|\Omega| \to \infty$, and boundary effects contribute non-negligible corrections to the energy. It is therefore crucial to choose the box size $\mathcal{L}$ sufficiently large, as a function of the diluteness parameter $\rho\mathfrak{a}^3$, in order not to affect the Lee–Huang–Yang correction.

We explain below how to quantify the energy shifts induced by the boundary conditions. Let us collect them here and explain the consequences on the choice of $\mathcal{L}$. Neumann boundary conditions modify the energy by a term of order $\mathcal{L}^{-1}\rho^2|\log\rho|$, which implies that, in order not to affect the Lee–Huang–Yang term, one must require $\mathcal{L} \gg \rho^{-1/2}|\log\rho|$, corresponding to $\varkappa > 0$. Meanwhile, Dirichlet boundary conditions produce an energy correction of order $\mathcal{L}^{-1}\rho^{3/2}$, which yields the stronger condition $\mathcal{L} \gg \rho^{-1}$, or equivalently $\varkappa > 1/2$. Choosing larger boxes, however, increases the particle number per box and reduces the local spectral gap, thus the analysis becomes more difficult. Balancing these competing effects determines the range of the parameter $\varkappa$, for which results are useful and manageable.

We emphasize that the notation differs between the lower and upper bound works.

> For the lower bound, the thermodynamic box size and particle number are denoted by L and N, respectively, while quantities associated with the fixed-size boxes are written as ℓ and n; in this case $\mathcal{L} = \ell$. Moreover, we set $\kappa := \varkappa$.
>
> For the upper bound the thermodynamic box and particle number are denoted by Ω and n, respectively, whereas L and N refer to the fixed-size boxes, so that $\mathcal{L} = L$. Here ℓ plays the role of a parameter in the localization procedure, see Figure 3. Moreover, we set $\gamma := 1/2 + \varkappa$, and $\kappa := (2\gamma - 1)/(3\gamma - 1)$ so that $L = N^{1-\kappa}$.

5.2 Lower bound

As discussed above, it is useful to analyze the problem on boxes whose size ℓ is independent of the thermodynamic limit. The localization for the lower-bound builds on ideas introduced in [65], but requires refinements in order to capture the Lee–Huang–Yang correction and to incorporate the entropy contribution. A difficulty that was already noted by Lieb and Yngvason arises from the fact that, after partitioning the thermodynamic box into smaller ones, the distribution of particles among the boxes is a priori unknown. From a physical perspective, one expects a uniform distribution, and in the thermodynamic limit this is indeed guaranteed by the convexity of the free energy density in ρ; see [84, Thm. 3.5.8]. However, since the analysis is performed at finite volume, this argument cannot be applied directly and must be replaced by a quantitative estimate.

The key ingredients are the superadditivity of the energy, which follows from the assumption $V \geqslant 0$ and the Neumann boundary conditions, and the subadditivity of the entropy. Combining these properties, and introducing a chemical potential $\mu \geqslant 0$, one obtains the lower bound

$$F_L(N) \;\geqslant\; -TM_B \log \sum_{n=0}^{N} e^{-\frac{1}{T}(F_\ell(n)-\mu n)} + \mu\rho L^3,$$

where L denotes the side length of the thermodynamic box, N the total number of particles, ℓ the side length of the small boxes, n the number of particles in a single small box, and M_B the total number of boxes, satisfying $M_B\ell^3 = L^3$. A detailed derivation of this inequality is given in Section 6.9.

The main input is a precise lower bound on the free energy of a single small box. Specifically, one shows that for particle numbers $n \leqslant C\rho\ell^3 =: n_0$, with $C > 0$,

$$F_\ell(n) \geqslant f_{\mathrm{Bog}}(n,l) + o(\ell^3(\rho\mathfrak{a})^{5/2})$$
$$f_{\mathrm{Bog}}(n,l) = 4\pi\frac{\mathfrak{a}}{\ell^3}n^2\left(1 + \frac{128}{15\sqrt{\pi}}n^{1/2}\frac{\mathfrak{a}^{3/2}}{\ell^{3/2}}\right) + T\sum_{p\in\pi\mathbb{N}_0^3\setminus\{0\}}\log\left(1 - e^{\frac{-1}{T\ell^2}\sqrt{p^4+16\pi\mathfrak{a}n\ell^{-1}p^2}}\right), \tag{5.2.1}$$

which is the content of Theorem 6.1. We postpone a discussion of the proof of this estimate and first explain how it is used to complete the lower bound.

Given that we expect $n \approx \rho\ell^3$, it is known that the natural choice is $\mu = 8\pi\mathfrak{a}\rho$. We deduce this in Section 6.9 from (5.2.1). We find that for the restricted sum

$$\log\sum_{n=0}^{n_0} e^{-\frac{1}{T}(F_\ell(n)-\mu n)} \leqslant -\frac{f_{\mathrm{Bog}}(\rho\ell^3,\ell) - 8\pi\mathfrak{a}\rho^2\ell^3}{T} + o\big(\ell^3(\rho\mathfrak{a})^{5/2}\big) + \log(n_0+1).$$

The contribution from particle numbers $n > n_0$ is controlled by using the subadditivity of the energy together with the non-negativity of the relative entropy. Physically speaking, if there are too many particles in one box it is energetically better to distribute them to other boxes. This allows to reduce this case to the previously treated one. Combining all estimates and using $M_B\ell^3 = L^3$, one obtains the desired lower bound on the free energy, including the Lee–Huang–Yang correction.

We now outline the strategy used to establish (5.2.1). Similar results have been obtained in earlier works with periodic boundary conditions at zero temperature, and it is plausible that some of those arguments could be extended to sufficiently small temperatures $T > 0$. In our setting, however, Neumann boundary conditions are essential, which leads to a Hamiltonian that differs from the periodic one and requires a separate analysis.

The core idea is to successively conjugate the Hamiltonian with suitably chosen unitary transformations in order to isolate the relevant contributions. More precisely, we employ a quadratic transformation, which we split into a high and a low momentum part $e^{\mathcal{B}_1}$ respectively $e^{\mathcal{B}_2}$, to extract the contribution of the quadratic term Q_2, and a cubic transformation $e^{\mathcal{B}_c}$ to handle the cubic term Q_3; see (6.1.7) to (6.1.12) for the definitions of Q_i. To motivate the choice of these transformations, we rely on the Duhamel type expansion

$$\begin{aligned}&e^{-\mathcal{B}_1}(\mathrm{d}\Gamma(-\Delta) + Q_2 + Q_4)e^{\mathcal{B}_1}\\&\quad= \mathrm{d}\Gamma(-\Delta) + Q_4 + \int_0^1 e^{-t\mathcal{B}_1}\Big([\mathrm{d}\Gamma(-\Delta) + Q_4, \mathcal{B}_1] + Q_2\Big)e^{t\mathcal{B}_1}\mathrm{d}t + \int_0^1\int_t^1 e^{-s\mathcal{B}_1}[Q_2,\mathcal{B}_1]e^{s\mathcal{B}_1}\mathrm{d}s\mathrm{d}t.\end{aligned}$$

This identity suggests choosing $\mathcal{B}_1$ such that

$$[\mathrm{d}\Gamma(-\Delta) + Q_4, \mathcal{B}_1] + Q_2 = 0 \tag{5.2.2}$$

and that the main contribution of $[Q_2, \mathcal{B}_1]$ to the energy is a constant. With this choice, one finds

$$e^{-\mathcal{B}_1}\big(\mathrm{d}\Gamma(-\Delta) + Q_2 + Q_4\big)e^{\mathcal{B}_1} \approx \mathrm{d}\Gamma(-\Delta) + Q_4 + \frac{1}{2}[Q_2, \mathcal{B}_1].$$

An analogous construction is used for the cubic term, where $\mathcal{B}_c$ is chosen such that

$$[\mathrm{d}\Gamma(-\Delta) + Q_4, \mathcal{B}_c] + Q_3 \approx 0.$$

In practice, we do not enforce (5.2.2) exactly. Allowing for a small mismatch allows to choose a softer cubic transformation, which significantly simplifies the control of the error terms. This is achieved by truncating the scattering solution at distances well beyond the support of the interaction potential. Equivalently, one could modify the transformation in momentum space to only act on large momenta. After the cubic step, a second quadratic transformation $e^{\mathcal{B}_2}$ is applied to renormalize the remaining quadratic part of the Hamiltonian.

A notable difference in the Neumann setting is that the linear term Q_1, corresponding to a single creation or annihilation operator outside the zero mode, no longer vanishes due to the lack of momentum conservation. Nevertheless, this term is also absorbed by the first quadratic transformation, in the sense that

$$[Q_3, \mathcal{B}_1] + Q_1 \approx 0.$$

The main issue concerns the treatment of boundary conditions, which are implicitly present in (5.2.2). We address this by implementing the boundary conditions directly into the kernels of the transformations. Instead of the standard choice

$$K(x,y) = -n\omega(x-y) = -n \sum_{p \in \frac{2\pi}{L}\mathbb{Z}^3} \widehat{\omega}(p) e^{ip(x-y)},$$

with ω denoting the scattering solution from (2.3.3) (or a suitable modification thereof), we use

$$K(x,y) = -n \sum_{p \in \frac{\pi}{L}\mathbb{N}_0^3} \widehat{\omega}(p)\, u_p(x) u_p(y),$$

where $\{u_p\}$ are the eigenfunctions of the Neumann Laplacian. Comparing the resulting effective scattering length $\mathfrak{a}_{\text{Neumann}}$, which is obtained from the usual definition (2.3.4) by using the Neumann version of ω from the previous equation, with the true scattering length $\mathfrak{a}$, one finds

$$|\mathfrak{a}_{\text{Neumann}} - \mathfrak{a}| \leqslant \frac{\log \ell}{\ell}.$$

Using the Neumann kernel to derive the spectrum on small boxes yields (5.2.1) with $\mathfrak{a}$ replaced by $\mathfrak{a}_{\text{Neumann}}$. Thus, considering a typical box with $n = \rho\ell^3$ particles and summing over the L^3/ℓ^3 boxes yields a total error per unit volume of order

$$\rho^2 \frac{\log \ell}{\ell}.$$

Requiring this to be negligible compared with the Lee–Huang–Yang term of order $\rho^{5/2}$ leads precisely to the condition $\ell \gg \rho^{-1/2}$, as stated earlier.

The way we obtain (5.2.1) is in the form of operator inequalities. This is necessary for the lower bound as the inequality has to be valid for a general class of density matrices. Indeed, the resulting errors are small on physically relevant states, in particular on those with a moderate number of excitations, given by the restriction $n \leqslant C\rho\ell^3$.

5.3 Upper Bound

The overall strategy for the upper bound is based on the variational principle on a fixed size box $\Lambda_L = [-L/2, L/2]^3$. Recalling the definition (3.2),

$$F_{\Lambda_L}(N) := \inf\Big\{ \operatorname{Tr}(H_N\Gamma) - TS(\Gamma) \,\Big|\, 0 \leqslant \Gamma,\ \operatorname{Tr}\Gamma = 1 \Big\},$$

an upper bound is obtained by constructing a suitable trial state whose free energy has the correct leading behavior. This task is considerably more subtle than it may first appear, for two main reasons.

First, correlations generated by the interaction term in H_N already contribute at leading order and the trial state must incorporate these correlations. From a technical perspective, this is comparable to approximately diagonalizing the Hamiltonian, with the simplification that error terms only need to be controlled when evaluated in the chosen trial state.

Second, as discussed in the introduction to this section, the size L of the small boxes required for the upper bound is substantially larger than for the lower-bound. This is due to the fact that for the upper bound, Dirichlet boundary conditions are the natural choice. To handle the resulting boundary effects, we proceed by considering slightly larger boxes of side length $L + \ell$ equipped with periodic boundary conditions. A periodic trial state defined on such a box is then extended to a Dirichlet trial state on the larger box. This construction is illustrated in Figure 3.

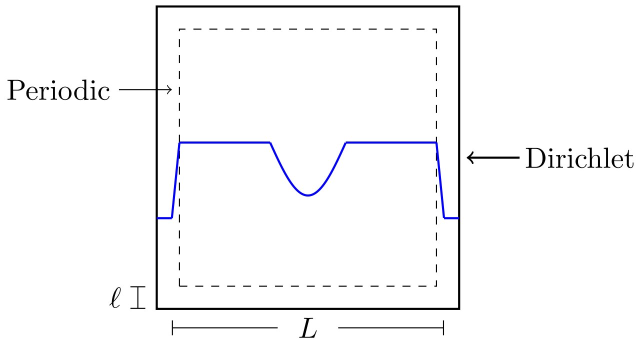

Figure 3: Extension of a trial state with periodic boundary conditions to one with Dirichlet boundary conditions. The dip in the middle corresponds to the influence of the potential as in Figure 1.

The extension of a normalized periodic wave function to a Dirichlet one comes with a kinetic energy cost. Indeed, the modification takes place at the boundary in a volume of order ℓL^2, and the wave function changes from magnitude $L^{-3/2}$ to zero over a length scale ℓ. The corresponding kinetic energy cost is therefore of order $\ell L^2 \times (L^{-3/2}/\ell)^2 = L^{-1}\ell^{-1}$. With N particles in the box, this leads to an error per unit volume of size

$$L^{-3}\, N \times L^{-1}\ell^{-1} = \rho\, L^{-1}\ell^{-1}.$$

A second source of error arises from the fact that placing N particles into the larger periodic box effectively lowers the density. Indeed, the density becomes $N/(L+\ell)^3$, which produces an error in the leading-order interaction energy of size

$$\rho^2 - \frac{N}{(L+\ell)^3} = \rho^2 \left(1 - \frac{1}{(1+\ell L^{-1})^3}\right) = \mathcal{O}(\rho^2 \ell L^{-1}).$$

Both contributions are rigorously derived in Proposition 7.1.

Balancing these two error terms leads to the optimal choice $\ell = \rho^{-1/2}$. If we require the resulting total error to be negligible compared with the Lee–Huang–Yang term of order $\rho^{5/2}$ this imposes the condition $L \gg \rho^{-1}$, or equivalently $\kappa > 1/2$. In order to patch the trial states on different boxes together we again increase the boxes by the range of the potential to rule out interactions between different boxes. The above analysis is unaffected since this can be done by an order 1 change of ℓ.

A novelty of our approach is its extension to mixed states, whereas earlier works were restricted to pure states. An even more substantial difference compared to related results, such as [6, 3], lies in the implementation of a unitary cubic transformation T_c in order to capture the cubic contributions of the Hamiltonian. The use of a unitary transformation offers two decisive advantages. First, the entropy is invariant under unitary conjugation, which greatly simplifies the control of the entropic term. Second, unitarity preserves the trace of the trial state, eliminating additional normalization issues. Both aspects lead to significant technical simplifications compared with the non-unitary framework, where these properties must be handled by more delicate arguments.

As in the aforementioned works, we introduce a cut-off Θ in the cubic transformation to control its action. On boxes of the size required for the upper bound, an unrestricted cubic transformation would otherwise create too many particles and the error terms would become uncontrollable.

Additionally, we make the analysis feasible by renormalizing only those cubic contributions of the form $a^*_{-r}a^*_{r+k}a_k$ with $k \in S$ and $r \in H_k$. Here, after resacling to boxes of size 1, the set S contains all shell momenta, that is, small momenta of order $N^{\kappa/2}$. These make up the relevant contribution in diagonal Bogoliubov-type Hamiltonians like (4.1.8). H_k is a suitable momentum set that enforces $|r|, |r+k| \gg |k|$, i.e., it restricts to processes where a momentum pair far out of the shell is created. We call such a pair a k-connection. We then treat each shell momentum k separately, which allows for a closed expression of $T_k := e^{\mathcal{B}_k}$ with

$$\mathcal{B}_k = \sum_{r \in H_k} N^{1/2}\, \varphi_r\, a^*_{-r}a^*_{r+k}a_k\, \Theta_{k,r} - \text{h.c.} =: \mathcal{B}^\sharp_k - \mathcal{B}^\circ_k,$$

Eventually, we define the cubic transformation as

$$T_c = \prod_{k \in S} e^{\mathcal{B}_k}.$$

Let us comment about the cut-off and how it contributes to the closed form of T_k. The cut-off $\Theta_{k,r}$, in particular, prevents the creation of a k-connection $a^*_{-r}a^*_{r+k}$ if one already exists. As a consequence, one has the nilpotency property

$$(\mathcal{B}^\sharp_k)^2 = 0 = (\mathcal{B}^\circ_k)^2,$$

which turns out to be extremely useful.

For instance one obtains, see Lemma 7.12,

$$X_k^2 := \mathcal{B}^\circ_k \mathcal{B}^\sharp_k = \sum_{r \in H_k} N\, \varphi_r(\varphi_r + \varphi_{r+k})\, a^*_k a_k\, \Theta_{k,r}.$$

Moreover, as shown in Lemma 7.13, the unitary transformation can be written as

$$e^{\mathcal{B}_k} = \cos X_k + \mathcal{B}^\sharp_k \frac{\sin X_k}{X_k} - \frac{\sin X_k}{X_k}\mathcal{B}^\circ_k + \mathcal{B}^\sharp_k \frac{\cos X_k - 1}{X_k^2}\mathcal{B}^\circ_k.$$

As mentioned before, trial states for diagonal Bogoliubov-type Hamiltonians, such as (4.1.8), contain their energy in the shell-momentum modes, while high-momentum excitations can be neglected. Thus, $\mathcal{B}^\circ_k \Gamma = 0$ holds for the relevant trial states, and the previous expression simplifies to

$$e^{\mathcal{B}_k}\Gamma = \left(\cos X_k + \mathcal{B}^\sharp_k \frac{\sin X_k}{X_k}\right)\Gamma;$$

an efficient tool for computing the action of the cubic transformation on the Hamiltonian.

A final novelty lies in the systematic exploitation of the special structure of the trial state. Since Gibbs states Γ of diagonalized Hamiltonians are quasi-free, many contributions vanish identically, for example

$$\mathrm{Tr}\,(Q_3\Gamma) = 0.$$

The main difficulty is that, after dressing the trial state with the cubic transformation, such cancellations no longer hold automatically: for generic cubic terms,

$$\mathrm{Tr}\,(Q_3\, T_c \Gamma T_c^*) \neq 0$$

in general. Nevertheless, by interpreting the cubic transformation as a quadratic operation that annihilates a low-momentum particle k and creates a corresponding k-connection, one finds that several terms remain identically zero, while others have vanishing leading contributions. This observation plays a crucial role in controlling error terms.

The following two sections reproduce material from the works [39, 40] with only the following minor adjustments. Introductory sections have been omitted, and minor changes were made to ensure consistency of notation. [39] is joint work with C. Hainzl, P. T. Nam, R. Seiringer and A. Triay and [40] is joint work with C. Hainzl, B. Schlein and A. Triay.

6 Proof of the Lower Bound

6.1 Introduction

6.1.1 Main result

Recall the main result Theorem 3.2

Theorem. *Let $V \in L^1(\mathbb{R}^3)$ be non-negative, spherically symmetric, compactly supported and radially decreasing. Let $\nu = 1/5000$ and $0 \leq T \leq \rho\mathfrak{a}(\rho\mathfrak{a}^3)^{-\nu}$. Then, in the dilute limit $\rho\mathfrak{a}^3 \to 0$, there exists $C > 0$ such that*

$$f(\rho, T) \geqslant 4\pi\mathfrak{a}\rho^2\left(1 + \frac{128}{15\sqrt{\pi}}\sqrt{\rho\mathfrak{a}^3}\right) + \frac{T^{5/2}}{(2\pi)^3}\int_{\mathbb{R}^3}\log\left(1 - e^{-\sqrt{p^4 + \frac{16\pi\rho\mathfrak{a}}{T}p^2}}\right)\mathrm{d}p$$
$$- C(\rho\mathfrak{a})^{5/2}(\rho\mathfrak{a}^3)^{\nu}.$$

Here the constant $C > 0$ depends only on V.

Here are some remarks on the main result Theorem 3.2.

1. The free energy formula (3.4) holds for $T \geq 0$, thus not only recovering the result on the ground state energy as established in [36] but also resolving the question on the excitation spectrum as predicted in [50]. Our condition $T \leq \rho\mathfrak{a}(\rho\mathfrak{a}^3)^{-\nu}$ allows the case $T \sim \rho\mathfrak{a}$, which is particularly interesting, since in this case the temperature correction is of the same order as the second order Lee–Huang–Yang correction to the ground state energy. An upper bound condition on T is not merely technical, but it is conceptually necessary. The formula (3.4) fails in the higher temperature regime $T \sim \rho^{2/3} = \rho\mathfrak{a}(\rho\mathfrak{a}^3)^{-1/3}$, and in this case deriving the correction to the leading order term in [87, 95] remains a very interesting open problem.

2. Our assumptions on the potential V can be relaxed in many ways. For example, if V is not decreasing but it is radial and satisfies $V(x) \leq CV(y)$ for $|x| \geq |y|$, then our proof applies equally well. In our analysis we fix V (and in particular the scattering length $\mathfrak{a}$) and consider the low-density and low-temperature limits $\rho \to 0$ and $T \to 0$. However, by simple scaling the relevant small parameters are the dimensionless quantities $\mathfrak{a}^3\rho$ and $\mathfrak{a}^2 T$. Our error terms will be bounded only in terms of the range R of V and its integral; more precisely, the constant C in Theorem 3.2 depends only on the dimensionless quantities $R/\mathfrak{a}$ and $\|V\|_{L^1(\mathbb{R}^3)}/\mathfrak{a}$.

Our proof strategy of Theorem 3.2 is different from the approach to the ground state energy problem in [36, 37]. There, the authors use a clever localization technique to reduce the analysis to local systems with periodic boundary conditions where the analysis is well understood. However this method does not seem to extend to the positive temperature case, as one would need to localize not only the energy but the entropy too. In an effort to obtain information on the excitation spectrum, we introduce a new method, compatible with superadditivity of the entropy and that also revolves around a detailed analysis of local systems but with Neumann boundary conditions. We use unitary transformations in the spirit of Bogoliubov's diagonalization idea [13] together with subtle renormalization techniques. While incorporating insights from recent developments [7, 69, 17, 43] on the excitation spectrum in the fixed volume setting, our analysis in the thermodynamic limit introduces several novel ingredients which serve to not only simplify but also extend existing approaches on a conceptual level.

To quickly explain the novelty of the methodology, let us mention that the Lee– Huang–Yang prediction [50] was based on the heuristic assumption of Bose–Einstein condensation (BEC), namely a macroscopic fraction of particles occupy the zero-momentum mode. Proving BEC in the thermodynamic limit is a major open problem in mathematical physics, but to compute the energy it is possible to consider localized systems in small boxes where BEC is easier to prove. Therefore, the localization method is of central importance. This idea was already used in 1998 by Lieb and Yngvason [65] in their proof of the leading order of the ground state energy, where they divided the thermodynamic box into smaller cells with Neumann boundary conditions on each cell, which is the appropriate method for a lower bound.

While this approach sounds plausible, the handling of the Neumann boundary conditions for the second order term of the ground state energy poses a major challenge compared to the typical periodic setting in unit volume [7, 17]. In [36, 37], Fournais and Solovej introduced a very subtle argument to localize the kinetic energy operator, which allows them to keep the calculation essentially in the periodic setting. The intricate analysis in [36, 37], however, does not seem to give access to the excitation spectrum. The main new contribution of the present work is to perform a rigorous analysis of the excitation spectrum on Neumann boxes, thus resolving the Lee–Huang–Yang prediction in a very natural way. Further details of our proof will be given below.

6.1.2 Outline of the proof

General ideas. Our proof strategy is inspired by Bogoliubov's 1947 approach [13] where he proposed an effective method to transform the Hamiltonian of an interacting Bose gas to a non-interacting one, thus enabling an approximation for not only the ground state energy but also the excitation spectrum (the latter is particularly interesting due to its connection to superfluidity). As mentioned already in [13], this method is reasonably good in a mean-field situation where the particles are more or less independent, but it is insufficient for dilute gases where the particles are highly correlated. In fact, a formal application of the Bogoliubov approximation produces an incomplete form of the energy density, see (4.1.12), where the first two terms in a Born approximation of the scattering length $\mathfrak{a}$ appear instead of $\mathfrak{a}$ itself [58]. Thus the main conceptual difficulty in our proof is to put the Bogoliubov approximation on a rigorous footing, including the subtle correction due to the correlation between particles.

Heuristically, an important input for the Bogoliubov approximation is BEC. Although proving BEC in the thermodynamic limit is a major open problem, we are able to prove BEC in localized systems in small boxes, which is sufficient to estimate the free energy. This idea has been carried out in the ground state problem [65, 36]. To be precise, we decompose the thermodynamic box $\Omega = [-L/2, L/2]^3 =: \Lambda_L$ into smaller cubes Λ_ℓ of side length

$$\ell = \frac{\mathfrak{a}}{(\rho\mathfrak{a}^3)^{1/2+\kappa}} \tag{6.1.1}$$

for some small parameter $\kappa > 0$ that will be chosen later. This length scale is chosen larger than the Gross–Pitaevskii length scale (also called healing length)

$$\ell_{\mathrm{GP}} = \frac{1}{\sqrt{\rho\mathfrak{a}}}.$$

At the Gross–Pitaevskii length scale, the gap of the kinetic energy operator is of the same order as the interaction energy of one particle, which makes the proof of BEC easier. On the other hand, at the Gross–Pitaevskii length scale, the contribution from boundary conditions affects the second order term of the energy [7]. Therefore, by focusing on the length scale ℓ slightly larger than the Gross–Pitaevskii length scale, we still have a reasonably good control on the number of excitations, and at the same time we control boundary effects caused by the localization procedure.

The Gross–Pitaevskii regime has been studied extensively in the literature, often in the equivalent formulation of having n particles in the unit box with the interaction potential of the form $n^2V(n(x-y))$. In this setting, the boundary of the domain matters. For periodic boundary conditions, BEC was first derived in [63], and the excitation spectrum was first computed in [7]. The key idea of [7] is that the Bogoliubov approximation can be justified rigorously by using suitable unitary transformations. Later, the excitation spectrum of inhomogeneous trapped Bose gases in $\mathbb{R}^3$ was derived independently in [69] and [17]. For us [69] is particularly relevant, as it contains several modifications of the strategy in [7]. This already led to a simplified proof in the periodic setting in [43] and will further be helpful for the analysis of the present paper.

For our purpose, we have to deal with the Gross–Pitaevskii regime with Neumann boundary conditions. In this case, BEC with an almost optimal bound was derived recently in [12], based on a suitable extension of the strategy in [7], but it turns out that the Neumann boundary conditions cause a serious problem in the computation of the ground state energy and the excitation spectrum. More precisely, in [12], a different choice of the scattering solution satisfying Neumann boundary conditions was made, which was however not explicit, and did not permit to implement the unitary transformation to the desired accuracy. In the study of the ground state problem in [36], a completely different localization technique has been used, which allows to avoid the Neumann boundary issue but requires a subtle modification of the kinetic energy operator.

Thus, while Neumann boundary conditions appear very naturally when seeking a lower bound, their are de facto incompatible with the translational invariant form of the interaction potential $V(x-y)$, making the justification of the Bogoliubov approximation in this case intricate. Solving that problem is the main new contribution of the present work. Roughly speaking, we will handle the Neumann boundary conditions by adapting the mirroring technique for the construction of the Neumann Green function to the context of the transformation kernels, thereby enabling the necessary extension of the strategy in [69, 43]. Moreover, while these works consider the Gross–Pitaesvskii regime, we need push the analysis to much larger length scales, where the interaction potential dominates the kinetic energy and the LHY term is visible compared to boundary effects. This makes the diagonalization of the Hamiltonian harder but is necessary to recover the correct free energy in the thermodynamic limit when summing up the local free energies in all small boxes.

Detailed setting. We shall now explain the proof strategy in detail. It is convenient to consider, for $n \geqslant 0$, the rescaled Hamiltonian

$$H_{n,\ell} = \sum_{i=1}^{n} -\Delta_{x_i} + \sum_{1 \leqslant i < j \leqslant n} \ell^2 V(\ell(x_i - x_j)) \tag{6.1.2}$$

acting on $L^2_s(\Lambda^n)$, the space of square integrable functions that are invariant under permutation of their variables, where Δ is the Neumann Laplacian on the unit box $\Lambda = [-1/2, 1/2]^3$.

The Hamiltonians H_n, defined as in (3.1) with (N, Λ_L) replaced by (n, Λ_ℓ), and $H_{n,\ell}$ defined in (6.1.2) are related via

$$H_n = \frac{1}{\ell^2} \mathcal{T}_\ell^* H_{n,\ell} \mathcal{T}_\ell$$

with the unitary scaling transformation $\mathcal{T}_\ell \Psi(\,\cdot\,) = \ell^{3n/2} \Psi(\ell\,\cdot\,)$. Hence, we are interested in the free energy

$$F_\ell(n) = -T \log \operatorname{Tr}\big(e^{-\frac{H_{n,\ell}}{T\ell^2}}\big)\,. \tag{6.1.3}$$

The main part of our work is devoted to the proof of the following theorem.

Theorem 6.1 (Free energy on small boxes)**.** *Let ℓ be given in* (6.1.1) *with $\kappa = 5\nu = 1/1000$. Let $0 \leq T \leqslant (\rho\mathfrak{a})(\rho\mathfrak{a}^3)^{-\nu}$ and $0 \leqslant n \leqslant C\rho\ell^3$ for some $C > 0$. Then, for $\rho\mathfrak{a}^3$ small enough,*

$$F_\ell(n) \geqslant f_{\mathrm{Bog}}(n, \ell) + \mathcal{O}(\ell^3 (\rho\mathfrak{a})^{5/2} (\rho\mathfrak{a}^3)^\nu), \tag{6.1.4}$$

where

$$f_{\mathrm{Bog}}(n,\ell) = 4\pi \frac{\mathfrak{a}}{\ell^3} n^2 \left(1 + \frac{128}{15\sqrt{\pi}} n^{1/2} \frac{\mathfrak{a}^{3/2}}{\ell^{3/2}}\right) + T \sum_{p \in \pi\mathbb{N}_0^3 \setminus \{0\}} \log\left(1 - e^{\frac{-1}{T\ell^2}\sqrt{p^4 + 16\pi\mathfrak{a} n \ell^{-1} p^2}}\right). \tag{6.1.5}$$

From Theorem 6.1, our main result in Theorem 3.2 then essentially follows from the superadditivity of the free energy.

We shall now explain the main ingredients in the proof of Theorem 6.1. In this introduction, to make the ideas transparent, we will not describe the error estimates in detail and simply write $A \approx B$ if the error is of order $\mathcal{O}(\ell^3(\rho\mathfrak{a})^{5/2}(\rho\mathfrak{a}^3)^\nu)$ which appears in (6.1.4).

We will use the Fock space formalism (see Section 6.2.2) and the unitary transformation $U : L^2_s(\Lambda^n) \to \mathcal{F}_+^{\leqslant n} = \bigoplus_{m=0}^n (u_0^\perp)^{\otimes_s m}$ introduced in [56], defined in (6.2.14), to factor out the contribution of the condensate described by the constant function $u_0 = 1 \in L^2(\Lambda)$. As explained in Lemma 6.3, using the projection $\mathbb{1}_+^{\leqslant n}$ onto $\mathcal{F}_+^{\leqslant n} \subset \mathcal{F} = \bigoplus_{m=0}^\infty L^2_s(\Lambda^m)$ we can write

$$U H_{n,\ell} U^* = \mathbb{1}_+^{\leqslant n} \mathcal{H} \mathbb{1}_+^{\leqslant n},$$

where

$$\mathcal{H} \approx \frac{n^2}{2} V_\ell^{0000} + Q_1 + \mathrm{d}\Gamma(-\Delta) + H_2^{(U)} + Q_2 + Q_3^{(U)} + Q_4 \tag{6.1.6}$$

is an operator on the full Fock space $\mathcal{F}$, with

$$V_\ell^{0000} = \int_{\Lambda^2} V_\ell(x-y)\mathrm{d}x\mathrm{d}y, \tag{6.1.7}$$

$$Q_1 = n^{3/2} \int_{\Lambda^2} V_\ell(x-y) a_x^* \mathrm{d}x\mathrm{d}y + \text{h.c.}, \tag{6.1.8}$$

$$Q_2 = \frac{n}{2} \int_{\Lambda^2} V_\ell(x-y) a_x^* a_y^* \mathrm{d}x\mathrm{d}y + \text{h.c.}, \tag{6.1.9}$$

$$Q_3^{(U)} = \sqrt{(n-\mathcal{N}+1)_+} \int_{\Lambda^2} V_\ell(x-y) a_x^* a_y^* a_x \mathrm{d}x\mathrm{d}y + \text{h.c.}, \tag{6.1.10}$$

$$Q_4 = \frac{1}{2} \int_{\Lambda^2} V_\ell(x-y) a_x^* a_y^* a_x a_y \mathrm{d}x\mathrm{d}y, \tag{6.1.11}$$

$$\begin{aligned} H_2^{(U)} &= n \int_{\Lambda^2} V_\ell(x-y)(a_x^* a_x + a_x^* a_y)\mathrm{d}x\mathrm{d}y - nV_\ell^{0000}\mathcal{N} \\ &\quad - \left(\frac{1}{2} \int_{\Lambda^2} V_\ell(x-y) a_x^* a_y^* \mathrm{d}x\mathrm{d}y\, \mathcal{N} + \text{h.c.} \right). \end{aligned} \tag{6.1.12}$$

Here $\mathcal{N}$ is the number operator on Fock space.

We then conjugate this excitation Hamiltonian with the unitary maps $e^{\mathcal{B}_1}, e^{\mathcal{B}_c}$ and $e^{\mathcal{B}_2}$, where the kernels $\mathcal{B}_1, \mathcal{B}_2$ are quadratic in creation and annihilation operators and $\mathcal{B}_c$ is cubic in those, such that

- The first quadratic transformation $e^{\mathcal{B}_1}$ extracts the leading order of the correlation, effectively renormalizing Q_2 where the short-range interaction V_ℓ gets replaced by a long-range one of mean-field type;

- The cubic transformation $e^{\mathcal{B}_c}$ removes the cubic term $Q_3^{(U)}$, and also renormalizes $H_2^{(U)}$ with a similar replacement for V_ℓ;

- The second quadratic transformation $e^{\mathcal{B}_2}$ diagonalizes the quadratic Hamiltonian emerging from the Bogoliubov approximation, thereby resulting in the correct ground state energy and excitation spectrum.

Note that the Hamiltonian $\mathcal{H}$ is defined on the full Fock space $\mathcal{F} = \mathcal{F}(L^2(\Lambda))$ even though $UH_{n,\ell}U^*$ is only defined on the subspace $\mathcal{F}_+^{\leqslant n}$. Lifting the restriction on the number of particles allows us to use the exact canonical commutation relations. Eventually, we will evaluate the error terms on the Gibbs state of the system, which lives on $\mathcal{F}_+^{\leqslant n}$. Moreover, our estimates will always hold on $\mathcal{F}_+$, which is left invariant under the unitary transformations. In particular, we will often say that two expressions agree on $\mathcal{F}_+$ when they agree in the sense of quadratic forms on $\mathcal{F}_+$.

In the mean-field regime, where V_ℓ is replaced by a long-range potential, only one quadratic transformation is needed to justify the Bogoliubov approximation. This was first done in [86] in the periodic setting and extended to trapped gases in $\mathbb{R}^3$ in [38, 56]. However, in the Gross–Pitaevskii regime, the use of a cubic transformation is crucial to effectively get back to the mean-field regime and capture correctly the excitation spectrum. This key idea was first implemented in [7] in the periodic setting and extended to general trapped cases in $\mathbb{R}^3$ in [69, 17]. An attempt of adapting this strategy to Neumann boundary conditions was given in [12], but it is insufficient to obtain the correct excitation spectrum. Here we will resolve this issue. The main challenge for us is to choose the correct kernels $\mathcal{B}_1$, $\mathcal{B}_c$, and $\mathcal{B}_2$ adapted to the Neumann boundary conditions and to be able to compute the action of the corresponding transformation to the LHY order.

Modified scattering solution. To define the kernels we use the zero-scattering solution ω_ℓ associated with V_ℓ (see Section 6.2.1). Following the approach in [69], we introduce a modified scattering solution

$$\omega_{\ell,\lambda}(x) = \omega_\ell(x)\chi_\lambda(x),$$

where $\omega_\ell(x) = \omega(\ell x)$ and $\chi_\lambda(x) = \chi(\lambda^{-1}x)$ with χ a fixed C^∞ radial function approximating $\mathbb{1}_{|x|\leq 1}$. The function $\omega_{\ell,\lambda}$ satisfies

$$-\Delta\omega_{\ell,\lambda} = \frac{1}{2}V_\ell(1-\omega_\ell) - \frac{1}{2}\epsilon_{\ell,\lambda}, \quad \frac{1}{2}\epsilon_{\ell,\lambda}(x) = \frac{\mathfrak{a}}{\ell}\lambda^{-3}\left(\frac{\chi''}{|\cdot|}\right)(\lambda^{-1}x). \tag{6.1.13}$$

In our final estimate we will eventually choose

$$\ell^{-1} \ll \lambda \ll 1.$$

The first constraint $\ell^{-1} \ll \lambda$, which is inspired by [7], ensures that the range of $\epsilon_{\ell,\lambda}$ in (6.1.13) is much longer than that of V_ℓ, and hence in our calculation it plays the role of a renormalized version of V_ℓ. Moreover, the second constraint $\lambda \ll 1$, which is inspired by [69], ensures that $\ell\epsilon_{\ell,\lambda}$ tends to a delta interaction, thus simplifying several estimates and also enabling us to go beyond the Gross–Pitaevskii regime.

Heuristically, as proposed in the previous works on the Gross–Pitaevskii regime [7, 69, 17], the correlation structure of particles can be encoded using two transformations $e^{\mathcal{B}_1}$ and $e^{\mathcal{B}_c}$. More precisely, by putting the scattering solution $-n\omega_{\ell,\lambda}$ in the kernels $\mathcal{B}_1$, $\mathcal{B}_c$, we hope to replace the short range potential V_ℓ by the longer-range one $\epsilon_{\ell,\lambda}$. The naive choice of $\mathcal{B}_1$

$$-n\int_{\Lambda^2}\omega_{\ell,\lambda}(x-y)a_x^*a_y^*\mathrm{d}x\mathrm{d}y - \text{h.c.},$$

does not work in our case since the function $-n\omega_{\ell,\lambda}$ does not satisfy the Neumann boundary conditions. To fix this issue, we use a symmetrization technique as follows.

Neumann symmetrization. We shall construct a kernel $\widetilde{K}(x,y)$ that can be interpreted as a symmetrized version of $-n\omega_{\ell,\lambda}(x-y)$ satisfying Neumann boundary conditions in an appropriate sense. It belongs to $H^1(\Lambda^2)$ and satisfies the following two useful properties:

$$\widetilde{K}(x,y) = -n\omega_{\ell,\lambda}(x-y), \quad \forall x,y \in \{z\in\Lambda : \operatorname{dist}(z,\partial\Lambda) > \lambda\} \tag{6.1.14}$$

and that the operator with kernel $\widetilde{K}(x,y)$ is diagonal in the Neumann basis, see (6.1.17).

The construction uses the same mirroring technique as in the construction of the Neumann Green's function. Denoting

$$\Lambda + z = \{x+z : x\in\Lambda\}, \quad z\in\mathbb{Z}^3$$

we define the transformation

$$P_z : \Lambda \to \Lambda + z, \quad (P_z(x))_i = (-1)^{z_i}x_i + z_i, \tag{6.1.15}$$

which maps a point $x\in\Lambda$ to its mirror point in the box $\Lambda + z$. For a visual illustration in 2D, we refer to Figure 4, where the mirror points of $x\in\Lambda$ are plotted in the neighboring boxes of Λ.

We define the function $\widetilde{K} : \Lambda^2 \to \mathbb{R}$ as

$$\widetilde{K}(x,y) = -\sum_{z\in\mathbb{Z}^3} n\omega_{\ell,\lambda}(P_z(x)-y). \tag{6.1.16}$$

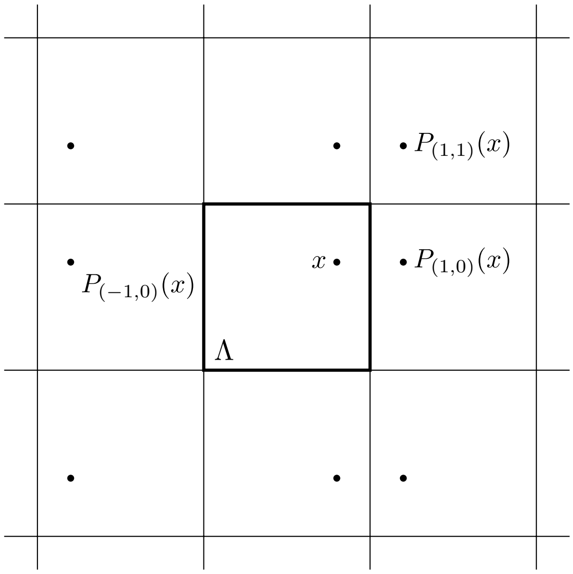

Figure 4: Relevant mirror points of x shown in two dimensions.

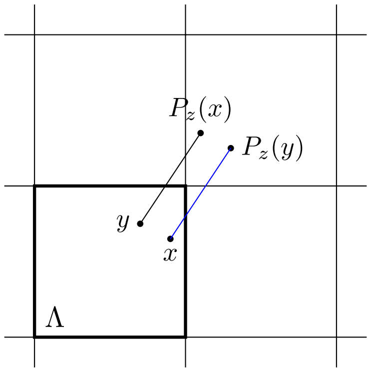

Figure 5: The distance is conserved.

Observe that while $\{\Lambda + z : z \in \mathbb{Z}^3\}$ covers all of $\mathbb{R}^3$, due to the cutoff χ_λ there is a contribution to the sum only if $|P_z(x) - y| \leqslant \lambda \ll 1$ and the property (6.1.14) follows immediately. Taking into account that $y \in \Lambda$ we find that in the last term of (6.1.16) only the summands with

$$z \in \mathbb{Z}^3_{\leqslant 1} := \{z \in \mathbb{Z}^3 : \max_i |z_i| \leqslant 1\}$$

are non-zero. Thus, the sum is finite and $\widetilde{K}$ is well-defined by (6.1.16). Moreover, $\widetilde{K}$ is symmetric, namely $\widetilde{K}(x,y) = \widetilde{K}(y,x)$, since $|P_z(x) - y| = |P_z(y) - x|$ for all $z \in \mathbb{Z}^3_{\leqslant 1}$ (see Figure 5 for a 2D illustration).

In fact, as we will see in Lemma 6.4, it is also diagonal in the Neumann basis

$$\widetilde{K}(x,y) = -\sum_{p \in \pi \mathbb{N}_0^3} n\widehat{\omega}_{\ell,\lambda}(p) u_p(x) u_p(y), \tag{6.1.17}$$

where $u_p \in L^2(\Lambda)$ are Neumann eigenfunctions given in (6.2.11) and we used the following convention of the Fourier transform

$$\widehat{f}(p) = \int_{\mathbb{R}^3} f(x) e^{-ip\cdot x} \mathrm{d}x. \tag{6.1.18}$$

Since the local property (6.1.14) does not obviously follow from (6.1.17), both the forms (6.1.16) and (6.1.17) will be useful in the following.

Next, we remove from the function $\widetilde{K}$ any contribution from the zero-momentum mode by using the projection $Q = 1 - |u_0\rangle\langle u_0|$. This results in the function

$$K(x,y) = (Q^{\otimes 2}\widetilde{K})(x,y) = \widetilde{K}(x,y) + n\widehat{\omega}_{\ell,\lambda}(0) = -\sum_{p\in\pi\mathbb{N}_0^3\setminus\{0\}} n\widehat{\omega}_{\ell,\lambda}(p)u_p(x)u_p(y), \tag{6.1.19}$$

which is the key tool to define the transformations $e^{\mathcal{B}_1}$ and $e^{\mathcal{B}_c}$.

First quadratic transformation. We define the first transformation kernel

$$\mathcal{B}_1 = \frac{1}{2}\int_{\Lambda^2} K(x,y)a_x^*a_y^*\mathrm{d}x\mathrm{d}y - \text{h.c.} \tag{6.1.20}$$

with K given in (6.1.19). We will show that by conjugating the excitation Hamiltonian $\mathcal{H}$ in (6.1.6) by the quadratic transformation $e^{\mathcal{B}_1}$, we essentially renormalize Q_2 and extract the leading order contribution $4\pi\mathfrak{a}n^2\ell^{-1}$ (see Lemma 6.7).

Note that thanks to the last identity in (6.1.19), we may rewrite (6.1.20) as

$$\mathcal{B}_1 = \frac{1}{2}\sum_{p\in\pi\mathbb{N}_0^3\setminus\{0\}} (-n\widehat{\omega}_{\ell,\lambda}(p))a_p^*a_p^* - \text{h.c.}, \tag{6.1.21}$$

where we denoted $a_p^* = a^*(u_p)$ the creation operator on Fock space. The formula (6.1.21) can be compared with the kernel in the translation-invariant case in [7, 43], where $a_p^*a_{-p}^*$ is used instead of $a_p^*a_p^*$. However, the algebraic structure is not as nice as in the translation-invariant case and it is often more convenient to work in configuration space where pointwise estimates, the identity (6.1.14) or the non-negativity of V are available.

We shall now explain some details of the action of the transformation $e^{\mathcal{B}_1}$. As we show in Lemma 6.10, we have

$$[\mathrm{d}\Gamma(-\Delta) + Q_4, \mathcal{B}_1] \approx \int_{\Lambda^2}\Big((-\Delta_2 K)(x,y) + \frac{1}{2}V_\ell(x-y)K(x,y)\Big)a_x^*a_y^*\mathrm{d}x\mathrm{d}y + \text{h.c.},$$

which, together with the definition (6.1.19) and the scattering equation (6.1.13), gives

$$[\mathrm{d}\Gamma(-\Delta) + Q_4, \mathcal{B}_1] + Q_2 \approx \widetilde{Q}_2 = \int_{\Lambda^2}\widetilde{Q}_2(x,y)a_x^*a_y^*\mathrm{d}x\mathrm{d}y + \text{h.c.}, \tag{6.1.22}$$

where

$$\widetilde{Q}_2(x,y) = \frac{n}{2}\sum_{z\in\mathbb{Z}^3}\epsilon_{\ell,\lambda}(P_z(x)-y) + \frac{n}{2}\sum_{z\in\mathbb{Z}^3\setminus\{0\}}(V_\ell(\omega_{\ell,\lambda}-1)(P_z(x)-y) - V_\ell(x-y)\omega_{\ell,\lambda}(P_z(x)-y)).$$

Here $\widetilde{Q}_2(x,y)$ contains the function $\epsilon_{\ell,\lambda}$ in the first sum, which can be interpreted as a renormalized version of the short-range potential V_ℓ and inherits the symmetrization of K, as well as some boundary contribution in the second sum which will disappear after the cubic transformation $e^{\mathcal{B}_c}$. The approximation (6.1.22) is exactly the motivation for the choice of the kernel $\mathcal{B}_1$, in the same spirit as in [69, 42].

From (6.1.22) and the Duhamel expansion (see (6.4.7) for an explanation) we can write

$$
\begin{aligned}
&e^{-\mathcal{B}_1}(\mathrm{d}\Gamma\,(-\Delta)+Q_2+Q_4)e^{\mathcal{B}_1}-\mathrm{d}\Gamma(-\Delta)-Q_4\\
&=\int_0^1 e^{-t\mathcal{B}_1}\Big([\mathrm{d}\Gamma\,(-\Delta)+Q_4,\mathcal{B}_1]+Q_2\Big)e^{t\mathcal{B}_1}\mathrm{d}t+\int_0^1\int_t^1 e^{-s\mathcal{B}_1}[Q_2,\mathcal{B}_1]e^{s\mathcal{B}_1}\mathrm{d}s\mathrm{d}t\\
&\approx\int_0^1 e^{-t\mathcal{B}_1}\widetilde{Q}_2e^{t\mathcal{B}_1}\mathrm{d}t+\int_0^1\int_t^1 e^{-s\mathcal{B}_1}[Q_2,\mathcal{B}_1]e^{s\mathcal{B}_1}\mathrm{d}s\mathrm{d}t\\
&=\widetilde{Q}_2+\int_0^1\int_0^t e^{-s\mathcal{B}_1}[\widetilde{Q}_2,\mathcal{B}_1]e^{s\mathcal{B}_1}\mathrm{d}s\mathrm{d}t+\int_0^1\int_t^1 e^{-s\mathcal{B}_1}[Q_2,\mathcal{B}_1]e^{s\mathcal{B}_1}\mathrm{d}s\mathrm{d}t.
\end{aligned}
\tag{6.1.23}
$$

As proved in Lemma 6.11, the last two terms in (6.1.23) are essentially two constant contributions. In particular the last term helps us to correct the constant in (6.1.6) and we recover the full leading order of the energy,

$$
\begin{aligned}
&\frac{1}{2}n^2V_\ell^{0000}+\int_0^1\int_t^1 e^{-s\mathcal{B}_1}[Q_2,\mathcal{B}_1]e^{s\mathcal{B}_1}\mathrm{d}s\mathrm{d}t\\
&\approx\frac{1}{2}n^2V_\ell^{0000}+\frac{1}{2}[Q_2,\mathcal{B}_1]\approx\frac{1}{2}n^2V_\ell^{0000}+\frac{n}{2}\int_{\Lambda^2}V_\ell(x-y)K(x,y)\mathrm{d}x\mathrm{d}y\approx 4\pi\mathfrak{a}n^2\ell^{-1}
\end{aligned}
$$

with an error smaller than the second order in the LHY formula. The other term is

$$
\int_0^1\int_0^t e^{-s\mathcal{B}_1}[\widetilde{Q}_2,\mathcal{B}_1]e^{s\mathcal{B}_1}\mathrm{d}s\mathrm{d}t\approx\frac{1}{2}[\widetilde{Q}_2,\mathcal{B}_1]\approx\sum_{p\in\pi\mathbb{N}_0^3\setminus\{0\}}\frac{|n\widehat{\epsilon}_{\ell,\lambda}(p)|^2}{2p^2},
\tag{6.1.24}
$$

which will be combined with another constant contribution coming from the transformation $e^{\mathcal{B}_2}e^{\mathcal{B}_c}$ to give the correct LHY second order term.

So far, we have seen that the quadratic transformation $e^{\mathcal{B}_1}$ essentially replaces $\mathrm{d}\Gamma(-\Delta)+Q_4+Q_2$ by $\mathrm{d}\Gamma(-\Delta)+Q_4+\widetilde{Q}_2$ plus some constants. Furthermore, we will show in Lemma 6.12 that

$$
e^{-\mathcal{B}_1}H_2^{(U)}e^{\mathcal{B}_1}\approx n\int_{\Lambda^2}V_\ell(x-y)(a_x^*a_x+a_x^*a_y)\mathrm{d}x\mathrm{d}y-8\pi\mathfrak{a}n\ell^{-1}\mathcal{N},
\tag{6.1.25}
$$

namely the term $\mathcal{N}nV_\ell^{0000}+\big(\frac{1}{2}\int_{\Lambda^2}V_\ell(x-y)a_x^*a_y^*\mathrm{d}x\mathrm{d}y\mathcal{N}+\text{h.c.}\big)$ in $H_2^{(U)}$ is replaced by $8\pi\mathfrak{a}\frac{n}{\ell}\mathcal{N}$. Moreover, as proved in Lemma 6.14 we have

$$
e^{-\mathcal{B}_1}(Q_1+Q_3^{(U)})e^{\mathcal{B}_1}\approx Q_3=\sqrt{n}\int_{\Lambda^2}V_\ell(x-y)a_x^*a_y^*a_x\mathrm{d}x\mathrm{d}y+\text{h.c.}
\tag{6.1.26}
$$

The cubic term Q_3 then will be handled by the cubic transformation $e^{\mathcal{B}_c}$ below. In summary we have

$$
\begin{aligned}
e^{-\mathcal{B}_1}\mathcal{H}e^{\mathcal{B}_1}\approx{}&4\pi\mathfrak{a}n^2\ell^{-1}+\mathrm{d}\Gamma(-\Delta)+Q_4+\widetilde{Q}_2+Q_3+n\int_{\Lambda^2}V_\ell(x-y)(a_x^*a_x+a_x^*a_y)\mathrm{d}x\mathrm{d}y\\
&-8\pi\mathfrak{a}n\ell^{-1}\mathcal{N}.
\end{aligned}
$$

Cubic transformation. Next, for the cubic transformation, we define

$$
\mathcal{B}_c=\frac{\theta_M(\mathcal{N})}{\sqrt{n}}\int_{\Lambda^2}K(x,y)q_x^*a_y^*q_x\mathrm{d}x\mathrm{d}y-\text{h.c.}
\tag{6.1.27}
$$

Here $q_x = a(Q_x)$, where $Q_x(y) = Q(x,y)$, is used instead of a_x to ensure that $\mathcal{B}_c$ leaves $\mathcal{F}_+$ invariant, and $\theta_M(\mathcal{N})$ is a smooth cut-off on the sector $\{\mathcal{N} \leq M\}$, with $1 \ll M \ll n$, which prevents $e^{\mathcal{B}_c}$ from creating too many excitations.

As proved in Lemma 6.15, by using $e^{\mathcal{B}_c}$ we can remove the cubic term Q_3 in (6.1.26) and also renormalize some quadratic terms. More precisely, using the Duhamel formula, we can expand

$$\begin{aligned} &e^{-\mathcal{B}_c}\Big(\mathrm{d}\Gamma(-\Delta) + Q_4 + Q_3\Big)e^{\mathcal{B}_c} - \mathrm{d}\Gamma(-\Delta) - Q_4 \\ &= \int_0^1 e^{-t\mathcal{B}_c}\Big([\mathrm{d}\Gamma(-\Delta) + Q_4, \mathcal{B}_c] + Q_3\Big)e^{t\mathcal{B}_c}\mathrm{d}t + \int_0^1\int_t^1 e^{-s\mathcal{B}_c}[Q_3, \mathcal{B}_c]e^{s\mathcal{B}_c}\mathrm{d}s\mathrm{d}t. \end{aligned} \tag{6.1.28}$$

We have chosen the cubic kernel $\mathcal{B}_c$ such that

$$[\mathrm{d}\Gamma(-\Delta) + Q_4, \mathcal{B}_c] + Q_3 \approx 0,$$

and hence the first term on the right-hand side of (6.1.28) is negligible. Moreover, the last term in (6.1.28) can be put together with the transformations of (6.1.25), and we can show that

$$e^{-\mathcal{B}_c}\Big(\int_{\Lambda^2} nV_\ell(x-y)(a_x^*a_x + a_x^*a_y)\mathrm{d}x\mathrm{d}y - 8\pi\mathfrak{a}n\ell^{-1}\mathcal{N}\Big)e^{\mathcal{B}_c} + \int_0^1\int_t^1 e^{-s\mathcal{B}_c}[Q_3, \mathcal{B}_c]e^{s\mathcal{B}_c}\mathrm{d}s\mathrm{d}t$$

is essentially $8\pi\mathfrak{a}n\ell^{-1}\mathcal{N}$. After the cubic transformation, we may remove the boundary contribution in $\widetilde{Q}_2$ and obtain the desired pairing term (see Lemma 6.22)

$$e^{-\mathcal{B}_c}\widetilde{Q}_2e^{\mathcal{B}_c} \approx \frac{n}{2}\int_{\Lambda^2}\sum_{z\in\mathbb{Z}^3}\epsilon_{\ell,\lambda}(P_z(x)-y)a_x^*a_y^*\mathrm{d}x\mathrm{d}y + \text{h.c.}$$

which coincides with

$$\frac{1}{2}\sum_{p\in\pi\mathbb{N}_0^3\setminus\{0\}} n\widehat{\epsilon}_{\ell,\lambda}(p)(a_p^*a_p^* + a_pa_p)$$

when restricted to $\mathcal{F}_+$. Thus we arrive at

$$e^{-\mathcal{B}_c}e^{-\mathcal{B}_1}\mathcal{H}e^{\mathcal{B}_1}e^{\mathcal{B}_c} \approx 4\pi\mathfrak{a}n^2\ell^{-1} + \mathbb{H}_{\mathrm{Bog}} + Q_4$$

with the quadratic Bogoliubov Hamiltonian

$$\begin{aligned} \mathbb{H}_{\mathrm{Bog}} = &\sum_{p\in\pi\mathbb{N}_0^3\setminus\{0\}}\Big(p^2 + 8\pi\mathfrak{a}\frac{n}{\ell}\Big)a_p^*a_p + \frac{1}{2}\sum_{p\in\pi\mathbb{N}_0^3\setminus\{0\}} n\widehat{\epsilon}_{\ell,\lambda}(p)(a_p^*a_p^* + a_pa_p) \\ &+ \frac{1}{2}\sum_{p\in\pi\mathbb{N}_0^3\setminus\{0\}}\frac{|n\widehat{\epsilon}_{\ell,\lambda}(p)|^2}{2p^2}. \end{aligned} \tag{6.1.29}$$

Second quadratic transformation. It is well-known that the quadratic operator in (6.1.29) can be diagonalized explicitly. To be precise, by choosing the second quadratic transformation $e^{\mathcal{B}_2}$ with

$$\mathcal{B}_2 = \frac{1}{2}\sum_{p\in\pi\mathbb{N}_0^3\setminus\{0\}}\varphi_p(a_p^*a_p^* - a_pa_p), \tag{6.1.30}$$

for suitable φ_p one can show that

$$e^{-\mathcal{B}_2}\mathbb{H}_{\mathrm{Bog}}e^{\mathcal{B}_2} + 4\pi\mathfrak{a}n^2\ell^{-1} \approx E_{n,\ell} + \mathrm{d}\Gamma(E_{\mathrm{Bog}})$$

on $\mathcal{F}_+$ with the ground state energy

$$E_{n,\ell} := 4\pi\mathfrak{a}n^2\ell^{-1} + \frac{1}{2}\sum_{p\in\pi\mathbb{N}_0^3\backslash\{0\}}\left[\sqrt{p^4+16\pi\mathfrak{a}n\ell^{-1}p^2} - p^2 - 8\pi\mathfrak{a}\frac{n}{\ell} + \frac{(8\pi\mathfrak{a}n\ell^{-1})^2}{2p^2}\right]$$

and the effective Hamiltonian

$$\mathrm{d}\Gamma(E_{\mathrm{Bog}}) = \sum_{p\in\pi\mathbb{N}_0^3\backslash\{0\}}\sqrt{p^4+16\pi\mathfrak{a}n\ell^{-1}p^2}\,a_p^*a_p.$$

In this way, we recover all information on the excitation spectrum predicted by the Bogoliubov approximation [13].

Localization on Fock space. On the technical level, we can only estimate the relevant errors in the above analysis on the low particle number sectors in $\mathcal{F}_+^{\leq n}$. The high particle number sectors have to be handled differently. By adapting the analysis in [63], we are able to prove BEC for the Gibbs state, i.e. there are only few excitations. In combination with the Gibbs variational principle, this allows to ignore the free energy coming from the high particle number sectors. Finally, using the localization method on the number of excited particles in the spirit of [59, 56], we put together the low and high particle number sectors, thus concluding the proof of Theorem 6.1.

Organization of the proof. In Section 6.2 we recall general properties of the scattering length $\mathfrak{a}$ and the scattering solution. We also introduce some notation on the Fock space formalism; in particular we use the excitation map U defined in [56] to link $H_{n,\ell}$ to an excitation Hamiltonian on the Fock space of excitations $\mathcal{F}(u_0^\perp)$. In Section 6.3, we explain in detail the construction of the Neumann kernel $K(x,y)$ by symmetrization. We then conjugate this excitation Hamiltonian with the unitary maps $e^{\mathcal{B}_1}, e^{\mathcal{B}_c}$ and $e^{\mathcal{B}_2}$. The actions of the transformations $e^{\mathcal{B}_1}, e^{\mathcal{B}_c}$ and $e^{\mathcal{B}_2}$ are carried out in Sections 6.4, 6.5 and 6.6, respectively. In Section 6.7, we prove BEC for the Gibbs state associated with $\mathbb{H}_{n,\ell}$ as well as derive some rough estimates for the kinetic and interaction energies, which are needed for the localization technique on the number of excited particles. Finally, we prove Theorem 6.1 in Section 6.8, and conclude Theorem 3.2 in Section 6.9.

Notation. We always use $C > 0$ to denote a general constant which depends only on V. We also write $A \lesssim B$ if $A \leq CB$, and write $A \ll B$ if $A/B \to 0$ when $\rho\mathfrak{a}^3 \to 0$. Moreover, all operator inequalities are interpreted as quadratic forms, namely we write $S \geq T$ on $\mathfrak{H}$, if $\langle u, Su\rangle \geq \langle u, Tu\rangle$ for all $u \in \mathfrak{H}$ (which is in particular convenient when S and T act on a larger Hilbert space and do not leave $\mathfrak{H}$ invariant). When writing an operator in terms of the distributional creation and annihilation operator, we omit the integration variable for shortness if it is unambiguous, e.g., we write $\int T(x,y)a_x^*a_y$ instead of $\int T(x,y)a_x^*a_y\mathrm{d}x\mathrm{d}y$.

6.2 Preliminaries

In this section we collect some standard tools, which are helpful to transform the Hamiltonian $H_{n,\ell}$ in (6.1.2).

6.2.1 Modified Scattering Problem

Recall from Lemma 2.3 that the equation

$$-\Delta\omega = \frac{1}{2}V(1-\omega) \text{ in } \mathbb{R}^3, \quad \lim_{|x|\to\infty}\omega(x) = 0 \tag{6.2.1}$$

has a unique solution ω satisfying $0 \leqslant \omega \leqslant 1$. The scattering length $\mathfrak{a}$ of V is given by

$$8\pi\mathfrak{a} = \int_{\mathbb{R}^3} V(1-\omega). \tag{6.2.2}$$

Since the scattering solution ω is harmonic outside the support of V, we have the exact formula for $x \in \mathbb{R}^3 \setminus \mathrm{Supp}(V)$:

$$\omega(x) = \frac{\mathfrak{a}}{|x|}. \tag{6.2.3}$$

In our application, we will consider a modified version of the scattering solution ω. Let ℓ be as in (6.1.1). Defining $\omega_\ell(x) = \omega(\ell x)$, and recalling that $V_\ell(x) = \ell^2 V(\ell x)$, obviously from (6.2.1) we have the rescaled equation

$$-\Delta\omega_\ell = \frac{1}{2}V_\ell(1-\omega_\ell). \tag{6.2.4}$$

Next, let us introduce a cut-off version of ω_ℓ. Following [69], for

$$2R/\ell < \lambda < 1/4, \tag{6.2.5}$$

we define

$$\omega_{\ell,\lambda}(x) = \omega_\ell(x)\chi_\lambda(x), \quad \chi_\lambda(x) = \chi(\lambda^{-1}x),$$

where χ is a fixed C^∞ radial function satisfying

$$\chi(x) = 0 \text{ for } |x| \geqslant 1 \quad \text{and} \quad \chi(x) = 1 \text{ for } |x| < \frac{1}{2}.$$

Under the assumption that $\mathrm{Supp}\,V \subset \{|x| \leqslant R\}$ and that $\lambda > 2R\ell^{-1}$, the truncated scattering solution $\omega_{\ell,\lambda}$ satisfies a modified scattering equation

$$-\Delta\omega_{\ell,\lambda} = \frac{1}{2}V_\ell(1-\omega_\ell) - \frac{1}{2}\epsilon_{\ell,\lambda}, \tag{6.2.6}$$

where

$$\frac{1}{2}\epsilon_{\ell,\lambda} = \Delta(\omega_{\ell,\lambda} - \omega_\ell) = 2\nabla\omega_\ell \cdot \nabla\chi_\lambda + \omega_\ell\Delta\chi_\lambda. \tag{6.2.7}$$

From (6.2.7) we see that $\epsilon_{\ell,\lambda}$ and V_ℓ have disjoint support. Therefore, we may use (6.2.3) in (6.2.7) and that χ is radial to arrive at

$$\frac{1}{2}\epsilon_{\ell,\lambda}(x) = \frac{\mathfrak{a}}{\ell}\lambda^{-3}\left(\frac{\chi''}{|\cdot|}\right)(\lambda^{-1}x), \tag{6.2.8}$$

where we interpreted $\chi(x) = \chi(|x|)$ when writing χ''.

Finally, we gather some of their properties in the following lemma.

Lemma 6.2. *Let $2R/\ell < \lambda$. Then for all $x \in \mathbb{R}^3$, we have the pointwise bounds*

$$0 \leqslant \omega_{\ell,\lambda}(x) \leqslant \frac{C\mathbb{1}_{\{|x|\leqslant\lambda\}}}{|\ell x|+1}, \quad |\nabla\omega_{\ell,\lambda}(x)| \leqslant \frac{C\ell\mathbb{1}_{\{|x|\leqslant\lambda\}}}{|\ell x|^2+1}, \quad |\epsilon_{\ell,\lambda}(x)| \leqslant \frac{C}{\ell}\lambda^{-3}\mathbb{1}_{\{\lambda/2\leqslant|x|\leqslant\lambda\}}. \tag{6.2.9}$$

Moreover,

$$\int_{\mathbb{R}^3} \epsilon_{\ell,\lambda} = 8\pi\mathfrak{a}\ell^{-1}. \tag{6.2.10}$$

Note that the last bound in (6.2.9) implies that $\epsilon_{\ell,\lambda}(P_z(x)-y)=0$ for $z\notin\mathbb{Z}^3_{\leqslant 1}$.

Proof. From (6.2.3) and $0\leqslant\omega\leqslant 1$ we obtain

$$0\leqslant\omega(x)\leqslant\frac{C}{|x|+1},\quad |\nabla\omega(x)|\leqslant\frac{C}{|x|^2+1}.$$

Moreover $\mathrm{Supp}\,(\chi_\lambda)\subset B_\lambda(0)$ and $|\nabla\chi_\lambda|\leqslant C\lambda^{-1}\mathbb{1}_{\{\lambda/2\leqslant|x|\leqslant\lambda\}}$, which implies the first two bounds in (6.2.9). The last bound in (6.2.9) follows from (6.2.7) and $\mathrm{Supp}(\chi'')\subset\{\lambda/2\leqslant|x|\leqslant\lambda\}$. Finally, since $\omega_{\ell,\lambda}$ is compactly supported, from (6.2.6) and (6.2.2) we have

$$0=2\int_{\mathbb{R}^3}\Delta\omega_{\ell,\lambda}=\int_{\mathbb{R}^3}V_\ell(1-\omega_\ell)-\int_{\mathbb{R}^3}\epsilon_{\ell,\lambda}=8\pi\mathfrak{a}\ell^{-1}-\int_{\mathbb{R}^3}\epsilon_{\ell,\lambda}.$$

This implies (6.2.10). □

6.2.2 Neumann Fock Space Formalism

For $m\in\pi\mathbb{N}_0^3=\pi\{0,1,2,...\}^3$, let us denote

$$u_m(x)=\prod_{i=1}^3 u_{m_i}(x_i),\quad u_{m_i}(x)=\left\{\begin{array}{cc}1, & m_i=0\\ \sqrt{2}\cos(m_i(x_i+1/2)), & m_i\neq 0\end{array}\right. . \tag{6.2.11}$$

The family $\{u_m\}_{m\in\pi\mathbb{N}_0^3}$ is an orthonormal basis of $L^2(\Lambda)$ satisfying Neumann boundary conditions. A special role is played by the condensate function $u_0=\mathbb{1}_\Lambda$.

Recall from Section 2.1 the notion of the Fock space for the Hilbert space $\mathfrak{H}$. We consider

$$\mathcal{F}(\mathfrak{H})=\bigoplus_{n\geqslant 0}\mathfrak{H}^{\otimes_s n},\quad \mathcal{F}^{\leqslant k}(\mathfrak{H})=\bigoplus_{n=0}^{k}\mathfrak{H}^{\otimes_s n},$$

the bosonic Fock space over $\mathfrak{H}$ and its truncated version, respectively. In our application, we focus on the cases where $\mathfrak{H}=L^2(\Lambda)$ or the subspace $u_0^\perp\subset L^2(\Lambda)$, and we will denote respectively the Fock spaces

$$\mathcal{F}=\mathcal{F}(L^2(\Lambda)),\quad \mathcal{F}_+=\mathcal{F}(u_0^\perp).$$

In particular, the particle number and the excitation number are denoted

$$\mathcal{N}=\mathrm{d}\Gamma(\mathbb{1})=\sum_{p\in\pi\mathbb{N}_0^3}a_p^*a_p,\qquad \mathcal{N}_+=\mathrm{d}\Gamma(Q)=\sum_{p\neq 0}a_p^*a_p,$$

where we introduced the notation $\sum_{p\neq 0}:=\sum_{p\in\pi\mathbb{N}_0^3\setminus\{0\}}$ and $Q=1-|u_0\rangle\langle u_0|$. Additionally, we denote the orthogonal projections onto the excitation Fock space $\mathcal{F}_+$ and onto the truncated Fock space $\mathcal{F}_+^{\leqslant n}$ by $\mathbb{1}_+=\mathbb{1}^{\{\mathcal{N}=\mathcal{N}_+\}}$ and $\mathbb{1}_+^{\leqslant n}=\mathbb{1}^{\{\mathcal{N}=\mathcal{N}_+\}}\mathbb{1}^{\{\mathcal{N}_+\leqslant n\}}$ for $n\geqslant 0$, respectively.

With this formalism, the $n-$particle Hamiltonian in (6.1.2) can be written as

$$\begin{aligned} H_{n,\ell}&=\sum_{p\in\pi\mathbb{N}_0^3}p^2a_p^*a_p+\frac{1}{2}\sum_{p,q,r,s\in\pi\mathbb{N}_0^3}V_\ell^{pqrs}a_p^*a_q^*a_ra_s &(6.2.12)\\ &=\int_\Lambda\nabla_xa_x^*\nabla_xa_x\mathrm{d}x+\frac{1}{2}\int_{\Lambda^2}V_\ell(x-y)a_x^*a_y^*a_xa_y\mathrm{d}x\mathrm{d}y, &(6.2.13)\end{aligned}$$

where we have denoted

$$V_\ell^{pqrs}=\langle u_p\otimes u_q,V_\ell u_r\otimes u_s\rangle_{L^2(\Lambda^2)}.$$

The right-hand side (6.2.13) is an operator on Fock space $\mathcal{F}=\mathcal{F}(L^2(\Lambda))$ but we will always consider its restriction to the n-particle sector which coincides with the expression in (6.1.2).

6.2.3 The Excitation Hamiltonian

In this section, we will rewrite the Hamiltonian $H_{n,\ell}$ in the Fock space of excitations $\mathcal{F}_+ = \mathcal{F}(u_0^\perp)$. We do so by using the unitary transformation $U : L^2_s(\Lambda^n) \to \mathcal{F}_+^{\leqslant n}$ introduced in [56]

$$U(\Psi) = \bigoplus_{j=0}^{n} \frac{1}{\sqrt{(n-j)!}} Q^{\otimes j} a_0^{n-j} \Psi. \tag{6.2.14}$$

On $\mathcal{F}_+^{\leqslant n}$ and for all $p, q \neq 0$, it satisfies

$$Ua_0^* a_0 U^* = n - \mathcal{N}_+, \qquad Ua_p^* a_q U^* = a_p^* a_q, \tag{6.2.15}$$

$$Ua_p^* a_0 U^* = a_p^* \sqrt{n - \mathcal{N}_+}, \qquad Ua_0^* a_q U^* = \sqrt{n - \mathcal{N}_+} a_q. \tag{6.2.16}$$

Implementing these transformations on $UH_{n,\ell}U^*$, we obtain the following lemma.

Lemma 6.3. *Let $H_{n,\ell}$ be as in (6.1.2). We have the following operator identity on $\mathcal{F}_+^{\leqslant n}$*

$$UH_{n,\ell}U^* = \mathbb{1}_+^{\leqslant n} \mathcal{H} \mathbb{1}_+^{\leqslant n},$$

where

$$\mathcal{H} = \frac{n^2}{2} V_\ell^{0000} + Q_1 + \mathrm{d}\Gamma(-\Delta) + H_2^{(U)} + Q_2 + Q_3^{(U)} + Q_4 + \mathcal{E}^{(U)} \tag{6.2.17}$$

is an operator on the full Fock space $\mathcal{F}$, V_ℓ^{0000}, Q_1, Q_2, $Q_3^{(U)}$, Q_4, $H_2^{(U)}$ are given in (6.1.7)–(6.1.12) *and the error term $\mathcal{E}^{(U)}$, given by* (6.2.19)*, satisfies*

$$\pm \mathcal{E}^{(U)} \leqslant C \frac{n^{\frac{1}{2}} (\mathcal{N}+1)^{\frac{3}{2}}}{\ell} + \varepsilon n^{-1} Q_4 + \varepsilon^{-1} C \frac{n}{\ell}, \quad \forall \varepsilon > 0, \tag{6.2.18}$$

on $\mathcal{F}$.

Proof. The computation of $\mathcal{E}^{(U)}$ is standard, see for instance [56, Section 4]: conjugating the Hamiltonian $H_{n,\ell}$ in (6.2.13) with U and applying the rules (6.2.16), we obtain $UH_{n,\ell}U^* = \mathbb{1}_+^{\leqslant n} \mathcal{H} \mathbb{1}_+^{\leqslant n}$ with $\mathcal{H}$ given by (6.2.17) and $\mathcal{E}^{(U)}$ by

$$\begin{aligned}
\mathcal{E}^{(U)} = \mathbb{1}_+^{\leqslant n} \Bigg(& \int_{\Lambda^2} V_\ell(x-y) \mathrm{d}x\mathrm{d}y \frac{\mathcal{N}^2 - n + \mathcal{N}}{2} - \int_{\Lambda^2} V_\ell(x-y) \left(a_x^* a_x + a_x^* a_y \right) \mathrm{d}x\mathrm{d}y\, \mathcal{N} \\
& + \int_{\Lambda^2} V_\ell(x-y) a_x^* \mathrm{d}x\mathrm{d}y \left((n - \mathcal{N} - 1)\sqrt{n - \mathcal{N}} - n^{\frac{3}{2}} \right) + \mathrm{h.c.} \\
& + \frac{1}{2} \int_{\Lambda^2} V_\ell(x-y) a_x^* a_y^* \mathrm{d}x\mathrm{d}y \left(\sqrt{n - \mathcal{N} - 1}\sqrt{n - \mathcal{N}} - n + \mathcal{N} \right) + \mathrm{h.c.} \Bigg) \mathbb{1}_+^{\leqslant n} \\
=: \mathbb{1}_+^{\leqslant n} & \left(\mathcal{E}^{(U,0)} + \mathcal{E}^{(U,1)} + \mathcal{E}^{(U,2)} \right) \mathbb{1}_+^{\leqslant n}.
\end{aligned} \tag{6.2.19}$$

We shall estimate the right-hand side of (6.2.19) term by term. Due to the projections it is enough to estimate $\mathcal{E}^{(U,0)}, \mathcal{E}^{(U,1)}$ and $\mathcal{E}^{(U,2)}$ on $\mathcal{F}_+^{\leqslant n}$. Using the Cauchy–Schwarz inequality we obtain

$$\begin{aligned}
\pm \mathcal{E}^{(U,0)} & \leqslant \int_{\Lambda^2} V_\ell(x-y) \mathrm{d}x\mathrm{d}y \left(\mathcal{N}^2 + \mathcal{N} + n \right) + 2 \int_{\Lambda^2} V_\ell(x-y) a_x^* a_x \mathrm{d}x\mathrm{d}y\, \mathcal{N} \\
& \leqslant C \frac{(\mathcal{N}+1)^2 + n}{\ell} \leqslant C \frac{n^{1/2} (\mathcal{N}+1)^{3/2} + n}{\ell}
\end{aligned}$$

on $\mathcal{F}_+^{\leqslant n}$, where we used that $\|V_\ell\|_1 \leqslant C\ell^{-1}$.

For $\mathcal{E}^{(U,1)}$ we use the elementary inequality $|\sqrt{1-t}-1| \leqslant Ct$ for $0 \leqslant t \leqslant 1$ to obtain

$$\begin{aligned}\pm\mathcal{E}^{(U,1)} &= \pm a^*(V_\ell * u_0^2)\left[n^{\frac{3}{2}}\left(\sqrt{1-\frac{\mathcal{N}}{n}}-1\right)-(\mathcal{N}+1)\sqrt{n-\mathcal{N}}\right]+\text{h.c.}\\ &\leqslant \varepsilon_1 a^*(V_\ell * u_0^2)\,(\mathcal{N}+1)^{1/2}\,a(V_\ell * u_0^2)+\varepsilon_1^{-1}n^3\left(\sqrt{1-\frac{\mathcal{N}}{n}}-1\right)^2(\mathcal{N}+1)^{-\frac{1}{2}}\\ &\quad+\varepsilon_1^{-1}\left((\mathcal{N}+1)\sqrt{n-\mathcal{N}}\right)^2(\mathcal{N}+1)^{-\frac{1}{2}}\\ &\leqslant C\varepsilon_1\ell^{-2}(\mathcal{N}+1)^{\frac{3}{2}}+\varepsilon_1^{-1}Cn(\mathcal{N}+1)^{3/2}\\ &\leqslant Cn^{\frac{1}{2}}\ell^{-1}(\mathcal{N}+1)^{\frac{3}{2}},\end{aligned}$$

on $\mathcal{F}_+^{\leqslant n}$, where we used that $\|V_\ell * u_0^2\|_2 \leqslant \|V_\ell\|_1 \leqslant C\ell^{-1}$ and optimized over $\varepsilon_1 > 0$. We proceed similarly for $\mathcal{E}^{(U,2)}$, using the elementary bound $|\sqrt{1-t-n^{-1}}\sqrt{1-t}-1+t| \leqslant n^{-1}$ for all $0 \leqslant t \leqslant 1-n^{-1}$. We obtain for all $\varepsilon > 0$

$$\pm\mathcal{E}^{(U,2)} \leqslant \varepsilon n^{-1}Q_4+\varepsilon^{-1}n^3\|V_\ell\|_1\left(\sqrt{1-\frac{\mathcal{N}+1}{n}}\sqrt{1-\frac{\mathcal{N}}{n}}-1+\frac{\mathcal{N}}{n}\right)^2 \leqslant \varepsilon n^{-1}Q_4+\varepsilon^{-1}C\frac{n}{\ell}$$

on $\mathcal{F}_+^{\leqslant n}$. The proof of Lemma 6.3 is complete. ☐

6.3 Symmetrization and Neumann Boundary Conditions

As already explained in the introduction, we cover $\mathbb{R}^3$ with copies of the box $\Lambda = [-\frac{1}{2},\frac{1}{2}]^3$ and label them canonically by $z+\Lambda$ with $z \in \mathbb{Z}^3$. Then we define $P_z : \Lambda \to \Lambda + z$ as in (6.1.15) and define $K, \widetilde{K} : \Lambda^2 \to \mathbb{R}$ as in (6.1.16) and (6.1.19),

$$K = Q^{\otimes 2}\widetilde{K}, \quad Q = 1-|u_0\rangle\langle u_0|, \quad \widetilde{K}(x,y) = -\sum_{z\in\mathbb{Z}^3} n\omega_{\ell,\lambda}(P_z(x)-y). \tag{6.3.1}$$

Let us now collect some useful bounds and properties of the function K. In particular we show that its L^2-norm is small if λ is, and that it is diagonal in the basis of Neumann eigenfunctions.

Lemma 6.4 (Properties of K)**.** *Assume $2R/\ell < \lambda < 1/4$. Then we have*

$$K(x,y) = \widetilde{K}(x,y)+n\widehat{\omega}_{\ell,\lambda}(0) = -\sum_{p\in\pi\mathbb{N}_0^3\setminus\{0\}} n\widehat{\omega}_{\ell,\lambda}(p)u_p(x)u_p(y). \tag{6.3.2}$$

Moreover, there is a constant $C > 0$ such that

$$\|K\|_\infty \leqslant Cn, \quad \|K\|_2^2 \leqslant C\lambda\left(\frac{n}{\ell}\right)^2, \quad \sup_{x\in\Lambda}\|K_x\|_2^2 \leqslant C\lambda\left(\frac{n}{\ell}\right)^2,$$

where $K_x(y) := K(x,y) = K(y,x)$.

Let us start with the following useful identity.

Lemma 6.5. *(Coefficients in the Neumann basis) Let $f : \mathbb{R}^3 \to \mathbb{R}$ be radial and integrable with* $\mathrm{Supp}(f) \subset \Lambda$*. Then for all $p, q \in \mathbb{N}_0^3$ we have*

$$\int_{\Lambda^2}\sum_{z\in\mathbb{Z}^3} f(P_z(x)-y)u_p(x)u_q(y)\mathrm{d}x\mathrm{d}y = \delta_{p,q}\widehat{f}(p)$$

with the Fourier transform defined in (6.1.18).

Proof. First note that terms with $\max\{|z_i|, i = 1,2,3\} \geqslant 2$ are zero due to our assumption on the support of f. Using simple coordinate transformations and $u_p(P_z(x)) = u_p(x)$ for all $p \in \pi\mathbb{N}_0^3$ we obtain for $y \in \Lambda$

$$\int_\Lambda u_p(x) \sum_{z\in\mathbb{Z}^3} f(P_z(x) - y)\mathrm{d}x = \int_{[-\frac{3}{2},\frac{3}{2}]^3} u_p(x) f(x-y)\mathrm{d}x = \int_\Lambda u_p(x+y) f(x)\mathrm{d}x,$$

where we used that $\Lambda \subset y + [-\frac{3}{2}, \frac{3}{2}]^3$. Thus, with the definition of u_p (6.2.11) we arrive at

$$\begin{aligned}\int_{\Lambda^2} \sum_{z\in\mathbb{Z}^3} f(P_z(x) - y) u_p(x) u_q(y)\mathrm{d}x\mathrm{d}y &= \int_\Lambda f(x) \int_\Lambda u_p(x+y) u_q(y)\mathrm{d}y\mathrm{d}x \\ = \int_\Lambda f(x) \prod_{i=1}^3 \int_{-\frac{1}{2}}^{\frac{1}{2}} &\left[\cos(p_i x_i) u_{p_i}(y_i) - \sqrt{2}\sin(p_i x_i)\sin(p_i(y_i + \frac{1}{2}))\right] u_{q_i}(y_i)\mathrm{d}y\mathrm{d}x.\end{aligned}$$

Observe that this formula trivially holds true for $p_i = 0$. The second term vanishes if we integrate over x since f is radial. We conclude that

$$\int_{\Lambda^2} \sum_{z\in\mathbb{Z}^3} f(P_z(x) - y) u_p(x) u_q(y)\mathrm{d}x\mathrm{d}y = \delta_{p,q} \int_\Lambda f(x) \prod_{i=1}^3 \cos(p_i x_i)\mathrm{d}x = \delta_{p,q} \int_{\mathbb{R}^3} f(x) e^{ip\cdot x}\mathrm{d}x$$

where in the second identity we used the fact that f is radial and supported in Λ. □

Proof of Lemma 6.4. From Lemma 6.5 we immediately have

$$\widetilde{K}(x,y) = -\sum_{p\in\pi\mathbb{N}_0^3} n\widehat{\omega}_{\ell,\lambda}(p) u_p(x) u_p(y)\ , \quad K(x,y) = -\sum_{p\in\pi\mathbb{N}_0^3\setminus\{0\}} n\widehat{\omega}_{\ell,\lambda}(p) u_p(x) u_p(y). \tag{6.3.3}$$

Moreover, Lemma 6.2 yields

$$0 \leq K_2 := K(x,y) - \widetilde{K}(x,y) = n\widehat{\omega}_{\ell,\lambda}(0) \leq C\lambda^2 \frac{n}{\ell}. \tag{6.3.4}$$

Let us emphasize that K_2 is a constant. Next, note that $|P_z(x) - y| \geqslant |x-y|$ for all $x, y \in \Lambda$. Together with the first bound in (6.2.9) and the finiteness of the sum this yields

$$|\widetilde{K}(x,y)| \leqslant \frac{Cn\mathbb{1}_{|x-y|\leqslant\lambda}}{1 + \ell|x-y|}. \tag{6.3.5}$$

From (6.3.5) and (6.3.4) we obtain

$$|K(x,y)| \leqslant \frac{Cn\mathbb{1}_{|x-y|\leqslant\lambda}}{1 + \ell|x-y|} + C\lambda^2 \frac{n}{\ell}. \tag{6.3.6}$$

The uniform bound $\|K\|_\infty \leqslant Cn$ follows immediately. For the L^2-norm we have

$$\begin{aligned}\|K\|_2^2 &\leqslant Cn^2 \int_{\Lambda^2} \frac{\mathbb{1}_{|x-y|\leqslant\lambda}\mathrm{d}x\mathrm{d}y}{(1 + \ell|x-y|)^2} + C\lambda^4 \left(\frac{n}{\ell}\right)^2 \\ &\leqslant Cn^2 \int_0^\lambda \frac{r^2}{(1+\ell r)^2}\mathrm{d}r + C\lambda^4 \left(\frac{n}{\ell}\right)^2 \leqslant C\lambda \left(\frac{n}{\ell}\right)^2.\end{aligned}$$

Similarly, $\|K_x\|_2^2 \leqslant C\lambda\,(n/\ell)^2$ independently of x. □

We may think of K as a modified scattering solution. Therefore, it is interesting to compare the scattering length $\mathfrak{a}$ with the one obtained by K. The following Lemma quantifies their difference. This will be used to extract the scattering length $\mathfrak{a}$ in computations in the upcoming sections.

Lemma 6.6. *(Boundary effects) The function*

$$h(x) = \int_\Lambda V_\ell(x-y)\,(n + K(x,y))\,\mathrm{d}y - 8\pi\mathfrak{a}\frac{n}{\ell}, \quad x \in \Lambda \tag{6.3.7}$$

satisfies

$$\|h\|_1 \lesssim \frac{n}{\ell}\frac{\log(\ell)}{\ell} \quad \textit{and} \quad \|h\|_p \lesssim \frac{n}{\ell}\ell^{-1/p}, \quad \forall p \in (1,\infty].$$

Consequently,

$$\left| nV_\ell^{0000} + \int_{\Lambda^2} V_\ell(x-y)K(x,y)\mathrm{d}x\mathrm{d}y - 8\pi\mathfrak{a}\frac{n}{\ell}\right| \leqslant Cn\ell^{-2}\log(\ell).$$

Proof. We choose $R > 0$ such that $\operatorname{supp}(V) \subset B_R(0)$. Using the uniform bound $|K(x,y)| \leqslant Cn$ from Lemma 6.4 and the obvious bound

$$\int_\Lambda V_\ell(x-y)\mathrm{d}y \leq \frac{1}{\ell}\int_{\mathbb{R}^3} V$$

we have

$$|h(x)| \leqslant C\frac{n}{\ell}, \quad \forall x \in \Lambda. \tag{6.3.8}$$

Moreover, this bound can be improved if x lies well within the interior of Λ. Indeed, for $x \in \Lambda$ satisfying $\operatorname{dist}(x,\partial\Lambda) > R\ell^{-1}$, we claim that

$$|h(x)| \leqslant C\frac{n}{\ell}\frac{1}{1+\ell\mathrm{d}(x,\partial\Lambda)} + C\frac{n}{\ell^2}. \tag{6.3.9}$$

From (6.3.8) and (6.3.9), it is straightforward to deduce the desired L^p bounds of h.

It remains to verify (6.3.9). Using the definition (6.3.1) and $V_\ell(1-\omega_{\ell,\lambda}) = V_\ell f_\ell$, we obtain

$$\begin{aligned}\int_\Lambda V_\ell(x-y)(n+K(x,y))\mathrm{d}y = \int_\Lambda n(V_\ell f_\ell)(x-y)\mathrm{d}y - \sum_{z\neq 0}\int_\Lambda V_\ell(x-y)n\omega_{\ell,\lambda}(P_z(x)-y)\mathrm{d}y \\ + K_2\int_\Lambda V_\ell(x-y)\mathrm{d}y\end{aligned} \tag{6.3.10}$$

with $K_2 = K - \widetilde{K}$. The last term of (6.3.10) is bounded easily by (6.3.4),

$$0 \leq K_2\int_\Lambda V_\ell(x-y)\mathrm{d}y \leqslant C\frac{n}{\ell}\lambda^2\|V_\ell\|_1 \leqslant C\frac{n}{\ell^2}.$$

For the first term on the right-hand side of (6.3.10), from the assumption $\operatorname{dist}(x,\partial\Lambda) > R\ell^{-1}$ we have $(\Lambda - x)\cap B_{R\ell^{-1}}(0) = B_{R\ell^{-1}}(0)$, which can be used together with the fact $\operatorname{supp}(V_\ell) \subset B_{R\ell^{-1}}(0)$ to deduce that

$$\int_\Lambda n(V_\ell f_\ell)(x-y)\mathrm{d}y = \int_{\Lambda - x} n(V_\ell f_\ell)(y)\mathrm{d}y = \int_{\mathbb{R}^3} n(V_\ell f_\ell)(y)\mathrm{d}y = 8\pi\mathfrak{a}\frac{n}{\ell}.$$

For the second term on the right-hand side of (6.3.10) we note that $P_z(x) \notin \Lambda$ for $x \in \Lambda$ and $z \neq 0$. In particular $|P_z(x) - y| \geqslant \mathrm{d}(x, \partial\Lambda)$. Together with the first bound in (6.2.9) this implies

$$\omega_{\ell,\lambda}(P_z(x) - y) \leqslant \frac{C}{1 + \ell|P_z(x) - y|} \leqslant \frac{C}{1 + \ell \mathrm{d}(x, \partial\Lambda)} \quad \forall z \in \mathbb{Z}^3 \setminus \{0\}. \tag{6.3.11}$$

Therefore, as only finitely many summands in this term are non-zero,

$$\begin{aligned}\sum_{z\neq 0} \int_\Lambda V_\ell(x-y) n \omega_{\ell,\lambda}(P_z(x) - y) \mathrm{d}y &\leqslant C \int_\Lambda n V_\ell(x-y) \frac{1}{1 + \ell \mathrm{d}(x, \partial\Lambda)} \mathrm{d}y \\ &\leqslant C \frac{n}{\ell} \frac{1}{1 + \ell \mathrm{d}(x, \partial\Lambda)}.\end{aligned}$$

This concludes (6.3.9) as well as the proof of Lemma 6.6. □

6.4 The First Quadratic Transformation

In this section we apply the first transformation $e^{\mathcal{B}_1}$ to the excitation Hamiltonian $\mathcal{H}$ in (6.2.17), where

$$\mathcal{B}_1 = \frac{1}{2} \int_{\Lambda^2} K(x,y) a_x^* a_y^* \mathrm{d}x \mathrm{d}y - \text{h.c.} \tag{6.4.1}$$

with K given in (6.3.1). The role of this transformation is to replace the quadratic term Q_2 in (6.2.17) by $\widetilde{Q}_2$, defined in (6.1.22), which is less singular, and extracts a scalar contribution leading to the full leading order energy $4\pi\mathfrak{a}n^2\ell^{-1}$. The main result of this section is the following lemma.

Lemma 6.7. *Assume that $\lambda \left(\frac{n}{\ell}\right)^2 \leqslant 1$, that $2R/\ell < \lambda < 1/4$, and that ℓ is large enough. Then we have*

$$\begin{aligned} e^{-\mathcal{B}_1} \mathcal{H} e^{\mathcal{B}_1} = 4\pi\mathfrak{a}n^2\ell^{-1} &+ \sum_{p \in \pi\mathbb{N}_0^3 \setminus \{0\}} \frac{|n\widehat{\epsilon}_{\ell,\lambda}(p)|^2}{2p^2} + \mathrm{d}\Gamma(-\Delta) + Q_4 \\ &+ n \int_{\Lambda^2} V_\ell(x-y)(a_x^* a_x + a_x^* a_y) \mathrm{d}x\mathrm{d}y - 8\pi\mathfrak{a}n\ell^{-1}\mathcal{N} \\ &+ \widetilde{Q}_2 + Q_3 + \mathcal{E}_1 \end{aligned} \tag{6.4.2}$$

on $\mathcal{F}_+$, with

$$\begin{aligned} Q_3 &= \sqrt{n} \int_{\Lambda^2} V_\ell(x-y) a_x^* a_y^* a_x \mathrm{d}x\mathrm{d}y + \text{h.c.}, \\ \widetilde{Q}_2 &= \int_{\Lambda^2} \widetilde{Q}_2(x,y) a_x^* a_y^* \mathrm{d}x\mathrm{d}y + \text{h.c.}, \\ \widetilde{Q}_2(x,y) &= \frac{n}{2} \sum_{z\in\mathbb{Z}^3} \epsilon_{\ell,\lambda}(P_z(x) - y) \\ &\quad + \frac{n}{2} \sum_{z \neq 0} \Big(V_\ell(\omega_\ell - 1)(P_z(x) - y) - V_\ell(x-y)\omega_{\ell,\lambda}(P_z(x) - y) \Big) \end{aligned}$$

and

$$\begin{aligned} \pm\mathcal{E}_1 \leqslant{}& C(\delta + \ell^{-1}\lambda^2 + \varepsilon n^{-1}) Q_4 + C\delta^{-1} \left(\frac{(\mathcal{N}+1)}{\ell} + \frac{(\mathcal{N}+1)^2}{n\ell} + \lambda \left(\frac{n}{\ell}\right)^3 \right) (\mathcal{N}+1) \\ &+ C\lambda^{\frac{1}{2}} \left(\left(\frac{n}{\ell}\right)^2 + \frac{n}{\ell} \right)(\mathcal{N}+1) + Cn^{\frac{1}{2}} \frac{(\mathcal{N}+1)^{\frac{3}{2}}}{\ell} \\ &+ C\frac{n^{1/2}}{\ell^{5/6}} \left(\mathrm{d}\Gamma(-\Delta) + \frac{n^2 \log(\ell)}{\ell^2} \right) + C\varepsilon^{-1}\frac{n}{\ell} + C\frac{n^2}{\ell^2}\log\ell \end{aligned} \tag{6.4.3}$$

for all $0 < \delta, \varepsilon \leqslant 1$.

The remainder of this section is dedicated to proving this lemma. Let us first make some remarks.

1. The condition $2R/\ell < \lambda$ was already introduced in (6.2.5), it ensures that $\omega_{\ell,\lambda} \equiv \omega_\ell$ on the support of V_ℓ. The condition $\lambda \left(\frac{n}{\ell}\right)^2 \leqslant 1$ ensures that $\|K\|_2$ remains bounded, so that the first quadratic transform preserves powers of the particle number, see Lemma 6.8 below. We will keep those constraints throughout the paper. Eventually, we will additionally ask $\lambda \ll 1$ so that only the first terms in the Duhamel expansion of $e^{\mathcal{B}_1}$ will contribute to the LHY order.

2. We will eventually choose $\delta = o(1)_{\rho\mathfrak{a}^3 \to 0}$. On the other hand, ε will be independent of $\rho\mathfrak{a}^3$.

3. We have chosen the transformation kernel of $\mathcal{B}_1$ in such a way that

$$[\mathrm{d}\Gamma(-\Delta) + Q_4, \mathcal{B}_1] + Q_2 \approx \widetilde{Q}_2. \tag{6.4.4}$$

The renormalized quadratic term $\widetilde{Q}_2$ defined in Lemma 6.7 consists of two parts,

$$\widetilde{Q}_2 = \widetilde{Q}_2^{(\epsilon)} + \widetilde{Q}_2^{(bc)} = \int_{\Lambda^2} \widetilde{Q}_2^{(\epsilon)}(x,y) a_x^* a_y^* \mathrm{d}x\mathrm{d}y + \text{h.c.} + \int_{\Lambda^2} \widetilde{Q}_2^{(bc)}(x,y) a_x^* a_y^* \mathrm{d}x\mathrm{d}y + \text{h.c.}$$

with

$$\begin{aligned} \widetilde{Q}_2^{(\epsilon)}(x,y) &= \frac{n}{2} \sum_{z \in \mathbb{Z}^3} \epsilon_{\ell,\lambda}(P_z(x) - y), \qquad (6.4.5) \\ \widetilde{Q}_2^{(bc)}(x,y) &= \frac{n}{2} \sum_{z \neq 0} \left[\Big(V_\ell(\omega_\ell - 1)(P_z(x) - y) \Big) - V_\ell(x-y)\omega_{\ell,\lambda}(P_z(x) - y) \right]. \end{aligned}$$

The part $\widetilde{Q}_2^{(\epsilon)}$ comes from the cutoff we introduced in $\omega_{\ell,\lambda}$, see (6.2.6), it is essentially the desired renormalized form of Q_2. The additional part $\widetilde{Q}_2^{(bc)}$ is a boundary effect that arises from the symmetrization of the kernel K. This is an error term, but for technical reasons we have to keep the boundary contribution $\widetilde{Q}_2^{(bc)}$ in $\widetilde{Q}_2$ in Lemma 6.7, and will eliminate it later after conjugating with the cubic transformation.

We shall need the following standard estimate.

Lemma 6.8. *Assume that* $\lambda \left(\frac{n}{\ell}\right)^2 \leqslant 1$ *and that* $2R/\ell < \lambda < 1/4$. *For all* $k \in \mathbb{N}$ *there is a constant* $C_k > 0$ *independent of* n, ℓ *and* λ *such that on* $\mathcal{F}$ *we have*

$$e^{-t\mathcal{B}_1}(\mathcal{N}+1)^k e^{t\mathcal{B}_1} \leqslant C_k(\mathcal{N}+1)^k, \quad \forall t \in [-1,1].$$

Proof. The proof that quadratic transformations preserve powers of the particle number is well known, see for instance [69, Lemma 4] from which we have

$$e^{-t\mathcal{B}_1}(\mathcal{N}+1)^k e^{t\mathcal{B}_1} \leqslant C_k \left(1 + \|K\|_2^2\right)^k (\mathcal{N}+1)^k.$$

Thanks to Lemma 6.4 and the assumption on λ, we have $\|K\|_2^2 \leqslant C\lambda(n/\ell)^2 \leqslant C$. □

From (6.2.17) we have

$$
\begin{aligned}
e^{-\mathcal{B}_1}\mathcal{H}e^{\mathcal{B}_1} &= \left(\frac{n^2}{2}V_\ell^{0000} + e^{-\mathcal{B}_1}(\mathrm{d}\Gamma(-\Delta) + Q_2 + Q_4)e^{\mathcal{B}_1}\right) + e^{-\mathcal{B}_1}H_2^{(U)}e^{\mathcal{B}_1} \\
&\quad + e^{-\mathcal{B}_1}(Q_1 + Q_3^{(U)})e^{\mathcal{B}_1} + e^{-\mathcal{B}_1}\mathcal{E}^{(U)}e^{\mathcal{B}_1} \\
&= (\mathrm{I})_1 + (\mathrm{II})_1 + (\mathrm{III})_1 + e^{-\mathcal{B}_1}\mathcal{E}^{(U)}e^{\mathcal{B}_1}\,. \qquad (6.4.6)
\end{aligned}
$$

We will estimate $(\mathrm{I})_1, (\mathrm{II})_1$ and $(\mathrm{III})_1$ in Sections 6.4.1, 6.4.2 and 6.4.3, respectively. Finally, in Section 6.4.4, we gather all previous estimates and complete the proof of Lemma 6.7.

6.4.1 Analysis of $(\mathrm{I})_1$

In this subsection we estimate the term $(\mathrm{I})_1$ appearing in (6.4.6).

Lemma 6.9. *Assume that $\lambda\left(\frac{n}{\ell}\right)^2 \leqslant 1$, that $2R/\ell < \lambda < 1/4$ and that ℓ is large enough. Then we have*

$$
\begin{aligned}
(\mathrm{I})_1 &= \frac{n^2}{2}V_\ell^{0000} + e^{-\mathcal{B}_1}(\mathrm{d}\Gamma\,(-\Delta) + Q_2 + Q_4)e^{\mathcal{B}_1} \\
&= 4\pi\mathfrak{a}n^2\ell^{-1} + \sum_{p\in\pi\mathbb{N}_0^3\setminus\{0\}} \frac{|n\widehat{\epsilon}_{\ell,\lambda}(p)|^2}{2p^2} + \mathrm{d}\Gamma(-\Delta) + Q_4 + \widetilde{Q}_2 + \mathcal{E}_1^{(Q_2)}
\end{aligned}
$$

on $\mathcal{F}_+$, with

$$
\pm\mathcal{E}_1^{(Q_2)} \leqslant (\delta + C\ell^{-1}\lambda^2)Q_4 + C\delta^{-1}\lambda\frac{n^2}{\ell^3}(\mathcal{N}+1)^2 + C\lambda^{\frac12}\frac{n^2}{\ell^2}(\mathcal{N}+1) + C\frac{n^2}{\ell^2}\log\ell,
$$

for all $0 < \delta \leqslant 1$.

To prove Lemma 6.9, we use the Duhamel-type identity

$$
\begin{aligned}
&e^{-\mathcal{B}_1}(\mathrm{d}\Gamma\,(-\Delta) + Q_2 + Q_4)e^{\mathcal{B}_1} - \mathrm{d}\Gamma(-\Delta) - Q_4 \\
&= \int_0^1 e^{-t\mathcal{B}_1}\Big([\mathrm{d}\Gamma\,(-\Delta) + Q_4, \mathcal{B}_1] + Q_2\Big)e^{t\mathcal{B}_1}\mathrm{d}t + \int_0^1\int_t^1 e^{-s\mathcal{B}_1}[Q_2,\mathcal{B}_1]e^{s\mathcal{B}_1}\mathrm{d}s\mathrm{d}t\,. \qquad (6.4.7)
\end{aligned}
$$

We deal with the two terms on the right-hand side of (6.4.7) by using Lemmata 6.10 and 6.11 below.

Lemma 6.10. *Assume that $\lambda\left(\frac{n}{\ell}\right)^2 \leqslant 1$, that $2R/\ell < \lambda < 1/4$ and that ℓ is large enough. Then we have*

$$
[\mathrm{d}\Gamma(-\Delta) + Q_4, \mathcal{B}_1] + Q_2 = \widetilde{Q}_2 + \mathcal{E} \qquad (6.4.8)
$$

on $\mathcal{F}_+$, where $\widetilde{Q}_2$ is given in Lemma 6.7 and $\mathcal{E}$ satisfies

$$
\pm\int_0^1 e^{-t\mathcal{B}_1}\mathcal{E}e^{t\mathcal{B}_1}\mathrm{d}t \leqslant (\delta + C\ell^{-1}\lambda^2)Q_4 + C\delta^{-1}\lambda\frac{n^2}{\ell^3}(\mathcal{N}+1)^2 + C\lambda^{\frac12}\frac{n^2}{\ell^2}(\mathcal{N}+1) \qquad (6.4.9)
$$

for all $0 < \delta \leqslant 1$. Moreover, it holds that

$$
e^{-t\mathcal{B}_1}Q_4e^{t\mathcal{B}_1} \leqslant C\left(Q_4 + \frac{n^2}{\ell} + \lambda\frac{n^2}{\ell^3}(\mathcal{N}+1)^2\right), \quad \forall t \in [-1,1]. \qquad (6.4.10)
$$

Proof. We use the momentum space representation from (6.3.3) and Lemma 6.5 and calculate

$$
\begin{aligned}
[\mathrm{d}\Gamma(-\Delta), \mathcal{B}_1] &= -n \sum_{p\neq 0} p^2 \widehat{w}_{\ell,\lambda}(p) a_p^* a_p^* + \text{h.c.} \\
&= n \sum_{z\in\mathbb{Z}^3} \int_{\Lambda^2} \Delta\omega_{\ell,\lambda}(P_z(x)-y) a_x^* a_y^* + \text{h.c.} \qquad (6.4.11)
\end{aligned}
$$

Moreover,

$$
[Q_4, \mathcal{B}_1] = \frac{1}{2} \int_{\Lambda^2} V_\ell(x-y) \widetilde{K}(x,y) a_x^* a_y^* + \text{h.c.} + \mathcal{E} \qquad (6.4.12)
$$

where

$$
\mathcal{E} = \frac{1}{2} K_2 \int_{\Lambda^2} V_\ell(x-y) a_x^* a_y^* + \int_{\Lambda^2} V_\ell(x-y) a_x^* a_y^* a^*(K_y) a_x + \text{h.c.} \qquad (6.4.13)
$$

with $K_2 = K - \widetilde{K}$ the constant given in (6.3.4). With the definition of $\widetilde{K}$ in (6.1.16) and the scattering equation (6.2.6) we compute

$$
\begin{aligned}
& n \sum_{z\in\mathbb{Z}^3} \Delta\omega_{\ell,\lambda}(P_z(x)-y) + \frac{1}{2} V_\ell(x-y) \widetilde{K}(x,y) \\
&= \frac{n}{2} \sum_{z\in\mathbb{Z}^3} \Big(\epsilon_{\ell,\lambda} - \big(V_\ell(1-\omega_\ell)\big)(P_z(x)-y) - V_\ell(x-y)\omega_{\ell,\lambda}(P_z(x)-y) \Big),
\end{aligned}
$$

which is exactly equal to $\widetilde{Q}_2(x,y)$ defined in Lemma 6.7 plus

$$
\frac{n}{2}\Big(- \big(V_\ell(1-\omega_\ell)\big)(P_z(x)-y) - V_\ell(x-y)\omega_{\ell,\lambda}(P_z(x)-y) \Big)|_{z=0} = -\frac{n}{2} V_\ell(x-y).
$$

Therefore, we deduce from (6.4.11) and (6.4.12) that

$$
[\mathrm{d}\Gamma(-\Delta) + Q_4, \mathcal{B}_1] = \int_{\Lambda^2} \Big(\widetilde{Q}_2(x,y) - \frac{n}{2} V_\ell(x-y) \Big) a_x^* a_y^* + \text{h.c.} + \mathcal{E} = \widetilde{Q}_2 - Q_2 + \mathcal{E}.
$$

We shall now prove the estimate (6.4.10). Recall the uniform bound $|K(x,y)| \leqslant Cn$ from Lemma 6.4. The Cauchy–Schwarz inequality yields

$$
\begin{aligned}
& \pm \int_{\Lambda^2} V_\ell(x-y) K(x,y) a_x^* a_y^* + \text{h.c.} \\
& \leqslant \int_{\Lambda^2} V_\ell(x-y) a_x^* a_y^* a_x a_y + \int_{\Lambda^2} V_\ell(x-y) K(x,y)^2 \leqslant Q_4 + Cn^2 \ell^{-1}.
\end{aligned}
$$

Moreover, the bound $\sup_{y\in\Lambda} \|K_y\|_2^2 \leqslant C\lambda n^2/\ell^2$ again from Lemma 6.4 gives

$$
\begin{aligned}
\pm & \int_{\Lambda^2} V_\ell(x-y) a_x^* a_y^* a^*(K_y) a_x + \text{h.c.} \\
& \leqslant \int_{\Lambda^2} V_\ell(x-y) a_x^* a_y^* a_x a_y + \int_{\Lambda^2} V_\ell(x-y) a_x^* a(K_y) a^*(K_y) a_x \\
& \leqslant Q_4 + C\lambda \frac{n^2}{\ell^3} \mathcal{N}^2. \qquad (6.4.14)
\end{aligned}
$$

Therefore, from (6.4.12) and (6.4.13) we have

$$
\pm[\mathcal{B}_1, Q_4] \leqslant 2Q_4 + Cn^2\ell^{-1} + C\lambda \frac{n^2}{\ell^3} \mathcal{N}^2.
$$

From this and Lemma 6.8, a standard Grönwall argument gives

$$e^{-t\mathcal{B}_1}Q_4e^{t\mathcal{B}_1} \leqslant C\left(Q_4+n^2\ell^{-1}+\lambda\frac{n^2}{\ell^3}(\mathcal{N}+1)^2\right), \quad \forall t\in[-1,1].$$

Now we have the tools to show the estimate (6.4.9) with $\mathcal{E}$ given in (6.4.13) as the sum of the two terms. For the first one, we use the Cauchy–Schwarz inequality and the inequality (6.3.4) to obtain

$$\pm\frac{1}{2}K_2\int_{\Lambda^2}V_\ell(x-y)a_x^*a_y^*+\text{h.c.} \leqslant (\ell^{-1}\lambda^2)Q_4+K_2^2(\ell^{-1}\lambda^2)^{-1}\|V_\ell\|_1 \leqslant \ell^{-1}\lambda^2Q_4+C\lambda^2\frac{n^2}{\ell^2}$$

and by (6.4.10)

$$\pm e^{-t\mathcal{B}_1}\left(\frac{1}{2}K_2\int_{\Lambda^2}V_\ell(x-y)a_x^*a_y^*+\text{h.c.}\right)e^{t\mathcal{B}_1} \leqslant C\ell^{-1}\lambda^2Q_4+C\lambda^3\frac{n^2}{\ell^4}(\mathcal{N}+1)^2+C\lambda^2\frac{n^2}{\ell^2}. \tag{6.4.15}$$

For the second term in $\mathcal{E}$ we write

$$e^{-t\mathcal{B}_1}a_x^*a_y^*e^{t\mathcal{B}_1}=a_x^*a_y^*+tK(x,y)+\int_0^t e^{-s\mathcal{B}_1}\big(a_x^*a(K_y)+a_y^*a(K_x)\big)e^{s\mathcal{B}_1}\mathrm{d}s. \tag{6.4.16}$$

We find

$$\begin{aligned}
&e^{-t\mathcal{B}_1}\left(\int_{\Lambda^2}V_\ell(x-y)a_x^*a_y^*a^*(K_y)a_x+\text{h.c.}\right)e^{t\mathcal{B}_1}\\
&=\int_{\Lambda^2}V_\ell(x-y)\left(a_x^*a_y^*+tK(x,y)+\int_0^t e^{-s\mathcal{B}_1}\big(a_x^*a(K_y)+a_y^*a(K_x)\big)e^{s\mathcal{B}_1}\mathrm{d}s\right)\\
&\qquad\qquad\times e^{-t\mathcal{B}_1}a^*(K_y)a_xe^{t\mathcal{B}_1}+\text{h.c.}
\end{aligned}$$

We may now bound each term with the Cauchy–Schwarz inequality while making use of Lemma 6.8. For $\delta>0$ we obtain

$$\pm\int_{\Lambda^2}V_\ell(x-y)a_x^*a_y^*e^{-t\mathcal{B}_1}a^*(K_y)a_xe^{t\mathcal{B}_1}+\text{h.c.} \leqslant \delta Q_4+\delta^{-1}C\|V_\ell\|_1\sup_y\|K_y\|_2^2(\mathcal{N}+1)^2,$$
$$\pm\int_{\Lambda^2}V_\ell(x-y)K(x,y)e^{-t\mathcal{B}_1}a^*(K_y)a_xe^{t\mathcal{B}_1}+\text{h.c.} \leqslant C\|V_\ell\|_1 n\sup_y\|K_y\|_2(\mathcal{N}+1)$$

and

$$\begin{aligned}
&\pm\int_{\Lambda^2}V_\ell(x-y)\int_0^t e^{-s\mathcal{B}_1}\big(a_x^*a(K_y)+a_y^*a(K_x)\big)e^{s\mathcal{B}_1}\mathrm{d}s\,e^{-t\mathcal{B}_1}a^*(K_y)a_xe^{t\mathcal{B}_1}+\text{h.c.}\\
&\leqslant C\|V_\ell\|_1\sup_y\|K_y\|_2^2(\mathcal{N}+1)^2.
\end{aligned}$$

Then, $\|K\|_\infty\leqslant Cn$ and $\sup_y\|K_y\|_2\leqslant C\lambda n^2\ell^{-2}$ from Lemma 6.4 yield

$$\begin{aligned}
&\pm e^{-t\mathcal{B}_1}\left(\int_{\Lambda^2}V_\ell(x-y)a_x^*a_y^*a^*(K_y)a_x+\text{h.c.}\right)e^{t\mathcal{B}_1}\\
&\quad\leqslant \delta Q_4+\delta^{-1}C\lambda\frac{n^2}{\ell^3}(\mathcal{N}+1)^2+C\lambda^{\frac{1}{2}}\frac{n^2}{\ell^2}(\mathcal{N}+1)+C\lambda\frac{n^2}{\ell^3}(\mathcal{N}+1)^2.
\end{aligned}$$

Combining this with (6.4.14), and $\lambda,\ell^{-1},\delta\leqslant 1$ to simplify some error terms, yields the desired error bound (6.4.9). □

From (6.4.8) and (6.4.7) we obtain the identity

$$\begin{aligned}
&e^{-\mathcal{B}_1}(\mathrm{d}\Gamma(-\Delta)+Q_2+Q_4)e^{\mathcal{B}_1}-\mathrm{d}\Gamma(-\Delta)-Q_4\\
&=\widetilde{Q}_2+\int_0^1\int_0^t e^{-s\mathcal{B}_1}[\widetilde{Q}_2,\mathcal{B}_1]e^{s\mathcal{B}_1}\mathrm{d}s\mathrm{d}t\\
&\quad+\int_0^1\int_t^1 e^{-s\mathcal{B}_1}[Q_2,\mathcal{B}_1]e^{s\mathcal{B}_1}\mathrm{d}s\mathrm{d}t+\int_0^1 e^{-t\mathcal{B}_1}\mathcal{E}e^{t\mathcal{B}_1}\mathrm{d}t,
\end{aligned}\tag{6.4.17}$$

where we again used the Duhamel formula. The last term in (6.4.17) is an error term that is controlled by (6.4.9).

As $Q_2,\widetilde{Q}_2$ and $\mathcal{B}_1$ are all quadratic, there are constant contributions in $[Q_2,\mathcal{B}_1]$ and $[\widetilde{Q}_2,\mathcal{B}_1]$. They are extracted in the following lemma.

Lemma 6.11. *Assume that $\lambda\left(\frac{n}{\ell}\right)^2\leqslant 1$, that $2R/\ell<\lambda<1/4$ and that ℓ is large enough. Then we have*

$$\frac{n^2}{2}V_\ell^{0000}+\frac{1}{2}[Q_2,\mathcal{B}_1]=4\pi\mathfrak{a}n^2\ell^{-1}+\Xi_1^{(a)},\tag{6.4.18}$$

$$\frac{1}{2}[\widetilde{Q}_2,\mathcal{B}_1]=\sum_{p\in\pi\mathbb{N}_0^3\setminus\{0\}}\frac{|n\widehat{\epsilon}_{\ell,\lambda}(p)|^2}{2p^2}+\Xi_1^{(b)}\tag{6.4.19}$$

on $\mathcal{F}_+$ where both of the error terms $\Xi_1^{(a)}$ and $\Xi_1^{(b)}$ are bounded by

$$\pm\Xi_1^{(a)},\pm\Xi_1^{(b)}\leq C\lambda^{\frac{1}{2}}\left(\frac{n}{\ell}\right)^2\mathcal{N}+C\frac{n^2}{\ell^2}\log\ell.$$

Consequently,

$$\begin{aligned}
&\frac{n^2}{2}V_\ell^{0000}+\int_0^1\int_t^1 e^{-s\mathcal{B}_1}[Q_2,\mathcal{B}_1]e^{s\mathcal{B}_1}\mathrm{d}s\mathrm{d}t+\int_0^1\int_0^t e^{-s\mathcal{B}_1}[\widetilde{Q}_2,\mathcal{B}_1]e^{s\mathcal{B}_1}\mathrm{d}s\mathrm{d}t\\
&\quad=4\pi\mathfrak{a}n^2\ell^{-1}+\sum_{p\in\pi\mathbb{N}_0^3\setminus\{0\}}\frac{|n\widehat{\epsilon}_{\ell,\lambda}(p)|^2}{2p^2}+\Xi_1
\end{aligned}\tag{6.4.20}$$

on $\mathcal{F}_+$, with

$$\pm\Xi_1\leqslant C\lambda^{\frac{1}{2}}\left(\frac{n}{\ell}\right)^2(\mathcal{N}+1)+C\frac{n^2}{\ell^2}\log\ell.$$

Proof. Let us start with (6.4.18). A simple calculation shows that

$$[Q_2,\mathcal{B}_1]=\int_{\Lambda^2}nV_\ell(x-y)K(x,y)+n\int_{\Lambda^2}V_\ell(x-y)a^*(K_x)a_y+\text{h.c.}\tag{6.4.21}$$

For the first term on the right hand-side of (6.4.21), which will be multiplied by a factor $1/2=\int_0^1\int_0^t\mathrm{d}s\mathrm{d}t$, we have by Lemma 6.6

$$\left|\frac{n^2}{2}V_\ell^{0000}+\frac{n}{2}\int_{\Lambda^2}V_\ell(x-y)K(x,y)-4\pi\mathfrak{a}n^2\ell^{-1}\right|\leqslant Cn^2\ell^{-2}\log\ell.$$

For the second term in (6.4.21) we use the Cauchy–Schwarz inequality and obtain

$$\pm n\int_{\Lambda^2}V_\ell(x-y)a^*(K_x)a_y+\text{h.c.}\leqslant Cn\|V_\ell\|_1\sup_y\|K_y\|_2\mathcal{N}\leqslant C\lambda^{\frac{1}{2}}\left(\frac{n}{\ell}\right)^2\mathcal{N}.$$

Thus (6.4.18) holds.

The proof of (6.4.19) is more involved. To estimate

$$[\widetilde{Q}_2, \mathcal{B}_1] = 2\int_{\Lambda^2} \widetilde{Q}_2(x,y)K(x,y) + 2\int_{\Lambda^2} \widetilde{Q}_2(x,y)a^*(K_x)a_y + \text{h.c.} \tag{6.4.22}$$

let us decompose

$$\widetilde{Q}_2(x,y) = \widetilde{Q}_2^{(\epsilon)}(x,y) + \widetilde{Q}_2^{(bc)}(x,y)$$

as in (6.4.5) and derive pointwise estimates for $\widetilde{Q}_2^{(\epsilon)}(x,y)$ and $\widetilde{Q}_2^{(bc)}(x,y)$. Note that in (6.4.5) both sums are finite (each sum contains at most $3^3 = 27$ non-zero summands). From Lemma 6.2 and the bound $|P_z(x) - y| \geqslant |x-y|$ for all $x, y \in \Lambda$ we have

$$\begin{aligned}|\widetilde{Q}_2^{(\epsilon)}(x,y)|\mathrm{d}y &\leq Cn\ell^{-1}\lambda^{-3}\sum_{z\in\mathbb{Z}^3}\mathbb{1}_{|P_z(x)-y|\leqslant\lambda}\\ &\leq Cn\ell^{-1}\lambda^{-3}\sup_{z\in\mathbb{Z}^3}\mathbb{1}_{|P_z(x)-y|\leqslant\lambda} \leq Cn\ell^{-1}\lambda^{-3}\mathbb{1}_{|x-y|\leqslant\lambda} \quad \forall x,y\in\Lambda.\end{aligned} \tag{6.4.23}$$

Moreover, for all $0 \neq z \in \mathbb{Z}^3$ we have

$$V_\ell(P_z(x)-y) = V_\ell(P_z(x)-y)\mathbb{1}_{\mathrm{d}(x,\partial\Lambda)\leqslant R\ell^{-1}} \leq \frac{CV_\ell(P_z(x)-y)}{1+\ell\mathrm{d}(x,\partial\Lambda)}$$

since $\mathrm{supp}(V_\ell) \subset B_{R\ell^{-1}}(0)$. In combination with (6.3.11) and $|P_z(x)-y| \geqslant |x-y|$, as well as the non-increasing assumption on $|x| \mapsto V(x)$, we arrive at the bound

$$|\widetilde{Q}_2^{(bc)}(x,y)| \leqslant Cn\sum_{z\in\mathbb{Z}^3}\frac{V_\ell(P_z(x)-y)}{1+\ell\mathrm{d}(x,\partial\Lambda)} \leq Cn\frac{V_\ell(x-y)}{1+\ell\mathrm{d}(x,\partial\Lambda)}. \tag{6.4.24}$$

Now we are ready to bound the last term in (6.4.22). From (6.4.23) and (6.4.24), we obtain the pointwise estimate

$$|\widetilde{Q}_2(x,y)| \leq Cn\left(\ell^{-1}\lambda^{-3}\mathbb{1}_{|x-y|\leq\lambda} + V_\ell(x-y)\right), \quad \forall x,y\in\Lambda.$$

Combining this with the uniform bound $\sup_{x\in\Lambda}\|K_x\|_2 \leqslant C\lambda^{1/2}n\ell^{-1}$ from Lemma 6.4 and the Cauchy–Schwarz inequality with $\delta = \ell/(\lambda^{1/2}n)$, we have

$$\begin{aligned}&\pm 2\int_{\Lambda^2}\widetilde{Q}_2(x,y)a^*(K_x)a_y + \text{h.c.}\\ &\leqslant \delta\int_{\Lambda^2}|\widetilde{Q}_2(x,y)|a^*(K_x)a(K_x) + \delta^{-1}\int_{\Lambda^2}|\widetilde{Q}_2(x,y)|a_y^*a_y\\ &\leqslant C\delta n\ell^{-1}\int_\Lambda a^*(K_x)a(K_x) + C\delta^{-1}n\ell^{-1}\int_\Lambda a_y^*a_y\\ &\leqslant C\delta n\ell^{-1}\sup_{x\in\Lambda}\|K_x\|_2^2\mathcal{N} + C\delta^{-1}n\ell^{-1}\mathcal{N} \leq C\lambda^{\frac{1}{2}}\left(\frac{n}{\ell}\right)^2\mathcal{N}.\end{aligned}$$

It remains to consider the constant term in (6.4.22). The contribution involving $\widetilde{Q}_2^{(bc)}$ is negligible and can be estimated using (6.4.24) and the uniform bound $\|K\|_\infty \leqslant Cn$ from Lemma 6.4 as

$$\begin{aligned}\left|2\int_{\Lambda^2}\widetilde{Q}_2^{(bc)}(x,y)K(x,y)\right| &\leqslant Cn^2\int_{\Lambda^2}\frac{V_\ell(x-y)}{1+\ell\mathrm{d}(x,\partial\Lambda)}\\ &\leq Cn^2\ell^{-1}\int_\Lambda\frac{1}{1+\ell\mathrm{d}(x,\partial\Lambda)} \leqslant C\frac{n^2}{\ell^2}\log\ell.\end{aligned}$$

Finally we consider the important constant contribution involving $\widetilde{Q}_2^{(\epsilon)}$. Combining (6.3.2) and (6.4.5) with Lemma 6.5 we obtain that

$$2\int_{\Lambda^2} \widetilde{Q}_2^{(\epsilon)}(x,y)K(x,y) = -n^2 \sum_{p\in\pi\mathbb{N}_0^3\setminus\{0\}} \widehat{\epsilon}_{\ell,\lambda}(p)\widehat{\omega}_{\ell,\lambda}(p) \tag{6.4.25}$$

Covering $\mathbb{Z}^3\setminus\{0\}$ with 8 rotations of $\mathbb{N}^3\setminus\{0\}$, we overcount the points in the hyperplanes $\{p_j=0\}$ for $j\in\{1,2,3\}$ at most 7 times. Recall from (6.2.8) that we can write

$$\epsilon_{\ell,\lambda}(x) = \frac{\mathfrak{a}}{\ell}\lambda^{-3}f(\lambda^{-1}x) \quad \text{with} \quad f = \frac{\chi''}{|\cdot|} \in C_c^\infty(\mathbb{R}^3). \tag{6.4.26}$$

Using that both $\epsilon_{\ell,\lambda}$ and $\omega_{\ell,\lambda}$ are radial (therefore so is f), we obtain from (6.4.25) that

$$\begin{aligned}
&\left| n^2 \sum_{p\in\pi\mathbb{N}_0^3\setminus\{0\}} \widehat{\epsilon}_{\ell,\lambda}(p)\widehat{\omega}_{\ell,\lambda}(p) - \frac{n^2}{8}\sum_{p\in\pi\mathbb{Z}^3} \widehat{\epsilon}_{\ell,\lambda}(p)\widehat{\omega}_{\ell,\lambda}(p)\right| \\
&\leqslant Cn^2 \sum_{q\in\pi\mathbb{Z}^2} |\widehat{\epsilon}_{\ell,\lambda}(q,0)\widehat{\omega}_{\ell,\lambda}(q,0)| \\
&\leqslant C\frac{n^2}{\ell^2}\lambda^2 \sum_{q\in\pi\mathbb{Z}^2} |\widehat{f}(\lambda q,0)| \leqslant C\left(\frac{n}{\ell}\right)^2,
\end{aligned}$$

where we used that $\|\widehat{\omega}_{\ell,\lambda}\|_\infty \leqslant \|\omega_{\ell,\lambda}\|_1 \leqslant C\lambda^2\ell^{-1}$, which follows from (6.2.9). Using that $\{\frac{1}{\sqrt{8}}e^{ip\cdot x}\}_{p\in\pi\mathbb{Z}^3}$ is an orthonormal basis of $L^2(2\Lambda)$, we obtain that

$$\left|2\int_{\Lambda^2} \widetilde{Q}_2^{(\epsilon)}(x,y)K(x,y) + n^2\int_{\mathbb{R}^3} \epsilon_{\ell,\lambda}(x)\omega_{\ell,\lambda}(x)\mathrm{d}x\right| \leqslant C\left(\frac{n}{\ell}\right)^2.$$

We shall now suitably rewrite the second term. Recall the scattering equation (6.2.6),

$$\frac{1}{2}\epsilon_{\ell,\lambda} = \Delta\left(\omega_{\ell,\lambda}-\omega_\ell\right) \qquad \text{on } \mathbb{R}^3,$$

and note that $\omega_{\ell,\lambda}-\omega_\ell$ and $\Delta\omega_\ell$ have disjoint supports. Therefore,

$$0 = 2\left\langle (\omega_{\ell,\lambda}-\omega_\ell),\Delta\omega_\ell\right\rangle_{L^2(\mathbb{R}^3)} = 2\left\langle \Delta(\omega_{\ell,\lambda}-\omega_\ell),\omega_\ell\right\rangle_{L^2(\mathbb{R}^3)} = \left\langle \epsilon_{\ell,\lambda},\omega_\ell\right\rangle_{L^2(\mathbb{R}^3)},$$

and hence

$$\begin{aligned}
-n^2\int_{\mathbb{R}^3} \epsilon_{\ell,\lambda}(x)\omega_{\ell,\lambda}(x)\mathrm{d}x &= -n^2\langle \epsilon_{\ell,\lambda},\omega_{\ell,\lambda}-\omega_\ell\rangle_{L^2(\mathbb{R}^3)} \\
&= n^2\left\langle \epsilon_{\ell,\lambda},\frac{1}{-2\Delta}\epsilon_{\ell,\lambda}\right\rangle_{L^2(\mathbb{R}^3)} = n^2(2\pi)^{-3}\int_{\mathbb{R}^3}\frac{|\widehat{\epsilon}_{\ell,\lambda}(p)|^2}{2p^2}\mathrm{d}p.
\end{aligned}$$

To conclude, we claim that the integral can be replaced by a corresponding Riemann sum, namely

$$\left| n^2(2\pi)^{-3}\int_{\mathbb{R}^3}\frac{|\widehat{\epsilon}_{\ell,\lambda}(p)|^2}{2p^2}\mathrm{d}p - \sum_{p\in\pi\mathbb{N}_0^3\setminus\{0\}} \frac{|n\widehat{\epsilon}_{\ell,\lambda}(p)|^2}{2p^2}\right| \leqslant C\left(\frac{n}{\ell}\right)^2. \tag{6.4.27}$$

Indeed, using (6.4.26) we see that (6.4.27) is equivalent to

$$\left| \int_{\mathbb{R}^3_{\geqslant 0}} g(\lambda z) \mathrm{d}z - \sum_{z \in \mathbb{N}^3 \setminus \{0\}} g(\lambda z) \right| \leqslant C\lambda^{-2} \quad \text{with} \quad g(z) = \frac{|\widehat{f}(\pi z)|^2}{|\pi z|^2}. \tag{6.4.28}$$

Since $f \in C_c^\infty(\mathbb{R}^3)$, it is straightforward to check that all second derivatives $D^\alpha g$, $|\alpha| = 2$, are bounded as

$$|D_z^\alpha g(z)| \leq C|z|^{-4}, \quad \forall z \in \mathbb{R}^3 \setminus \{0\}.$$

Therefore, for every $z \in \mathbb{N}^3 \setminus \{0\}$ and $\xi \in \Lambda + z$, we have the Taylor expansion

$$g(\lambda \xi) = g(\lambda z) + \lambda(\xi - z) \cdot (\nabla g)(\lambda z) + \mathcal{O}(\lambda^{-2})|z|^{-4}.$$

Integrating over $\xi \in \Lambda + z$ and using $\int_{\Lambda + z} \xi \mathrm{d}\xi = z$ we find that

$$\int_{\Lambda + z} g(\lambda \xi) \mathrm{d}\xi = g(\lambda z) + \mathcal{O}(\lambda^{-2})|z|^{-4}, \quad \forall z \in \mathbb{N}^3 \setminus \{0\}.$$

Summing up these bounds over $z \in \mathbb{N}^3 \setminus \{0\}$ and combining with

$$\int_\Lambda g(\lambda z) \mathrm{d}z \leq \int_\Lambda \frac{C}{|\lambda z|^2} \mathrm{d}z \leq C\lambda^{-2}$$

we obtain (6.4.28). Thus the proof of (6.4.19) is complete.

The last statement (6.4.20) in Lemma 6.11 follows from (6.4.18), (6.4.19) and Lemma 6.8. □

Conclusion of Lemma 6.9. Inserting (6.4.20) in (6.4.17) we obtain the claim. □

6.4.2 Analysis of $(\mathrm{II})_1$

Here we estimate the term

$$(\mathrm{II})_1 = e^{-\mathcal{B}_1} H_2^{(U)} e^{\mathcal{B}_1}$$

appearing in (6.4.6). We recall from (6.1.12) that

$$H_2^{(U)} = n \, \mathrm{d}\Gamma(V_\ell * u_0^2 + \widehat{V}_\ell - V_\ell^{0000}) - \left(\frac{1}{2} \int_{\Lambda^2} V_\ell(x-y) a_x^* a_y^* \mathrm{d}x \mathrm{d}y \, \mathcal{N} + \mathrm{h.c.} \right), \tag{6.4.29}$$

where $nV_\ell * u_0^2$ is a multiplication operator and $\widehat{V}_\ell$ denotes the operator with integral kernel $V_\ell(x-y)$.

Lemma 6.12. *Assume that $\lambda \left(\frac{n}{\ell}\right)^2 \leqslant 1$, that $2R/\ell < \lambda < 1/4$ and that ℓ is large enough. Then we have*

$$e^{-\mathcal{B}_1} H_2^{(U)} e^{\mathcal{B}_1} = \mathrm{d}\Gamma \left(nV_\ell * u_0^2 + n\widehat{V}_\ell - 8\pi \mathfrak{a} \frac{n}{\ell} \right) + \mathcal{E}_1^{(H_2^{(U)})}$$

on $\mathcal{F}_+$, with

$$\pm \mathcal{E}_1^{(H_2^{(U)})} \leqslant \delta Q_4 + \delta^{-1} C \frac{(\mathcal{N}+1)^2}{\ell} + C\lambda^{\frac{1}{2}} \left(\left(\frac{n}{\ell}\right)^2 + \frac{n}{\ell} \right) (\mathcal{N}+1)$$

for all $0 < \delta \leqslant 1$.

To control the diagonal terms in (6.4.29) we use the following lemma.

Lemma 6.13. *Assume that $\lambda\left(\frac{n}{\ell}\right)^2 \leqslant 1$ and that $2R/\ell < \lambda < 1/4$. Let $A : L^2(\Lambda) \to L^2(\Lambda)$ be a bounded, self-adjoint linear operator. Then on $\mathcal{F}$ we have*

$$\pm\left(e^{-\mathcal{B}_1}\mathrm{d}\Gamma(A)e^{\mathcal{B}_1} - \mathrm{d}\Gamma(A)\right) \leqslant C\|A\|_{\mathrm{op}}\|K\|_2\,(\mathcal{N}+1) \leqslant C\|A\|_{\mathrm{op}}\lambda^{1/2}\frac{n}{\ell}\,(\mathcal{N}+1)\,.$$

Proof. Applying the Duhamel formula yields

$$e^{-\mathcal{B}_1}\mathrm{d}\Gamma(A)e^{\mathcal{B}_1} - \mathrm{d}\Gamma(A) = \int_0^1 e^{-t\mathcal{B}_1}[\mathrm{d}\Gamma(A),\mathcal{B}_1]e^{t\mathcal{B}_1}\mathrm{d}t.$$

Let us denote by K the operator with kernel $K(x,y)$ so that $\mathcal{B}_1 = \frac{1}{2}\sum_{m\neq 0} a_m^* a^*(Ku_m) - \text{h.c.}$ From the Cauchy–Schwarz inequality we find

$$\pm[\mathrm{d}\Gamma(A),\mathcal{B}_1] = \pm\sum_{m\neq 0} a^*(AKu_m)a_m^* + \text{h.c.} \leqslant C\|AK\|_2(\mathcal{N}+1) \leqslant C\|A\|_{\mathrm{op}}\|K\|_2(\mathcal{N}+1).$$

The first inequality in Lemma 6.13 then follows from Lemma 6.8 and the second one from Lemma 6.4. ☐

Proof of Lemma 6.12. For the last term of $H_2^{(U)}$ we find with the aid of (6.4.16)

$$\begin{aligned}
&e^{-\mathcal{B}_1}\left(\frac{1}{2}\int_{\Lambda^2} V_\ell(x-y)a_x^*a_y^*\mathcal{N} + \text{h.c.}\right)e^{\mathcal{B}_1}\\
&\quad= \frac{1}{2}\int_{\Lambda^2} V_\ell(x-y)a_x^*a_y^*e^{-\mathcal{B}_1}\mathcal{N}e^{\mathcal{B}_1} + \text{h.c.}\\
&\qquad+ \int_{\Lambda^2} V_\ell(x-y)K(x,y)e^{-\mathcal{B}_1}\mathcal{N}e^{\mathcal{B}_1}\\
&\qquad+ \int_{\Lambda^2} V_\ell(x-y)\int_0^1 e^{-s\mathcal{B}_1}a_x^*a(K_y)e^{s\mathcal{B}_1}\mathrm{d}s\, e^{-\mathcal{B}_1}\mathcal{N}e^{\mathcal{B}_1} + \text{h.c.}
\end{aligned}$$

The second term on the right-hand side is the main term. The first term is controlled by Q_4 with the Cauchy–Schwarz inequality and Lemma 6.8,

$$\begin{aligned}
\pm\int_{\Lambda^2} V_\ell(x-y)a_x^*a_y^*e^{-\mathcal{B}_1}\mathcal{N}e^{\mathcal{B}_1} + \text{h.c.} &\leqslant \delta Q_4 + C\delta^{-1}\int_{\Lambda^2} V_\ell(x-y)e^{-\mathcal{B}_1}\mathcal{N}^2e^{\mathcal{B}_1}\\
&\leqslant \delta Q_4 + C\delta^{-1}\frac{(\mathcal{N}+1)^2}{\ell}.
\end{aligned}$$

For the third term we find similarly

$$\begin{aligned}
&\pm\int_{\Lambda^2} V_\ell(x-y)\int_0^1 e^{-s\mathcal{B}_1}a_x^*a(K_y)e^{s\mathcal{B}_1}\mathrm{d}s\, e^{-\mathcal{B}_1}\mathcal{N}e^{\mathcal{B}_1} + \text{h.c.}\\
&\leqslant \int_{\Lambda^2} V_\ell(x-y)\int_0^1 \left(\|K\|_2^{-1}e^{-s\mathcal{B}_1}a_x^*a(K_y)a^*(K_y)a_xe^{s\mathcal{B}_1} + \|K\|_2e^{-\mathcal{B}_1}\mathcal{N}^2e^{\mathcal{B}_1}\right)\mathrm{d}s\\
&\leqslant C\lambda^{\frac{1}{2}}\frac{n}{\ell^2}(\mathcal{N}+1)^2 \leqslant C\frac{(\mathcal{N}+1)^2}{\ell},
\end{aligned}$$

where we used $\lambda^{\frac{1}{2}}(n/\ell) \leq 1$ in the last estimate. The above bounds show that

$$e^{-\mathcal{B}_1}H_2^{(U)}e^{\mathcal{B}_1} = e^{-\mathcal{B}_1}\mathrm{d}\Gamma\left(nV_\ell * u_0^2 + n\widehat{V}_\ell - \int_{\Lambda^2} V_\ell(x-y)(n+K(x,y)\right)e^{\mathcal{B}_1} + \widetilde{\mathcal{E}}_1^{(H_2^{(U)})} \tag{6.4.30}$$

with

$$\pm\widetilde{\mathcal{E}}_1^{(H_2^{(U)})} \leqslant C\lambda^{\frac{1}{2}}\left(\frac{n}{\ell}\right)^2(\mathcal{N}+1)+\delta Q_4+C\delta^{-1}\frac{(\mathcal{N}+1)^2}{\ell}.$$

From Lemma 6.6 we find

$$\pm\left(\int_{\Lambda^2}V_\ell(x-y)(n+K(x,y))-8\pi\mathfrak{a}\frac{n}{\ell}\right)\leq Cn\ell^{-2}\log(\ell)\leq C\lambda^{\frac{1}{2}}\frac{n}{\ell},$$

where we used $\lambda\geqslant C\ell^{-1}\geqslant(\log(\ell)/\ell)^2$ in the last estimate. Note that the operator in the bracket in the first line of (6.4.30) is bounded by $Cn\ell^{-1}$. We now apply the previous estimate together with Lemma 6.13 to the first line of (6.4.30) and find the statement from Lemma 6.12. □

6.4.3 Analysis of $(\mathrm{III})_1$

Here we analyze

$$(\mathrm{III})_1=e^{-\mathcal{B}_1}(Q_1+Q_3^{(U)})e^{\mathcal{B}_1}$$

appearing in (6.4.6), where we recall that

$$\begin{aligned}
Q_1&=n^{3/2}\int_{\Lambda^2}V_\ell(x-y)a_x^*\mathrm{d}x\mathrm{d}y+\text{h.c.}\,,\\
Q_3^{(U)}&=\sqrt{(n-\mathcal{N}+1)_+}\int_{\Lambda^2}V_\ell(x-y)a_x^*a_y^*a_x\mathrm{d}x\mathrm{d}y+\text{h.c.},\\
Q_3&=n^{\frac{1}{2}}\int_{\Lambda^2}V_\ell(x-y)a_x^*a_y^*a_x\mathrm{d}x\mathrm{d}y+\text{h.c.}
\end{aligned}$$

Lemma 6.14. *Assume that $\lambda\left(\frac{n}{\ell}\right)^2\leqslant 1$, that $2R/\ell<\lambda<1/4$ and that ℓ is large enough. Then we have*

$$(\mathrm{III})_1=Q_3+\mathcal{E}_1^{(Q_3)}$$

on $\mathcal{F}_+$ where the error term satisfies

$$\begin{aligned}
\pm\mathcal{E}_1^{(Q_3)}\leqslant{}& C\delta Q_4+\delta^{-1}C\left(\frac{(\mathcal{N}+1)^2}{n\ell}+\lambda\left(\frac{n}{\ell}\right)^3\right)(\mathcal{N}+1)+Cn^{\frac{1}{2}}\frac{(\mathcal{N}+1)^{\frac{3}{2}}}{\ell}\\
&+C\frac{n^{1/2}}{\ell^{5/6}}\left(\mathrm{d}\Gamma(-\Delta)+\frac{n^2\log(\ell)}{\ell^2}\right)
\end{aligned}$$

for any $0<\delta\leqslant 1$.

Proof. We expand $e^{-\mathcal{B}_1}a_x^*a_y^*e^{\mathcal{B}_1}$ as in (6.4.16) to obtain

$$\begin{aligned}
e^{-\mathcal{B}_1}Q_3^{(U)}e^{\mathcal{B}_1}={}&\int_{\Lambda^2}V_\ell(x-y)a_x^*a_y^*e^{-\mathcal{B}_1}a_x\sqrt{(n-\mathcal{N})_+}e^{\mathcal{B}_1}+\text{h.c.}\\
&+\int_{\Lambda^2}V_\ell(x-y)K(x,y)e^{-\mathcal{B}_1}a_x\sqrt{(n-\mathcal{N})_+}e^{\mathcal{B}_1}+\text{h.c.}\\
&+\int_{\Lambda^2}V_\ell(x-y)\int_0^1e^{-t\mathcal{B}_1}\big(a_x^*a(K_y)+a_y^*a(K_x)\big)e^{t\mathcal{B}_1}\mathrm{d}t\times\\
&\qquad\times e^{-\mathcal{B}_1}a_x\sqrt{(n-\mathcal{N})_+}e^{\mathcal{B}_1}+\text{h.c.}
\end{aligned}\tag{6.4.31}$$

The last term is an error term. In fact, using the Cauchy–Schwarz inequality (for an appropriate choice of $\eta > 0$) we obtain

$$\begin{aligned}
&\pm \int_{\Lambda^2} V_\ell(x-y) \int_0^1 e^{-t\mathcal{B}_1} a_x^* a(K_y) e^{t\mathcal{B}_1} \mathrm{d}t\, e^{-\mathcal{B}_1} a_x \sqrt{(n-\mathcal{N})_+} e^{\mathcal{B}_1} + \text{h.c.} \\
&\quad \leqslant \eta \int_{\Lambda^2} V_\ell(x-y) \int_0^1 \Big[e^{-t\mathcal{B}_1} a_x^* a(K_y) e^{(t-1)\mathcal{B}_1} (\mathcal{N}+1)^{-\frac{1}{2}} e^{-(t-1)\mathcal{B}_1} a^*(K_y) a_x e^{t\mathcal{B}_1} \\
&\qquad + \eta^{-1} C e^{-\mathcal{B}_1} \sqrt{(n-\mathcal{N})_+} a_x^* (\mathcal{N}+1)^{\frac{1}{2}} a_x \sqrt{(n-\mathcal{N})_+} e^{\mathcal{B}_1} \Big] \mathrm{d}t \\
&\quad \leqslant \ell^{-1} \left(\eta \sup_y \|K_y\|_2^2 + \eta^{-1} C n \right) (\mathcal{N}+1)^{\frac{3}{2}} \\
&\quad \leqslant C \lambda^{\frac{1}{2}} \frac{n^{\frac{3}{2}}}{\ell^2} (\mathcal{N}+1)^{\frac{3}{2}} \leqslant C \frac{n^{\frac{1}{2}}}{\ell} (\mathcal{N}+1)^{\frac{3}{2}}.
\end{aligned}$$

In the first two lines of (6.4.31) we may replace $\sqrt{(n-\mathcal{N})_+}$ by $\sqrt{n}$, using

$$\sqrt{n} - \sqrt{(n-\mathcal{N})_+} \leqslant \frac{\mathcal{N}}{\sqrt{n}},$$

which follows from the elementary inequality $1 - \sqrt{(1-x)_+} \leqslant x$ for all $x \geqslant 0$. With the aid of the Cauchy–Schwarz inequality we obtain

$$\begin{aligned}
&\pm \int_{\Lambda^2} V_\ell(x-y) K(x,y) e^{-\mathcal{B}_1} a_x \left(\sqrt{n} - \sqrt{(n-\mathcal{N})_+} \right) e^{\mathcal{B}_1} + \text{h.c.} \\
&\leqslant n \int_{\Lambda^2} V_\ell(x-y) e^{-\mathcal{B}_1} \left(n^{-\frac{1}{2}} a_x^* (\mathcal{N}+1)^{\frac{1}{2}} a_x + n^{\frac{1}{2}} \left(\sqrt{n} - \sqrt{(n-\mathcal{N}-1)_+} \right)^2 (\mathcal{N}+1)^{-\frac{1}{2}} \right) e^{\mathcal{B}_1} \\
&\leqslant C \frac{\sqrt{n}}{\ell} (\mathcal{N}+1)^{\frac{3}{2}}.
\end{aligned}$$

In a similar way one shows that

$$\begin{aligned}
&\pm \int_{\Lambda^2} V_\ell(x-y) a_x^* a_y^* e^{-\mathcal{B}_1} a_x \left(\sqrt{n} - \sqrt{(n-\mathcal{N})_+} \right) e^{\mathcal{B}_1} + \text{h.c.} \\
&\leqslant \delta Q_4 + \delta^{-1} C \int_{\Lambda^2} V_\ell(x-y) e^{-\mathcal{B}_1} (\sqrt{n} - \sqrt{(n-\mathcal{N}+1)_+}) a_x^* a_x (\sqrt{n} - \sqrt{(n-\mathcal{N}+1)_+}) e^{\mathcal{B}_1} \\
&\leqslant \delta Q_4 + \delta^{-1} C \ell^{-1} \frac{(\mathcal{N}+1)^3}{n}
\end{aligned}$$

for all $\delta > 0$. In particular, we have

$$\begin{aligned}
e^{-\mathcal{B}_1} Q_3^{(U)} e^{\mathcal{B}_1} = {} & \sqrt{n} \int_{\Lambda^2} V_\ell(x-y) a_x^* a_y^* e^{-\mathcal{B}_1} a_x e^{\mathcal{B}_1} + \text{h.c.} \\
& + \sqrt{n} \int_{\Lambda^2} V_\ell(x-y) K(x,y) e^{-\mathcal{B}_1} a_x e^{\mathcal{B}_1} + \text{h.c.} + \widetilde{\mathcal{E}}_1^{(Q_3)}
\end{aligned} \tag{6.4.32}$$

with

$$\pm \widetilde{\mathcal{E}}_1^{(Q_3)} \leqslant C n^{\frac{1}{2}} \frac{(\mathcal{N}+1)^{\frac{3}{2}}}{\ell} + \delta Q_4 + \delta^{-1} C \frac{(\mathcal{N}+1)^3}{n\ell}.$$

The second term of (6.4.32) cancels with $e^{-\mathcal{B}_1}Q_1e^{\mathcal{B}_1}$ as we will see below, whereas the first line equals Q_3 up to negligible errors. Indeed,

$$\begin{aligned}&\sqrt{n}\int_{\Lambda^2}V_\ell(x-y)a_x^*a_y^*e^{-\mathcal{B}_1}a_xe^{\mathcal{B}_1}+\text{h.c.}-Q_3\\&=\sqrt{n}\int_{\Lambda^2}V_\ell(x-y)a_x^*a_y^*\int_0^1e^{-t\mathcal{B}_1}[a_x,\mathcal{B}_1]e^{t\mathcal{B}_1}\mathrm{d}t+\text{h.c.}\\&=\sqrt{n}\int_{\Lambda^2}V_\ell(x-y)a_x^*a_y^*\int_0^1e^{-t\mathcal{B}_1}a^*(K_x)e^{t\mathcal{B}_1}\mathrm{d}t+\text{h.c.}\end{aligned}$$

so that with the Cauchy–Schwarz inequality for all $\delta>0$

$$\begin{aligned}&\pm\left(\int_{\Lambda^2}n^{\frac{1}{2}}V_\ell(x-y)a_x^*a_y^*e^{-\mathcal{B}_1}a_xe^{\mathcal{B}_1}+\text{h.c.}-Q_3\right)\\&\leqslant\delta Q_4+\delta^{-1}Cn\sup_x\|K_x\|_2^2\|V_\ell\|_1(\mathcal{N}+1)\\&\leqslant\delta Q_4+\delta^{-1}C\lambda\left(\frac{n}{\ell}\right)^3(\mathcal{N}+1).\end{aligned}\tag{6.4.33}$$

In order to control the second term in (6.4.32) we recall the definition of h in Lemma 6.6 and use $\langle\xi,\int_\Lambda a_x\xi\rangle=0$ for $\xi\in\mathcal{F}_+$ as well as that $e^{-\mathcal{B}_1}$ leaves $\mathcal{F}_+$ invariant to obtain

$$\begin{aligned}&n^{\frac{1}{2}}\int_{\Lambda^2}V_\ell(x-y)K(x,y)e^{-\mathcal{B}_1}a_xe^{\mathcal{B}_1}+\text{h.c.}+e^{-\mathcal{B}_1}Q_1e^{\mathcal{B}_1}\\&=n^{\frac{1}{2}}\int_\Lambda h(x)e^{-\mathcal{B}_1}a_xe^{\mathcal{B}_1}+\text{h.c.}\\&=n^{\frac{1}{2}}\int_\Lambda h(x)a_x+\text{h.c.}+n^{\frac{1}{2}}\int_\Lambda h(x)\int_0^1e^{-t\mathcal{B}_1}a^*(K_x)e^{t\mathcal{B}_1}\mathrm{d}t+\text{h.c.}\end{aligned}\tag{6.4.34}$$

on $\mathcal{F}_+$. Both terms on the right hand side are small. Indeed, the Cauchy–Schwarz inequality and the estimates on h in Lemma 6.6 yield

$$\begin{aligned}&\pm n^{\frac{1}{2}}\int_\Lambda h(x)\int_0^1e^{-t\mathcal{B}_1}a^*(K_x)e^{t\mathcal{B}_1}\mathrm{d}t+\text{h.c.}\leqslant Cn^{\frac{1}{2}}\|h\|_1\sup_x\|K_x\|_2(\mathcal{N}+1)^{\frac{1}{2}}\\&\leqslant Cn^{\frac{1}{2}}\frac{n\log(\ell)}{\ell^2}\lambda^{\frac{1}{2}}\frac{n}{\ell}(\mathcal{N}+1)^{\frac{1}{2}}\leqslant\lambda\left(\frac{n}{\ell}\right)^3(\mathcal{N}+1)+C\frac{n^2\log(\ell)^2}{\ell^3}.\end{aligned}\tag{6.4.35}$$

Moreover, by the Cauchy–Schwarz inequality we have for all $\eta>0$

$$\begin{aligned}\pm n^{\frac{1}{2}}\int_\Lambda h(x)a_x+\text{h.c.}&\leqslant C\eta n^{1/2}\int_\Lambda|h(x)|a_x^*a_x+C\eta^{-1}n^{1/2}\int_\Lambda|h(x)|\\&\leqslant C\eta n^{1/2}\|h\|_{3/2}\mathrm{d}\Gamma(-\Delta)+C\eta^{-1}n^{1/2}\|h\|_1\\&\leqslant C\eta n^{1/2}\ell^{-2/3}\frac{n}{\ell}\mathrm{d}\Gamma(-\Delta)+C\eta^{-1}n^{1/2}\ell^{-1}\frac{n}{\ell}\log\ell\\&\leqslant C\frac{n^{1/2}}{\ell^{5/6}}\left(\mathrm{d}\Gamma(-\Delta)+\frac{n^2\log(\ell)}{\ell^2}\right),\end{aligned}\tag{6.4.36}$$

where we chose $\eta=\ell^{5/6}/n$ in the last step. For the second inequality we used that on $\mathcal{F}_+$

$$\mathrm{d}\Gamma(\Phi)\leqslant C\|\Phi\|_{3/2}\mathrm{d}\Gamma(-\Delta),\tag{6.4.37}$$

for $\Phi\in L^{3/2}(\Lambda)$. This follows from the Hölder and Sobolev inequalities as

$$\langle f,\Phi f\rangle=\int_\Lambda\Phi(x)|f(x)|^2\leqslant C\|\Phi\|_{3/2}\|f\|_6^2\leqslant C\|\Phi\|_{3/2}\left(\|f\|_2^2+\|\nabla f\|_2^2\right),\ f\in H^1(\Lambda)$$

and $\mathcal{N} \leqslant \pi^{-2}\mathrm{d}\Gamma(-\Delta)$ on $\mathcal{F}_+$.

Inserting (6.4.35) and (6.4.36) into (6.4.34), and subsequently (6.4.33) and (6.4.34) into (6.4.32), yields

$$e^{-\mathcal{B}_1}\left(Q_1 + Q_3^{(U)}\right)e^{\mathcal{B}_1} = Q_3 + \mathcal{E}_1^{(Q_3)}$$

with

$$\begin{aligned}\pm\mathcal{E}_1^{(Q_3)} \leqslant{}& Cn^{\frac{1}{2}}\frac{(\mathcal{N}+1)^{\frac{3}{2}}}{\ell} + \delta Q_4 + \delta^{-1}C\frac{(\mathcal{N}+1)^3}{n\ell} + \delta Q_4 + \delta^{-1}C\lambda\left(\frac{n}{\ell}\right)^3(\mathcal{N}+1)\\ &+ \lambda\left(\frac{n}{\ell}\right)^3(\mathcal{N}+1) + C\frac{n^2\log(\ell)^2}{\ell^3} + C\frac{n^{1/2}}{\ell^{5/6}}\left(\mathrm{d}\Gamma(-\Delta) + \frac{n^2\log(\ell)}{\ell^2}\right).\end{aligned}$$

We readily deduce Lemma 6.14 via simplifications due to $\delta \leqslant 1$ and $\log(\ell)\ell^{-1} \lesssim \ell^{-5/6}$. □

6.4.4 Proof of Lemma 6.7

Proof. Inserting Lemmata 6.9, 6.12 and 6.14 in (6.4.6) we obtain

$$\begin{aligned}e^{-\mathcal{B}_1}\mathcal{H}e^{\mathcal{B}_1} ={}& 4\pi\mathfrak{a}n^2\ell^{-1} + \sum_{p\in\pi\mathbb{N}_0^3\setminus\{0\}}\frac{|n\widehat{\epsilon}_{\ell,\lambda}(p)|^2}{2p^2} + \mathrm{d}\Gamma(-\Delta) + Q_4 + \widetilde{Q}_2 + \mathcal{E}_1^{(Q_2)}\\ &+ \mathrm{d}\Gamma\left(nV_\ell * u_0^2 + n\widehat{V}_\ell - 8\pi\mathfrak{a}\frac{n}{\ell}\right) + \mathcal{E}_1^{(H_2^{(U)})} + Q_3 + \mathcal{E}_1^{(Q_3)} + e^{-\mathcal{B}_1}\mathcal{E}^{(U)}e^{\mathcal{B}_1}.\end{aligned}$$

We apply Lemma 6.8 and (6.4.10) to (6.2.18) and find

$$\pm e^{-\mathcal{B}_1}\mathcal{E}^{(U)}e^{\mathcal{B}_1} \leqslant \varepsilon n^{-1}CQ_4 + \varepsilon^{-1}C\frac{n}{\ell} + C\lambda\frac{n}{\ell^3}(\mathcal{N}+1)^2 + Cn^{\frac{1}{2}}\ell^{-1}(\mathcal{N}+1)^{\frac{3}{2}},$$

were some terms simplified due to the condition $\varepsilon \leqslant 1$. Collecting all the error terms and using $\lambda n^2\ell^{-2} \leqslant 1$ and $\delta \leqslant 1$ yields Lemma 6.7. □

6.5 The Cubic Transformation

In this section we apply the cubic transformation $e^{\mathcal{B}_c}$ to $e^{\mathcal{B}_1}\mathcal{H}e^{-\mathcal{B}_1}$ with

$$\mathcal{B}_c = \frac{\theta_M(\mathcal{N})}{\sqrt{n}}\int_{\Lambda^2} q_x^* a^*(K_x)q_x\mathrm{d}x\mathrm{d}y - \text{h.c.} \tag{6.5.1}$$

Recall that

$$q_x = \int_\Lambda Q(x,y)a_y\mathrm{d}y = a(Q_x).$$

where $Q = 1 - |u_0\rangle\langle u_0|$ and $Q(x,y)$ is its integral kernel. In particular

$$q(f) = a(Qf) = a(f) - \langle f, u_0\rangle a(u_0), \quad \forall f \in L^2(\Lambda).$$

The use of q_x instead of a_x in the definition of $\mathcal{B}_c$ in (6.5.1) ensures that $\mathcal{B}_c$ leaves $\mathcal{F}_+$ invariant. Note that the commutation relations of these operators with the usual creation and annihilation operators are given by

$$[q_x, a_y^*] = \delta_{x,y} - u_0(y) = \delta_{x,y} - 1, \quad \forall x, y \in \Lambda.$$

In all normal ordered expressions, q_x may be replaced by a_x on $\mathcal{F}_+$ since $q_x|\xi\rangle = a_x|\xi\rangle$ for all $\xi \in \mathcal{F}_+$.

For $1 \leqslant M \leqslant n$ we define

$$\theta_M(\mathcal{N}) := \theta(\mathcal{N}/M),$$

where $\theta \in C^\infty(\mathbb{R}_{\geqslant 0}, [0,1])$ satisfies $\theta(x) = 1$ for $x \leqslant \frac{1}{2}$ and $\theta(x) = 0$ for $x \geqslant 1$. The cut-off θ_M in $\mathcal{B}_c$ ensures that $\mathcal{B}_c$ does not create too many excitations, thereby allowing us to close some Grönwall estimates in the computation of $e^{-\mathcal{B}_c}(\mathrm{d}\Gamma(-\Delta)+Q_3+Q_4)e^{\mathcal{B}_c}$. Effectively, with this we only renormalize the Q_3 term on the sector with particle number $\mathcal{N} \lesssim M$. In Proposition 6.28, M is chosen of the order of $n^{1-68\kappa}$, which is sufficient to compute the free energy of the system up to the second order for small κ. We will write θ_M instead of $\theta_M(\mathcal{N})$ in the following.

The main purpose of the transformation $e^{\mathcal{B}_c}$ is to remove the cubic term Q_3 in (6.4.2). This also renormalizes the second line in (6.4.2), which is essentially $(2\widehat{V}(0) - 8\pi\mathfrak{a})n\ell^{-1}\mathcal{N}$, into $8\pi\mathfrak{a}n\ell^{-1}\mathcal{N}$. Eventually, we obtain the Bogoliubov Hamiltonian $\mathbb{H}_{\mathrm{Bog}}$ on $\mathcal{F}_+$ defined in (6.1.29).

The following lemma is the main result of this section.

Lemma 6.15. *Assume that $\lambda \left(\frac{n}{\ell}\right)^2 \leqslant 1$, that $2R/\ell < \lambda < 1/4$, that ℓ is large enough and that*

$$\sigma := \max\{n^{1/2}\ell^{-5/6}, n^{1/2}M\ell^{-3/2}, \lambda^{-1/2}n^{1/2}M^{1/2}\ell^{-1}\} \leqslant 1.$$

Then we have

$$e^{-\mathcal{B}_c}e^{-\mathcal{B}_1}\mathcal{H}e^{\mathcal{B}_1}e^{\mathcal{B}_c} = 4\pi\mathfrak{a}n^2\ell^{-1} + \mathbb{H}_{\mathrm{Bog}} + Q_4 + \mathcal{E}_c \tag{6.5.2}$$

on $\mathcal{F}_+$ where the error term satisfies

$$\begin{aligned}\pm\mathcal{E}_c \leqslant{}& C\sigma\left(Q_4 + \mathrm{d}\Gamma(-\Delta) + \frac{n}{\ell}(\mathcal{N}+1)\right) + \frac{1}{2}Q_4\\ &+ C\delta\left(Q_4 + \frac{n}{\ell}(\mathcal{N}+1)\right) + \delta^{-1}C\left[\frac{n}{\ell}\frac{\mathcal{N}+1}{M} + \frac{(\mathcal{N}+1)}{\ell} + \frac{(\mathcal{N}+1)^2}{n\ell} + \lambda\left(\frac{n}{\ell}\right)^3\right](\mathcal{N}+1)\\ &+ C\left[\lambda^{\frac{1}{2}}\left(\left(\frac{n}{\ell}\right)^2 + \frac{n}{\ell}\right) + \lambda^{-1/2}\frac{n^{3/2}}{\ell^2} + \frac{n}{\ell}\frac{(\mathcal{N}+1)^{1/2}}{n^{1/2}}\right](\mathcal{N}+1) + C\left(\left(\frac{n}{\ell}\right)^2\log\ell + \frac{n}{\ell}\right)\end{aligned}$$

on $\mathcal{F}_+$, for all $0 < \delta \leqslant 1$.

To prove Lemma 6.15, we start with Lemma 6.7 and the quadratic form identity

$$\begin{aligned}e^{-\mathcal{B}_c}e^{-\mathcal{B}_1}\mathcal{H}e^{\mathcal{B}_1}e^{\mathcal{B}_c} - 4\pi\mathfrak{a}n^2\ell^{-1} - \frac{1}{2}\sum_{p\neq 0}\frac{|n\widehat{\epsilon}_{\ell,\lambda}(p)|^2}{2p^2} &= e^{-\mathcal{B}_c}\Big(\mathrm{d}\Gamma(-\Delta) + Q_4 + Q_3\Big)e^{\mathcal{B}_c}\\ + e^{-\mathcal{B}_c}\mathrm{d}\Gamma\left(nV_\ell * u_0^2 + n\widehat{V}_\ell - 8\pi\mathfrak{a}\frac{n}{\ell}\right)e^{\mathcal{B}_c} &+ e^{-\mathcal{B}_c}\widetilde{Q}_2e^{\mathcal{B}_c} + e^{-\mathcal{B}_c}\mathcal{E}_1e^{\mathcal{B}_c}\end{aligned} \tag{6.5.3}$$

on $\mathcal{F}_+$. Recall that $V_\ell * u_0^2$ is a multiplication operator and that $\widehat{V}_\ell$ is the operator with integral kernel $V_\ell(x-y)$. Using the Duhamel formula, we can expand the term on the third line above as

$$\begin{aligned}e^{-\mathcal{B}_c}\Big(\mathrm{d}\Gamma(-\Delta) + Q_4 + Q_3\Big)e^{\mathcal{B}_c} = \mathrm{d}\Gamma(-\Delta) + Q_4 + \int_0^1\int_t^1 e^{-s\mathcal{B}_c}[Q_3, \mathcal{B}_c]e^{s\mathcal{B}_c}\mathrm{d}s\mathrm{d}t\\ + \int_0^1 e^{-t\mathcal{B}_c}\Big(Q_3 + [\mathrm{d}\Gamma(-\Delta) + Q_4, \mathcal{B}_c]\Big)e^{t\mathcal{B}_c}\mathrm{d}t.\end{aligned}$$

Plugging the above equation into (6.5.3), we obtain

$$
\begin{aligned}
&e^{-\mathcal{B}_c}e^{-\mathcal{B}_1}\mathcal{H}e^{\mathcal{B}_1}e^{\mathcal{B}_c} - 4\pi\mathfrak{a}n^2\ell^{-1} - \frac{1}{2}\sum_{p\neq 0}\frac{|n\widehat{\epsilon}_{\ell,\lambda}(p)|^2}{2p^2} - \mathrm{d}\Gamma(-\Delta) - Q_4 \\
&= \Big\{e^{-\mathcal{B}_c}\mathrm{d}\Gamma\left(nV_\ell * u_0^2 + n\widehat{V}_\ell - 8\pi\mathfrak{a}\frac{n}{\ell}\right)e^{\mathcal{B}_c} + \int_0^1\int_t^1 e^{-s\mathcal{B}_c}[Q_3,\mathcal{B}_c]e^{s\mathcal{B}_c}\mathrm{d}s\mathrm{d}t\Big\} \\
&\quad + \Big\{e^{-\mathcal{B}_c}\widetilde{Q}_2e^{\mathcal{B}_c}\Big\} + \Big\{\int_0^1 e^{-t\mathcal{B}_c}\Big(Q_3 + [\mathrm{d}\Gamma(-\Delta)+Q_4,\mathcal{B}_c]\Big)e^{t\mathcal{B}_c}\mathrm{d}t + e^{-\mathcal{B}_c}\mathcal{E}_1e^{\mathcal{B}_c}\Big\} \\
&= (\mathrm{I})_c + (\mathrm{II})_c + (\mathrm{III})_c.
\end{aligned}
\tag{6.5.4}
$$

In Section 6.5.1 we compute the action of $e^{\mathcal{B}_c}$ on $\mathrm{d}\Gamma(-\Delta)$ and Q_4. Then we show that $(\mathrm{I})_c$ is essentially $8\pi\mathfrak{a}n\ell^{-1}\mathcal{N}$, while $(\mathrm{II})_c$ gives the pairing term involving $(a_p^*a_p^* + \text{h.c.})$ in the Bogoliubov Hamiltonian in Section 6.5.2 and Section 6.5.3, respectively. Finally, in Section 6.5.4, we estimate the error term $(\mathrm{III})_c$ and conclude the proof of Lemma 6.15.

We end this subsection with an estimate of the action of $e^{\mathcal{B}_c}$ on $\mathcal{N}^k$ analogous to Lemma 6.8.

Lemma 6.16. *Assume that $\lambda\left(\frac{n}{\ell}\right)^2 \leqslant 1$ and that $2R/\ell < \lambda < 1/4$. For all $k\in\mathbb{N}$ there is a constant $C_k > 0$ such that on $\mathcal{F}_+$*

$$e^{-t\mathcal{B}_c}\mathcal{N}^ke^{t\mathcal{B}_c} \leqslant C_k(\mathcal{N}+1)^k, \quad \forall t\in[-1,1].$$

Proof. From the Duhamel formula we have

$$e^{-t\mathcal{B}_c}(\mathcal{N}+1)^ke^{t\mathcal{B}_c} - (\mathcal{N}+1)^k = \int_0^t e^{-s\mathcal{B}_c}[(\mathcal{N}+1)^k,\mathcal{B}_c]e^{s\mathcal{B}_c}\mathrm{d}s$$

Let us estimate the commutator. Recall that in normal ordered expressions we can replace q_x by a_x on $\mathcal{F}_+$. Therefore, using the Cauchy–Schwarz inequality, we have

$$
\begin{aligned}
&[(\mathcal{N}+1)^k,\mathcal{B}_c] = n^{-\frac12}\int_{\Lambda^2}[(\mathcal{N}+1)^k,\theta_MK(x,y)q_x^*a_y^*q_x] + \text{h.c.} \\
&= n^{-\frac12}\int_{\Lambda^2}((\mathcal{N}+1)^k - \mathcal{N}^k)\theta_MK(x,y)a_x^*a_y^*a_x + \text{h.c.} \\
&= n^{-\frac12}\int_{\Lambda^2}((\mathcal{N}+1)^k - \mathcal{N}^k)(\mathcal{N}+1)^{-\frac{k-1}{2}}\theta_Ma_x^*a^*(K_x)a_x(\mathcal{N}+2)^{\frac{k-1}{2}} + \text{h.c.} \\
&\le n^{-1}((\mathcal{N}+1)^k - \mathcal{N}^k)(\mathcal{N}+1)^{-\frac{k-1}{2}}\theta_M\sup_x\|K_x\|_2^2\mathcal{N}^2\theta_M(\mathcal{N}+1)^{-\frac{k-1}{2}}((\mathcal{N}+1)^k - \mathcal{N}^k) \\
&\quad + (\mathcal{N}+2)^{\frac{k-1}{2}}\mathcal{N}(\mathcal{N}+2)^{\frac{k-1}{2}} \\
&\le C_kn^{-1}(\mathcal{N}+1)^{k+1}\theta_M + C(\mathcal{N}+1)^k \le C_k(\mathcal{N}+1)^k.
\end{aligned}
$$

Here we used that $\sup_x\|K_x\|_2^2 \le \lambda n^2\ell^2 \leqslant 1$ and that $n^{-1}\theta_M(\mathcal{N}+1) \leqslant n^{-1}(M+1) \leqslant 2$. Therefore, we obtain

$$e^{-t\mathcal{B}_c}(\mathcal{N}+1)^ke^{t\mathcal{B}_c} - (\mathcal{N}+1)^k \leqslant C_k\int_0^t e^{-s\mathcal{B}_c}(\mathcal{N}+1)^ke^{s\mathcal{B}_c}\mathrm{d}s.$$

Applying the Grönwall lemma concludes the proof. □

6.5.1 Actions on $\mathrm{d}\Gamma(-\Delta)$ and Q_4

In this section, we estimate the actions of $e^{\mathcal{B}_c}$ on $\mathrm{d}\Gamma(-\Delta)$ and Q_4.

Lemma 6.17. *Assume that $\lambda\left(\frac{n}{\ell}\right)^2 \leqslant 1$, that $2R/\ell < \lambda < 1/4$ and that ℓ is large enough. Let $\sigma \le 1$ be as in Lemma 6.15. For all $t \in [-1,1]$ we have on $\mathcal{F}_+$*

$$e^{-t\mathcal{B}_c}\mathrm{d}\Gamma(-\Delta)e^{t\mathcal{B}_c} \leqslant C\left(\mathrm{d}\Gamma(-\Delta) + Q_4 + \frac{n}{\ell}(\mathcal{N}+1)\right),$$
$$e^{-t\mathcal{B}_c}Q_4e^{t\mathcal{B}_c} \leqslant C\left(Q_4 + \frac{n}{\ell}(\mathcal{N}+1) + \sigma\mathrm{d}\Gamma(-\Delta)\right).$$

As an intermediate step, we need to compute accurately the commutators $[\mathrm{d}\Gamma(-\Delta), \mathcal{B}_c]$ and $[Q_4, \mathcal{B}_c]$, which is done in Lemmata 6.18 and 6.19. This will further be useful in order to bound the term $(\mathrm{II})_c$ in the proof of Lemma 6.15 in Section 6.5.4.

Lemma 6.18. *Assume that $\lambda\left(\frac{n}{\ell}\right)^2 \leqslant 1$, that $2R/\ell < \lambda < 1/4$ and that ℓ is large enough. Then, on $\mathcal{F}_+$ we have*

$$[\mathrm{d}\Gamma(-\Delta), \mathcal{B}_c] = \theta_M n^{\frac{1}{2}} \int_{\Lambda^2} \left(V_\ell(\omega_\ell - 1)\right)(x-y) a_x^* a_y^* a_x \mathrm{d}x\mathrm{d}y + \text{h.c.} + \mathcal{E}_c^{(\mathrm{d}\Gamma(-\Delta))}$$

with

$$\pm\mathcal{E}_c^{(\mathrm{d}\Gamma(-\Delta))} \leqslant Cn^{\frac{1}{2}}\ell^{-\frac{5}{6}}\left(Q_4 + \mathrm{d}\Gamma(-\Delta)\right) + C\lambda^{-\frac{1}{2}}\frac{n^{\frac{1}{2}}M^{\frac{1}{2}}}{\ell}\mathrm{d}\Gamma(-\Delta).$$

Lemma 6.19. *Assume that $\lambda\left(\frac{n}{\ell}\right)^2 \leqslant 1$, that $2R/\ell < \lambda < 1/4$ and that ℓ is large enough. Then, on $\mathcal{F}_+$ we have*

$$[Q_4, \mathcal{B}_c] = -\theta_M n^{\frac{1}{2}} \int_{\Lambda^2} (V_\ell\omega_\ell)(x-y) a_x^* a_y^* a_x \mathrm{d}x\mathrm{d}y + \text{h.c.} + \mathcal{E}_c^{(Q_4)}$$

with

$$\pm\mathcal{E}_c^{(Q_4)} \leqslant C\left(n^{\frac{1}{2}}\ell^{-\frac{5}{6}} + \frac{n^{\frac{1}{2}}M}{\ell^{\frac{3}{2}}}\right)\left(Q_4 + \mathrm{d}\Gamma(-\Delta)\right).$$

We have defined σ in Lemma 6.15 in such a way that the error terms in Lemmata 6.18 and 6.19 are bounded by

$$\pm\left(\mathcal{E}_c^{(\mathrm{d}\Gamma(-\Delta))} + \mathcal{E}_c^{(Q_4)}\right) \leqslant C\sigma(Q_4 + \mathrm{d}\Gamma(-\Delta)). \tag{6.5.5}$$

Proof of Lemma 6.18. Clearly $[\mathrm{d}\Gamma(-\Delta), \theta_M] = 0$. From (6.3.2) we find

$$\mathcal{B}_c = -n\frac{\theta_M}{\sqrt{n}} \sum_{m,p,q\neq 0} \widehat{\omega}_{\ell,\lambda}(p) a_m^* a_p^* a_q \int_\Lambda u_m(x)u_p(x)u_q(x) - \text{h.c.}$$

We compute

$$\begin{aligned}
[\mathrm{d}\Gamma(-\Delta), \mathcal{B}_c] &= -n^{1/2}\theta_M \sum_{m,p,q\neq 0} \widehat{\omega}_{\ell,\lambda}(p) a_m^* a_p^* a_q (m^2 + p^2 - q^2) \int_\Lambda u_m(x)u_p(x)u_q(x) + \text{h.c.} \\
&= -2n^{1/2}\theta_M \sum_{m,p,q\neq 0} p^2 \widehat{\omega}_{\ell,\lambda}(p) a_m^* a_p^* a_q \int_\Lambda u_m(x)u_p(x)u_q(x) + \text{h.c.} \\
&\quad - 2n^{1/2}\theta_M \sum_{m,p,q\neq 0} \widehat{\omega}_{\ell,\lambda}(p) a_m^* a_p^* a_q \int_\Lambda (\nabla u_m)(x)u_p(x)(\nabla u_q)(x) + \text{h.c.} \\
&= 2\frac{\theta_M}{\sqrt{n}} \int_{\Lambda^2} (-\Delta_2 K)(x,y) q_x^* a_y^* q_x + \text{h.c.} - 2\frac{\theta_M}{n^{1/2}} \int_{\Lambda^2} (\nabla_1 K)(x,y) q_x^* a_y^* \nabla_x q_x + \text{h.c.},
\end{aligned}$$

where for the last equality we used (6.3.2). Moreover,

$$-\Delta_2 K(x,y) = n \sum_{z\in\mathbb{Z}^3} (\Delta\omega_\ell)(P_z(x)-y) + \frac{n}{2} \sum_{z\in\mathbb{Z}^3} \epsilon_{\ell,\lambda}(P_z(x)-y).$$

On $\mathcal{F}_+$, we can replace q_x by a_x, and we have

$$\begin{aligned}
[\mathrm{d}\Gamma(-\Delta), \mathcal{B}_c] = \theta_M n^{\frac12} &\int_{\Lambda^2} (2\Delta\omega_\ell)(x-y) a_x^* a_y^* a_x + \text{h.c.} \\
&+ \theta_M n^{\frac12} \sum_{z\neq 0} \int_{\Lambda^2} (2\Delta\omega_\ell)(P_z(x)-y) a_x^* a_y^* a_x + \text{h.c.} \\
&+ \theta_M n^{\frac12} \sum_{z\in\mathbb{Z}^3} \int_{\Lambda^2} \epsilon_{\ell,\lambda}(P_z(x)-y) a_x^* a_y^* a_x + \text{h.c.} \\
&- \left(2n^{-\frac12}\theta_M \int_{\Lambda^2} \nabla_x K(x,y)\cdot a_x^* a_y^* \nabla_x a_x + \text{h.c.}\right) \\
=:\ & \theta_M n^{\frac12} \int_{\Lambda^2} (2\Delta\omega_\ell)(x-y) a_x^* a_y^* a_x + \text{h.c.} + \sum_{i=1}^3 G_i.
\end{aligned}$$

The scattering equation $2\Delta\omega_\ell + V_\ell - V_\ell\omega_\ell = 0$ now gives the correct main term in Lemma 6.18 and we conclude the proof by estimating the error $\mathcal{E}_c^{(\mathrm{d}\Gamma(-\Delta))} := \sum_{i=1}^3 G_i$ term by term.

For G_1, we use $|1-\omega_\ell| \leqslant 1$ and that for $z\neq 0$ we have

$$V_\ell(P_z(x)-y) \leqslant V_\ell(x-y)\mathbb{1}_{\mathrm{d}(x,\partial\Lambda)\leqslant R\ell^{-1}}$$

since $|x-y| \leqslant |P_z(x)-y|$ and V is decreasing and supported on a ball of radius R. Together with $\theta_M \leqslant 1$ and the Cauchy–Schwarz inequality we obtain on $\mathcal{F}_+$

$$\begin{aligned}
\pm G_1 &= \pm n^{\frac12}\theta_M \sum_{z\neq 0} \int_{\Lambda^2} \big(V_\ell(\omega_\ell - 1)\big)(P_z(x)-y) a_x^* a_y^* a_x + \text{h.c.} \\
&\leqslant \delta Q_4 + C\delta^{-1} n \int_{\Lambda^2} V_\ell(x-y)\mathbb{1}_{\mathrm{d}(x,\partial\Lambda)\leqslant R\ell^{-1}} a_x^* a_x \\
&\leqslant \delta Q_4 + C\delta^{-1} n \ell^{-\frac53} \mathrm{d}\Gamma(-\Delta)
\end{aligned}$$

for all $\delta > 0$. In the last inequality we applied (6.4.37) to $\Phi = \mathbb{1}_{\mathrm{d}(x,\partial\Lambda)\leqslant R\ell^{-1}}$ with $\|\Phi\|_{3/2} \leqslant C\ell^{-2/3}$. The choice $\delta = n^{1/2}\ell^{-5/6}$ gives the first error term in Lemma 6.18.

In order to bound G_2, we again use (6.4.37), this time applied to $\Phi(y) = \epsilon_{\ell,\lambda}(P_z(x)-y)$ for fixed x. We may estimate the L^p-norms of $\epsilon_{\ell,\lambda}$ using

$$|\epsilon_{\ell,\lambda}(P_z(x)-y)| \leqslant C\ell^{-1}\lambda^{-3}\mathbb{1}_{|x-y|\leqslant\lambda},$$

which follows from Lemma 6.2 and $|x-y| \leqslant |P_z(x)-y|$. The Cauchy–Schwarz inequality, $\theta_M(\mathcal{N}+1)^k\theta_M \leqslant CM^k$ for $k\geqslant 0$, $\mathcal{N} \leqslant \pi^{-2}\mathrm{d}\Gamma(-\Delta)$ on $\mathcal{F}_+$ and an appropriate choice for $\delta_M > 0$ yield on $\mathcal{F}_+$

$$\begin{aligned}
\pm G_2 &\leqslant n^{\frac12} \sum_{z\in\mathbb{Z}^3} \left(\int_{\Lambda^2} \delta_M |\epsilon_{\ell,\lambda}(P_z(x)-y)| \theta_M a_x^* a_y^* a_y a_x \theta_M + \delta_M^{-1} |\epsilon_{\ell,\lambda}(P_z(x)-y)| a_x^* a_x \right) \\
&\leqslant C n^{\frac12} \left(\delta_M \|\epsilon_{\ell,\lambda}\|_{3/2} \theta_M(\mathcal{N}+1)\mathrm{d}\Gamma(-\Delta)\theta_M + \delta_M^{-1}\|\epsilon_{\ell,\lambda}\|_1 \mathcal{N}\right) \\
&\leqslant C n^{\frac12}\ell^{-1}\lambda^{-3} \left(\delta_M M\lambda^2 + \delta_M^{-1}\lambda^3\right) \mathrm{d}\Gamma(-\Delta) \\
&\leqslant C\frac{n^{\frac12}M^{\frac12}}{\ell}\lambda^{-\frac12}\mathrm{d}\Gamma(-\Delta).
\end{aligned}$$

For G_3 we readily check that

$$|\nabla_x K(x,y)| \leqslant C\frac{n}{\ell}\frac{1}{|x-y|^2}$$

from Lemma 6.2 and (6.3.1), so that on $\mathcal{F}_+$

$$\begin{aligned}\pm\frac{1}{2}G_3 &\leqslant n^{-\frac{1}{2}}\left(\delta_M\int_{\Lambda^2}\theta_M a_x^*a_y^*a_ya_x\theta_M|\nabla_x K(x,y)| + \delta_M^{-1}\int_{\Lambda^2}\nabla_x a_x^*\nabla_x a_x|\nabla_x K(x,y)|\right)\\ &\leqslant Cn^{-\frac{1}{2}}\left(\delta_M\int_{\Lambda^2}\theta_M a_x^*a_y^*a_ya_x\theta_M\frac{n}{\ell|x-y|^2} + \delta_M^{-1}\int_{\Lambda}\nabla_x a_x^*\nabla_x a_x\frac{n}{\ell}\right).\end{aligned}$$

We now use the Hardy inequality on Λ

$$\int_\Lambda \frac{|f(x,y)|^2}{|x-y|^2}\mathrm{d}x \leqslant C\|f(\cdot,y)\|^2_{H^1(\Lambda)},\ \forall f\in H^1(\Lambda^2), y\in\Lambda. \tag{6.5.6}$$

Consequently, together with $\mathcal{N}\leqslant \pi^{-2}\mathrm{d}\Gamma(-\Delta)$ on $\mathcal{F}_+$, we have

$$\int_{\Lambda^2} a_x^*a_y^*a_xa_y\frac{1}{|x-y|^2} \leqslant C(\mathcal{N}-1)\mathrm{d}\Gamma(-\Delta).$$

With the aid of this bound we obtain

$$\pm G_3 \leqslant Cn^{-\frac{1}{2}}\frac{n}{\ell}\left(\delta_M\theta_M(\mathcal{N}-1)\mathrm{d}\Gamma(-\Delta)\theta_M + \delta_M^{-1}\mathrm{d}\Gamma(-\Delta)\right) \leqslant C\frac{n^{\frac{1}{2}}M^{\frac{1}{2}}}{\ell}\mathrm{d}\Gamma(-\Delta),$$

which completes the proof of Lemma 6.18 since $\lambda\leqslant 1$. □

Proof of Lemma 6.19. With the definition of K in (6.3.1), and recalling that $q_x = a_x$ on $\mathcal{F}_+$, we compute

$$\begin{aligned} n^{\frac{1}{2}}[Q_4,\mathcal{B}_c] = {}&\theta_M\int_{\Lambda^2}V_\ell(x-y)\big(-n\omega_\ell(x-y) - \sum_{z\neq 0}n\omega_{\ell,\lambda}(P_z(x)-y) + K_2\big)a_x^*a_y^*a_x + \text{h.c.}\\ &-\left(\theta_M\int_{\Lambda^2}V_\ell(x-y)a_x^*a_y^*a(K_x) + \text{h.c.}\right)\\ &+\theta_M\int_{\Lambda^2}V_\ell(x-y)a_x^*a_y^*\int_\Lambda a_v^*K(v,x)a_va_y + \text{h.c.}\\ &+\theta_M\int_{\Lambda^3}V_\ell(x-y)a_x^*a_v^*a^*(K_v)a_xa_y + \text{h.c.}\\ &-\left(\theta_M\int_{\Lambda^2}V_\ell(x-y)a_x^*a_y^*\int_\Lambda a^*(K_v)a_xa_v + \text{h.c.}\right)\\ =: {}&-\theta_M\int_{\Lambda^2}n(V_\ell\omega_\ell)(x-y)a_x^*a_y^*a_x + \text{h.c.} + n^{\frac{1}{2}}\sum_{i=1}^{6}I_i.\end{aligned}$$

Here we extracted the main term and it remains to estimate all the I_i. From (6.3.11) we have

$$\sum_{z\neq 0}|\omega_{\ell,\lambda}(P_z(x)-y)| \leqslant \frac{C}{1+\ell\mathrm{d}(x,\partial\Lambda)}.$$

With this and (6.4.37) we find

$$\begin{aligned}
\pm I_1 &= \mp\theta_M n^{\frac{1}{2}} \sum_{z\neq 0} \int_{\Lambda^2} V_\ell(x-y)\omega_{\ell,\lambda}(P_z(x)-y)a_x^* a_y^* a_x + \text{h.c.} \\
&\leqslant \delta Q_4 + C\delta^{-1} n\|V_\ell\|_1 \mathrm{d}\Gamma\left((1+\ell \mathrm{d}(\,\cdot\,,\partial\Lambda))^{-2}\right) \\
&\leqslant \delta Q_4 + C\delta^{-1}\frac{n}{\ell}\|(1+\ell\mathrm{d}(\,\cdot\,,\partial\Lambda))^{-2}\|_{3/2}\mathrm{d}\Gamma(-\Delta) \\
&\leqslant \delta Q_4 + C\delta^{-1} n\ell^{-\frac{5}{3}}\mathrm{d}\Gamma(-\Delta)
\end{aligned}$$

for all $\delta > 0$. Recalling the bound (6.3.4) we obtain

$$\pm I_2 = \pm\theta_M n^{-\frac{1}{2}} \int_{\Lambda^2} V_\ell(x-y)K_2 a_x^* a_y^* a_x + \text{h.c.} \leqslant \delta Q_4 + C\delta^{-1}\lambda^4\frac{n}{\ell^3}\mathcal{N}.$$

The term I_3 can be bounded by a simple Cauchy–Schwarz estimate as

$$\pm I_3 \leqslant \delta Q_4 + C\delta^{-1}\lambda\frac{n}{\ell^3}\mathcal{N}.$$

The choice $\delta = n^{1/2}\ell^{-5/6}$ and $\mathcal{N} \leqslant \pi^{-2}\mathrm{d}\Gamma(-\Delta)$ on $\mathcal{F}_+$ yields that $I_1 + I_2 + I_3$ may be bounded as stated in the lemma. For the remaining terms we set $\eta = n^{1/2}M\ell^{-3/2}$. The Cauchy–Schwarz inequality gives

$$\begin{aligned}
\pm I_4 \leqslant \eta M^{-2} &\int_{\Lambda^3} V_\ell(x-y)\theta_M a_x^* a_y^* a_v^* (\mathcal{N}+1) a_v a_x a_y \theta_M \\
&+ n^{-1}\eta^{-1}M^2 \int_{\Lambda^3} V_\ell(x-y)K(v,x)^2 a_y^* a_v^* (\mathcal{N}+1)^{-1} a_v a_y.
\end{aligned}$$

From Lemma 6.2 and (6.3.1) we find that $|K(x,v)| \leqslant C\frac{n}{\ell}|x-v|^{-1}$. Combining this with the Hardy inequality as in (6.5.6) we obtain

$$\int_{\Lambda^3} f(y,v)^2 V_\ell(x-y)K(v,x)^2 \mathrm{d}v\mathrm{d}x\mathrm{d}y \leqslant C\frac{n^2}{\ell^3}\|f\|^2_{H^1(\Lambda^2)}$$

for all $f \in H^1(\Lambda^2)$ so that

$$\int_{\Lambda^3} V_\ell(x-y)K(v,x)^2 a_y^* a_v^* a_v a_y \leqslant C\frac{n^2}{\ell^3}(\mathcal{N}-1)\mathrm{d}\Gamma(-\Delta). \tag{6.5.7}$$

We hence obtain

$$\pm I_4 \leqslant \eta M^{-2}\theta_M Q_4 \mathcal{N}^2\theta_M + Cn^{-1}\eta^{-1}M^2\frac{n^2}{\ell^3}\mathrm{d}\Gamma(-\Delta) \leqslant C\frac{n^{\frac{1}{2}}M}{\ell^{\frac{3}{2}}}\left(Q_4 + \mathrm{d}\Gamma(-\Delta)\right).$$

The remaining terms are bounded via simple Cauchy–Schwarz estimates, as

$$\begin{aligned}
\pm I_5 &= \pm\theta_M n^{-\frac{1}{2}} \int_{\Lambda^3} V_\ell(x-y) a_x^* a_v^* a^*(K_v) a_x a_y + \text{h.c.} \\
&\leqslant n^{-1}\eta^{-1}\|V_\ell\|_1 \sup_v \|K_v\|_2^2 \theta_M \mathcal{N}^3 \theta_M + \eta Q_4 \\
&\leqslant \eta Q_4 + Cn^{-1}\eta^{-1}\frac{n^2M^2}{\ell^3}\lambda\mathcal{N} \leqslant C\frac{n^{\frac{1}{2}}M}{\ell^{\frac{3}{2}}}\left(Q_4 + \mathrm{d}\Gamma(-\Delta)\right). \\
\pm I_6 &\leqslant \eta Q_4 + C\eta^{-1}\lambda\frac{n^2}{\ell^2}\frac{M^2}{n\ell}\mathcal{N} \leqslant C\frac{n^{\frac{1}{2}}M}{\ell^{\frac{3}{2}}}\left(Q_4 + \mathrm{d}\Gamma(-\Delta)\right).
\end{aligned}$$

The proof of Lemma 6.19 is complete. □

Now we are ready to give the proof of Lemma 6.17.

Proof of Lemma 6.17. Let us start by showing that

$$e^{-t\mathcal{B}_c}(Q_4 + \mathrm{d}\Gamma(-\Delta))e^{t\mathcal{B}_c} \leqslant C(Q_4 + \mathrm{d}\Gamma(-\Delta) + \frac{n}{\ell}(\mathcal{N}+1)) \tag{6.5.8}$$

We shall do this for $0 \leqslant t \leqslant 1$, the proof in the case $-1 \leqslant t < 0$ works the same. We first use the Duhamel formula as well as Lemmata 6.18 and 6.19, and subsequently the Cauchy–Schwarz inequality together with Lemma 6.16, $\theta_M \leqslant 1$ and (6.5.5) with $\sigma \leqslant 1$ to obtain

$$\begin{aligned}
&e^{-t\mathcal{B}_c}\big(Q_4 + \mathrm{d}\Gamma(-\Delta)\big)e^{t\mathcal{B}_c} - Q_4 - \mathrm{d}\Gamma(-\Delta) = \int_0^t e^{-s\mathcal{B}_c}[Q_4 + \mathrm{d}\Gamma(-\Delta), \mathcal{B}_c]e^{s\mathcal{B}_c}\mathrm{d}s \\
&= -\int_0^t e^{-s\mathcal{B}_c}\left(\theta_M \int_{\Lambda^2} n^{\frac{1}{2}} V_\ell(x-y)a_x^* a_y^* a_x + \text{h.c.} - \mathcal{E}_c^{(Q_4)} - \mathcal{E}_c^{(\mathrm{d}\Gamma(-\Delta))}\right)e^{s\mathcal{B}_c}\mathrm{d}s \\
&\leqslant \int_0^t e^{-s\mathcal{B}_c}\left(Q_4 + C\frac{n}{\ell}\mathcal{N}\right)e^{s\mathcal{B}_c}\mathrm{d}s + C\int_0^t e^{-s\mathcal{B}_c}\Big(Q_4 + \mathrm{d}\Gamma(-\Delta)\Big)e^{s\mathcal{B}_c}\mathrm{d}s \\
&\leqslant C\int_0^t e^{-s\mathcal{B}_c}\big(Q_4 + \mathrm{d}\Gamma(-\Delta)\big)e^{s\mathcal{B}_c}\mathrm{d}s + C\frac{n}{\ell}(\mathcal{N}+1).
\end{aligned}$$

The Grönwall lemma then yields (6.5.8). This immediately implies the result for the kinetic operator $\mathrm{d}\Gamma(-\Delta)$ in Lemma 6.17. For the quartic operator Q_4 we repeat the previous argument by solely considering Q_4. The Duhamel formula, Lemma 6.19 and the Cauchy–Schwarz inequality yield

$$e^{-t\mathcal{B}_c}Q_4 e^{t\mathcal{B}_c} - Q_4 = \int_0^t e^{-s\mathcal{B}_c}[Q_4, \mathcal{B}_c]e^{s\mathcal{B}_c}\mathrm{d}s \leqslant \int_0^t e^{-s\mathcal{B}_c}\left(Q_4 + C\frac{n}{\ell}\mathcal{N} + \mathcal{E}_c^{(Q_4)}\right)e^{s\mathcal{B}_c}\mathrm{d}s.$$

We then use the estimate of the error term in Lemma 6.19 together with Lemma 6.16 and (6.5.8) to find

$$\begin{aligned}
e^{-t\mathcal{B}_c}Q_4 e^{t\mathcal{B}_c} - Q_4 &\leqslant C\int_0^t e^{-s\mathcal{B}_c}\left(Q_4 + \sigma\mathrm{d}\Gamma(-\Delta)\right)e^{s\mathcal{B}_c}\mathrm{d}s + C\frac{n}{\ell}(\mathcal{N}+1) \\
&\leqslant C\int_0^t e^{-s\mathcal{B}_c}Q_4 e^{s\mathcal{B}_c}\mathrm{d}s + C\sigma\Big(Q_4 + \mathrm{d}\Gamma(-\Delta) + \frac{n}{\ell}(\mathcal{N}+1)\Big) + C\frac{n}{\ell}(\mathcal{N}+1) \\
&\leqslant C\int_0^t e^{-s\mathcal{B}_c}Q_4 e^{s\mathcal{B}_c}\mathrm{d}s + C\big(Q_4 + \frac{n}{\ell}(\mathcal{N}+1) + \sigma\mathrm{d}\Gamma(-\Delta)\big).
\end{aligned}$$

In the last inequality we gathered some terms due to $\sigma \leqslant 1$. Now Lemma 6.17 follows again by the Grönwall lemma. □

6.5.2 Analysis of $(\mathrm{I})_\mathrm{c}$

In this section we analyze the term

$$(\mathrm{I})_c = e^{-\mathcal{B}_c}\mathrm{d}\Gamma\left(nV_\ell * u_0^2 + n\widehat{V}_\ell - 8\pi\mathfrak{a}\frac{n}{\ell}\right)e^{\mathcal{B}_c} + \int_0^1\int_t^1 e^{-s\mathcal{B}_c}[Q_3, \mathcal{B}_c]e^{s\mathcal{B}_c}\mathrm{d}s\mathrm{d}t \tag{6.5.9}$$

appearing in (6.5.4). We prove that the main contribution of this term is $8\pi\mathfrak{a}\mathcal{N}n\ell^{-1}$. Prior to this let us show a lemma that will be used to handle the diagonal terms in (6.5.9). It is the cubic analogue of Lemma 6.13.

Lemma 6.20. *Assume that $\lambda\left(\frac{n}{\ell}\right)^2 \leqslant 1$ and that $2R/\ell < \lambda < 1/4$. Let $A : L^2(\Lambda) \to L^2(\Lambda)$ be a bounded hermitian operator. For all $t \in [-1,1]$ we have on $\mathcal{F}$*

$$\pm\left(e^{-t\mathcal{B}_c}\mathrm{d}\Gamma(A)e^{t\mathcal{B}_c} - \mathrm{d}\Gamma(A)\right) \leqslant C\|A\|_{\mathrm{op}}\|K\|_2(\mathcal{N}+1) \leqslant C\|A\|_{\mathrm{op}}\lambda^{\frac{1}{2}}\frac{n}{\ell}(\mathcal{N}+1).$$

Proof. One easily checks that for a bounded operator $T : L^2(\Lambda) \to L^2_{\mathrm{s}}(\Lambda^2)$ with integral kernel $T(x_1, x_2, ; y_1)$ and for any $\xi, \xi' \in \mathcal{F}$, the following inequality holds

$$\pm\int_{\Lambda^3} T(x_1, x_2; y_1)\langle \xi', a^*_{x_1}a^*_{x_2}a_{y_1}\xi\rangle + \mathrm{h.c.} \leqslant C\|T\|_{\mathrm{op}}\|\left(\mathcal{N}+1\right)^{3/4}\xi'\|\|\left(\mathcal{N}+1\right)^{3/4}\xi\|. \quad (6.5.10)$$

Define the operator $B_c : L^2(\Lambda) \to L^2_{\mathrm{s}}(\Lambda^2)$ by

$$\langle g, B_c f\rangle = n^{-1/2}\int_{\Lambda^2} \overline{(Q^{\otimes 2}g)}(x_1, x_2)K(x_1, x_2)(Qf)(x_2)\mathrm{d}x_1\mathrm{d}x_2, \quad (6.5.11)$$

for all $f \in L^2(\Lambda)$ and $g \in L^2_{\mathrm{s}}(\Lambda^2)$, so that

$$\mathcal{B}_c = \theta_M\int_{\Lambda^3} B_c(x_1, x_2; y_1)a^*_{x_1}a^*_{x_2}a_{y_1}\mathrm{d}x_1\mathrm{d}x_2\mathrm{d}y_1 - \mathrm{h.c.}$$

From the Cauchy–Schwarz inequality, we have

$$\|B_c\|_{\mathrm{op}} \leqslant n^{-1/2}\sup_{x\in\Lambda}\|K_x\|_2 \leqslant C\lambda^{\frac{1}{2}}\frac{n^{1/2}}{\ell},$$

where the second inequality is a consequence of Lemma 6.4.

With the aid of the Duhamel formula we can write

$$e^{-t\mathcal{B}_c}\mathrm{d}\Gamma(A)e^{t\mathcal{B}_c} - \mathrm{d}\Gamma(A) = \int_0^t e^{-s\mathcal{B}_c}[\mathrm{d}\Gamma(A), \mathcal{B}_c]e^{s\mathcal{B}_c}\mathrm{d}s. \quad (6.5.12)$$

Applying (6.5.10) and that $M \leqslant n$ we can bound the commutator as

$$\begin{aligned}\pm[\mathrm{d}\Gamma(A), \mathcal{B}_c] &= \pm\theta_M\int_{\Lambda^2}(A_1B_c + A_2B_c - B_cA)(x_1, x_2; y_1)a^*_{x_1}a^*_{x_2}a_{y_1} + \mathrm{h.c.}\\ &\leqslant C\|A\|_{\mathrm{op}}\|B_c\|_{\mathrm{op}}\theta_M\left(\mathcal{N}+1\right)^{3/2}\\ &\leqslant C\|A\|_{\mathrm{op}}M^{1/2}\lambda^{\frac{1}{2}}\frac{n^{1/2}}{\ell}\left(\mathcal{N}+1\right) \leqslant C\|A\|_{\mathrm{op}}\lambda^{\frac{1}{2}}\frac{n}{\ell}\left(\mathcal{N}+1\right).\end{aligned}$$

Here we have denoted by A_1B_c, A_2B_c and B_cA the composition of applications, where A_i is the operator A acting on the variable i. Now plugging this estimate into (6.5.12) and applying Lemma 6.16 we obtain the claim of the lemma. □

Lemma 6.21. *Assume that $\lambda\left(\frac{n}{\ell}\right)^2 \leqslant 1$, that $2R/\ell < \lambda < 1/4$ and that ℓ is large enough. Let $\sigma \leqslant 1$ as in Lemma 6.15. On $\mathcal{F}_+$ we have*

$$(\mathrm{I})_c = 8\pi\mathfrak{a}\mathcal{N}\frac{n}{\ell} + \Xi_c$$

with

$$\begin{aligned}\pm\Xi_c \leqslant{}& C\delta\left(Q_4 + \frac{n}{\ell}(\mathcal{N}+1)\right) + C\delta^{-1}\frac{n}{\ell}\frac{(\mathcal{N}+1)^2}{M} + C\delta^{-1}\frac{M}{n}\lambda\left(\frac{n}{\ell}\right)^3(\mathcal{N}+1)\\ &+ C\sigma\left(Q_4 + \mathrm{d}\Gamma(-\Delta) + \frac{n}{\ell}(\mathcal{N}+1)\right) + C\lambda^{\frac{1}{2}}\left(\frac{n}{\ell}\right)^2(\mathcal{N}+1)\end{aligned}$$

for all $0 < \delta \leqslant 1$.

Proof. We start with computing the commutator $[Q_3, \mathcal{B}_c]$. A lengthy but straightforward computation shows that

$$
\begin{aligned}
[Q_3, \mathcal{B}_c] &= \theta_M \int_{\Lambda^2} V_\ell(x-y) K(x,y)(a_x^* a_x + a_x^* a_y) + \text{h.c.} \\
&\quad + \Big\{ \theta_M \Big(- \int_{\Lambda^2} V_\ell(x-y) a_x^* (a(K_x) + a(K_y)) + \text{h.c.} \Big) \Big\} \\
&\quad + \Big\{ \theta_M \Big[\int_{\Lambda^2} V_\ell(x-y) a_x^* a^*(K_y) a_x a_y + \int_{\Lambda^3} V_\ell(x-y) a_v^* a^*(K_v) a_y a_x \\
&\qquad\qquad + \int_{\Lambda^3} V_\ell(x-y) a_x^* a_y^* a_v^* K(v,x) a_v - \int_{\Lambda^2} V_\ell(x-y) a_y^* a_x^* a^*(K_x) a_y \\
&\qquad\qquad - \int_{\Lambda^3} V_\ell(x-y) a_x^* a_y^* a^*(K_v) a_v \Big] + \text{h.c.} \Big\} \\
&\quad + \Big\{ \theta_M \Big[- \int_{\Lambda^3} V_\ell(x-y) a_x^* a^*(K_v) a_v (a_y + a_x) \\
&\qquad\qquad + \int_{\Lambda^3} V_\ell(x-y) a_y^* a_v^* a^*(K_v)(a_x + a_y) \Big] + \text{h.c.} \Big\} \\
&\quad + \Big\{ \theta_M \int_{\Lambda^3} V_\ell(x-y) a_x^* a_v^* (K(v,x) a_y + K(v,y) a_x) a_v + \text{h.c.} \Big\} \\
&\quad + \Big\{ \int_{\Lambda^3} V_\ell(x-y) \left([a_x^* a_y^* a_x, \theta_M] + [a_x^* a_y a_x, \theta_M] \right) a_v^* a^*(K_v) a_v + \text{h.c.} \Big\} \\
&=: \int_{\Lambda^2} V_\ell(x-y) K(x,y)(a_x^* a_x + a_x^* a_y) + \text{h.c.} + \sum_{i=1}^{6} J_i
\end{aligned}
\tag{6.5.13}
$$

where we set

$$
J_1 = (\theta_M - 1) \int_{\Lambda^2} V_\ell(x-y) K(x,y)(a_x^* a_x + a_x^* a_y) + \text{h.c.}
$$

and $J_2, \ldots, J_6$ denotes the remaining expressions in curly brackets. For the error term J_1 we use that

$$
\pm (\theta_M - 1) \leqslant \mathbb{1}^{\mathcal{N} \geqslant M/2}.
$$

Hence, by the Cauchy–Schwarz inequality

$$
\begin{aligned}
\pm J_1 &\leqslant \delta \|K\|_\infty \int_{\Lambda^2} V_\ell(x-y) a_x^* a_x + \delta^{-1} \|K\|_\infty \int_{\Lambda^2} V_\ell(x-y)(\theta_M - 1) a_x^* a_x (\theta_M - 1) \\
&\leqslant C\delta \frac{n}{\ell} \mathcal{N} + C\delta^{-1} \frac{n}{\ell} \mathcal{N} \mathbb{1}^{\mathcal{N} \geqslant M/2} \leqslant C\delta \frac{n}{\ell} \mathcal{N} + C\delta^{-1} \frac{n}{\ell} \frac{\mathcal{N}^2}{M}
\end{aligned}
\tag{6.5.14}
$$

for all $\delta > 0$. Similarly we bound the error terms J_2 through J_6 with the aid of the Cauchy–Schwarz inequality using that $\lambda, \ell^{-1}, Mn^{-1} \leqslant 1$. For any $\delta > 0$ we obtain

$$
\begin{aligned}
\pm J_2 &\leqslant C\ell^{-1} \sup_x \|K_x\|_2 \mathcal{N} \leqslant C\lambda \frac{n^2}{\ell^3} \mathcal{N} \leqslant C\lambda^{\frac{1}{2}} \left(\frac{n}{\ell}\right)^2 \mathcal{N}, \\
\pm J_3 &\leqslant C\delta^{-1} \|V_\ell\|_1 \sup_y \|K_y\|_2^2 \theta_M (\mathcal{N}+1)^2 \theta_M + \delta Q_4, \\
&\leqslant \delta Q_4 + C\delta^{-1} \frac{M}{\ell} \lambda \left(\frac{n}{\ell}\right)^2 (\mathcal{N}+1) \\
\pm J_4 &\leqslant C\theta_M \|V_\ell\|_1 \sup_v \|K_v\|_2 (\mathcal{N}+1)^2 \leqslant C\lambda^{\frac{1}{2}} \left(\frac{n}{\ell}\right)^2 (\mathcal{N}+1).
\end{aligned}
$$

For J_5 recall the bound (6.5.7). With $\delta_5 > 0$ appropriately chosen

$$\begin{aligned}
\pm J_5 &\leqslant C\delta_5^{-1} \int_{\Lambda^3} V_\ell(x-y)\theta_M a_x^* a_v^* (\mathcal{N}+1) a_v a_x \theta_M \\
&\quad + \delta_5 \int_{\Lambda^3} V_\ell(x-y) a_y^* a_v^* (\mathcal{N}+1)^{-1} a_v a_y K(v,x)^2 \\
&\leqslant C\delta_5 \frac{n^2}{\ell^3} \mathrm{d}\Gamma(-\Delta) + C\delta_5^{-1}\ell^{-1}\theta_M(\mathcal{N}+1)^3\theta_M \\
&= \eta \mathrm{d}\Gamma(-\Delta) + C\eta^{-1}\frac{n^2M^2}{\ell^4}(\mathcal{N}+1).
\end{aligned}$$

for any $\eta > 0$. For J_6 we use the pull-through formula $a_x\theta_M(\mathcal{N}) = \theta_M(\mathcal{N}+1)a_x$ which yields

$$\begin{aligned}
[a_x^* a_y^* a_x, \theta_M] a_v^* a^*(K_v) a_v &= a_x^* a_y^* \big(\theta_M(\mathcal{N}+1) - \theta_M(\mathcal{N}+2)\big) a_x a_v^* a^*(K_v) a_v \\
&= a_x^* a_y^* \big(\theta_M(\mathcal{N}+1) - \theta_M(\mathcal{N}+2)\big)(\delta_{x,v} + a_v^* a_x) a^*(K_v) a_v \\
&= \delta_{x,v} a_x^* a_y^* \big(\theta_M(\mathcal{N}+1) - \theta_M(\mathcal{N}+2)\big) a^*(K_v) a_v \\
&\quad + a_x^* a_y^* a_v^* \big(\theta_M(\mathcal{N}+2) - \theta_M(\mathcal{N}+3)\big) a_x a^*(K_v) a_v.
\end{aligned}$$

By the smoothness assumption on θ_M we can bound

$$\big\|\theta_M(\mathcal{N}+i) - \theta_M(\mathcal{N}+j)\big\|_{\mathrm{op}} \leqslant CM^{-1}|i-j|,\ i,j \in \mathbb{N}_0, \tag{6.5.15}$$

for some constant $C > 0$. Therefore,

$$\begin{aligned}
&\int_{\Lambda^3} V_\ell(x-y)[a_x^* a_y^* a_x, \theta_M] a_v^* a^*(K_v) a_v + \text{h.c.} \\
&= \int_{\Lambda^2} V_\ell(x-y) a_x^* a_y^* \big(\theta_M(\mathcal{N}+1) - \theta_M(\mathcal{N}+2)\big) a^*(K_x) a_x + \text{h.c.} \\
&\quad + \int_{\Lambda^3} V_\ell(x-y) a_x^* a_y^* a_v^* \big(\theta_M(\mathcal{N}+2) - \theta_M(\mathcal{N}+3)\big) a_x a^*(K_v) a_v + \text{h.c.} \\
&\leqslant \delta Q_4 + \delta^{-1} \int_{\Lambda^2} V_\ell(x-y) a_x^* a(K_x) \big(\theta_M(\mathcal{N}+1) - \theta_M(\mathcal{N}+2)\big)^2 a^*(K_x) a_x \\
&\quad + \delta Q_4 + \delta^{-1} \int_{\Lambda^3} V_\ell(x-y) a_v^* a(K_v) a_x^* \big(\theta_M(\mathcal{N}+2) - \theta_M(\mathcal{N}+3)\big)(\mathcal{N}+1) \times \\
&\qquad \times \big(\theta_M(\mathcal{N}+2) - \theta_M(\mathcal{N}+3)\big) a_x a^*(K_v) a_v \\
&\leqslant 2\delta Q_4 + C\delta^{-1}\|V_\ell\|_1 M^{-2}\lambda\left(\frac{n}{\ell}\right)^2 \Big(\mathbb{1}(\mathcal{N} \leqslant 2M)(\mathcal{N}+1)^2\mathbb{1}(\mathcal{N} \leqslant 2M) \\
&\qquad + \mathbb{1}(\mathcal{N}-1 \leqslant 2M)(\mathcal{N}+1)^4\mathbb{1}(\mathcal{N}-1 \leqslant 2M)\Big) \\
&\leqslant 2\delta Q_4 + C\delta^{-1}\frac{M}{\ell}\lambda\left(\frac{n}{\ell}\right)^2(\mathcal{N}+1).
\end{aligned}$$

Let us now consider the second part of J_6 containing $[a_x^* a_y a_x, \theta_M]$. Computing the commutator and normal ordering the expression one sees three terms appearing. One may be bounded as above and the other two as

$$\pm\left(\theta_M(\mathcal{N}+1) - \theta_M(\mathcal{N})\right) \int_{\Lambda^2} V_\ell(x-y) K(x,y) a_x^*(a_x + a_y) + \text{h.c.} \leqslant C\frac{n}{\ell}\frac{\mathcal{N}}{M}$$

with the Cauchy–Schwarz inequality and $\|K\|_\infty \leqslant Cn$ and

$$\begin{aligned}
&\pm \left(\theta_M(\mathcal{N}+1)-\theta_M(\mathcal{N})\right)\int_{\Lambda^3} V_\ell(x-y)a_x^*a_v^*a_v\left(a_xK(v,y)+a_yK(v,x)\right)+\text{h.c.}\\
&\leqslant C\delta_6^{-1}M\ell^{-1}+\delta_6\int_{\Lambda^3} V_\ell(x-y)a_x^*a_v^*(\mathcal{N}+1)^{-1}a_xa_vK(v,y)^2\\
&\leqslant C\delta_6\frac{n^2}{\ell^3}\mathrm{d}\Gamma(-\Delta)+C\delta_6^{-1}M\ell^{-1}\\
&=\eta\mathrm{d}\Gamma(-\Delta)+C\eta^{-1}n^2M\ell^{-4}.
\end{aligned}$$

for any $\eta>0$ using (6.5.7) as in the analysis of J_5. We conclude that

$$\pm J_6 \leqslant C\delta Q_4 + C\delta^{-1}\frac{M}{\ell}\lambda\left(\frac{n}{\ell}\right)^2(\mathcal{N}+1)+\eta\mathrm{d}\Gamma(-\Delta)+C\eta^{-1}n^2M\ell^{-4}+C\frac{n}{\ell}\frac{\mathcal{N}}{M}.$$

With (6.5.13) we have

$$\begin{aligned}
&\int_0^1\int_t^1 e^{-s\mathcal{B}_c}[Q_3,\mathcal{B}_c]e^{s\mathcal{B}_c}\mathrm{d}s\mathrm{d}t\\
&=2\int_0^1\int_t^1 e^{-s\mathcal{B}_c}\left(\int_{\Lambda^2}V_\ell(x-y)K(x,y)(a_x^*a_x+a_x^*a_y)\right)e^{s\mathcal{B}_c}\mathrm{d}s\mathrm{d}t\\
&\quad+\int_0^1\int_t^1 e^{-s\mathcal{B}_c}\sum_{i=1}^6 J_ie^{s\mathcal{B}_c}\mathrm{d}s\mathrm{d}t. \qquad (6.5.16)
\end{aligned}$$

Collecting the bounds on the error terms, we obtain with the aid of Lemma 6.16 and Lemma 6.17

$$\begin{aligned}
&\pm\int_0^1\int_t^1 e^{-s\mathcal{B}_c}\sum_{i=1}^6 J_ie^{s\mathcal{B}_c}\mathrm{d}s\mathrm{d}t\\
&\leqslant C\delta\left(Q_4+\frac{n}{\ell}(\mathcal{N}+1)+\sigma\mathrm{d}\Gamma(-\Delta)\right)+C\delta^{-1}\frac{n}{\ell}\frac{(\mathcal{N}+1)^2}{M}+C\delta^{-1}\frac{M}{n}\lambda\left(\frac{n}{\ell}\right)^3(\mathcal{N}+1)\\
&\quad+C\eta\left(Q_4+\mathrm{d}\Gamma(-\Delta)+\frac{n}{\ell}(\mathcal{N}+1)\right)+C\eta^{-1}\frac{n^2M^2}{\ell^4}(\mathcal{N}+1)+C\lambda^{\frac12}\left(\frac{n}{\ell}\right)^2(\mathcal{N}+1)
\end{aligned}$$

where we have used that $\delta, M^{-1}\leqslant 1$. We choose $\eta=\sigma$. In particular $\eta^{-1}n^2M^2\ell^{-4}\leqslant\sigma n\ell^{-1}$ so that with $\delta\leqslant 1$ we find

$$\begin{aligned}
&\pm\int_0^1\int_t^1 e^{-s\mathcal{B}_c}\sum_{i=1}^6 J_ie^{s\mathcal{B}_c}\mathrm{d}s\mathrm{d}t\\
&\leqslant C\delta\left(Q_4+\frac{n}{\ell}(\mathcal{N}+1)\right)+C\delta^{-1}\frac{n}{\ell}\frac{(\mathcal{N}+1)^2}{M}+C\delta^{-1}\frac{M}{n}\lambda\left(\frac{n}{\ell}\right)^3(\mathcal{N}+1)\\
&\quad+C\sigma\left(Q_4+\mathrm{d}\Gamma(-\Delta)+\frac{n}{\ell}(\mathcal{N}+1)\right)+C\lambda^{\frac12}\left(\frac{n}{\ell}\right)^2(\mathcal{N}+1).
\end{aligned}$$

The first line of (6.5.16) as well as the first term in (6.5.9) can be estimated with the aid of Lemma 6.20. One readily checks from the elementary properties of K in Lemma 6.4 that the various operators (taking the place of A in Lemma 6.20) are bounded by $Cn\ell^{-1}$. Therefore,

$$\begin{aligned}
(\mathrm{I})_c&=\int_{\Lambda^2}V_\ell(x-y)K(x,y)(a_x^*a_x+a_x^*a_y)+\mathrm{d}\Gamma\left(nV_\ell*u_0^2+n\widehat{V}_\ell-8\pi a\frac{n}{\ell}\right)\\
&\quad+\int_0^1\int_t^1 e^{-s\mathcal{B}_c}\sum_{i=1}^6 J_ie^{s\mathcal{B}_c}\mathrm{d}s\mathrm{d}t+J_7 \qquad (6.5.17)
\end{aligned}$$

with

$$\pm J_7 \leqslant C\lambda^{\frac{1}{2}} \left(\frac{n}{\ell}\right)^2 (\mathcal{N}+1).$$

The first line of (6.5.17) can equivalently be written as

$$\begin{aligned}&\int_{\Lambda^2} V_\ell(x-y)K(x,y)(a_x^*a_x + a_x^*a_y) + \mathrm{d}\Gamma\left(nV_\ell * u_0^2 + n\widehat{V}_\ell - 8\pi\mathfrak{a}\frac{n}{\ell}\right)\\ &= 8\pi\mathfrak{a}\frac{n}{\ell}\mathcal{N} + 2\mathrm{d}\Gamma(h) + J_8\end{aligned} \tag{6.5.18}$$

where h stands for multiplication with the function h in (6.3.7) and

$$J_8 = \int_{\Lambda^2} V_\ell(x-y)(n+K(x,y))\,(a_x^*a_y - a_x^*a_x)\,\mathrm{d}x\mathrm{d}y \tag{6.5.19}$$

Using the bound on h from Lemma 6.6 and the Sobolev inequality (6.4.37) we find

$$\pm\mathrm{d}\Gamma(h) \leqslant C\|h\|_{3/2}\mathrm{d}\Gamma(-\Delta) \leqslant C\sigma\mathrm{d}\Gamma(-\Delta).$$

For J_8 we shall show that operator inequality

$$\pm J_8 \leqslant C\frac{n}{\ell^3}\mathrm{d}\Gamma(-\Delta).$$

Indeed, $J_8 = \mathrm{d}\Gamma(S)$ and for $f \in H^1(\Lambda)$

$$\begin{aligned}\langle f, Sf\rangle &= -\frac{1}{2}\int_{\Lambda^2} V_\ell(x-y)(n+K(x,y))|f(x)-f(y)|^2\mathrm{d}x\mathrm{d}y\\ &\leqslant Cn\int_{\Lambda^2} V_\ell(x-y)\left|\int_0^1 \nabla f(x+t(y-x))\cdot(y-x)\mathrm{d}t\right|^2\mathrm{d}x\mathrm{d}y\\ &\leqslant Cn\int_0^1\int_{\Lambda^2}|x-y|^2V_\ell(x-y)|\nabla f(x+t(y-x))|^2\mathrm{d}x\mathrm{d}y\mathrm{d}t\\ &\leqslant Cn\ell^{-2}\int_0^1\int_{\mathbb{R}^3\times\mathbb{R}^3}\mathbb{1}_\Lambda(x+y)\mathbb{1}_\Lambda(y)V_\ell(x)|\nabla f(x+y-tx)|^2\mathrm{d}x\mathrm{d}y\mathrm{d}t\\ &\leqslant Cn\ell^{-3}\|\nabla f\|_2^2.\end{aligned} \tag{6.5.20}$$

Combining all the estimates, we conclude the proof of Lemma 6.21. □

6.5.3 Analysis of $(\mathrm{II})_{\mathrm{c}}$

In this section we analyze the term

$$(\mathrm{II})_c = e^{-\mathcal{B}_c}\widetilde{Q}_2 e^{\mathcal{B}_c} = e^{-\mathcal{B}_c}\widetilde{Q}_2^{(\epsilon)}e^{\mathcal{B}_c} + e^{-\mathcal{B}_c}\widetilde{Q}_2^{(bc)}e^{\mathcal{B}_c}$$

appearing in (6.5.4), where we decompose $\widetilde{Q}_2 = \widetilde{Q}_2^{(\epsilon)} + \widetilde{Q}_2^{(bc)}$ as in (6.4.5). As we will show below, the cubic transformation leaves $\widetilde{Q}_2$ essentially unchanged. However, after its action the boundary term $\widetilde{Q}_2^{(bc)}$ can be absorbed into the error terms. More precisely, we have the following lemma.

Lemma 6.22. *Assume that $\lambda\left(\frac{n}{\ell}\right)^2 \leqslant 1$, that $2R/\ell < \lambda < 1/4$ and that ℓ is large enough. Let $\sigma \leqslant 1$ as in Lemma 6.15. On $\mathcal{F}_+$ we have*

$$(\mathrm{II})_c = \widetilde{Q}_2^{(\epsilon)} + \mathcal{E}_c^{(\widetilde{Q}_2)}$$

with

$$\pm\mathcal{E}_c^{(\widetilde{Q}_2)} \leqslant \frac{1}{4}Q_4 + C\sigma\Big(\mathrm{d}\Gamma(-\Delta) + Q_4 + \frac{n}{\ell}(\mathcal{N}+1)\Big) + \delta\Big(Q_4 + \frac{n}{\ell}(\mathcal{N}+1)\Big) + \delta^{-1}C\lambda\Big(\frac{n}{\ell}\Big)^3(\mathcal{N}+1) + C\lambda^{-1}\frac{n^{3/2}}{\ell^2}(\mathcal{N}+1) + C\frac{n^2}{\ell^2}$$

for all $0<\delta\leqslant 1$.

Proof. With the aid of the Duhamel formula we can write

$$e^{-\mathcal{B}_c}\widetilde{Q}_2 e^{\mathcal{B}_c} = \widetilde{Q}_2^{(\epsilon)} + \widetilde{Q}_2^{(bc)} + \int_0^1 e^{-t\mathcal{B}_c}[\widetilde{Q}_2,\mathcal{B}_c]e^{t\mathcal{B}_c}\mathrm{d}t.$$

We will bound all terms except the main one $\widetilde{Q}_2^{(\epsilon)}$. Let us start with $\widetilde{Q}_2^{(bc)}$. With the aid of the pointwise bound (6.4.24) and the Cauchy–Schwarz inequality we obtain

$$\pm\widetilde{Q}_2^{(bc)} = \pm\Big(\int_{\Lambda^2}\widetilde{Q}_2^{(bc)}(x,y)a_x^*a_y^* + \mathrm{h.c.}\Big) \leqslant \frac{1}{4}Q_4 + C\frac{n^2}{\ell^2}$$

where we used that $\int_{\Lambda^2}V_\ell(x-y)[1+\ell d(x,\partial\Lambda)]^{-2}\leqslant C\ell^{-2}$. The explicit prefactor 1/4 is chosen for later convenience. Next, consider the commutator

$$[\widetilde{Q}_2,\mathcal{B}_c] = n^{-\frac{1}{2}}\theta_M\int_{\Lambda^2}K(v,w)[\widetilde{Q}_2,q_v^*a_w^*q_v] + \mathrm{h.c.} + n^{-\frac{1}{2}}[\widetilde{Q}_2,\theta_M]\int_{\Lambda^2}K(v,w)q_v^*a_w^*q_v + \mathrm{h.c.} \tag{6.5.21}$$

The first term of (6.5.21) equals

$$n^{-\frac{1}{2}}\theta_M\int_{\Lambda^4}\widetilde{Q}_2(x,y)K(v,w)[a_x^*a_y^* + a_xa_y, q_v^*a_w^*q_v] + \mathrm{h.c.} = \sum_{i=1}^3 R_i$$

with

$$\begin{aligned}
R_1 &= 2n^{-\frac{1}{2}}\int_{\Lambda^2}\widetilde{Q}_2^{(\epsilon)}(x,y)\theta_M\Big(a^*(K_y)a_xq_y - q_y^*a_x^*a^*(K_y)\\
&\quad + \int_\Lambda q_v^*a^*(K_v)a_x^* - \int_\Lambda a^*(K_v)a_xq_v + \int_\Lambda q_v^*K(v,x)a_yq_v + K(x,y)q_y - q(K_x)\Big) + \mathrm{h.c.}\\
R_2 &= 2n^{-\frac{1}{2}}\int_{\Lambda^2}\widetilde{Q}_2^{(bc)}(x,y)\theta_M\Big(a^*(K_x)a_xq_y - q_y^*a^*(K_y)a_x^*\Big) + \mathrm{h.c.}\\
R_3 &= 2n^{-\frac{1}{2}}\int_{\Lambda^2}\widetilde{Q}_2^{(bc)}(x,y)\theta_M\Big(\int_\Lambda q_v^*a^*(K_v)a_x^* + \int_\Lambda q_v^*K(v,x)a_yq_v - \int_\Lambda a^*(K_v)a_xq_v\\
&\qquad + K(x,y)q_y - q(K_x)\Big) + \mathrm{h.c.}
\end{aligned}$$

Since all expressions are normal ordered, we can again replace q_x by a_x on $\mathcal{F}_+$.

Let us start with estimating R_1. Recall the bound (6.4.23). For $x\in\Lambda$ fixed we have $\mathrm{d}\Gamma(\mathbb{1}_{|x-\cdot|\leqslant\lambda})\leqslant C\lambda^2\mathrm{d}\Gamma(-\Delta)$ on $\mathcal{F}_+$ by (6.4.37). Using this and $\sup_x\|K_x\|_2\leqslant C\lambda^{1/2}n/\ell$ from Lemma 6.4, we can bound all the cubic terms in a similar way. Let us bound for example the first one. Recall that $\theta_M=\theta_M(\mathcal{N})$ and note that $\theta_M(\mathcal{N})a^*(f) = a^*(f)\theta_M(\mathcal{N}+1)$. On $\mathcal{F}_+$ we have

$$
\begin{aligned}
&\pm 2n^{-1/2}\int_{\Lambda^2}\widetilde{Q}_2^{(\epsilon)}(x,y)\theta_M a^*(K_y)a_xa_y+\text{h.c.}\\
&\leqslant Cn^{1/2}\lambda^{-3}\ell^{-1}\left(\delta\int_{\Lambda^2}a^*(K_y)a(K_y)\mathbb{1}_{|x-y|\leqslant\lambda}+\delta^{-1}\theta_M(\mathcal{N}+1)\int_{\Lambda^2}\mathbb{1}_{|x-y|\leqslant\lambda}a_x^*a_y^*a_ya_x\right)\\
&\leqslant Cn^{1/2}\lambda^{-3}\ell^{-1}\left(\delta\lambda^4n^2\ell^{-2}\mathcal{N}+\delta^{-1}M\lambda^2\mathrm{d}\Gamma(-\Delta)\right)\\
&\leqslant CnM^{1/2}\ell^{-3/2}\left(\mathrm{d}\Gamma(-\Delta)+\frac{n}{\ell}\mathcal{N}\right)\\
&\leqslant C\sigma\left(\mathrm{d}\Gamma(-\Delta)+\frac{n}{\ell}\mathcal{N}\right),
\end{aligned}
$$

where we chose $\delta=\lambda^{-1}n^{-1/2}\ell^{1/2}M^{1/2}$ and used $\lambda n^2\ell^{-2}\leqslant 1$. The other cubic terms can be bounded in a similar way. We proceed with the linear terms in R_1. We find

$$
\begin{aligned}
&\pm 2n^{-1/2}\int_{\Lambda^2}\widetilde{Q}_2^{(\epsilon)}(x,y)K(x,y)\theta_M a_y+\text{h.c.}\\
&\quad\leqslant Cn^{1/2}\lambda^{-3}\ell^{-1}\left(\delta\int_{\Lambda^2}\mathbb{1}_{|x-y|\leqslant\lambda}a_y^*a_y+\delta^{-1}\int_{\Lambda^2}K(x,y)^2\right)\leqslant C\lambda^{-1}n^{3/2}\ell^{-2}(\mathcal{N}+1).
\end{aligned}
$$

Finally, for the last term in R_1 we have by the Cauchy–Schwarz inequality

$$
\begin{aligned}
\pm 2n^{-\frac{1}{2}}\int_{\Lambda^2}\widetilde{Q}_2^{(\varepsilon)}(x,y)\theta_M a(K_x)+\text{h.c.}&\leqslant Cn^{1/2}\ell^{-1}\lambda^{-3}\|\mathbb{1}_{|\cdot|\leqslant\lambda}\|_1\sup_x\|K_x\|_2\,(\mathcal{N}+1)\\
&\leqslant C\lambda^{1/2}n^{3/2}\ell^{-2}\,(\mathcal{N}+1)\leqslant C\sigma\frac{n}{\ell}(\mathcal{N}+1).
\end{aligned}
$$

This in particular shows that $\pm R_1\leqslant C\sigma(\mathrm{d}\Gamma(-\Delta)+\frac{n}{\ell}(\mathcal{N}+1))+C\lambda^{-1}n^{3/2}\ell^{-2}(\mathcal{N}+1)$.

Let us proceed with the analysis of R_2. Using the pointwise bound $|\widetilde{Q}_2^{(bc)}(x,y)|\leqslant CnV_\ell(x-y)$, we see that we can bound the two terms in R_2 using Q_4 because of the presence of a_xa_y or $a_y^*a_x^*$. From the Cauchy–Schwarz inequality, we obtain

$$
\pm R_2\leqslant\delta Q_4+\delta^{-1}Cn\sup_y\|K_y\|_2^2\|V_\ell\|_1(\mathcal{N}+1)\leqslant\delta Q_4+\delta^{-1}C\lambda\frac{n^3}{\ell^3}(\mathcal{N}+1).
$$

It remains to study R_3. The first three terms in R_3 are bounded similarly as their counterpart in R_1, that is

$$
\begin{aligned}
&\pm 2n^{-\frac{1}{2}}\int_{\Lambda^3}\widetilde{Q}_2^{(bc)}(x,y)\theta_M(a_v^*a^*(K_v)a_x^*+a_v^*K(v,x)a_ya_v-a^*(K_v)a_xa_v)+\text{h.c.}\\
&\leqslant CM^{1/2}n^{1/2}\sup_v\|K_v\|_2\sup_y\|V_\ell\|_1(\mathcal{N}+1)\\
&\leqslant C\lambda^{\frac{1}{2}}\frac{n^{\frac{3}{2}}M^{\frac{1}{2}}}{\ell^2}(\mathcal{N}+1)\leqslant C\sigma\frac{n}{\ell}\,(\mathcal{N}+1)\,.
\end{aligned}
$$

For last term in R_3 the Cauchy–Schwarz inequality yields

$$
\begin{aligned}
\pm 2n^{-\frac{1}{2}}\int_{\Lambda^2}\widetilde{Q}_2^{(bc)}(x,y)\theta_M a(K_x)+\text{h.c.}&\leqslant Cn^{1/2}\sup_x\|K_x\|_2\sup_y\|V_\ell\|_1(\mathcal{N}+1)\\
&\leqslant C\lambda^{1/2}\frac{n^{3/2}}{\ell^2}\mathcal{N}\leqslant C\sigma\frac{n}{\ell}(\mathcal{N}+1).
\end{aligned}
$$

Finally, for the fourth term in R_3, we use the more elaborate pointwise estimate (6.4.24) on $\widetilde{Q}_2^{(bc)}(x,y)$ and the Sobolev inequality from (6.4.37) for $\Phi(y) = (1+\ell d(y,\partial\Lambda))^{-5/6}$ so that $\|\Phi\|_{3/2} \leqslant C\ell^{-2/3}$. With $\|K\|_\infty \lesssim n$ we obtain

$$\begin{aligned}
&\pm 2n^{-1/2} \int_{\Lambda^2} \widetilde{Q}_2^{(bc)}(x,y) K(x,y) \theta_M a_y + \text{h.c.} \\
&\leqslant Cn^{3/2} \left(\delta \int_{\Lambda^2} V_\ell(x-y) \frac{a_y^* a_y}{(1+\ell d(y,\partial\Lambda))^{5/6}} + \delta^{-1} \int_{\Lambda^2} \frac{V_\ell(x-y)}{(1+\ell d(y,\partial\Lambda))^{7/6}} \right) \\
&\leqslant Cn^{3/2} \left(\delta \ell^{-5/3} \mathrm{d}\Gamma(-\Delta) + \delta^{-1}\ell^{-2} \right) \leqslant C \frac{n^{1/2}}{\ell^{5/6}} \left(\mathrm{d}\Gamma(-\Delta) + \left(\frac{n}{\ell}\right)^2 \right) \\
&\leqslant C\sigma \left(\mathrm{d}\Gamma(-\Delta) + \left(\frac{n}{\ell}\right)^2 \right).
\end{aligned}$$

In combination, we obtain

$$\pm R_3 \leqslant C\sigma \left(\frac{n}{\ell}(\mathcal{N}+1) + \mathrm{d}\Gamma(-\Delta) + \left(\frac{n}{\ell}\right)^2 \right),$$

which concludes the bound of the first term of (6.5.21).

We now bound the second term in (6.5.21), given by

$$\begin{aligned}
&n^{-\frac{1}{2}} [\widetilde{Q}_2, \theta_M] \int_\Lambda a_v^* a^*(K_v) a_v + \text{h.c.} \\
&= n^{-\frac{1}{2}} \int_{\Lambda^2} \widetilde{Q}_2^{(\epsilon)}(x,y) \Big(\big(\theta_M(\mathcal{N}-2) - \theta_M(\mathcal{N})\big) a_x^* a_y^* + \text{h.c.} \Big) \int_\Lambda q_v^* a^*(K_v) q_v + \text{h.c.} \\
&\quad + n^{-\frac{1}{2}} \int_{\Lambda^2} \widetilde{Q}_2^{(bc)}(x,y) \Big(\big(\theta_M(\mathcal{N}-2) - \theta_M(\mathcal{N})\big) a_x^* a_y^* + \text{h.c.} \Big) \int_\Lambda q_v^* a^*(K_v) q_v + \text{h.c.} \\
&=: R_4 + R_5.
\end{aligned}$$

For the analysis of R_4, recall (6.5.15) as well as the pointwise bound (6.4.23) on $\widetilde{Q}_2^{(\epsilon)}$ and $\mathrm{d}\Gamma(\mathbb{1}_{|x-\cdot|\leqslant\lambda}) \leqslant C\lambda^2 \mathrm{d}\Gamma(-\Delta)$ on $\mathcal{F}_+$, from which we obtain

$$\begin{aligned}
&\pm n^{-\frac{1}{2}} \int_{\Lambda^2} \widetilde{Q}_2^{(\epsilon)}(x,y) \big(\theta_M(\mathcal{N}-2) - \theta_M(\mathcal{N})\big) a_x^* a_y^* \int_\Lambda a_v^* a^*(K_v) a_v + \text{h.c.} \\
&\leqslant C\delta \int_{\Lambda^3} \big(\theta_M(\mathcal{N}-2) - \theta_M(\mathcal{N})\big)^2 |\widetilde{Q}_2^{(\epsilon)}(x,y)| a_x^* a_y^* a_v^* (\mathcal{N}+1) a_v a_y a_x \\
&\quad + \delta^{-1} n^{-1} \int_{\Lambda^3} |\widetilde{Q}_2^{(\epsilon)}(x,y)| a_v^* a(K_v) (\mathcal{N}+1)^{-1} a^*(K_v) a_v \\
&\leqslant C\delta M^{-2} \mathbb{1}\,(\mathcal{N}-2 \leqslant 2M)\, n\ell^{-1}\lambda^{-1} (\mathcal{N}+1)^3 \mathrm{d}\Gamma(-\Delta) + C\delta^{-1}\ell^{-1} \sup_{x\in\Lambda} \|K_x\|_2^2 (\mathcal{N}+1) m \\
&\leqslant C\delta M n \ell^{-1} \lambda^{-1} \mathrm{d}\Gamma(-\Delta) + C\delta^{-1} \lambda n^2 \ell^{-3} (\mathcal{N}+1) \\
&\leqslant CM^{1/2} n \ell^{-3/2} \left(\mathrm{d}\Gamma(-\Delta) + \frac{n}{\ell}(\mathcal{N}+1) \right) \leqslant C\sigma \left(\mathrm{d}\Gamma(-\Delta) + \frac{n}{\ell}(\mathcal{N}+1) \right).
\end{aligned}$$

The same estimate holds for the $a_x a_y$ term in R_4 after normal ordering the expression. The terms generated by the commutators are similar to the ones already appearing in R_1 and satisfy the same bound. Therefore we obtain

$$\pm R_4 \leqslant C\sigma \left(\mathrm{d}\Gamma(-\Delta) + \frac{n}{\ell}(\mathcal{N}+1) + \lambda^{-1} \frac{n^{3/2}}{\ell^2} M^{-1} (\mathcal{N}+1) \right).$$

For R_5 we use the pointwise bound $|\widetilde{Q}_2^{(bc)}(x,y)| \leqslant CnV_\ell(x-y)$ and the Cauchy–Schwarz inequality to obtain

$$\begin{aligned}
&n^{-\frac{1}{2}} \int_{\Lambda^2} \widetilde{Q}_2^{(bc)}(x,y)\big(\theta_M(\mathcal{N}-2)-\theta_M(\mathcal{N})\big)a_x^* a_y^* \int_\Lambda a_v^* a^*(K_v) a_v + \text{h.c.} \\
&\leqslant \delta \int_{\Lambda^3} V_\ell(x-y)\big(\theta_M(\mathcal{N}-2)-\theta_M(\mathcal{N})\big)^2 a_x^* a_y^* a_v^* (\mathcal{N}+1) a_v a_y a_x \\
&\quad + C\delta^{-1} n \int_{\Lambda^3} V_\ell(x-y) a_v^* a(K_v)(\mathcal{N}+1)^{-1} a^*(K_v) a_v \\
&\leqslant C\delta M^{-2} \mathbb{1}(\mathcal{N}-2 \leqslant 2M)(\mathcal{N}+1)^2 Q_4 + C\delta^{-1}\lambda \frac{n^3}{\ell^3}(\mathcal{N}+1) \\
&\leqslant C\delta Q_4 + \delta^{-1} C\lambda \frac{n^3}{\ell^3}(\mathcal{N}+1).
\end{aligned}$$

As in the case of R_4, the $a_x a_y$ term of R_5 is bounded similarly as the term above after normal ordering. The terms arising from the commutators are of the of type of the ones appearing in R_2 and R_3, we therefore omit their treatment. In total, we find for all $\delta > 0$

$$\pm R_5 \leqslant \delta Q_4 + C\delta^{-1}\lambda \frac{n^3}{\ell^3}(\mathcal{N}+1) + C\sigma\left(\frac{n}{\ell}(\mathcal{N}+1) + \mathrm{d}\Gamma(-\Delta) + \left(\frac{n}{\ell}\right)^2\right),$$

which is the desired bound for the second term of (6.5.21).

In summary, we have shown the lemma with

$$\mathcal{E}_c^{(\widetilde{Q}_2)} = \widetilde{Q}_2^{(bc)} + \int_0^1 e^{-t\mathcal{B}_c} \sum_{i=1}^5 R_i e^{t\mathcal{B}_c} \mathrm{d}t.$$

Applying Lemma 6.17 and Lemma 6.16 to the R_i and simplifying the error terms using $\delta \leqslant 1$, we conclude the bound on the error term $\mathcal{E}_c^{(\widetilde{Q}_2)}$ as stated in Lemma 6.22. □

6.5.4 Proof of Lemma 6.15

We are now ready to give the proof of Lemma 6.15.

Proof. Recall the notation introduced in (6.5.4). The two main terms $(\mathrm{I})_\mathrm{c}$ and $(\mathrm{II})_\mathrm{c}$ were analyzed in Lemma 6.21 and Lemma 6.22 respectively. Recall that

$$\mathrm{d}\Gamma(-\Delta) = \sum_{p \in \pi\mathbb{N}_0^3 \setminus \{0\}} p^2 a_p^* a_p.$$

Moreover, by (6.4.5) and Lemma 6.5

$$\widetilde{Q}_2^{(\epsilon)} = \int_{\Lambda^2} Q_2^{(\epsilon)}(x,y) a_x^* a_y^* + \text{h.c.} = \frac{n}{2} \sum_{p \in \pi\mathbb{N}_0^3} \widehat{\epsilon}_{\ell,\lambda}(p) a_p^* a_p^* + \text{h.c.},$$

which becomes the pairing term in the Bogoliubov Hamiltonian (6.1.29) when restricted to $\mathcal{F}_+$. Hence we have

$$e^{-\mathcal{B}_c} e^{-\mathcal{B}_1} \mathcal{H} e^{\mathcal{B}_1} e^{\mathcal{B}_c} = 4\pi\mathfrak{a} n^2 \ell^{-1} + \mathbb{H}_{\text{Bog}} + Q_4 + \Xi_c + \mathcal{E}_c^{(\widetilde{Q}_2)} + (\mathrm{III})_c$$

with the two error terms Ξ_c and $\mathcal{E}_c^{(\widetilde{Q}_2)}$ estimated in Lemma 6.21 and Lemma 6.22, respectively. It thus remains to estimate

$$(\mathrm{III})_c = \int_0^1 e^{-t\mathcal{B}_c}\Big(Q_3 + [\mathrm{d}\Gamma(-\Delta) + Q_4, \mathcal{B}_c]\Big)e^{t\mathcal{B}_c}\mathrm{d}t + e^{-\mathcal{B}_c}\mathcal{E}_1 e^{\mathcal{B}_c} = (\mathrm{III})_{c_1} + (\mathrm{III})_{c_2},$$

where we recall that $\mathcal{E}_1$ satisfies (6.4.3). We deal with the two terms separately.

Estimating $(\mathrm{III})_{c_1}$. From Lemmata 6.18 and 6.19, we obtain

$$Q_3 + [\mathrm{d}\Gamma(-\Delta) + Q_4, \mathcal{B}_c] = (1-\theta_M)\int_{\Lambda^2} V_\ell(x-y)a_x^* a_y^* a_x + \text{h.c.} + \mathcal{E}_c^{(\mathrm{d}\Gamma(-\Delta))} + \mathcal{E}_c^{(Q_4)}.$$

As in (6.5.14), we use that $(1-\theta_M)\mathbb{1}^{\{\mathcal{N}<M/2\}} = 0$ to obtain

$$\pm(1-\theta_M)n^{1/2}\int_{\Lambda^2} V_\ell(x-y)a_x^* a_y^* a_x + \text{h.c.} \leqslant \delta Q_4 + C\delta^{-1}\frac{n}{\ell}\frac{\mathcal{N}^2}{M}.$$

We may now combine Lemma 6.16 and Lemma 6.17 with (6.5.5) to bound $(\mathrm{III})_{c_1}$ as

$$\begin{aligned}
\pm(\mathrm{III})_{c_1} &\leqslant C\delta\left(Q_4 + \frac{n}{\ell}(\mathcal{N}+1) + \sigma\mathrm{d}\Gamma(-\Delta)\right) + C\delta^{-1}\frac{n}{\ell}\frac{(\mathcal{N}+1)^2}{M}\\
&\quad + C\sigma\left(Q_4 + \mathrm{d}\Gamma(-\Delta) + \frac{n}{\ell}(\mathcal{N}+1)\right)\\
&\leqslant C\sigma\left(Q_4 + \mathrm{d}\Gamma(-\Delta) + \frac{n}{\ell}(\mathcal{N}+1)\right) + C\delta\left(Q_4 + \frac{n}{\ell}(\mathcal{N}+1)\right) + C\delta^{-1}\frac{n}{\ell}\frac{(\mathcal{N}+1)^2}{M}.
\end{aligned}$$

Estimating $(\mathrm{III})_{c_2}$. We apply Lemmata 6.16 and 6.17 to (6.4.3) and find

$$\begin{aligned}
\pm\, e^{-\mathcal{B}_c}\mathcal{E}_1 e^{\mathcal{B}_c} &\leqslant C(\delta + \ell^{-1}\lambda^2 + \varepsilon n^{-1})\left(Q_4 + \frac{n}{\ell}(\mathcal{N}+1) + \sigma\mathrm{d}\Gamma(-\Delta)\right)\\
&\quad + C\delta^{-1}\left(\frac{(\mathcal{N}+1)}{\ell} + \frac{(\mathcal{N}+1)^2}{n\ell} + \lambda\left(\frac{n}{\ell}\right)^3\right)(\mathcal{N}+1) + C\lambda^{\frac12}\big((\frac{n}{\ell})^2 + \frac{n}{\ell}\big)(\mathcal{N}+1)\\
&\quad + Cn^{\frac12}\frac{(\mathcal{N}+1)^{\frac32}}{\ell} + C\sigma\left(Q_4 + \mathrm{d}\Gamma(-\Delta) + \frac{n}{\ell}(\mathcal{N}+1)\right)\\
&\quad + C\varepsilon^{-1}\frac{n}{\ell} + C\left(\frac{n}{\ell}\right)^2\log\ell\\
&\leqslant \frac14 Q_4 + C\delta\left(Q_4 + \frac{n}{\ell}(\mathcal{N}+1)\right) + \delta^{-1}C\left(\frac{(\mathcal{N}+1)}{\ell} + \frac{(\mathcal{N}+1)^2}{n\ell} + \lambda\left(\frac{n}{\ell}\right)^3\right)(\mathcal{N}+1)\\
&\quad + C\lambda^{\frac12}\left(\left(\frac{n}{\ell}\right)^2 + \frac{n}{\ell}\right)(\mathcal{N}+1) + Cn^{\frac12}\frac{(\mathcal{N}+1)^{\frac32}}{\ell} + C\sigma\left(Q_4 + \mathrm{d}\Gamma(-\Delta) + \frac{n}{\ell}(\mathcal{N}+1)\right)\\
&\quad + C\left(\left(\frac{n}{\ell}\right)^2\log\ell + \frac{n}{\ell}\right).
\end{aligned}$$

Here we used $\delta \leqslant 1$ for the second inequality and we set $\varepsilon = (5C)^{-1}$ so that for ℓ large enough we have $C(\ell^{-1}\lambda^2 + \varepsilon n^{-1}) \leqslant 1/4$.

We now have obtained the necessary bounds on $(\mathrm{III})_c = (\mathrm{III})_{c_1} + (\mathrm{III})_{c_2}$. Combining them with the estimates of $(\mathrm{I})_c$ and $(\mathrm{II})_c$ given by Lemmata 6.21 and 6.22, respectively, and using $M \leqslant n$, we conclude the proof of Lemma 6.15. □

6.6 The Second Quadratic Transformation

In this section, we diagonalize explicitly the Bogoliubov Hamiltonian in (6.1.29),

$$\mathbb{H}_{\mathrm{Bog}} = \sum_{p\neq 0}\left(p^2 + 8\pi\mathfrak{a}\frac{n}{\ell}\right)a_p^*a_p + \frac{1}{2}\sum_{p\neq 0} n\widehat{\epsilon_{\ell,\lambda}}(p)(a_p^*a_p^* + a_pa_p) + \frac{1}{2}\sum_{p\neq 0}\frac{|n\widehat{\epsilon_{\ell,\lambda}}(p)|^2}{2p^2}.$$

We define

$$\mathcal{B}_2 = \frac{1}{2}\sum_{p\neq 0}\varphi_p(a_p^*a_p^* - a_pa_p), \tag{6.6.1}$$

where

$$\varphi_p = \sinh^{-1}(\nu_p),\ \nu_p = -\sqrt{\frac{1}{2}\left(\frac{A_p}{\sqrt{A_p^2 - B_p^2}} - 1\right)}, \tag{6.6.2}$$

$$A_p = p^2 + 8\pi\mathfrak{a}n\ell^{-1},\ B_p = n\widehat{\epsilon_{\ell,\lambda}}(p). \tag{6.6.3}$$

Note that we have

$$|B_p - 8\pi\mathfrak{a}n\ell^{-1}| = |n\widehat{\epsilon_{\ell,\lambda}}(p) - n\widehat{\epsilon_{\ell,\lambda}}(0)| \leq C\min\{1, \lambda^2p^2\}n\ell^{-1}, \tag{6.6.4}$$

which follows from the radial symmetry of ϵ and $|\epsilon_{\ell,\lambda}(x)| \leqslant C\lambda^{-3}\ell^{-1}\mathbb{1}_{|x|\leqslant\lambda}$, see (6.2.9). In particular for $\lambda^2n\ell^{-1}$ small enough we have $A_p > |B_p|$ for all $p \neq 0$, and the formula of ν_p in (6.6.2) is therefore well-defined.

The main result of this section is the following lemma.

Lemma 6.23. *Let $\lambda, n, \ell, \sigma, \mathcal{E}_c$ as in Lemma 6.15, assume that λ is small enough and let $\mathcal{W} = e^{\mathcal{B}_1}e^{\mathcal{B}_c}e^{\mathcal{B}_2}$. Then*

$$\mathcal{W}^*\mathcal{H}\mathcal{W} = E_{n,\ell} + \mathrm{d}\Gamma(E_{\mathrm{Bog}}) + e^{-\mathcal{B}_2}\left(Q_4 + \mathcal{E}_c + \mathcal{E}_2\right)e^{\mathcal{B}_2}$$

on $\mathcal{F}_+$ with

$$\mathrm{d}\Gamma(E_{\mathrm{Bog}}) = \sum_{p\neq 0}\sqrt{p^4 + 16\pi\mathfrak{a}n\ell^{-1}p^2}\,a_p^*a_p,$$

$$E_{n,\ell} = 4\pi\mathfrak{a}n^2\ell^{-1} + \frac{1}{2}\sum_{p\neq 0}\left[\sqrt{p^4 + 16\pi\mathfrak{a}n\ell^{-1}p^2} - p^2 - 8\pi\mathfrak{a}\frac{n}{\ell} + \frac{(8\pi\mathfrak{a}n\ell^{-1})^2}{2p^2}\right] \tag{6.6.5}$$

and

$$\pm\mathcal{E}_2 \leqslant C\lambda\left(\left(\frac{n}{\ell}\right)^{\frac{1}{2}} + 1\right)\mathcal{N} + C\lambda\left(\frac{n}{\ell}\right)^3 + C\lambda^2\left(\frac{n}{\ell}\right)^{5/2}.$$

Let us first state the following lemma, which will be proved at the end of this section.

Lemma 6.24. *Let $\lambda\left(\frac{n}{\ell}\right)^2 \leqslant 1$, $2R/\ell < \lambda$ and λ be small enough. Then we have*

$$e^{\pm\mathcal{B}_2}(\mathcal{N}+1)e^{\mp\mathcal{B}_2} \leqslant C\left(\left(\frac{n}{\ell}\right)^{\frac{1}{2}} + 1\right)\mathcal{N} + C\left(\frac{n}{\ell}\right)^{\frac{3}{2}} \tag{6.6.6}$$

and

$$e^{-\mathcal{B}_2}\mathrm{d}\Gamma(-\Delta)e^{\mathcal{B}_2} \leqslant C\left(\left(\frac{n}{\ell}\right)^{\frac{1}{2}} + 1\right)\mathrm{d}\Gamma(-\Delta) + C\lambda^{-1}\left(\frac{n}{\ell}\right)^2. \tag{6.6.7}$$

Proof of Lemma 6.23. From the assumptions on $\lambda(\frac{n}{\ell})^2$ and λ we conclude that $\lambda^2(\frac{n}{\ell})$ is sufficiently small for φ_p in (6.6.2) to be well defined. Given (6.1.29) and (6.6.1), the action of the transformation $e^{\mathcal{B}_2}$ on $\mathbb{H}_{\mathrm{Bog}}$ is standard, see e.g. [86, Section 3]. It gives

$$e^{-\mathcal{B}_2}\mathbb{H}_{\mathrm{Bog}}e^{\mathcal{B}_2} = e_{\mathrm{Bog}} + \sum_{p\neq 0} e_p a_p^* a_p \tag{6.6.8}$$

with

$$e_p = \sqrt{A_p^2 - B_p^2}, \quad e_{\mathrm{Bog}} = \frac{1}{2}\sum_{p\neq 0}\left[\sqrt{A_p^2 - B_p^2} - A_p\right] + \frac{1}{2}\sum_{p\neq 0}\frac{(n\widehat{\epsilon}_{\ell,\lambda}(p))^2}{2p^2},$$

where we recall that A_p and B_p are defined in (6.6.3). We will use the following lemma that we show after the proof of Lemma 6.23.

Lemma 6.25. *Let $\lambda\left(\frac{n}{\ell}\right)^2 \leqslant 1$, $2R/\ell < \lambda$ and λ be small enough. We have the uniform bound*

$$\sup_{p\in\mathbb{R}^3}\left|e_p - \sqrt{p^4 + 16\pi\mathfrak{a}n\ell^{-1}p^2}\right| \leqslant C\lambda^2\frac{n^2}{\ell^2} \tag{6.6.9}$$

as well as

$$\left|e_{\mathrm{Bog}} - \frac{1}{2}\sum_{p\neq 0}\left[\sqrt{p^4 + 16\pi\mathfrak{a}n\ell^{-1}p^2} - p^2 - 8\pi\mathfrak{a}\frac{n}{\ell} + \frac{(8\pi\mathfrak{a}n\ell^{-1})^2}{2p^2}\right]\right| \leqslant C\lambda\frac{n^3}{\ell^3}. \tag{6.6.10}$$

Starting from (6.5.2), using the identity (6.6.8), the estimates of Lemma 6.25 and the bounds of Lemma 6.24, readily imply the statement of Lemma 6.23. □

We end this section with the proofs of Lemmata 6.25 and 6.24.

Proof of Lemma 6.25. Let us start by showing (6.6.9). Using $|\sqrt{1+x} - 1| \leqslant |x|$ for all $x \geqslant -1$ and (6.6.4) we find

$$\begin{aligned}
&\left|e_p - \sqrt{p^4 + 16\pi\mathfrak{a}n\ell^{-1}p^2}\right| \\
&\leqslant \left(p^4 + 16\pi\mathfrak{a}n\ell^{-1}p^2\right)^{-\frac{1}{2}}|8\pi\mathfrak{a}\frac{n}{\ell} + n\widehat{\epsilon}_{\ell,\lambda}(p)||8\pi\mathfrak{a}\frac{n}{\ell} - n\widehat{\epsilon}_{\ell,\lambda}(p)| \\
&\leqslant C\left(p^4 + 16\pi\mathfrak{a}n\ell^{-1}p^2\right)^{-\frac{1}{2}}\lambda^2 p^2\frac{n^2}{\ell^2} \leqslant C\lambda^2\frac{n^2}{\ell^2},
\end{aligned}$$

which shows (6.6.9). To prove (6.6.10) note that

$$\begin{aligned}
\tau &:= 2e_{\mathrm{Bog}} - \left[\sum_{p\neq 0}\sqrt{p^4 + 16\pi\mathfrak{a}n\ell^{-1}p^2} - p^2 - 8\pi\mathfrak{a}\frac{n}{\ell} + \frac{(8\pi\mathfrak{a}n/\ell)^2}{2p^2}\right] \\
&= \sum_{p\neq 0}p^2\left(\sqrt{1 + \frac{16\pi\mathfrak{a}n/\ell}{p^2} + \frac{(8\pi\mathfrak{a}n/\ell)^2 - (n\widehat{\epsilon}_{\ell,\lambda}(p))^2}{p^4}}\right. \\
&\qquad\qquad \left. - \sqrt{1 + \frac{16\pi\mathfrak{a}n/\ell}{p^2} - \frac{(8\pi\mathfrak{a}n/\ell)^2 - (n\widehat{\epsilon}_{\ell,\lambda}(p))^2}{2p^4}}\right).
\end{aligned}$$

The Taylor formula readily gives

$$|v(x) - v(y) - v'(0)(x-y)| \leqslant C\|v''\|_\infty|x-y|(|x|+|y|)$$

for $v \in C^2(U), U \subset \mathbb{R}$ open. Applying this inequality to

$$v(z) = \sqrt{1+z} \text{ with } x = \frac{16\pi\mathfrak{a}n/\ell}{p^2} + \frac{(8\pi\mathfrak{a}n/\ell)^2 - (n\widehat{\epsilon}_{\ell,\lambda}(p))^2}{p^4},\ y = \frac{16\pi\mathfrak{a}n/\ell}{p^2}$$

and using (6.6.4) yields

$$\begin{aligned}
|\tau| &\leqslant C\sum_{p\neq 0} p^2 \frac{|(8\pi\mathfrak{a}n/\ell)^2 - (n\widehat{\epsilon}_{\ell,\lambda}(p))^2|}{p^4}\left(2\frac{16\pi\mathfrak{a}n/\ell}{p^2} + \frac{|(8\pi\mathfrak{a}n/\ell)^2 - (n\widehat{\epsilon}_{\ell,\lambda}(p))^2|}{p^4}\right)\\
&\leqslant C\sum_{p\neq 0} p^2\frac{n/\ell}{p^4}|8\pi\mathfrak{a}\frac{n}{\ell} - n\widehat{\epsilon}_{\ell,\lambda}(p)|\left(\frac{n/\ell+\lambda^2(n/\ell)^2}{p^2}\right)\\
&\leqslant C(\frac{n}{\ell})^2\sum_{p\neq 0}|8\pi\mathfrak{a}\frac{n}{\ell} - n\widehat{\epsilon}_{\ell,\lambda}(p)|p^{-4}\\
&\leqslant C(\frac{n}{\ell})^2\sum_{p\neq 0}\min\{1,\lambda^2p^2\}\frac{n}{\ell}p^{-4} \leqslant C\lambda(\frac{n}{\ell})^3,
\end{aligned}$$

which concludes the proof of (6.6.10). □

Proof of Lemma 6.24. The action of the quadratic transformation $\mathcal{B}_2$ on the creation and annihilation operators is given by

$$e^{\mp\mathcal{B}_2}a_p^*e^{\pm\mathcal{B}_2} = \cosh(\varphi_p)a_p^* \pm \sinh(\varphi_p)a_p.$$

Thus

$$\begin{aligned}
e^{\pm\mathcal{B}_2}\mathcal{N}e^{\mp\mathcal{B}_2} &= \sum_{p\neq 0}\left(\cosh(\varphi_p)a_p^* \pm \sinh(\varphi_p)a_p\right)\left(\cosh(\varphi_p)a_p \pm \sinh(\varphi_p)a_p^*\right)\\
&= \sum_{p\neq 0}\left[\left(\cosh(\varphi_p)^2 + \sinh(\varphi_p)^2\right)a_p^*a_p \pm \cosh(\varphi_p)\sinh(\varphi_p)(a_p^*a_p^* + a_pa_p) + \sinh(\varphi_p)^2\right]\\
&\leqslant 2\sum_{p\neq 0}\left[(\cosh(\varphi_p)^2 + \sinh(\varphi_p)^2)a_p^*a_p + \sinh(\varphi_p)^2\right]. \qquad (6.6.11)
\end{aligned}$$

To verify (6.6.6) it remains to show that

$$\cosh(\varphi_p)^2 + \sinh(\varphi_p)^2 \leqslant C\left(\left(\frac{n}{\ell}\right)^{\frac{1}{2}} + 1\right), \qquad (6.6.12)$$

$$\sum_{p\neq 0}\sinh(\varphi_p)^2 \leqslant C\left(\frac{n}{\ell}\right)^{\frac{3}{2}}. \qquad (6.6.13)$$

Let us prove (6.6.12). From (6.6.2) we have

$$\begin{aligned}
\cosh(\varphi_p)^2 + \sinh(\varphi_p)^2 &= 2\sinh(\varphi_p)^2 + 1\\
&= |p|^{-1}\frac{p^2 + 8\pi\mathfrak{a}n/\ell}{\sqrt{p^2 + 16\pi\mathfrak{a}n/\ell + \frac{(8\pi\mathfrak{a}n/\ell)^2 - (n\widehat{\epsilon}_{\ell,\lambda}(p))^2}{p^2}}}\\
&\leqslant |p|^{-1}\frac{p^2 + 8\pi\mathfrak{a}n/\ell}{\sqrt{p^2 + 8\pi\mathfrak{a}n/\ell}} = \sqrt{1 + 8\pi\mathfrak{a}\frac{n}{\ell}p^{-2}} \leqslant C\left(\left(\frac{n}{\ell}\right)^{\frac{1}{2}} + 1\right).
\end{aligned}$$

Here we used $p^{-2}\left((8\pi\mathfrak{a}n/\ell)^2 - (n\widehat{\epsilon}_{\ell,\lambda}(p))^2\right) \geqslant -8\pi\mathfrak{a}n\ell^{-1}$, which follows from (6.6.4).

To prove (6.6.13) we use again (6.6.2) and divide the sum into momenta $|p|$ less or bigger than $(n/\ell)^{\frac{1}{2}}$. For small momenta we have

$$\begin{aligned}\sum_{0<|p|\leqslant(\frac{n}{\ell})^{\frac{1}{2}}}\sinh(\varphi_p)^2 &\leqslant C\sum_{0<|p|\leqslant(\frac{n}{\ell})^{\frac{1}{2}}}\left(\sqrt{1+8\pi\mathfrak{a}n/\ell p^{-2}}+1\right)\\ &\leqslant C\sum_{0<|p|\leqslant(\frac{n}{\ell})^{\frac{1}{2}}}\left(1+8\pi\mathfrak{a}n/\ell p^{-2}\right)\leqslant C\left(\frac{n}{\ell}\right)^{\frac{3}{2}}. \qquad (6.6.14)\end{aligned}$$

For large momenta we use $|\sqrt{1+z}-1-z|\leqslant z^2$ for $z\geqslant -1$ as well as and $|\sqrt{1+x}-\sqrt{1+y}|\leqslant C|x-y|$ for $x,y\geqslant-\frac{1}{2}$ to obtain

$$\begin{aligned}\sum_{|p|>(\frac{n}{\ell})^{\frac{1}{2}}}\sinh(\varphi_p)^2 &\leqslant \sum_{|p|>(\frac{n}{\ell})^{\frac{1}{2}}} p^{-2}\left|p^2+8\pi\mathfrak{a}\frac{n}{\ell}-p^2\sqrt{1+\frac{16\pi\mathfrak{a}n/\ell}{p^2}+\frac{(8\pi\mathfrak{a}n/\ell)^2-(n\widehat{\epsilon}_{\ell,\lambda}(p))^2}{p^4}}\right|\\ &\leqslant \sum_{|p|>(\frac{n}{\ell})^{\frac{1}{2}}}\left|1+\frac{8\pi\mathfrak{a}n/\ell}{p^2}-\sqrt{1+\frac{16\pi\mathfrak{a}n/\ell}{p^2}}\right|\\ &\quad+\sum_{|p|>(\frac{n}{\ell})^{\frac{1}{2}}}\left|\sqrt{1+\frac{16\pi\mathfrak{a}n/\ell}{p^2}+\frac{(8\pi\mathfrak{a}n/\ell)^2-(n\widehat{\epsilon}_{\ell,\lambda}(p))^2}{p^4}}-\sqrt{1+\frac{16\pi\mathfrak{a}n/\ell}{p^2}}\right|\\ &\leqslant C\frac{n^2}{\ell^2}\sum_{|p|>(\frac{n}{\ell})^{\frac{1}{2}}}p^{-4}\leqslant C\left(\frac{n}{\ell}\right)^{\frac{3}{2}}.\end{aligned}$$

This concludes the proof of (6.6.6). The bound (6.6.7) is proved similarly. Proceeding as in (6.6.11) we obtain

$$\begin{aligned}e^{-\mathcal{B}_2}\mathrm{d}\Gamma(-\Delta)e^{\mathcal{B}_2} &\leqslant 2\sum_{p\neq 0}\left[p^2(\cosh(\varphi_p))^2+\sinh(\varphi_p))^2)a_p^*a_p+p^2\sinh(\varphi_p)^2\right]\\ &\leqslant C\left(\left(\frac{n}{\ell}\right)^{\frac{1}{2}}+1\right)\mathrm{d}\Gamma(-\Delta)+C\left(\frac{n}{\ell}\right)^2\lambda^{-1}\end{aligned}$$

given that

$$\sum_{p\neq 0}p^2\sinh(\varphi_p)^2\leqslant C\left(\frac{n}{\ell}\right)^2\lambda^{-1}, \qquad (6.6.15)$$

which remains to be shown. We have

$$2p^2\sinh(\varphi_p)^2=p^2\frac{1+8\pi\mathfrak{a}(n/\ell)p^{-2}-\sqrt{1+16\pi\mathfrak{a}(n/\ell)p^{-2}+\frac{(8\pi\mathfrak{a}(n/\ell))^2-(n\widehat{\epsilon}_{\ell,\lambda}(p))^2}{p^4}}}{\sqrt{1+16\pi\mathfrak{a}(n/\ell)p^{-2}+\frac{(8\pi\mathfrak{a}(n/\ell))^2-(n\widehat{\epsilon}_{\ell,\lambda}(p))^2}{p^4}}}.$$

Let us define

$$v(x)=1+8\pi\mathfrak{a}(n/\ell)x-\left(1+16\pi\mathfrak{a}(n/\ell)x+((8\pi\mathfrak{a}(n/\ell))^2-(n\widehat{\epsilon}_{\ell,\lambda}(p))^2)x^2\right)^{\frac{1}{2}}.$$

Taylor expanding at $x = p^{-2}$, we obtain

$$v(x) = \frac{(n\widehat{\epsilon}_{\ell,\lambda}(p))^2}{2} x^2 + R(x)$$

with

$$|R(x)| \leqslant \sup_{0 \leqslant y \leqslant p^{-2}} |v'''(y)| x^2 \leqslant C \left(\frac{n}{\ell}\right)^3 x^2.$$

Thus

$$2p^2 \sinh(\varphi_p)^2 \leqslant \frac{(n\widehat{\epsilon}_{\ell,\lambda}(p))^2}{2p^2} + C \left(\frac{n}{\ell}\right)^3 p^{-4},$$

which immediately implies

$$\sum_{p \neq 0} p^2 \sinh(\varphi_p)^2 \leqslant \sum_{p \neq 0} \frac{(n\widehat{\epsilon}_{\ell,\lambda}(p))^2}{2p^2} + C \left(\frac{n}{\ell}\right)^3.$$

From the assumptions $\lambda \left(\frac{n}{\ell}\right)^2 \leqslant 1$ and λ small enough, we find $(n/\ell)^3 \leq \lambda^{-1}(n/\ell)^2$.

As we argued in the proof of (6.4.27), we have $\widehat{\epsilon}_{\ell,\lambda}(p) = \mathfrak{a}\ell^{-1}\widehat{f}(\lambda p)$ for a fixed function $f \in C_c^\infty(\mathbb{R}^3)$, and hence

$$\begin{aligned} \sum_{p \neq 0} \frac{(n\widehat{\epsilon}_{\ell,\lambda}(p))^2}{2p^2} &\leqslant \left| \sum_{p \neq 0} \frac{(n\widehat{\epsilon}_{\ell,\lambda}(p))^2}{2p^2} - \frac{1}{(2\pi)} \int_{\mathbb{R}^3} \frac{(n\widehat{\epsilon}_{\ell,\lambda}(p))^2}{2p^2} \right| + \frac{1}{(2\pi)} \int_{\mathbb{R}^3} \frac{(n\widehat{\epsilon}_{\ell,\lambda}(p))^2}{2p^2} \\ &\leqslant C \left(\frac{n}{\ell}\right)^2 + C\lambda^{-1} \left(\frac{n}{\ell}\right)^2 \leqslant C\lambda^{-1} \left(\frac{n}{\ell}\right)^2. \end{aligned} \tag{6.6.16}$$

This shows (6.6.15) and consequently completes the proof of Lemma 6.24. □

6.7 A-Priori Estimates for Gibbs States

Recall the definition (6.1.2) of $H_{n,\ell}$, and the one of U in Section 6.2.3. We introduce the Gibbs state on $\mathcal{F}_+^{\leqslant n}$

$$\Gamma = e^{-\frac{\mathbb{H}_{n,\ell}}{T\ell^2}} / \mathrm{Tr}\, e^{-\frac{\mathbb{H}_{n,\ell}}{T\ell^2}}, \quad \mathbb{H}_{n,\ell} = U H_{n,\ell} U^* \tag{6.7.1}$$

It minimizes the Gibbs variational principle and yields the free energy on the box Λ_ℓ as in (6.1.3).

The analysis of $\mathcal{H}$ in the previous sections will be used in Section 6.8 to control Γ on the sector of few excited particles. This section, on the other hand, provides rough a priori estimates on the kinetic and interaction operator, which are helpful to control the sector of high particle number. Moreover, we derive complete BEC for Γ given that the thermal contribution to the free energy is subleading. We shall see that this is the case as long as n is not too small.

6.7.1 Rough Kinetic and Interaction Energy Estimates

Lemma 6.26. *Let $0 \leqslant n \leqslant C\rho\ell^3$ and $\ell = \mathfrak{a}(\rho\mathfrak{a}^3)^{-1/2-\kappa}$. Then we have*

$$\mathbb{H}_{n,\ell} \lesssim \left(\mathrm{d}\Gamma(-\Delta) + Q_4 + n^2\mathfrak{a}\ell^{-1}\right) \lesssim \mathbb{H}_{n,\ell} + n^2\mathfrak{a}\ell^{-1} \tag{6.7.2}$$

on $\mathcal{F}_+^{\leqslant n}$.

Proof. Recall from Lemma 6.3 that $\mathbb{H}_{n,\ell} = \mathbb{1}_+^{\leqslant n}\mathcal{H}\mathbb{1}_+^{\leqslant n}$, where $\mathcal{H}$ is an operator on $\mathcal{F}$ defined in (6.2.17). We shall show that all the terms $n^2V_\ell^{0000}$, Q_1, $H_2^{(U)}$, Q_2, $Q_3^{(U)}$ and $\mathcal{E}^{(U)}$, when restricted to $\mathcal{F}_+^{\leqslant n}$, are bounded by $\varepsilon Q_4 + C_\varepsilon n^2\ell^{-1}$ with $\varepsilon > 0$ arbitrarily small .

First, the constant $n^2V_\ell^{0000}$ is bounded by $n^2\|V_\ell\|_{L^1} \leq Cn^2\ell^{-1}$. Next, from the bound (6.2.18) in Lemma 6.3, with ε replaced by $n\varepsilon$, we have

$$\pm\mathcal{E}^{(U)} \leq Cn^{\frac{1}{2}}(\mathcal{N}+1)^{\frac{3}{2}}\ell^{-1} + \varepsilon Q_4 + C\varepsilon^{-1}\ell^{-1} \tag{6.7.3}$$

on $\mathcal{F}$ for all $\varepsilon > 0$. For $H_2^{(U)}$ we have $\mathcal{N}nV_\ell^{0000} \leq C\mathcal{N}n\ell^{-1}$ and

$$\begin{aligned}
\pm\int_{\Lambda^2} nV_\ell(x-y)a_x^*a_x &\leq n\|V_\ell\|_{L^1}\mathcal{N} \leq Cn\ell^{-1}\mathcal{N},\\
\pm\int_{\Lambda^2} nV_\ell(x-y)a_x^*a_y &\leq \frac{1}{2}\int_{\Lambda^2} nV_\ell(x-y)(a_x^*a_x + a_y^*a_y) \leq Cn\ell^{-1}\mathcal{N},\\
\pm\left(\frac{1}{2}\int_{\Lambda^2} V_\ell(x-y)a_x^*a_y^*\mathcal{N} + \text{h.c.}\right) &\leq \frac{\varepsilon}{2}\int_{\Lambda^2} V_\ell(x-y)a_x^*a_y^*a_xa_y + \frac{1}{2\varepsilon}\int_{\Lambda^2} V_\ell(x-y)\mathcal{N}^2\\
&\leq \varepsilon Q_4 + C\varepsilon^{-1}\ell^{-1}\mathcal{N}^2
\end{aligned}$$

so that

$$\pm H_2^{(U)} \leqslant Cn\ell^{-1}\mathcal{N} + \varepsilon Q_4 + C\varepsilon^{-1}\ell^{-1}\mathcal{N}^2 \tag{6.7.4}$$

on $\mathcal{F}$ for all $\varepsilon > 0$. Moreover, by the Cauchy–Schwarz inequality

$$\begin{aligned}
\pm Q_1 &\leq \int_{\Lambda^2} nV_\ell(x-y)(\mathcal{N}+1)^{-1/4}a_x^*a_x(\mathcal{N}+1)^{-1/4} + \int_{\Lambda^2} n^2V_\ell(x-y)(\mathcal{N}+1)^{1/2}\\
&\leq Cn^{3/2}\ell^{-1}(\mathcal{N}+1)^{1/2}, \qquad (6.7.5)\\
\pm Q_2 &\leq \frac{\varepsilon}{2}\int_{\Lambda^2} V_\ell(x-y)a_x^*a_y^*a_xa_y + \frac{\varepsilon^{-1}}{2}n^2\int_{\Lambda^2} V_\ell(x-y)\\
&\leq \varepsilon Q_4 + C\varepsilon^{-1}n^2\ell^{-1}, \qquad (6.7.6)\\
\pm Q_3^{(U)} &\leq \frac{\varepsilon}{2}\int_{\Lambda^2} V_\ell(x-y)a_x^*a_y^*a_xa_y + 2\varepsilon^{-1}n\int_{\Lambda^2} V_\ell(x-y)a_x^*a_x\\
&\leq \varepsilon Q_4 + C\varepsilon^{-1}n\ell^{-1}\mathcal{N} \qquad (6.7.7)
\end{aligned}$$

on $\mathcal{F}$ for all $\varepsilon > 0$. Restricting these bounds to $\mathcal{F}_+^{\leqslant n}$ where $\mathcal{N} \leq n$ we find that

$$\pm(\mathbb{H}_{n,\ell} - \mathrm{d}\Gamma(-\Delta) - Q_4) \leq \varepsilon Q_4 + C\varepsilon^{-1}n^2\ell^{-1}$$

on $\mathcal{F}_+^{\leqslant n}$ for all $0 < \varepsilon \leqslant 1$, which implies (6.7.2). □

6.7.2 Bose–Einstein Condensation

Lemma 6.27. *Let Γ be as in (6.7.1) with $(\rho\mathfrak{a}^3)^{1/4+\nu/2}(\rho\ell^3) \leqslant n \leqslant C(\rho\ell^3)$, $\ell = \mathfrak{a}(\rho\mathfrak{a}^3)^{-1/2-\kappa}$ with $0 < \kappa < 1/34$ and $0 \leqslant T \leqslant (\rho\mathfrak{a})(\rho\mathfrak{a}^3)^{-\nu}$ with $0 < \nu < 1/12 - 5\kappa/3$. Then we have*

$$\mathrm{Tr}\,(\mathcal{N}_+\Gamma) \leqslant Cn(\rho\mathfrak{a}^3)^\gamma, \tag{6.7.8}$$

with $\gamma = \min\{1/10 - 2\kappa - 6\nu/5, 1/17 - 2\kappa\} > 0$.

In the dilute limit $\rho\mathfrak{a}^3 \to 0$, Lemma 6.27 implies that $\mathrm{Tr}\,(\mathcal{N}_+\Gamma)$ is much smaller than n, the total number of particles. This is equivalent to complete condensation of Γ, namely all but $o(n)$ particles occupy the zero-momentum mode.

Proof. From the method in [63] (see also [58, Lemma 5.2]) we have the a priori knowledge of condensation on $L^2_s(\Lambda^n)$

$$H_{n,\ell} \geqslant 4\pi\mathfrak{a}\ell^{-1}n^2 + C^{-1}\mathcal{N}_+ - Cn\rho\mathfrak{a}\ell^2(\rho\mathfrak{a}^3)^{1/17}. \tag{6.7.9}$$

Since $U\mathcal{N}_+U^* = \mathcal{N}_+$, the same bound holds with $H_{n,\ell}$ replaced by $\mathbb{H}_{n,\ell} = UH_{n,\ell}U^*$. We obtain

$$C^{-1}\mathrm{Tr}\,(\mathcal{N}_+\Gamma) \leqslant \mathrm{Tr}\,(\mathbb{H}_{n,\ell}\Gamma) - 4\pi\mathfrak{a}\ell^{-1}n^2 + Cn\rho\mathfrak{a}\ell^2(\rho\mathfrak{a}^3)^{1/17}.$$

Therefore, it is enough to show that

$$\mathrm{Tr}\,(\mathbb{H}_{n,\ell}\Gamma) - 4\pi\mathfrak{a}\ell^{-1}n^2 \leqslant Cn(\rho\mathfrak{a}^3)^{1/10-2\kappa-6\nu/5}. \tag{6.7.10}$$

In order to prove (6.7.10), we will use the following upper bound on the ground state energy [58, Theorem 2.2]

$$\ell^2F_\ell(n) \leqslant \inf\sigma(\mathbb{H}_{n,\ell}) \leqslant 4\pi\mathfrak{a}n^2\ell^{-1} + Cn(\rho\mathfrak{a}^3)^{1/3}. \tag{6.7.11}$$

From the Gibbs variational principle, we have that for all $\varepsilon > 0$

$$\varepsilon\mathrm{Tr}\,(\mathrm{d}\Gamma(-\Delta)\Gamma) - T\ell^2S(\Gamma) \geqslant -T\ell^2\log\mathrm{Tr}\,e^{-\frac{\varepsilon}{T\ell^2}\mathrm{d}\Gamma(-\Delta)} \geqslant -CT^{5/2}\ell^5\varepsilon^{-3/2},$$

which follows from the bound

$$\beta^{-1}\log\mathrm{Tr}\,e^{-\beta\mathrm{d}\Gamma(-\Delta)} = -\beta^{-1}\sum_{p\in\pi\mathbb{N}_0^3\setminus\{0\}}\log\left(1-e^{-\beta p^2}\right) \leqslant C\beta^{-5/2} \tag{6.7.12}$$

for some $C > 0$ and all $\beta > 0$.

We can now prove (6.7.10). From the Gibbs variational principle we have for all $0 < \varepsilon \leqslant 1$

$$\begin{aligned}
\mathrm{Tr}\,(\mathbb{H}_{n,\ell}\Gamma) &= (1+\varepsilon)\left(\mathrm{Tr}\,(\mathbb{H}_{n,\ell}\Gamma) - T\ell^2S(\Gamma)\right) - \left(\varepsilon\mathrm{Tr}\,(\mathbb{H}_{n,\ell}\Gamma) - (1+\varepsilon)T\ell^2S(\Gamma)\right) \\
&\leqslant (1+\varepsilon)\ell^2F_\ell(n) - \left(\varepsilon\mathrm{Tr}\,(\mathrm{d}\Gamma(-\Delta)\Gamma) - 2T\ell^2S(\Gamma)\right) \\
&\leqslant (1+\varepsilon)\inf\sigma(\mathbb{H}_{n,\ell}) - \left(\varepsilon\mathrm{Tr}\,(\mathrm{d}\Gamma(-\Delta)\Gamma) - 2T\ell^2S(\Gamma)\right) \\
&\leqslant (1+\varepsilon)\left(4\pi\mathfrak{a}n^2\ell^{-1} + Cn(\rho\mathfrak{a}^3)^{1/3}\right) + C\varepsilon^{-3/2}T^{5/2}\ell^5.
\end{aligned}$$

Taking $\varepsilon = (\rho\mathfrak{a}^3)^{1/10-6\nu/5}$, using that $(\rho\mathfrak{a}^3)^{1/4+\nu/2}(\rho\ell^3) \leqslant n$ and our assumptions on ℓ and T, we obtain (6.7.10) from which Lemma 6.27 follows. □

6.8 Proof of Theorem 6.1

In this section we shall give the proof of Theorem 6.1. We denote $Y = \rho\mathfrak{a}^3$ and set

$$M_0 = n^{1-80\kappa}, M = n^{1-68\kappa}, \lambda = Y^{10\kappa}, \delta = Y^{3\kappa} \tag{6.8.1}$$

with $\kappa = 1/1000$. Recall that $T \leq \rho\mathfrak{a}(\rho\mathfrak{a}^3)^{-\nu}$ and $\ell = \mathfrak{a}/(\rho\mathfrak{a}^3)^{1/2+\kappa}$ as in (6.1.1) with $\nu = \kappa/5$. Moreover, let us first focus on the case $(\rho\mathfrak{a}^3)^{1/4+\nu/2}(\rho\ell^3) \leqslant n \leqslant C(\rho\ell^3)$, which allows us to use condensation in the sense of Lemma 6.27. The case of smaller n will be considered afterwards.

Case $(\rho\mathfrak{a}^3)^{1/4+\nu/2}(\rho\ell^3) \leqslant n \leqslant C(\rho\ell^3)$**:** We will combine the estimates in the previous sections with the localization method on the number of excited particles in the spirit of [59, 56]. To be precise, we fix smooth functions $f, g : \mathbb{R}_{\geqslant 0} \to [0,1]$ such that

$$f^2 + g^2 = 1, \quad f(x) = 1 \text{ for } x < \frac{1}{2}, \quad f(x) = 0 \text{ for } x > 1$$

and define

$$f_{M_0} = f(\mathcal{N}_+/M_0), \quad g_{M_0} = g(\mathcal{N}_+/M_0).$$

Recall the definition of the Hamiltonian $\mathbb{H}_{n,\ell}$ and the Gibbs state Γ in (6.7.1). Applying [56, Proposition 6.1], we can write

$$\mathbb{H}_{n,\ell} = f_{M_0}\mathbb{H}_{n,\ell}f_{M_0} + g_{M_0}\mathbb{H}_{n,\ell}g_{M_0} + \mathcal{E}_{M_0}, \tag{6.8.2}$$

where

$$\pm\mathcal{E}_{M_0} = \pm\left(\frac{1}{2}[f_{M_0},[f_{M_0},\mathbb{H}_{n,\ell}]] + \frac{1}{2}[g_{M_0},[g_{M_0},\mathbb{H}_{n,\ell}]]\right) \leq \frac{C}{M_0^2}[H_{n,\ell}]_{\text{diag}}. \tag{6.8.3}$$

Here $[H_{n,\ell}]_{\text{diag}}$ is the diagonal part of $\mathbb{H}_{n,\ell}$, i.e. $[H_{n,\ell}]_{\text{diag}}$ contains the terms in $\mathbb{H}_{n,\ell}$ that commute with the number operator $\mathcal{N}$. Recall the rough estimate (6.7.2)

$$\mathbb{H}_{n,\ell} \lesssim \mathrm{d}\Gamma(-\Delta) + Q_4 + Cn^2\mathfrak{a}\ell^{-1}. \tag{6.8.4}$$

The diagonal part $[H_{n,\ell}]_{\text{diag}}$ satisfies the same bound since the right-hand side of (6.8.4) is diagonal. Thus we deduce from (6.8.3) that the localization error can be controlled by

$$\pm\mathcal{E}_{M_0} \leq \frac{C}{M_0^2}\left(\mathrm{d}\Gamma(-\Delta) + Q_4 + Cn^2\mathfrak{a}\ell^{-1}\right). \tag{6.8.5}$$

Applying again (6.7.2) together with (6.7.10) yields

$$\mathrm{Tr}\,((Q_4 + \mathrm{d}\Gamma(-\Delta))\,\Gamma) \leqslant C\mathrm{Tr}\,(\mathbb{H}_{n,\ell}\Gamma) + Cn^2\mathfrak{a}\ell^{-1} \leqslant Cn^2\mathfrak{a}\ell^{-1} + nY^{1/10-2\kappa-6\nu/5}. \tag{6.8.6}$$

With the choice of M_0 in (6.8.1) and the assumption $n \leq C\rho\ell^3$, a combination of (6.8.5) and (6.8.6) gives

$$\pm\mathrm{Tr}\,(\mathcal{E}_{M_0}\Gamma) \lesssim n\mathfrak{a}\ell^{-1} + Y^{1/10-2\kappa-6\nu/5} \lesssim Y^{-2\kappa} = \mathcal{O}((\rho\mathfrak{a})^{5/2}\ell^5Y^{3\kappa}). \tag{6.8.7}$$

Let us introduce the notation

$$\Gamma_{f_{M_0}} = f_{M_0}\Gamma f_{M_0}, \quad \Gamma_{g_{M_0}} = g_{M_0}\Gamma g_{M_0}, \quad \alpha = \mathrm{Tr}\,(\Gamma_{g_{M_0}}) = \mathrm{Tr}\,(g_{M_0}^2\Gamma).$$

We will see later that $\alpha \geq 0$ is small. If $\alpha = 0$, then the analysis below can be simplified greatly. Here we focus on the case $\alpha > 0$. Note that $(1-\alpha)^{-1}\Gamma_{f_{M_0}}$ and $\alpha^{-1}\Gamma_{g_{M_0}}$ are normalized states. Combining (6.8.2) with the subadditivity of the entropy (see, e.g., [21, Theorem 14]) $S(\Gamma) \leq S(\Gamma_{f_{M_0}}) + S(\Gamma_{g_{M_0}})$ and (6.8.7) we have

$$\begin{aligned} F_\ell(n) &= \ell^{-2}\mathrm{Tr}\,(\mathbb{H}_{n,\ell}\Gamma) - TS(\Gamma) \\ &\geq \ell^{-2}\mathrm{Tr}\,(\mathbb{H}_{n,\ell}\Gamma_{f_{M_0}}) - TS(\Gamma_{f_{M_0}}) + \ell^{-2}\mathrm{Tr}\,(\mathbb{H}_{n,\ell}\Gamma_{g_{M_0}}) - TS(\Gamma_{g_{M_0}}) - C(\rho\mathfrak{a})^{5/2}\ell^3Y^{3\kappa}. \end{aligned} \tag{6.8.8}$$

By the Gibbs variational principle we can bound

$$\begin{aligned}\ell^{-2}\mathrm{Tr}\,(\mathbb{H}_{n,\ell}\Gamma_{g_{M_0}}) - TS(\Gamma_{g_{M_0}}) &= \alpha\left(\ell^{-2}\mathrm{Tr}\,(\mathbb{H}_{n,\ell}\alpha^{-1}\Gamma_{g_{M_0}}) - T\mathcal{S}(\alpha^{-1}\Gamma_{g_{M_0}})\right) + T\alpha\log\alpha \\ &\geq \alpha F_\ell(n) + T\alpha\log\alpha. \end{aligned} \tag{6.8.9}$$

To analyze the terms involving $\Gamma_{f_{M_0}}$ on the right-hand side of (6.8.8), we use the following formulation of the Bogoliubov approximation in the sector of few excited particles, which is a consequence of the analysis in the previous sections.

Proposition 6.28. *Under the choice of parameters in* (6.8.1) *we have*

$$\mathbb{H}_{n,\ell} \geqslant (1 - CY^\kappa)\mathcal{W}\mathrm{d}\Gamma(E_{\mathrm{Bog}})\mathcal{W}^* + E_{n,\ell} + \mathcal{O}((\rho\mathfrak{a})^{5/2}\ell^5 Y^{\kappa/2})$$

on $\mathcal{F}_+^{\leqslant M_0}$, *where* $\mathcal{W}, E_{\mathrm{Bog}}$ *and* $E_{n,\ell}$ *are defined in Lemma 6.23.*

We postpone the proof of Proposition 6.28 to the end of this section. Let us introduce a normalized state on $\mathcal{F}_+$

$$\widetilde{\Gamma} = (1-\alpha)^{-1}\mathcal{W}^*\Gamma_{f_{M_0}}\mathcal{W}.$$

With Proposition 6.28 and the identity $S(\Gamma_{f_{M_0}}) = S(\mathcal{W}^*\Gamma_{f_{M_0}}\mathcal{W})$ we can bound

$$\begin{aligned}&\ell^{-2}\mathrm{Tr}\,(\mathbb{H}_{n,\ell}\Gamma_{f_{M_0}}) - TS(\Gamma_{f_{M_0}}) \geqslant -T(1-\alpha)S(\widetilde{\Gamma}) + T(1-\alpha)\log(1-\alpha) \\ &\quad + (1-\alpha)\left[\ell^{-2}(1-CY^{5\nu})\mathrm{Tr}\,(\mathrm{d}\Gamma(E_{\mathrm{Bog}})\widetilde{\Gamma}) + \ell^{-2}E_{n,\ell} + \mathcal{O}((\rho\mathfrak{a})^{5/2}\ell^3 Y^\nu)\right].\end{aligned}$$

We use the Gibbs variational principle to obtain

$$\begin{aligned}\ell^{-2}(1-CY^{5\nu})\mathrm{Tr}\,(\mathrm{d}\Gamma(E_{\mathrm{Bog}})\widetilde{\Gamma}) - TS(\widetilde{\Gamma}) &\geq \ell^{-2}(1-CY^{5\nu})\mathrm{Tr}\,(\mathrm{d}\Gamma(E_{\mathrm{Bog}})\Gamma_\nu) - TS(\Gamma_\nu) \\ &\geqslant -T\log\mathrm{Tr}\, e^{-\frac{1}{T\ell^2}\mathrm{d}\Gamma(E_{\mathrm{Bog}})} - C\ell^{-2}Y^{5\nu}\mathrm{Tr}\,(\mathrm{d}\Gamma(E_{\mathrm{Bog}})\Gamma_\nu),\end{aligned}$$

with

$$\Gamma_\nu = e^{-\frac{1-CY^{5\nu}}{T\ell^2}\mathrm{d}\Gamma(E_{\mathrm{Bog}})}/\mathrm{Tr}\, e^{-\frac{1-CY^{5\nu}}{T\ell^2}\mathrm{d}\Gamma(E_{\mathrm{Bog}})}.$$

We find that

$$\begin{aligned}&\ell^{-2}(1-CY^{5\nu})\mathrm{Tr}\,(\mathrm{d}\Gamma(E_{\mathrm{Bog}})\Gamma_\nu) \\ &= 2\ell^{-2}(1-CY^{5\nu})(\mathrm{Tr}\,(\mathrm{d}\Gamma(E_{\mathrm{Bog}})\Gamma_\nu) - 2TS(\Gamma_\nu) \\ &\quad - \left(\ell^{-2}(1-CY^{5\nu})\mathrm{Tr}\,(\mathrm{d}\Gamma(E_{\mathrm{Bog}})\Gamma_\nu) - 2TS(\Gamma_\nu)\right) \\ &\leqslant 2\inf\sigma\left(\ell^{-2}(1-CY^{5\nu})\mathrm{d}\Gamma(E_{\mathrm{Bog}})\right) + 2T\log\mathrm{Tr}\, e^{-\frac{1-CY^{5\nu}}{2T\ell^2}\mathrm{d}\Gamma(E_{\mathrm{Bog}})} \\ &\leqslant CT^{5/2}\ell^3,\end{aligned}$$

where for the last inequality we used that $\inf\sigma(\mathrm{d}\Gamma(E_{\mathrm{Bog}})) = 0$ and (6.7.12) together with $\mathrm{d}\Gamma(E_{\mathrm{Bog}}) \geqslant \mathrm{d}\Gamma(-\Delta)$. Again with a calculation as in (6.7.12) we find

$$\begin{aligned}&\ell^{-2}\mathrm{Tr}\,(\mathbb{H}_{n,\ell}\Gamma_{f_{M_0}}) - TS(\Gamma_{f_{M_0}}) \\ &\geq (1-\alpha)\left(\ell^{-2}E_{n,\ell} + T\sum_{p\in\pi\mathbb{N}_0^3\setminus\{0\}}\log\left(1 - e^{-\frac{1}{T\ell^2}\sqrt{p^4+16\pi\mathfrak{a}n\ell^{-1}p^2}}\right)\right) \\ &\quad + T(1-\alpha)\log(1-\alpha) + \mathcal{O}(\ell^3(\rho\mathfrak{a})^{5/2}Y^\nu).\end{aligned} \tag{6.8.10}$$

We claim that from (6.6.5) we have

$$\left| E_{n,\ell} - 4\pi\mathfrak{a}n^2\ell^{-1} - 4\pi\frac{128}{15\sqrt{\pi}}\left(\mathfrak{a}\frac{n}{\ell}\right)^{5/2}\right| \leqslant C\Big(\frac{n\mathfrak{a}}{\ell}\Big)^2. \tag{6.8.11}$$

Indeed, for $p \in \mathbb{R}^3$ denote $g(p) = \sqrt{p^4 + 16p^2} - 8 - p^2 + \frac{8^2}{2p^2}$ and observe that

$$\frac{1}{2}\int_{\mathbb{R}^3_{\geqslant 0}} g(z)\mathrm{d}^3 z = 4\pi\frac{128}{15}.$$

Then with $\hbar = (\pi\mathfrak{a}\frac{n}{\ell})^{-1/2}$ we have

$$2\hbar^5 \left| E_{n,\ell} - 4\pi\mathfrak{a}n^2\ell^{-1} - 4\pi\frac{128}{15\sqrt{\pi}}\left(\mathfrak{a}\frac{n}{\ell}\right)^{5/2}\right| = \left|\hbar^3 \sum_{p\in\pi\mathbb{N}_0^3\setminus\{0\}} g(p\hbar) - \pi^{-3}\int_{\mathbb{R}^3_{\geqslant 0}} g(z)\mathrm{d}^3 z\right|. \tag{6.8.12}$$

Elementary calculations show that

$$|\partial_i\partial_j g(p)| = \left|256 p_i p_j \left(\frac{-1}{p^3(16+p^2)^{3/2}} + \frac{1}{p^6}\right) + \delta_{ij}\left(\frac{2p^2+16}{\sqrt{p^4+16p^2}} - 2 - \frac{64}{p^4}\right)\right| \leqslant Cp^{-4}.$$

With this we may compare the sum and the integral in boxes of size $(\pi\hbar)^3$ as in (6.4.27) to bound the right hand side of (6.8.12) by $C\hbar$. Multiplying with $\hbar^{-5}$ yields (6.8.11).

We can now insert (6.8.9), (6.8.10) and (6.8.11) in (6.8.8) and find

$$F_\ell(n) \geq f_{\mathrm{Bog}}(n,\ell) - (1-\alpha)^{-1}\left[C\ell^3(\rho\mathfrak{a})^{5/2}Y^\nu + T\alpha|\log\alpha| + T(1-\alpha)|\log(1-\alpha)|\right], \tag{6.8.13}$$

with $f_{\mathrm{Bog}}(n,\ell)$ defined in (6.1.5). From the BEC estimate in Lemma 6.27 and the assumption $T \leqslant (\rho\mathfrak{a})Y^{-\nu}$ we obtain

$$\alpha = \mathrm{Tr}\,(g_{M_0}^2\Gamma) \leqslant CM_0^{-1}\mathrm{Tr}\,(\mathcal{N}_+\Gamma) \leqslant Cn^{80\kappa}Y^\gamma \leq CY^{4\nu}.$$

The last inequality follows from an elementary computation using that $n \leq C\rho\ell^3 = CY^{-1/2-3\kappa}$ and the definition of $\gamma = \min\{1/10 - 2\kappa - 6\nu/5, 1/17 - 2\kappa\} = 1/17 - 2\kappa$ (for our choice of parameters). In particular $(1-\alpha)^{-1} \leqslant C$. Moreover, the last error term in (6.8.13) can be bounded by

$$T\alpha|\log\alpha| + T(1-\alpha)|\log(1-\alpha)| \leq CT\alpha^{1/2} \leqslant CTY^{2\nu} \leq C(\rho\mathfrak{a})^{5/2}\ell^3 Y^\nu, \tag{6.8.14}$$

concluding the proof of Theorem 6.1 in the case $(\rho\mathfrak{a}^3)^{1/4+\nu/2}(\rho\ell^3) \leqslant n \leqslant C(\rho\ell^3)$.

Case $n \leqslant (\rho\mathfrak{a}^3)^{1/4+\nu/2}(\rho\ell^3)$: For $n = 0$ the statement is trivial as the thermal contribution is negative. For $1 \leqslant n < (\rho\mathfrak{a}^3)^{1/4+\nu/2}(\rho\ell^3)$ we shall show that the thermal contribution dominates. One easily checks that

$$f_{\mathrm{Bog}}(n,\ell) = T\sum_{p\neq 0}\log\left(1 - e^{\frac{-1}{T\ell^2}\sqrt{p^4+16\pi\mathfrak{a}n\ell^{-1}p^2}}\right) + \mathcal{O}(\ell^3(\rho\mathfrak{a})^{5/2}Y^\nu).$$

in this case. Therefore, we ignore the interaction in the computation of the free energy for a lower bound, which we are allowed to do since $V \geqslant 0$. The Gibbs variational principle and the calculation in (6.7.12) yield

$$F_\ell(n) \geqslant T\sum_{p\neq 0}\log\left(1 - e^{-\frac{p^2}{T\ell^2}}\right).$$

It remains to compare this quantity with the thermal contribution that appears in f_{Bog}. For $p \in \mathbb{R}^3, q \in \mathbb{R}_{\geqslant 0}$ we define the function

$$g(p,q) = \log\left(1 - e^{-\sqrt{p^4+qp^2}}\right). \tag{6.8.15}$$

Then

$$|\partial_q g(p,q)| = \left|\frac{1}{e^{\sqrt{p^4+qp^2}}-1}\frac{p^2}{2\sqrt{p^4+qp^2}}\right| \leqslant \frac{1}{2}\frac{1}{e^{p^2}-1}. \tag{6.8.16}$$

Note that the upper bound is independent of q so that by a first order Taylor expansion

$$\begin{aligned}
0 &\leqslant T\sum_{p\neq 0}\log\left(1 - e^{\frac{-1}{T\ell^2}\sqrt{p^4+16\pi\mathfrak{a}n\ell^{-1}p^2}}\right) - T\sum_{p\neq 0}\log\left(1-e^{-\frac{p^2}{T\ell^2}}\right)\\
&= T\sum_{p\neq 0} g\left(\frac{p}{T^{1/2}\ell}, \frac{16\pi\mathfrak{a}n\ell^{-1}}{T\ell^2}\right) - g\left(\frac{p}{T^{1/2}\ell}, 0\right)\\
&\leqslant \frac{8\pi\mathfrak{a}n\ell^{-1}}{T\ell^2}T\sum_{p\neq 0}\frac{1}{e^{\frac{p^2}{T\ell^2}}-1} \leqslant C\frac{\mathfrak{a}n}{T\ell^3}T^{5/2}\ell^3 = \mathcal{O}((\rho\mathfrak{a})^{5/2}\ell^3 Y^{1/4-\nu}).
\end{aligned}$$

This proves the desired bound. □

We conclude this section by giving the proof of Proposition 6.28.

Proof of Proposition 6.28. From Lemma 6.15 and Lemma 6.23 we have

$$\mathcal{H} = E_{n,\ell} + \mathcal{W}\mathrm{d}\Gamma(E_{\mathrm{Bog}})\mathcal{W}^* + e^{\mathcal{B}_1}e^{\mathcal{B}_c}(Q_4 + \mathcal{E}_c + \mathcal{E}_2)e^{-\mathcal{B}_c}e^{-\mathcal{B}_1} \tag{6.8.17}$$

on $\mathcal{F}_+$, where

$$\begin{aligned}
Q_4 + \mathcal{E}_c + \mathcal{E}_2 \geq{}& \left(\frac{1}{2} - C(\sigma+\delta)\right)Q_4 - C\sigma\mathrm{d}\Gamma(-\Delta)\\
&- C\left[(\sigma+\delta)\frac{n}{\ell} + \lambda\Big(\left(\frac{n}{\ell}\right)^{1/2}+1\Big) + \lambda^{\frac{1}{2}}\Big(\left(\frac{n}{\ell}\right)^2 + \frac{n}{\ell}\Big) + \lambda^{-1}\frac{n^{3/2}}{\ell^2}\right](\mathcal{N}+1)\\
&- C\delta^{-1}\left[\frac{n}{\ell}\frac{\mathcal{N}+1}{M} + \frac{(\mathcal{N}+1)}{\ell} + \frac{(\mathcal{N}+1)^2}{n\ell} + \lambda\left(\frac{n}{\ell}\right)^3\right](\mathcal{N}+1)\\
&- C\frac{n}{\ell}\frac{(\mathcal{N}+1)^{1/2}}{n^{1/2}}(\mathcal{N}+1) - C\left(\left(\frac{n}{\ell}\right)^2\log\ell + \frac{n}{\ell} + \lambda^2\left(\frac{n}{\ell}\right)^{5/2}\right)
\end{aligned} \tag{6.8.18}$$

on $\mathcal{F}_+$. The condition $n \leq C\rho\ell^3$ and the choice $\ell = \mathfrak{a}Y^{-1/2-\kappa}$ in (6.1.1) imply that $n\mathfrak{a}\ell^{-1} \leq C\rho\mathfrak{a}\ell^2 = CY^{-2\kappa}$. Moreover, with the choice of the parameters in (6.8.1), we have

$$\frac{M}{\ell} \leqslant CY^{32\kappa}, \quad \frac{M_0}{\ell} \leqslant CY^{38\kappa}, \quad \frac{n}{\ell}\frac{M_0}{M} \leqslant CY^{4\kappa},$$

from which one easily checks that

$$\begin{aligned}
&\sigma = \max\{n^{1/2}\ell^{-5/6}, n^{1/2}M\ell^{-3/2}, \lambda^{-1/2}n^{1/2}M^{1/2}\ell^{-1}\} \leqslant CY^{10\kappa},\\
&(\sigma+\delta)\frac{n}{\ell} + \lambda\Big(\left(\frac{n}{\ell}\right)^{1/2}+1\Big) + \lambda^{\frac{1}{2}}\Big(\left(\frac{n}{\ell}\right)^2 + \frac{n}{\ell}\Big) + \lambda^{-1}\frac{n^{3/2}}{\ell^2} \leq CY^{\kappa},\\
&\delta^{-1}\left[\frac{n}{\ell}\frac{M_0}{M} + \frac{M_0}{\ell} + \frac{M_0^2}{n\ell} + \lambda\left(\frac{n}{\ell}\right)^3\right] + \frac{n}{\ell}\frac{M_0^{1/2}}{n^{1/2}} \leq CY^{\kappa}.
\end{aligned}$$

Hence, (6.8.18) reduces to

$$Q_4+\mathcal{E}_c+\mathcal{E}_2 \geq \left(\frac{1}{2}-CY^{3\kappa}\right) Q_4 - CY^{10\kappa}\mathrm{d}\Gamma(-\Delta) - CY^{\kappa}\left(1+\frac{(\mathcal{N}+1)^2}{M_0^2}\right)(\mathcal{N}+1) - CY^{-4\kappa}|\log Y|. \tag{6.8.19}$$

On the right-hand side of (6.8.19), the term involving Q_4 is positive and can be dropped for a lower bound. Now let us apply the transformation $e^{\mathcal{B}_1}e^{\mathcal{B}_c}(\cdots)e^{-\mathcal{B}_c}e^{-\mathcal{B}_1}$ and additionally restrict to $\mathcal{F}_+^{\leq M_0}$. We have

$$\begin{aligned}
&\mathbb{1}^{\{\mathcal{N}_+\leqslant M_0\}}e^{\mathcal{B}_1}e^{\mathcal{B}_c}\left(1+\frac{(\mathcal{N}+1)^2}{M_0^2}\right)(\mathcal{N}+1)e^{-\mathcal{B}_c}e^{-\mathcal{B}_1}\mathbb{1}^{\{\mathcal{N}_+\leqslant M_0\}}\\
&\leq C\mathbb{1}^{\{\mathcal{N}_+\leqslant M_0\}}\left(1+\frac{(\mathcal{N}+1)^2}{M_0^2}\right)(\mathcal{N}+1)\mathbb{1}^{\{\mathcal{N}_+\leqslant M_0\}} \leq C\mathbb{1}^{\{\mathcal{N}_+\leqslant M_0\}}(\mathcal{N}+1)\mathbb{1}^{\{\mathcal{N}_+\leqslant M_0\}}\\
&\leqslant C\left(\left(\frac{n}{\ell}\right)^{1/2}+1\right)\mathbb{1}^{\{\mathcal{N}_+\leqslant M_0\}}\mathcal{W}(\mathcal{N}+1)\mathcal{W}^*\mathbb{1}^{\{\mathcal{N}_+\leqslant M_0\}} + C\left(\frac{n}{\ell}\right)^{3/2}\\
&\leq C\mathbb{1}^{\{\mathcal{N}_+\leqslant M_0\}}\left(\mathcal{W}\mathrm{d}\Gamma(E_{\mathrm{Bog}})\mathcal{W}^*+Y^{-3\kappa}\right)\mathbb{1}^{\{\mathcal{N}_+\leqslant M_0\}}
\end{aligned}$$

by Lemma 6.8, Lemma 6.16, the first bound in Lemma 6.24 and the fact that $\left(\left(\frac{n}{\ell}\right)^{1/2}+1\right)\mathcal{N}$ is bounded by $\mathrm{d}\Gamma(E_{\mathrm{Bog}})$. Moreover, we find

$$\begin{aligned}
Y^{10\kappa}e^{\mathcal{B}_1}e^{\mathcal{B}_c}\mathrm{d}\Gamma(-\Delta)e^{-\mathcal{B}_c}e^{-\mathcal{B}_1} &\leqslant CY^{10\kappa}\left(\left(\frac{n}{\ell}\right)^{1/2}+1\right)\mathcal{W}\mathrm{d}\Gamma(-\Delta)\mathcal{W}^* + CY^{10\kappa}\lambda^{-1}\left(\frac{n}{\ell}\right)^2\\
&\leq CY^{9\kappa}\mathcal{W}\mathrm{d}\Gamma(E_{\mathrm{Bog}})\mathcal{W}^* + CY^{-4\kappa}
\end{aligned}$$

by the second bound in Lemma 6.24 and $\mathrm{d}\Gamma(-\Delta)\leqslant \mathrm{d}\Gamma(E_{\mathrm{Bog}})$.

In combination with (6.8.19) it follows that

$$e^{\mathcal{B}_1}e^{\mathcal{B}_c}(Q_4+\mathcal{E}_c+\mathcal{E}_2)e^{-\mathcal{B}_c}e^{-\mathcal{B}_1} \geq -CY^{\kappa}\mathcal{W}\mathrm{d}\Gamma(E_{\mathrm{Bog}})\mathcal{W}^* - CY^{-4\kappa}|\log Y| \tag{6.8.20}$$

on $\mathcal{F}^{\{\mathcal{N}_+\leqslant M_0\}}$. Inserting (6.8.20) in (6.8.17) and using $\mathbb{H}_{n,\ell}=\mathbb{1}_+^{\leq n}\mathcal{H}\mathbb{1}_+^{\leq n}$ we obtain

$$\mathbb{H}_{n,\ell} \geqslant E_{n,\ell} + (1-CY^{\kappa})\,\mathcal{W}^*\mathrm{d}\Gamma(E_{\mathrm{Bog}})\mathcal{W} - CY^{-4\kappa}|\log Y|$$

on $\mathcal{F}^{\{\mathcal{N}_+\leqslant M_0\}}$. The claim then follows from

$$Y^{-4\kappa}|\log Y| = \ell^5(\rho\mathfrak{a})^{5/2}Y^{\kappa}|\log Y| \leqslant C\ell^5(\rho\mathfrak{a})^{5/2}Y^{\kappa/2}.$$

□

6.9 Proof of Theorem 3.2

Let $\kappa=5\nu=1/1000$ as in the assumptions of Theorem 6.1 and let $Y=\rho\mathfrak{a}^3$ so that $\ell=\mathfrak{a}Y^{-1/2-\kappa}$ as in (6.1.1). Since the limit $F_L(N)/L^3$ does not depend on the sequence of $N\to\infty$ with $N/L^3\to\rho$, we may assume without loss of generality that L/ℓ is an integer and take $N=\lfloor\rho L^3\rfloor+1$. This is helpful since we shall divide the big box Λ_L into M_B smaller boxes Λ_ℓ, where now $M_B=(L/\ell)^3$ is an integer.

We claim that

$$\frac{F_L(N)}{L^3} \geqslant \frac{1}{\ell^3}f_{\mathrm{Bog}}(\rho\ell^3,\ell) - C(\rho\mathfrak{a})^{5/2}Y^{\nu}, \tag{6.9.1}$$

where we recall that $f_{\rm Bog}$ is defined in (6.1.5). Assuming (6.9.1), Theorem 3.2 follows readily from approximating the sum in the definition of $f_{\rm Bog}$ in (6.1.5) by an integral. This is done in (6.9.3) in the following lemma. Furthermore, Lemma 6.29 contains a second estimate (6.9.4), which measures the error made in replacing n by $\rho\ell^3$ in the thermal contribution of the free energy $f_{\rm Bog}$. It will be used in the proof of (6.9.1) below.

Lemma 6.29. *Under the assumptions of Theorem 6.1 consider*

$$f^{\rm th}_{\rm Bog}(n,\ell) = T \sum_{p\in\pi\mathbb{N}_0^3\setminus\{0\}} \log\left(1 - e^{\frac{-1}{T\ell^2}\sqrt{p^4+16\pi\frac{\mathfrak{a}n}{\ell}p^2}}\right). \tag{6.9.2}$$

Then we have

$$\left|\frac{f^{\rm th}_{\rm Bog}(\rho\ell^3,\ell)}{\ell^3} - \frac{T^{5/2}}{(2\pi)^3}\int_{\mathbb{R}^3}\log\left(1-e^{-\sqrt{p^4+16\pi\frac{\rho\mathfrak{a}}{T}p^2}}\right)\mathrm{d}p\right| \leqslant C(\rho\mathfrak{a})^{5/2}Y^{3\nu} \tag{6.9.3}$$

and, for all $0\leqslant n\leqslant C\rho\ell^3$,

$$\left|f^{\rm th}_{\rm Bog}(n,\ell) - f^{\rm th}_{\rm Bog}(\rho\ell^3,\ell)\right| \leqslant C\frac{\mathfrak{a}}{\ell^3}(n-\rho\ell^3)^2Y^{1/4} + C\ell^3(\rho\mathfrak{a})^{5/2}Y^{1/4-3\nu}. \tag{6.9.4}$$

We postpone the proof of Lemma 6.29 to the end of this section.

Proof of (6.9.1). Let Γ be the Gibbs state of H_N, satisfying

$$F_L(N) = \operatorname{Tr} H_N\Gamma - TS(\Gamma),$$

where we recall that $S(\Gamma) = -\operatorname{Tr}\Gamma\log\Gamma$ is the entropy of the state Γ. We want to localize Γ in smaller boxes. For this purpose we introduce a collection of disjoint cubes $(B_i)_{1\leqslant j\leqslant M_B}$ of side length ℓ forming a partition of Λ, that is $\Lambda = \bigcup_{j=1}^{M_B} B_j$. Using that $V\geqslant 0$ and the bosonic symmetry of Γ we have

$$\begin{aligned}
&\operatorname{Tr} H_N\Gamma \\
&\geqslant \sum_{j=1}^{M_B}\left[N\operatorname{Tr}_{L^2_s(\Lambda_L^N)}(i\nabla)_{x_1}\mathbb{1}_{B_j}(x_1)(i\nabla)_{x_1}\Gamma + \frac{N(N-1)}{2}\operatorname{Tr}_{L^2_s(\Lambda_L^N)}V(x_1-x_2)\mathbb{1}_{B_j}(x_1)\mathbb{1}_{B_j}(x_2)\Gamma\right] \\
&= \sum_{j=1}^{M_B}\sum_{n=0}^{N}\left[n\operatorname{Tr}_{L^2_s(\Lambda_L)}(-\Delta)\Gamma^{(1)}_{j,n} + \frac{n(n-1)}{2}\operatorname{Tr}_{L^2_s(\Lambda_L^2)}V(x-y)\Gamma^{(2)}_{j,n}\right] \\
&= \sum_{j=1}^{M_B}\sum_{n=0}^{N}\operatorname{Tr}_{L^2_s(\Lambda_L^n)}H_n\Gamma_{j,n},
\end{aligned}$$

where we have denoted, for $0\leqslant n\leqslant N$,

$$\Gamma_{j,n} = \binom{N}{n}\operatorname{Tr}_{n+1\to N}\left(\mathbb{1}_{B_j}^{\otimes n}\mathbb{1}_{B_j^c}^{\otimes N-n}\Gamma\mathbb{1}_{B_j}^{\otimes n}\mathbb{1}_{B_j^c}^{\otimes N-n}\right), \tag{6.9.5}$$

with the notation $B_j^c = \Lambda\setminus B_j$, and where $\Gamma^{(k)}_{j,n} = \operatorname{Tr}_{k+1\to n}\Gamma_{j,n}$. It is understood that $H_0 = 0$ and $H_1 = -\Delta$. Here $\operatorname{Tr} H_n\Gamma_{j,n}$ has to be interpreted in terms of quadratic forms. Indeed, the range of $\Gamma_{j,n}$ does not belong to the domain of the Neumann Laplacian, but it does belong to $H^1((B_j)^n)$, the domain of the associated quadratic form $Q(\Psi) = \sum_{k=0}^n\int_{(B_j)^n}|\nabla_{x_k}\Psi|^2$.

We will now use the subadditivity of the entropy [57]. Following the notation of [53, Proposition 7], the state $\Gamma_j = \bigoplus_{n=0}^{N} \Gamma_{j,n}$ is the $\mathbb{1}_{B_j}$-localization of Γ. Since $\sum_{j=1}^{M_B} \mathbb{1}_{B_j} = \mathbb{1}_{\Lambda_L}$, we obtain that

$$S(\Gamma) \leqslant \sum_{j=1}^{M_B} S(\Gamma_j) = \sum_{j=1}^{M_B} \sum_{n=0}^{N} S(\Gamma_{j,n})$$

(see e.g. [87, Lemma 4] and [41, Remark 25]).

Let us denote

$$\alpha_{j,n} = \operatorname{Tr} \Gamma_{j,n}, \quad \widetilde{\Gamma}_{j,n} = \alpha_{j,n}^{-1} \Gamma_{j,n} ,$$

which satisfy

$$\operatorname{Tr} \widetilde{\Gamma}_{j,n} = 1, \quad \sum_{n=0}^{N} \alpha_{j,n} = 1, \quad \sum_{j=1}^{M_B} \sum_{n=0}^{N} \alpha_{j,n} = M_B, \quad \sum_{j=1}^{M_B} \sum_{n=0}^{N} n\alpha_{j,n} = N.$$

From this we obtain that for all $\mu \geqslant 0$

$$\begin{aligned} F_L(N) &\geqslant \sum_{j=1}^{M_B} \sum_{n=0}^{N} \left[\alpha_{j,n} \left(\operatorname{Tr} (H_n - \mu n) \widetilde{\Gamma}_{j,n} - TS(\widetilde{\Gamma}_{j,n}) \right) + T\alpha_{j,n} \log \alpha_{j,n} \right] + \mu N \\ &\geqslant \sum_{j=1}^{M_B} \sum_{n=0}^{N} \left[\alpha_{j,n} (F_\ell(n) - \mu n) + T\alpha_{j,n} \log \alpha_{j,n} \right] + \mu\rho L^3 \\ &\geqslant -TM_B \log \sum_{n=0}^{N} e^{-\frac{1}{T}(F_\ell(n) - \mu n)} + \mu\rho L^3, \end{aligned} \tag{6.9.6}$$

where the last inequality follows from the Gibbs variational principle.

Let us take $\mu = 8\pi\mathfrak{a}\rho$ and denote $n_0 := \lfloor 20\rho\ell^3 \rfloor$. For $n \leqslant n_0$, we use Theorem 6.1 to estimate $F_\ell(n)$. We obtain

$$\begin{aligned} F_\ell(n) - 8\pi\mathfrak{a}\rho n &\geqslant f_{\mathrm{Bog}}(n,\ell) - 8\pi\mathfrak{a}\rho n - C\ell^3(\rho\mathfrak{a})^{5/2} Y^\nu \\ &= f_{\mathrm{Bog}}(\rho\ell^3,\ell) - 8\pi\mathfrak{a}\rho^2\ell^3 + 4\pi\frac{\mathfrak{a}}{\ell^3}\left((n-\rho\ell^3)^2 + \frac{128}{15\sqrt{\pi}} \frac{\mathfrak{a}^{3/2}}{\ell^{3/2}} \left(n^{5/2} - (\rho\ell^3)^{5/2} \right) \right) \\ &\quad + \left(f_{\mathrm{Bog}}^{\mathrm{th}}(n,\ell) - f_{\mathrm{Bog}}^{\mathrm{th}}(\rho\ell^3,\ell) \right) - C\ell^3(\rho\mathfrak{a})^{5/2} Y^\nu \qquad (6.9.7) \\ &\geqslant f_{\mathrm{Bog}}(\rho\ell^3,\ell) - 8\pi\mathfrak{a}\rho^2\ell^3 + 2\pi\frac{\mathfrak{a}}{\ell^3}(n-\rho\ell^3)^2 - C\ell^3(\rho\mathfrak{a})^{5/2} Y^\nu. \qquad (6.9.8) \end{aligned}$$

To obtain (6.9.7), we inserted the definitions of f_{Bog} and $f_{\mathrm{Bog}}^{\mathrm{th}}$ in (6.1.5) and (6.9.2), respectively, and completed the square in the leading order of the free energy. The inequality (6.9.8) is obtained, for Y small enough, by using (6.9.4) to estimate $f_{\mathrm{Bog}}^{\mathrm{th}}(n,\ell) - f_{\mathrm{Bog}}^{\mathrm{th}}(\rho\ell^3,\ell)$ and by bounding

$$\begin{aligned} &\left| 4\pi \frac{128}{15\sqrt{\pi}} \frac{\mathfrak{a}^{5/2}}{\ell^{9/2}} \left(n^{5/2} - (\rho\ell^3)^{5/2} \right) \right| \leqslant C\frac{\mathfrak{a}^{5/2}}{\ell^{9/2}} |n-\rho\ell^3| (\rho\ell^3)^{3/2} \\ &\leqslant \pi\frac{\mathfrak{a}}{\ell^3}(n-\rho\ell^3)^2 + C\frac{\mathfrak{a}^4}{\ell^6}(\rho\ell^3)^3 \leqslant \pi\frac{\mathfrak{a}}{\ell^3}(n-\rho\ell^3)^2 + CY^\nu\ell^3(\rho\mathfrak{a})^{5/2}, \end{aligned}$$

where we used the choice of ℓ and that $\nu < 1/2$.

To deal with contributions from $n > n_0$, we use the superadditivity of the free energy $F_\ell(n)$,

$$F_\ell(n) \geqslant \left\lfloor \frac{n}{n_0} \right\rfloor F_\ell(n_0) + F_\ell(r)\,, \tag{6.9.9}$$

which follows from grouping the n particles into $\lfloor n/n_0 \rfloor$ subgroups of n_0 particles and one group of $0 \leqslant r := n - n_0\lfloor n/n_0 \rfloor < n_0$ particles, and dropping the interactions as well as the symmetry constraint between particles in different groups. More precisely, since $V \geqslant 0$ we have for all states Γ in $L^2_s(\Lambda^n)$,

$$\mathrm{Tr}\, H_{n,\ell}\Gamma \geqslant \lfloor n/n_0 \rfloor \mathrm{Tr}\,(H_{n_0,\ell}\Gamma^{(n_0)}) + \mathrm{Tr}\,(H_{r,\ell}\Gamma^{(r)}), \tag{6.9.10}$$

where we have denoted $\Gamma^{(k)} = \mathrm{Tr}_{\,k+1\to n}\Gamma$ for $0 \leqslant k \leqslant n$. On the other hand, denoting $\Gamma' = (\Gamma^{(n_0)})^{\otimes \lfloor n/n_0 \rfloor} \otimes \Gamma^{(r)}$ and using the non-negativity of the relative entropy we have

$$S(\Gamma) = -\mathrm{Tr}\,\Gamma \log \Gamma \leqslant -\mathrm{Tr}\,\Gamma \log \Gamma' = \lfloor n/n_0 \rfloor S(\Gamma^{(n_0)}) + S(\Gamma^{(r)}), \tag{6.9.11}$$

where we used that $\mathrm{Tr}_{\,x_{i_1},\dots,x_{i_k}}\Gamma = \mathrm{Tr}_{\,1\to k}\Gamma$ for any $1 \leqslant i_1 < \cdots < i_k \leqslant n$ because of the bosonic symmetry of Γ. Combining (6.9.10) and (6.9.11), (6.9.9) follows from the Gibbs variational principle. Therefore, for $n > n_0$

$$\begin{aligned} F_\ell(n) - 8\pi\mathfrak{a}\rho n \geqslant{}& \left\lfloor \frac{n}{n_0} \right\rfloor (F_\ell(n_0) - 8\pi\mathfrak{a}\rho n_0) + F_\ell(r) - 8\pi\mathfrak{a}\rho r \\ \geqslant{}& \left\lfloor \frac{n}{n_0} \right\rfloor \Big(f_{\mathrm{Bog}}(\rho\ell^3, \ell) - 8\pi\mathfrak{a}\rho^2\ell^3 + \pi\frac{\mathfrak{a}}{\ell^3}(n_0 - \rho\ell^3)^2 - C\ell^3(\rho\mathfrak{a})^{5/2}Y^\nu \Big) \\ &+ \left\lfloor \frac{n}{n_0} \right\rfloor \pi\frac{\mathfrak{a}}{\ell^3}(n_0 - \rho\ell^3)^2 - 8\pi\mathfrak{a}\rho r - C\ell^3(\rho\mathfrak{a})^{5/2}, \end{aligned}$$

where we used the lower bound for $n \leqslant n_0$ in (6.9.8) and that by Theorem 6.1

$$F_\ell(r) \geqslant f^{\mathrm{th}}_{\mathrm{Bog}}(0, \ell) - C\ell^3(\rho\mathfrak{a})^{5/2}Y^\nu \geqslant -C\ell^3(\rho\mathfrak{a})^{5/2}$$

with $f^{\mathrm{th}}_{\mathrm{Bog}}$ defined in (6.9.2) and bounded as in (6.7.12). Now using that $19\rho\ell^3 \leqslant n_0 \leqslant 20\rho\ell^3$, so that in particular

$$\left\lfloor \frac{n}{n_0} \right\rfloor \geqslant \frac{n}{2n_0} \geqslant \frac{n}{40\rho\ell^3},$$

we obtain

$$\begin{aligned} F_\ell(n) - 8\pi\mathfrak{a}\rho n \geqslant{}& \left\lfloor \frac{n}{n_0} \right\rfloor \Big(f_{\mathrm{Bog}}(\rho\ell^3, \ell) - 8\pi\mathfrak{a}\rho^2\ell^3 + 18^2\pi\mathfrak{a}\rho^2\ell^3 - C\ell^3(\rho\mathfrak{a})^{5/2}Y^\nu \Big) \\ &+ \pi\frac{n}{40\rho\ell^3}\frac{\mathfrak{a}}{\ell^3}18^2(\rho\ell^3)^2 - 8\pi\mathfrak{a}\rho n - C\ell^3(\rho\mathfrak{a})^{5/2}. \end{aligned}$$

Since the term in parentheses in the first line is non-negative, we may replace the prefactor $\lfloor \frac{n}{n_0} \rfloor$ by 1 to obtain a lower bound. The result is then

$$\begin{aligned} F_\ell(n) - 8\pi\mathfrak{a}\rho n \geqslant{}& f_{\mathrm{Bog}}(\rho\ell^3, \ell) - 8\pi\mathfrak{a}\rho^2\ell^3 + \frac{\pi}{10}\rho\mathfrak{a}n - C\ell^3(\rho\mathfrak{a})^{5/2} \\ \geqslant{}& f_{\mathrm{Bog}}(\rho\ell^3, \ell) - 8\pi\mathfrak{a}\rho^2\ell^3 + \frac{\pi}{20}\rho\mathfrak{a}n - C\ell^3(\rho\mathfrak{a})^{5/2}Y^\nu, \end{aligned} \tag{6.9.12}$$

where we first used that $18^2/40 - 8 = 1/10$ and then that $\rho\mathfrak{a}n - C\ell^3(\rho\mathfrak{a})^{5/2} \geqslant -C\ell^3(\rho\mathfrak{a})^{5/2}Y^\nu$ for $n > \rho\ell^3$.

Let us combine the cases $n \leqslant n_0$ and $n > n_0$ by inserting (6.9.8) and (6.9.12) into (6.9.6). Using that $L^3 = \ell^3 M_B$, we obtain

$$\begin{aligned}\frac{1}{L^3} F_L(N) \geqslant& \frac{1}{\ell^3} f_{\mathrm{Bog}}(\rho\ell^3, \ell) - C(\rho\mathfrak{a})^{5/2}(\rho\mathfrak{a}^3)^\nu \\ &- \frac{T}{\ell^3}\log\bigg(\sum_{n\leqslant n_0} e^{-2\pi\frac{\mathfrak{a}}{T\ell^3}(n-\rho\ell^3)^2} + \sum_{n>n_0} e^{-\frac{\pi}{20}\frac{\rho\mathfrak{a}}{T}n}\bigg).\end{aligned}$$

It remains to estimate the last term above. We have

$$\begin{aligned}&\frac{T}{\ell^3}\log\bigg(\sum_{n\leqslant n_0} e^{-2\pi\frac{\mathfrak{a}}{T\ell^3}(n-\rho\ell^3)^2} + \sum_{n>n_0} e^{-\frac{\pi}{20}\frac{\rho\mathfrak{a}}{T}n}\bigg) \leqslant C\frac{T}{\ell^3}\log\Big(n_0 + C(\rho\mathfrak{a}/T)^{-1}e^{-C\frac{\rho\mathfrak{a}}{T}n_0}\Big) \\ &\leqslant C\frac{T}{\ell^3}\log\Big(CY^{-1/2-3\kappa} + CY^{-\nu}e^{-CY^{-1/2-3\kappa+\nu}}\Big) \leqslant C(\rho\mathfrak{a})^{5/2}Y^{3\kappa-\nu}|\log Y|.\end{aligned}$$

For the first inequality, we used that $e^{-\theta} \leqslant 1$ for $\theta \geqslant 0$ and that

$$\sum_{n>n_0} e^{-\theta n} = \frac{e^{-\theta(n_0+1)}}{1-e^{-\theta}} \leqslant \theta^{-1}e^{-\theta n_0}$$

for $\theta > 0$. The second inequality follows from $\rho\ell^3 \lesssim n_0 \lesssim \rho\ell^3 = Y^{-1/2-3\kappa}$ and $T \leq (\rho\mathfrak{a})Y^{-\nu}$. To obtain the last inequality, it was used that $-1/2 - 3\kappa + \nu < 0$ and that $T\ell^{-3} \leqslant (\rho\mathfrak{a})^{5/2}Y^{3\kappa-\nu}$. The choice of ν concludes the proof of Theorem 3.2. □

Finally, let us provide the proof of Lemma 6.29.

Proof of Lemma 6.29. Recall the definition of g in (6.8.15). Let us start by proving (6.9.3). With the notation $\hbar = (T\ell^2)^{-1/2}$ we have

$$\begin{aligned}&\bigg|\frac{1}{(T\ell^2)^{3/2}}\sum_{p\in\pi\mathbb{N}_0^3\setminus\{0\}}\log(1-e^{\frac{-1}{T\ell^2}\sqrt{p^4+16\pi\rho\mathfrak{a}\ell^2p^2}}) - \frac{1}{(2\pi)^3}\int_{\mathbb{R}^3}\log\Big(1-e^{-\sqrt{p^4+16\pi\frac{\rho\mathfrak{a}}{T}p^2}}\Big)\,\mathrm{d}p\bigg| \\ &\leqslant C\hbar^4\sum_{p\in\pi\mathbb{N}_0^3\setminus\{0\}}|\hbar p|^{-1}e^{-\frac{(\hbar p)^2}{2}} \leqslant C\hbar. \qquad (6.9.13)\end{aligned}$$

Here we used that $\nabla_1 g$ satisfies the bound

$$|\nabla_1 g(p,q)| = \left|\frac{2p^2p+qp}{\sqrt{p^4+qp^2}}\frac{1}{e^{\sqrt{p^4+qp^2}}-1}\right| \leqslant \frac{2\sqrt{p^4+qp^2}}{|p|\Big(e^{\sqrt{p^4+qp^2}}-1\Big)} \leqslant 2|p|^{-1}e^{-\frac{p^2}{2}},$$

since $z(e^z-1)^{-1} \leqslant e^{-z/2}$ for $z > 0$. Note that the estimate (6.9.13) is uniform in $\hbar > 0$ and in particular does not require $\hbar$ to be small. The desired estimate (6.9.3) is obtained by multiplying (6.9.13) with $T^{5/2}$.

Let us now turn to (6.9.4) and recall the bound (6.8.16) on $\partial_q g(p,q)$. Again with $\hbar =$

$(T\ell^2)^{-1/2}$ we have

$$\begin{aligned}
&\Big| T \sum_{p\in\pi\mathbb{N}_0^3\setminus\{0\}} \log(1-e^{\frac{-1}{T\ell^2}\sqrt{p^4+n\mathfrak{a}\ell^{-1}p^2}}) - T \sum_{p\in\pi\mathbb{N}_0^3\setminus\{0\}} \log(1-e^{\frac{-1}{T\ell^2}\sqrt{p^4+\rho\mathfrak{a}\ell^2p^2}}) \Big| \\
&\leqslant T \sum_{p\in\pi\mathbb{N}_0^3\setminus\{0\}} \Big| g\Big(\hbar p, \frac{n\mathfrak{a}}{T\ell^3}\Big) - g\Big(\hbar p, \frac{\rho\mathfrak{a}}{T}\Big)\Big| \\
&\leqslant \frac{\mathfrak{a}}{\ell^3}\big|n-\rho\ell^3\big| \sum_{p\in\pi\mathbb{N}_0^3\setminus\{0\}} \sup_{q>0} \big|\partial_q g(\hbar p, q)\big| \\
&\leqslant CT^{3/2}\mathfrak{a}\big|n-\rho\ell^3\big| \\
&\leqslant C\frac{\mathfrak{a}}{\ell^3}(n-\rho\ell^3)^2 Y^{1/4} + C\ell^3T^3\mathfrak{a}Y^{-1/4} \leqslant C\frac{\mathfrak{a}}{\ell^3}(n-\rho\ell^3)^2Y^{1/4} + C\ell^3(\rho\mathfrak{a})^{5/2}Y^{1/4-3\nu}.
\end{aligned}$$

In the second to last inequality, we used the Cauchy–Schwarz inequality and in the last one we used that $T \leqslant (\rho\mathfrak{a})Y^{-\nu}$. This concludes the proof of (6.9.4). □

7 Proof of the Upper Bound

7.1 Introduction

Recall the main result Theorem 3.3

Theorem. *Let $V \in L^2(\mathbb{R}^3)$ be non-negative, spherically symmetric and compactly supported. Let $0 \leqslant T \leqslant C\rho\mathfrak{a}$ for some $C > 0$. Then, in the dilute limit $\rho\mathfrak{a}^3 \to 0$, there exist $c, \epsilon > 0$ such that*

$$\begin{aligned}
f(\rho, T) \leqslant\ & 4\pi\mathfrak{a}\rho^2\left(1 + \frac{128}{15\sqrt{\pi}}\sqrt{\rho\mathfrak{a}^3}\right) + \frac{T^{5/2}}{(2\pi)^3}\int_{\mathbb{R}^3} \log\left(1 - e^{-\sqrt{p^4+\frac{16\pi\rho\mathfrak{a}}{T}p^2}}\right)\mathrm{d}p. \\
&+ c(\rho\mathfrak{a})^{5/2}(\rho\mathfrak{a}^3)^{\varepsilon}.
\end{aligned}$$

We remark that the the proof of the main result Theorem 3.3, similarly as for the result on the lower bound [39], also allows to take slightly larger temperatures, that is $T \leqslant C\rho\mathfrak{a}(\rho\mathfrak{a}^3)^{-\nu}$ for some $\nu > 0$ small enough. For the sake of simplicity we restrict our attention to $T \leqslant C\rho\mathfrak{a}$.

We have slightly relaxed the integrability condition on the interaction potential of [6] which assumes $V \in L^3(\mathbb{R}^3)$. This improvement comes from a different treatment of the scattering problem: we solve the equation on the torus and our analysis only requires $V \in L^2(\mathbb{R}^3)$ (see Lemma 7.3). The restriction $V \in L^2(\mathbb{R}^3)$ is also needed in the many-body analysis to prove that several error terms are negligible.

7.1.1 Localization into small boxes and grand canonical ensemble

To show Theorem 3.3, it is convenient to consider a system confined in a smaller box $\Lambda_L = [-L/2; L/2]^3$, with $L = \rho^{-\gamma}$ and with periodic boundary conditions, in the grand canonical setting, where the number of particles is allowed to fluctuate. If $\gamma > 1$, we will show that an upper bound on the small periodic box Λ_L implies an upper bound in the thermodynamic limit by patching small boxes together, see Fig. 6. To work in the grand canonical ensemble, we recall from Section 2.1 the bosonic Fock space

$$\mathcal{F}(\Lambda_L) = \bigoplus_{k\geqslant 0} L^2(\Lambda_L)^{\otimes_s k}$$

and consider the Hamiltonian

$$\mathcal{H} = \sum_{p\in\frac{2\pi}{L}\mathbb{Z}^3} p^2 a_p^* a_p + \frac{1}{2}\sum_{p,q,r\in\frac{2\pi}{L}\mathbb{Z}^3} \widehat{V}(r) a_{p+r}^* a_q^* a_{q+r} a_p \tag{7.1.1}$$

on $\mathcal{F}(\Lambda_L)$. Here, for a momentum $p \in \frac{2\pi}{L}\mathbb{Z}^3$, a_p^* and a_p are the usual creation and annihilation operators satisfying canonical commutation relations.

Localization to the small periodic box Λ_L is achieved through the following standard proposition, which is proven similarly to [6, Prop. 1.2], see also Figure 6. For the sake of completeness, we sketch the proof in Appendix 7.B, stressing the changes due to the fact that we work at positive temperature.

Proposition 7.1 (Comparison to small periodic boxes). *Let $0 < R < \ell < L$ such that $V(x) = 0$ for all $|x| \geqslant R$. Let Γ_L be a density matrix on the Fock space $\mathcal{F}(\Lambda_L)$, i.e. a non-negative operator on $\mathcal{F}(\Lambda_L)$ with $\operatorname{Tr}\Gamma_L = 1$, satisfying periodic boundary conditions and the bound $\operatorname{Tr}\mathcal{N}\Gamma_L < \infty$. Let*

$$\widetilde{\rho} := \frac{1}{(L+2\ell+R)^3}\operatorname{Tr}\mathcal{N}\Gamma_L. \tag{7.1.2}$$

Then there exists a constant $c > 0$ such that

$$f(\widetilde{\rho}, T) \leqslant \frac{1}{(L+2\ell+R)^3}\Big[\operatorname{Tr}\mathcal{H}\Gamma_L - TS(\Gamma_L)\Big] + \frac{c}{L\ell}\widetilde{\rho} \tag{7.1.3}$$

for all $T \leqslant C\rho\mathfrak{a}$.

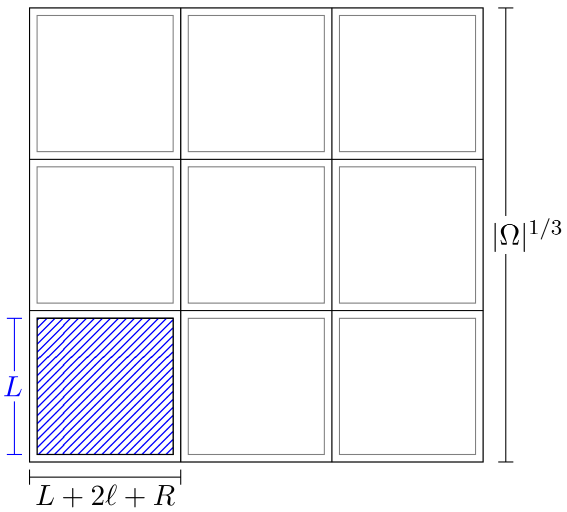

Figure 6: We obtain a trial state on the thermodynamic box Ω by first taking the periodic state Γ_L on Λ_L from Prop. 7.2 and placing it in a slightly bigger box of sidelength $L + 2\ell$. On this box, we modify Γ_L such that it satisfies Dirichlet boundary conditions, while also not changing its free energy significantly. Finally, we copy this state into boxes of sidelength $L + 2\ell + R$, where the slight increase of the box sidelength by R prevents interactions among them.

Taking into account Prop. 7.1, our main challenge is the construction of the trial state Γ_L for the free energy functional on the small periodic box Λ_L with $L = \rho^{-\gamma}$. As discussed above, to make sure that the localization error on the right-hand side of (7.1.3) is smaller than the resolution we want to achieve, we will need to choose $\gamma > 1$. In the next proposition, whose proof occupies the bulk of the paper, we construct the trial state Γ_L. Its particle density is slightly bigger than the desired density ρ in order to compensate for the extension of the box Λ_L that was needed in Prop. 7.1 to switch to Dirichlet boundary conditions and to avoid interactions among boxes.

Proposition 7.2 (Trial state on small periodic boxes)**.** *For $\rho > 0$ and $\gamma > 1$ we set $L = \rho^{-\gamma}$. Then, if γ is sufficiently close to 1, there exists $\epsilon > 0$ and a density matrix Γ_L on $\mathcal{F}(\Lambda_L)$, i.e. a non-negative operator on $\mathcal{F}(\Lambda_L)$ with* $\mathrm{Tr}\,\Gamma_L = 1$, *that satisfies periodic boundary conditions and is such that*

$$c_1\rho^{(\gamma+2)/2} \leqslant \frac{1}{L^3}\mathrm{Tr}\,\mathcal{N}\Gamma_L - \rho \leqslant c_2\rho^{3/2} \tag{7.1.4}$$

for some $c_1, c_2 > 0$, and

$$\begin{aligned}\frac{1}{L^3}\Big[\mathrm{Tr}\,\mathcal{H}\Gamma_L - TS(\Gamma_L)\Big] \leqslant\; & 4\pi\mathfrak{a}\rho^2\Big(1 + \frac{128}{15\sqrt{\pi}}(\rho\mathfrak{a}^3)^{1/2} + c(\rho\mathfrak{a}^3)^{1/2+\epsilon}\Big) \\ & + \frac{T^{5/2}}{(2\pi)^3}\int_{\mathbb{R}^3}\log\left(1 - e^{-\sqrt{|p|^4 + \frac{16\pi\rho\mathfrak{a}}{T}p^2}}\right)dp\end{aligned} \tag{7.1.5}$$

for some $c > 0$ and for all $T \leqslant C\rho\mathfrak{a}$.

Combining Proposition 7.1 and 7.2 we are ready to prove Theorem 3.3.

7.1.2 Proof of Theorem 3.3

Let $\gamma > 1$ be sufficiently close to 1. Putting $L = \rho^{-\gamma}$, we conclude from Prop. 7.2 that there exists a density matrix Γ_L on $\mathcal{F}(\Gamma_L)$, satisfying periodic boundary conditions and the above estimates (7.1.4) and (7.1.5). Setting now $\ell = L^\alpha = \rho^{-\gamma\alpha}$ for some $\alpha \in (0,1)$ and defining $\widetilde{\rho}$ as in (7.1.2), Prop. 7.1 implies that

$$\begin{aligned}f(\widetilde{\rho}, T) \leqslant\; & 4\pi\mathfrak{a}\rho^2\Big(1 + \frac{128}{15\sqrt{\pi}}(\rho\mathfrak{a}^3)^{1/2}\Big) + \frac{T^{5/2}}{(2\pi)^3}\int_{\mathbb{R}^3}\log\left(1 - e^{-\sqrt{|p|^4 + \frac{16\pi\mathfrak{a}\rho}{T}p^2}}\right)dp \\ & + C\big[\rho^{5/2+\epsilon} + \rho^{1+\gamma+\alpha\gamma}\big].\end{aligned}$$

Moreover, by (7.1.4) there exists $c_1 > 0$ such that

$$\widetilde{\rho} = \frac{\mathrm{Tr}\,\mathcal{N}\Gamma_L}{(L + 2\ell + R)^3} \geqslant (\rho + c_1\rho^{(\gamma+2)/2})(1 - C\rho^{\gamma-\alpha\gamma}) \geqslant \rho + c_1\rho^{(\gamma+2)/2} - C\rho^{1+\gamma-\alpha\gamma} \geqslant \rho$$

for ρ small enough, if we assume $\alpha < 1/2$. Here, we used that $RL^{-1} \leqslant \ell L^{-1} = \rho^{\gamma-\alpha\gamma}$.

Using that $r \mapsto f(r, T)$ is convex (see [84]), that $f(0, T) = 0$ and that $f(\widetilde{\rho}, T) \geqslant 0$ for our range of parameters (see [39]), we have $f(\rho, T) \leqslant f(\widetilde{\rho}, T)$. Taking into account that $\gamma > 1$ and choosing $\alpha = 1/2 - \eta$ for a sufficiently small $\eta > 0$, this concludes the proof of Theorem 3.3. □

7.1.3 Strategy of the proof of Proposition 7.2

The remainder of the paper is devoted to the proof of Proposition 7.2. In order to show (7.1.5), it is convenient to rescale variables $x_j \mapsto x_j/L$. Particles then move in the unit torus Λ, i.e. the unit box $[-1/2, 1/2]^3$ with periodic boundary conditions. For convenience, we introduce $N := \rho L^3 = \rho^{1-3\gamma}$ or, equivalently, $L = N^{1-\kappa}$, with $\kappa = (2\gamma - 1)/(3\gamma - 1)$. The constraint on the temperature becomes $T \leqslant CN^{-2+3\kappa}$. We conclude that the Hamilton operator (7.1.1), acting on $\mathcal{F}(\Lambda_L)$, is unitarily equivalent to $L^{-2}\mathcal{H}_N$, with the new Hamiltonian

$$\mathcal{H}_N = \sum_{p\in\Lambda^*} p^2 a_p^* a_p + \frac{1}{2}\sum_{p,q,r\in\Lambda^*}\widehat{V}_N(r)a_{p+r}^* a_q^* a_{q+r} a_p \tag{7.1.6}$$

acting on $\mathcal{F}(\Lambda)$. Here, we introduced the notation $\widehat{V}_N(r) = N^{-1+\kappa}\widehat{V}(r/N^{1-\kappa})$ and we denoted by $\Lambda^* = 2\pi\mathbb{Z}^3$ the set of momenta on the torus Λ. The condition $\gamma > 1$ is equivalent to $\kappa > 1/2$.

In the next sections, we will construct a density matrix Γ_N on $\mathcal{F}(\Lambda)$ that has the correct expected number of particles and the correct energy. That is, we have the bound

$$c_1 N^{3\kappa/2-(\kappa-1/2)} \leqslant \operatorname{Tr}\mathcal{N}\Gamma_N - N \leqslant c_2 N^{3\kappa/2}, \tag{7.1.7}$$

which is equivalent to (7.1.4) and also

$$\begin{aligned}
&\operatorname{Tr}\mathcal{H}_N\Gamma_N - TL^2 S(\Gamma_N) \\
&\leqslant 4\pi\mathfrak{a}N^{1+\kappa}\left(1 + \frac{128}{15\sqrt{\pi}}(N^{-2+3\kappa}\mathfrak{a}^3)^{1/2}\right) \\
&\quad + TN^{2-2\kappa}\sum_{N^{\kappa/2-\varepsilon}<|p|\leqslant N^{\kappa/2+\varepsilon}} \log\left[1 - \exp\Big(-\frac{1}{TN^{2-2\kappa}}\sqrt{|p|^4 + 16\pi\mathfrak{a}N^\kappa p^2}\Big)\right] + CN^{5\kappa/2-\varepsilon/2}
\end{aligned} \tag{7.1.8}$$

for all $T \leqslant CN^{-2+3\kappa}$ and some fixed $\varepsilon > 0$. Note that the restricted sum can be extended to include all momenta up to a negligible error. Hence, rescaling and approximating the sum with an integral, (7.1.8) leads us to the statement of Prop. 7.2. Note that, after rescaling to the unit torus, the effective temperature is given by $TL^2 = TN^{2-2\kappa}$.

To construct the trial state Γ_N, we will apply a strategy similar to the one used in [6] to prove an upper bound for the ground state energy at temperature $T = 0$. The work [6] was partly motivated by the results of [10, 7], establishing the validity of Bogoliubov theory in the Gross–Pitaevskii regime, where the Hamiltonian takes the form (7.1.6), with $\kappa = 0$ (see [43, 19] for alternative approaches). The main observation is that (7.1.6) can be reduced, through a series of unitary transformations, to a Hamilton operator that can be approximated by a linear combination of decoupled harmonic oscillators when evaluated in our trial state.

Let us explain the procedure a bit more precisely; the mathematical details will follow in the next section. First of all, since the temperatures under consideration are below the critical temperature, we need to factor out the Bose–Einstein condensate. To this end, we conjugate (7.1.6) with a Weyl operator W_{N_0}, producing a condensate with N_0 particles. The parameter $N_0 \in \mathbb{R}_+$ will be fixed later on; it will be chosen so that $0 \leqslant N - N_0 \lesssim N^{3\kappa/2}$. Let us introduce the momentum sets

$$\begin{aligned}
&\text{High momenta:}\quad H = \{p \in \Lambda^* : |p| > N^{1-\kappa-\varepsilon}\}, \\
&\text{Shell momenta:}\quad S = \{p \in \Lambda^* : N^{\kappa/2-\varepsilon} < |p| \leqslant N^{\kappa/2+\varepsilon}\} \\
&\quad\text{with}\quad \varepsilon > 0 \quad \text{s.t.}\quad -2 + 3\kappa + 4\varepsilon < 0.
\end{aligned} \tag{7.1.9}$$

In particular the sets do not overlap. To approximate $W_{N_0}^*\mathcal{H}_N W_{N_0}$ with a quadratic Hamiltonian, we first remove the short-range correlation structure. This renormalization is achieved by conjugating $W_{N_0}^*\mathcal{H}_N W_{N_0}$ with a Bogoliubov transformation $e^{\mathcal{B}_1}$, acting only on momenta $|p| > N^{\kappa/2+\varepsilon}$. Unfortunately, to reach the correct energy, quasi-free states constructed by quadratic transformations are not enough. Therefore, we conjugate the resulting renormalized excitation Hamiltonian with a unitary cubic operator T_c; the choice of T_c is the crucial step in our analysis. The Hamiltonian $T_c^* e^{-\mathcal{B}_1} W_{N_0}^*\mathcal{H}_N W_{N_0} e^{\mathcal{B}_1} T_c$ is well approximated by a quadratic operator, which can be diagonalized by a second Bogoliubov transformation $e^{\mathcal{B}_2}$, acting on momenta in the shell S. Up to error terms, that are negligible in an appropriate sense, we find

$$\begin{aligned}
&e^{-\mathcal{B}_2}T_c^* e^{-\mathcal{B}_1} W_{N_0}^*\mathcal{H}_N W_{N_0} e^{\mathcal{B}_1} T_c e^{\mathcal{B}_2} \\
&\qquad \simeq 4\pi\mathfrak{a}N^{1+\kappa}\left(1 + \frac{128}{15\sqrt{\pi}}(N^{-2+3\kappa}\mathfrak{a}^3)^{1/2}\right) + \sum_{p\in S}\sqrt{|p|^4 + 16\pi\mathfrak{a}N^\kappa p^2}\, a_p^* a_p,
\end{aligned} \tag{7.1.10}$$

provided that $\kappa > 1/2$ is sufficiently close to 1/2. At temperature $TN^{2-2\kappa}$, the Gibbs state associated with the quadratic operator on the right hand side of (7.1.10) has the form

$$\Gamma_0 = Z^{-1}\mathbb{1}_{\{\mathcal{N}_{S^c}=0\}} \exp\bigg(- \frac{1}{TN^{2-2\kappa}} \sum_{p\in S} \sqrt{|p|^4 + 16\pi\mathfrak{a}N^\kappa p^2}\, a_p^* a_p \bigg) \tag{7.1.11}$$

with the normalization constant $Z > 0$ chosen so that $\operatorname{Tr}\Gamma_0 = 1$ and where, for any $F \subset \Lambda^*$, we introduced the notation

$$\mathcal{N}_F = \sum_{p\in F} a_p^* a_p$$

for the operator measuring the number of particles with momentum in the set F. Therefore, we use

$$\Gamma_N = Z^{-1} W_{N_0} e^{\mathcal{B}_1} T_c e^{\mathcal{B}_2} \Gamma_0 e^{-\mathcal{B}_2} T_c^* e^{-\mathcal{B}_1} W_{N_0}^* \tag{7.1.12}$$

as a trial state for the Hamiltonian (7.1.6). With the approximation (7.1.10), it is then not difficult to check that this trial state has indeed the correct free energy, completing the proof of (7.1.8).

We now highlight the main novelties with respect to [6], where a trial state was constructed to estimate the ground state energy of (7.1.6). Since we work at positive temperature, Γ_0 must be chosen as a mixed state that describes thermal excitations. In contrast, at zero temperature it is sufficient to take Γ_0 as the projection onto the vacuum vector in the Fock space $\mathcal{F}(\Lambda)$. The analysis of [6] strongly relied on the fact that the cubic transformation that is needed to create the correct correlation structure acted directly on the vacuum. For this reason, it was possible to implement this transformation through a non-unitary operator, given by the exponential of a cubic expression involving only creation operators, and to compute its action almost explicitly. Here, we follow a different strategy and implement a unitary transformation mainly for two reasons. First, the action of the cubic transformation on Γ_0 is more involved than its action on the vacuum and explicit computations are the exception. Second, to estimate the entropy of Γ_N we need to compute the spectral distribution of the transformed state, which is considerably simpler if T_c is unitary.

Let us briefly explain why it is challenging to control the action of a unitary cubic transformation in the current setting. The action of a unitary operator $e^{\mathcal{B}}$ can be formally computed via the commutator expansion

$$e^{-\mathcal{B}} X e^{\mathcal{B}} = \sum_{n\geqslant 0} \frac{(-1)^n}{n!} \mathrm{ad}_{\mathcal{B}}^{(n)}(X), \tag{7.1.13}$$

with $\mathrm{ad}_{\mathcal{B}}(X) = [\mathcal{B}, X]$ and where $\mathrm{ad}_{\mathcal{B}}^{(n)}$ denotes its n−fold iteration. For quadratic transformations, say $\mathcal{B} = \frac{1}{2}\sum_{k\in\Lambda^*} \eta_k a_k^* a_{-k}^* - \text{h.c.}$ with some real numbers $\eta_k = \eta_{-k}$, it is well known that (7.1.13) yields a closed formula. For example for $X = a_p^*, p \in \Lambda^*$, it leads to the explicit formula

$$e^{-\mathcal{B}} a_p^* e^{\mathcal{B}} = \mathrm{ch}(\eta_p) a_p^* + \mathrm{sh}(\eta_p) a_p.$$

Cubic transformations, however, do not enjoy the same algebraic structure. In the Gross–Pitaevskii regime ($\kappa = 0$) considered in [10, 17, 69], or in slightly more singular regimes ($\kappa > 0$ small), as in [1, 16, 39], the coefficients of the cubic transformation $\mathcal{B} = \sum_{k,r\in\Lambda^*} \eta_r a_{k+r}^* a_{-r}^* a_k - \text{h.c.}$ can be taken to be small enough in N (in appropriate ℓ^p norm for example) so that the expansion (7.1.13) can be truncated after a few iterations. In our case, since we consider $\kappa > 1/2$, the trial state Γ_0 has too many excitations and the terms in the expansion (7.1.13) cannot be adequately controlled in expectation as $N \to \infty$, in the sense that higher order terms are larger than lower order terms, already for simple observables like the particle number operator $X = \mathcal{N}$.

To deal with this problem, we implement the cubic renormalization as product of many "smaller" unitary operators, constructed in such a way that the expansion (7.1.13) is controllable and yields a closed formula, similar to the one obtained for quadratic transformations. To achieve this goal, we introduce cutoff functions analogous to the ones used in [6], to make sure that for a given momentum k in the shell S, we only create one pair $(-r, k+r)$ of particles with high momentum in H. For $k \in S$, we say that a pair (p, q) of momenta in H forms a k-connection if $p+q=k$. We define $\mathcal{B}_k = \mathcal{B}_k^\sharp - \mathcal{B}_k^\circ$, see (7.2.10) below, so that $\mathcal{B}_k^\sharp$ only creates a k-connection if it acts on a state with no k-connection, and it cannot create k'-connections, for $k' \neq k$. Note that $\mathcal{B}_k^\sharp$ and $\mathcal{B}_k^\circ$ are adjoints to each other so that $\mathcal{B}_k$ is skew-adjoint. Thanks to these exclusion rules, we will show in Lemma 7.4.3 below that the unitary transformation $e^{\mathcal{B}_k}$ is explicitly given by

$$e^{\mathcal{B}_k} = \cos X_k + \mathcal{B}_k^\sharp \frac{\sin X_k}{X_k} - \frac{\sin X_k}{X_k} \mathcal{B}_k^\circ + \mathcal{B}_k^\sharp \frac{\cos X_k - 1}{X_k^2} \mathcal{B}_k^\circ,$$

where $X_k = |\mathcal{B}_k^\sharp|$. Using that X_k is small in average on the trial state, we will be able to iteratively combine the action of $e^{\mathcal{B}_k}$, for all momenta in the shell S. Additionally, we will show that the cubic transformation preserves some properties of the trial state, which is used to simplify computations.

Organization of the paper. In Section 7.2, we precisely define the previously discussed unitary transformations and our trial state. In Lemma 7.4 and in Lemma 7.5, we describe the action of the Bogoliubov transformation $e^{\mathcal{B}_1}$ and of the cubic transformation T_c, respectively. Using these lemmas, we may conclude the proof of Prop. 7.2. Section 7.3 is devoted to the proof of Lemma 7.4 and Section 7.4 to the proof of Lemma 7.5. Finally, in the appendix, we show properties of the kernel of the transformations and we give a proof of Prop. 7.1.

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7.2 The trial state

This section provides an explicit description of the trial state Γ_N introduced in (7.1.12). In particular, we construct the unitary transformations appearing in its definition and compute their actions on the Hamiltonian.

7.2.1 The Weyl transformation W_{N_0}

To generate the Bose-Einstein condensate we use the Weyl operator

$$W_{N_0} = \exp\left[\sqrt{N_0}(a_0^* - a_0)\right],$$

with a parameter $N_0 \in \mathbb{N}$, which will be specified later on, see (7.2.28). The Weyl operator leaves a_p, a_p^* invariant for all $p \in \Lambda^* \setminus \{0\}$. On a_0, a_0^*, it acts as a shift, i.e.

$$W_{N_0}^* a_0 W_{N_0} = a_0 + \sqrt{N_0}, \quad W_{N_0}^* a_0^* W_{N_0} = a_0^* + \sqrt{N_0}. \tag{7.2.1}$$

We obtain the excitation Hamiltonian

$$W_{N_0}^* \mathcal{H}_N W_{N_0} = \frac{N_0^2}{2} \widehat{V}_N(0) + Q_1 + Q_2 + Q_3 + Q_4 + \sum_{p \in \Lambda^*} \left(p^2 + N_0 \widehat{V}_N(0) + N_0 \widehat{V}_N(p)\right) a_p^* a_p \tag{7.2.2}$$

with

$$Q_1 = N_0^{3/2}\widehat{V}_N(0)a_0 + \text{h.c.} \qquad\qquad Q_2 = \frac{N_0}{2}\sum_{p\in\Lambda^*}\widehat{V}_N(p)a_p^*a_{-p}^* + \text{h.c.}$$

$$Q_3 = N_0^{1/2}\sum_{p,r\in\Lambda^*}\widehat{V}_N(r)a_{-r}^*a_{r+p}^*a_p + \text{h.c.} \qquad Q_4 = \frac{1}{2}\sum_{p,q,r\in\Lambda^*}\widehat{V}_N(r)a_{p+r}^*a_q^*a_{q+r}a_p$$

7.2.2 Quadratic transformation $e^{\mathcal{B}_1}$ on momenta $|p| > N^{\kappa/2+\varepsilon}$

To factor out the short-range correlations, we conjugate $W_{N_0}^*\mathcal{H}_N W_{N_0}$ with a Bogoliubov transformation that acts on momenta that are higher than the shell momenta. For $p \in \Lambda^* \setminus \{0\}$, we define φ_p as the unique solution to the box scattering equation

$$p^2\varphi_p + \frac{1}{2}\sum_{q\neq 0}\widehat{V}_N(p-q)\varphi_q = -\frac{1}{2}\widehat{V}_N(p), \tag{7.2.3}$$

where we introduced the notation "$q \neq 0$" for $q \in \Lambda^* \setminus \{0\}$. The existence and the uniqueness of a solution to this equation was established in [43]. For the sake of completeness we provide the proof in Section 7.A. Next, we define the box scattering length $\mathfrak{a}_N$, which appears more naturally in our setting and, as we will show, is close to the full space scattering length $\mathfrak{a}$.

$$8\pi\mathfrak{a}_N := \widehat{V}(0) + N^{1-\kappa}\sum_{p\neq 0}\widehat{V}_N(p)\varphi_p. \tag{7.2.4}$$

Important properties of the function $\varphi\colon p \mapsto \varphi_p$ with $\varphi_0 = 0$ and of the box scattering length $\mathfrak{a}_N$ are stated in the next lemma. Its proof is given in Section 7.A, see also [43], [19, Appendix] or [48, Appendix] for alternative proofs.

Lemma 7.3. *For $p \in \Lambda^* \setminus \{0\}$, we have the pointwise bound*

$$\varphi_p \lesssim p^{-2}N^{-1+\kappa}.$$

Moreover, we have the estimates

$$\|\varphi\|_1 \lesssim 1, \qquad \|\varphi\|_2 \lesssim N^{-1+\kappa}, \qquad \|\varphi\|_\infty \lesssim N^{-1+\kappa}, \qquad \|p\varphi\|_2^2 \lesssim N^{-1+\kappa}.$$

For $\varphi_p^{(\alpha)} = \varphi_p\mathbb{1}_{|p|>N^\alpha}, \alpha > 0$, we obtain

$$\|\varphi^{(\alpha)}\|_2 \lesssim N^{-1+\kappa-\alpha/2}, \qquad \|\varphi^{(\alpha)}\|_\infty \lesssim N^{-1+\kappa-2\alpha}.$$

Moreover,

$$|\mathfrak{a}_N - \mathfrak{a}| \lesssim N^{-1+\kappa}. \tag{7.2.5}$$

Using the solution φ_p, we define the unitary Bogoliubov transformation $e^{\mathcal{B}_1}$, with the antisymmetric operator

$$\mathcal{B}_1 = \frac{1}{2}\sum_{|p|>N^{\kappa/2+\varepsilon}}\sinh^{-1}(N_0\varphi_p)a_p^*a_{-p}^* - \text{h.c.}$$

Recall that the parameter $\varepsilon > 0$ was introduced in (7.1.9). For $p \in \Lambda^*$, the action of $e^{\mathcal{B}_1}$ on an annihilation operator is given by

$$e^{-\mathcal{B}_1}a_p e^{\mathcal{B}_1} = c_p a_p + s_p a_{-p}^*, \tag{7.2.6}$$

where we denote

$$c_p = \cosh\big(\sinh^{-1}(N_0\varphi_p)\big) = \sqrt{1+N_0^2\varphi_p^2}, \qquad s_p = \sinh\big(\sinh^{-1}(N_0\varphi_p)\big) = N_0\varphi_p \tag{7.2.7}$$

for all $|p| > N^{\kappa/2+\varepsilon}$, while the transformation acts trivially otherwise, i.e. $c_p = 1$ and $s_p = 0$ for $|p| \leqslant N^{\kappa/2+\varepsilon}$.

Conjugating (7.2.2) with the Bogoliubov transformation $e^{\mathcal{B}_1}$ we obtain a new, renormalized excitation Hamiltonian. Its form is described in the next lemma, whose proof is deferred to Section 7.3. Here we introduce the orthogonal projection

$$\Xi := \mathbb{1}_{\{\mathcal{N}_{(S\cup H)^c}=0\}}\mathbb{1}_{\{\mathcal{N}_H\in 2\mathbb{N}_0\}}.$$

Since the state that we are going to use to estimate the free energy of $e^{-\mathcal{B}_1}W_{N_0}^*\mathcal{H}_N W_{N_0}e^{\mathcal{B}_1}$ will be in the range of Ξ (because (7.1.11) is clearly in Ran Ξ and because Ξ commutes with T_c and $e^{\mathcal{B}_2}$), it is enough for us to estimate the error arising from conjugation with $e^{\mathcal{B}_1}$ on this subspace.

Lemma 7.4. *Suppose that $0 \leqslant N - N_0 \leqslant CN^{3\kappa/2}$ for some constant $C > 0$. Then we have*

$$\begin{aligned} &e^{-\mathcal{B}_1}W_{N_0}^*\mathcal{H}_N W_{N_0}e^{\mathcal{B}_1} \\ &\qquad = 4\pi\mathfrak{a}N^{1+\kappa} - 8\pi\mathfrak{a}N^{\kappa}(N-N_0) + \sum_{p\in S}\frac{(4\pi\mathfrak{a}N^{\kappa})^2}{p^2} \\ &\qquad\quad + \sum_{p\in\Lambda^*}p^2a_p^*a_p + 2\widehat{V}(0)N^{\kappa}\mathcal{N} + \sum_{p\in S}4\pi\mathfrak{a}N^{\kappa}\big(a_p^*a_{-p}^* + \text{h.c.}\big) + Q_3 + Q_4 + \mathcal{E}_1, \end{aligned} \tag{7.2.8}$$

where the error term $\mathcal{E}_1$ is bounded, on the range of the projection Ξ, by

$$\begin{aligned} \mathcal{E}_1 \lesssim{}& N^{-3\varepsilon}\sum_{p\in\Lambda^*}p^2a_p^*a_p + N^{-5\varepsilon/2}Q_4 + N^{-\kappa/2-\varepsilon/2}\mathcal{N}^2 + N^{-3+7\kappa+4\varepsilon}\mathcal{N}_H^2 + N^{2-2\kappa-2\varepsilon}\mathcal{N}_H \\ &+ N^{5\kappa/2-\varepsilon/2} \end{aligned} \tag{7.2.9}$$

if $1/2 < \kappa < 8/15 - 2\varepsilon/3$ and $\varepsilon > 0$ is chosen as in (7.1.9).

Remark. We will show that the trial state that we are going to use for the Hamiltonian $e^{-\mathcal{B}_1}W_{N_0}^*\mathcal{H}_N W_{N_0}e^{\mathcal{B}_1}$ is such that, for $j = 1, 2$,

$$\mathcal{N}_H^j \lesssim N^{(-2+9\kappa/2+\varepsilon)j}; \qquad \mathcal{N}^j \lesssim N^{j3\kappa/2}; \qquad Q_4, \sum p^2a_p^*a_p \lesssim N^{5\kappa/2}$$

in expectation. This explains why, for $1/2 < \kappa < 14/27 - \varepsilon$, all terms on the right-hand side of (7.2.9) are subleading, i.e. they are smaller than $N^{5\kappa/2}$, which is the resolution we are trying to achieve.

Note that the operator inequality (7.2.9), as well as subsequent ones, should be understood in the sense of quadratic forms. In particular, "on the range of the projection" means that the inequality holds after taking expectations in a vector $\psi \in \Xi\mathcal{F}(\Lambda)$.

7.2.3 The cubic transformation T_c

Next, we conjugate the renormalized excitation Hamiltonian $e^{-\mathcal{B}_1}W_{N_0}^*\mathcal{H}_N W_{N_0}e^{\mathcal{B}_1}$ with cubic transformations, annihilating a particle with shell momentum $k \in S$ and creating a pair of particles with high momenta $-r, k+r \in H$, or, vice versa, annihilating a pair of particles with high momenta $-r, k+r \in H$ and creating a particle with shell momentum $k \in S$. Instead of a single cubic transformation, we consider a product of unitary operators, one for each low momentum $k \in S$. More precisely, for $k \in S$, we define

$$\mathcal{B}_k^\sharp = \sum_{r \in H_k} N^{1/2} \varphi_r a_{-r}^* a_{r+k}^* a_k \Theta_{k,r}, \qquad \mathcal{B}_k^\circ = \left(\mathcal{B}_k^\sharp\right)^*, \qquad \mathcal{B}_k = \mathcal{B}_k^\sharp - \mathcal{B}_k^\circ, \tag{7.2.10}$$

with $H_k = \{r \in H \,|\, r+k \in H\}$ and where the cutoff $\Theta_{k,r}$ is defined, similarly as in [6], by

$$\begin{aligned} &\Theta_{k,r} = \Theta_k^{(1)} \times \Theta_{k,r}^{(2)}, \\ &\Theta_k^{(1)} = \prod_{t \in H} (1 - \mathbb{1}_{\{\mathcal{N}_{-t}>0\}} \mathbb{1}_{\{\mathcal{N}_{t+k}>0\}}), \qquad \Theta_{k,r}^{(2)} = \prod_{q \in S} (1 - \mathbb{1}_{\{\mathcal{N}_{r+q} + \mathcal{N}_{-(k+r)+q} > 0\}}). \end{aligned} \tag{7.2.11}$$

Here and in the following we use the notation $\mathcal{N}_q = a_q^* a_q$, $q \in \Lambda^*$, for the operator measuring the number of particles with momentum q. Thanks to the cutoffs, the operators $\mathcal{B}_k^\sharp$ and $\mathcal{B}_k^\circ$ are well defined on the domain of $\mathcal{N}$ (see Lemma 7.12). It is easy to check that they are closable and their closures are adjoints of each other. Moreover, from [81, Theorem X.36] we obtain that $i\mathcal{B}_k$ is essentially self-adjoint on the domain of $\mathcal{N}$. We will make the usual abuse of notations and use the same notation for the operators $\mathcal{B}_k^\sharp$, $\mathcal{B}_k^\circ$ and $i\mathcal{B}_k$ and their respective closures or self-adjoint extension. We can now define the unitary operator $T_k = e^{\mathcal{B}_k}$ for every $k \in S$, and the product

$$T_c = \prod_{k \in S} T_k. \tag{7.2.12}$$

In fact, since $[T_k, T_{k'}] \neq 0$, for $k' \neq k$, we need to choose an order in the finite set S to define T_c. However, our analysis will not depend on this choice.

We say that a pair of high momenta $(r,t) \in H^2$ is a *k-connection* if $r + t = k$. The cut-off $\Theta_{k,r}$ has two roles. The first factor $\Theta_k^{(1)}$ ensures that $\mathcal{B}_k^\sharp$ only creates a k-connection if there is not already one. The second factor $\Theta_{k,r}^{(2)}$ ensures that $\mathcal{B}_k^\sharp$ does not create any q-connection, for $q \neq k$. This latter condition is implemented by asking that the *shell-neighborhoods* of r and $-(k+r)$ are empty, that is, that there is no occupied mode with momentum $t \in r + S$ or $t \in -(k+r) + S$.

In the next lemma we describe the action of T_c on the renormalized excitation Hamiltonian $e^{-\mathcal{B}_1} W_{N_0}^* \mathcal{H}_N W_{N_0} e^{\mathcal{B}_1}$. When applying the lemma, we will only be interested in controlling the action of T_c on a specific trial state Γ. For this reason, we are going to restrict our attention to states with certain additional properties, which will be satisfied by the Γ that we are going to choose. First of all, we can restrict our attention to the range of the projection $\mathbb{1}_{\{\mathcal{N}_{S^c}=0\}}$ (because the trial state will not have particles with momentum outside S). Additionally, we can focus on states that commute with the parity operator for the sum of the number of particles with momentum $\pm k$ and the number of $\pm k$-connections. For $k \in S$, consider

$$\mathcal{M}_k = \mathcal{N}_k + \frac{1}{2} \sum_{t \in H_k} \mathcal{N}_{-t} \mathcal{N}_{t+k} \tag{7.2.13}$$

and the parity operators

$$\begin{aligned} \mathbb{P}_k &= \mathbb{1}_{\{\mathcal{M}_k + \mathcal{M}_{-k} \in 2\mathbb{N}_0\}}, \\ \mathbb{Q}_k &= 1 - \mathbb{P}_k = \mathbb{1}_{\{\mathcal{M}_k + \mathcal{M}_{-k} \in 2\mathbb{N}_0 + 1\}}. \end{aligned} \tag{7.2.14}$$

In accordance with the intuition that $\mathcal{B}_k^\sharp$ annihilates a particle with momentum k while creating a k-connection, one readily checks that $[\mathcal{B}_q^\sharp, \mathcal{M}_k] = 0$ for all $q \in S$. Therefore we find that

$[T_c, \mathcal{M}_k] = [T_c, \mathbb{P}_k] = [T_c, \mathbb{Q}_k] = 0$ for all $k \in S$. For this reason, restricting to Γ such that $[\Gamma, \mathbb{P}_k] = [\Gamma, \mathbb{Q}_k] = 0$ for all $k \in S$, we will be able to neglect all terms in the renormalized excitation Hamiltonian $e^{-\mathcal{B}_1} W_{N_0}^* \mathcal{H}_N W_{N_0} e^{\mathcal{B}_1}$ that do not preserve parity.

Lemma 7.5. *Let Γ be a normalized density matrix on $\mathcal{F}(\Lambda)$ with $\Gamma = \mathbb{1}_{\{\mathcal{N}_{S^c}=0\}} \Gamma \mathbb{1}_{\{\mathcal{N}_{S^c}=0\}}$ and such that $[\Gamma, \mathbb{P}_k] = 0$ for all $k \in S$. Assume $0 \leqslant N - N_0 \lesssim N^{3\kappa/2}$. Then we have*

$$\begin{aligned} &\operatorname{Tr} T_c^* e^{-\mathcal{B}_1} W_{N_0}^* \mathcal{H}_N W_{N_0} e^{\mathcal{B}_1} T_c \Gamma \\ &\quad \leqslant 4\pi \mathfrak{a} N^{1+\kappa} - 8\pi \mathfrak{a} N^{\kappa} (N - N_0) + \sum_{p \in S} \frac{(4\pi \mathfrak{a} N^{\kappa})^2}{p^2} \\ &\qquad + \operatorname{Tr} \Big[\sum_{p \in S} p^2 a_p^* a_p + 16\pi \mathfrak{a} N^{\kappa} \mathcal{N}_S + \sum_{p \in S} 4\pi \mathfrak{a} N^{\kappa} \big(a_p^* a_{-p}^* + \text{h.c.} \big) \Big] \Gamma + \delta(\Gamma) \end{aligned} \tag{7.2.15}$$

where

$$\begin{aligned} \delta(\Gamma) \lesssim\; & N^{-1+\kappa+6\varepsilon} \operatorname{Tr} \big(\mathcal{N}_S + N^{3\kappa/2+3\varepsilon} \big) \sum_{k \in S} \mathcal{N}_k^2 \, \Gamma \\ & + \big(N^{-\kappa/2-\varepsilon/2} + N^{-7+13\kappa+6\varepsilon} \big) \operatorname{Tr} \mathcal{N}_S^2 \Gamma + N^{5\kappa/2-\varepsilon/2} \end{aligned} \tag{7.2.16}$$

if $1/2 < \kappa < 8/15 - 2\varepsilon/3$ and $\varepsilon > 0$ is chosen as in (7.1.9).

This lemma is the main novelty of the paper. We defer its proof to Section 7.4.

7.2.4 Quadratic transformation $e^{\mathcal{B}_2}$ on shell momenta

Consider now the quadratic Hamiltonian in (7.2.15). Since we are going to choose N_0 such that $N - N_0 = \operatorname{Tr} \mathcal{N}_S \Gamma + o(N^{3\kappa/2})$, see (7.2.28) below, we are effectively left with a factor $8\pi \mathfrak{a} N^{\kappa} \mathcal{N}_S$ in the last line of (7.2.15). With the aim of diagonalizing this quadratic operator, we define the coefficients $\tau_p \in \mathbb{R}$, for $p \in S$, via

$$\tanh(2\tau_p) = -\frac{8\pi \mathfrak{a} N^{\kappa}}{p^2 + 8\pi \mathfrak{a} N^{\kappa}}.$$

The action of the unitary Bogoliubov transformation $e^{\mathcal{B}_2}$, with the antisymmetric operator

$$\mathcal{B}_2 = \frac{1}{2} \sum_{p \in S} \tau_p a_p^* a_{-p}^* - \text{h.c.},$$

is given explicitly, similarly to (7.2.6), by

$$e^{-\mathcal{B}_2} a_p e^{\mathcal{B}_2} = \gamma_p a_p + \sigma_p a_{-p}^*, \qquad e^{-\mathcal{B}_2} a_p^* e^{\mathcal{B}_2} = \gamma_p a_p^* + \sigma_p a_{-p} \tag{7.2.17}$$

with $\gamma_p = \cosh \tau_p$, $\sigma_p = \sinh \tau_p$, for all $p \in S$. A straightforward calculation shows that

$$\begin{aligned} & e^{-\mathcal{B}_2} \Big[\sum_{p \in S} p^2 a_p^* a_p + 8\pi \mathfrak{a} N^{\kappa} \mathcal{N}_S + \sum_{p \in S} 4\pi \mathfrak{a} N^{\kappa} \big(a_p^* a_{-p}^* + \text{h.c.} \big) \Big] e^{\mathcal{B}_2} \\ &\quad = \frac{1}{2} \sum_{p \in S} \big[\sqrt{|p|^4 + 16\pi \mathfrak{a} N^{\kappa} p^2} - p^2 - 8\pi \mathfrak{a} N^{\kappa} \big] + \sum_{p \in S} \sqrt{|p|^4 + 16\pi \mathfrak{a} N^{\kappa} p^2} \, a_p^* a_p. \end{aligned} \tag{7.2.18}$$

We may now precisely define the trial state of the transformed Hamiltonian as the Gibbs state of the diagonal quadratic Hamiltonian in (7.2.18). We set

$$\Gamma_0 = Z^{-1} \mathbb{1}_{\{\mathcal{N}_{S^c}=0\}} \exp \Big(- \frac{1}{T N^{2-2\kappa}} \sum_{p \in S} \sqrt{|p|^4 + 16\pi \mathfrak{a} N^{\kappa} p^2} \, a_p^* a_p \Big), \tag{7.2.19}$$

with the normalization constant

$$Z = \mathrm{Tr}\ \mathbb{1}_{\{\mathcal{N}_{S^c}=0\}}\ \exp\bigg(- \frac{1}{TN^{2-2\kappa}} \sum_{p\in S} \sqrt{|p|^4 + 16\pi\mathfrak{a}N^\kappa p^2}\, a_p^* a_p \bigg).$$

Furthermore, we define

$$\Gamma = e^{\mathcal{B}_2}\Gamma_0 e^{-\mathcal{B}_2} \tag{7.2.20}$$

as the trial state for the Hamiltonian appearing in Lemma 7.5. Some important properties of Γ are listed in the following lemma.

Lemma 7.6. *Let Γ be defined as in (7.2.20). Then $\Gamma \geqslant 0$ with $\mathrm{Tr}\,\Gamma = 1$. Moreover, we have $\Gamma = \mathbb{1}_{\{\mathcal{N}_{S^c}=0\}}\Gamma\mathbb{1}_{\{\mathcal{N}_{S^c}=0\}}$ and $[\Gamma,\mathbb{P}_k] = [\Gamma,\mathbb{Q}_k] = 0$ for all $k \in S$ and with the parity operators $\mathbb{P}_k, \mathbb{Q}_k$ defined in (7.2.14). Furthermore, for $j = 1, 2$, there exist positive constants $c < C$ such that*

$$\begin{aligned} cN^{3j\kappa/2} &\leqslant \mathrm{Tr}\ \mathcal{N}_S^j\Gamma \leqslant CN^{3j\kappa/2} \\ \mathrm{Tr}\,\mathcal{N}_S^{j-1}\sum_{k\in S}\mathcal{N}_k^2\Gamma &\leqslant CN^{j(3\kappa/2+2\varepsilon)}. \end{aligned} \tag{7.2.21}$$

Proof. The fact that $\Gamma \geqslant 0$, $\mathrm{Tr}\,\Gamma = 1$, $\Gamma = \mathbb{1}_{\{\mathcal{N}_{S^c}=0\}}\Gamma\mathbb{1}_{\{\mathcal{N}_{S^c}=0\}}$ and $[\Gamma,\mathbb{P}_k] = [\Gamma,\mathbb{Q}_k] = 0$ for all $k \in S$ follows readily from the definition of Γ. It remains to show the inequalities (7.2.21). We begin with $j = 1$. From the definition of Γ_0 a standard ideal gas computation gives

$$\begin{aligned} \mathrm{Tr}\,\mathcal{N}_p\Gamma_0 &= \frac{1}{\exp\big(\frac{1}{TN^{2-2\kappa}}\sqrt{|p|^4+16\pi\mathfrak{a}N^\kappa p^2}\big)-1} \\ \mathrm{Tr}\,\mathcal{N}_p^2\Gamma_0 &= \frac{2}{\Big[\exp\big(\frac{1}{TN^{2-2\kappa}}\sqrt{|p|^4+16\pi\mathfrak{a}N^\kappa p^2}\big)-1\Big]^2} + \frac{1}{\exp\big(\frac{1}{TN^{2-2\kappa}}\sqrt{|p|^4+16\pi\mathfrak{a}N^\kappa p^2}\big)-1} \end{aligned} \tag{7.2.22}$$

and, by symmetry,

$$\mathrm{Tr}\,a_p^*a_{-p}^*\Gamma_0 = \mathrm{Tr}\,a_p a_{-p}\Gamma_0 = 0$$

for all $p \in S$. With (7.2.17), we find

$$\begin{aligned} \mathrm{Tr}\,\mathcal{N}_S\Gamma &= \sum_{p\in S}\mathrm{Tr}\ (\gamma_p a_p^* + \sigma_p a_{-p})(\gamma_p a_p + \sigma_p a_{-p}^*)\Gamma_0 \\ &= \sum_{p\in S}\frac{p^2+8\pi\mathfrak{a}N^\kappa}{\sqrt{|p|^4+16\pi\mathfrak{a}N^\kappa p^2}}\frac{1}{\exp\big(\frac{1}{TN^{2-2\kappa}}\sqrt{|p|^4+16\pi\mathfrak{a}N^\kappa p^2}\big)-1} \\ &\qquad + \frac{1}{2}\sum_{p\in S}\Big[\frac{p^2+8\pi\mathfrak{a}N^\kappa}{\sqrt{|p|^4+16\pi\mathfrak{a}N^\kappa p^2}}-1\Big]. \end{aligned} \tag{7.2.23}$$

Scaling $p \mapsto p/N^{\kappa/2}$, interpreting the sums as Riemann sums, approximating them with integrals over $\mathbb{R}^3$, and using the restriction $TN^{2-3\kappa} \leqslant C$, we conclude that $cN^{3\kappa/2} \leqslant \mathrm{Tr}\,\mathcal{N}_S\Gamma \leqslant CN^{3\kappa/2}$ (both terms are positive, the second term is of order $N^{3\kappa/2}$, independently of T and the first term is at most of order $N^{3\kappa/2}$, for $TN^{2-3\kappa} \leqslant C$).

To prove the second bound in (7.2.21), we proceed similarly. Also here, we use the fact that only observables preserving the number of particles have non-trivial expectation w.r.t. Γ_0.

$$
\begin{aligned}
\mathrm{Tr}\, \sum_{p\in S} \mathcal{N}_p^2 \Gamma &= \sum_{p\in S} \mathrm{Tr}\, (\gamma_p a_p^* + \sigma_p a_{-p})(\gamma_p a_p + \sigma_p a_{-p}^*)(\gamma_p a_p^* + \sigma_p a_{-p})(\gamma_p a_p + \sigma_p a_{-p}^*)\Gamma_0 \\
&\lesssim \sum_{p\in S} (\gamma_p^2 + \sigma_p^2)^2 \,\mathrm{Tr}\,(\mathcal{N}_p^2 + \mathcal{N}_{-p}^2)\Gamma_0 + \sum_{p\in S} \sigma_p^2 (\gamma_p^2 + \sigma_p^2) \\
&\lesssim \sum_{p\in S} \frac{\left[p^2 + 8\pi \mathfrak{a} N^\kappa\right]^2}{|p|^4 + 16\pi \mathfrak{a} N^\kappa p^2} \,\mathrm{Tr}\, \mathcal{N}_p^2 \Gamma_0 \\
&\quad + \frac{1}{2} \sum_{p\in S} \Big[\frac{p^2 + 8\pi \mathfrak{a} N^\kappa}{\sqrt{|p|^4 + 16\pi \mathfrak{a} N^\kappa p^2}} - 1 \Big] \frac{p^2 + 8\pi \mathfrak{a} N^\kappa}{\sqrt{|p|^4 + 16\pi \mathfrak{a} N^\kappa p^2}}
\end{aligned}
\tag{7.2.24}
$$

Inserting (7.2.22), we can again scale $p \mapsto p/N^{\kappa/2}$ and we can approximate with an integral. Compared with (7.2.23), however, the singularity at $p/N^{\kappa/2} \simeq 0$ is more severe since there $\mathrm{Tr}\, \mathcal{N}_p^2 \Gamma_0 \simeq (p/N^{\kappa/2})^{-2}$. For this reason, in the region $N^{-\varepsilon} \leqslant |p|/N^{\kappa/2} \leqslant c$, we estimate $\mathrm{Tr}\, \mathcal{N}_p^2 \Gamma_0 \lesssim N^{2\varepsilon}$. We conclude that $\sum_{p\in S} \mathrm{Tr}\, \mathcal{N}_p^2 \Gamma \lesssim N^{3\kappa/2 + 2\varepsilon}$.

Let us now consider the case $j = 2$. We have

$$
\mathrm{Tr}\, \mathcal{N}_S^2 \Gamma = \sum_{p,q\in S} \mathrm{Tr}\, (\gamma_p a_p^* + \sigma_p a_{-p})(\gamma_p a_p + \sigma_p a_{-p}^*)(\gamma_q a_q^* + \sigma_q a_{-q})(\gamma_q a_q + \sigma_q a_{-q}^*)\Gamma_0 \tag{7.2.25}
$$

Since the Gibbs state Γ_0 factorizes, we find that $\mathrm{Tr}\, \mathcal{N}_S^2 \Gamma$ is the same as $(\mathrm{Tr}\, \mathcal{N}_S \Gamma)^2$, up to terms that are associated with $p = q$ on the right-hand side of (7.2.25) and that can be handled as we did in (7.2.24), producing errors of order $N^{3\kappa/2 + 2\varepsilon} \ll N^{3\kappa}$. We conclude that $cN^{3\kappa} \leqslant \mathrm{Tr}\, \mathcal{N}_S^2 \Gamma \leqslant CN^{3\kappa}$. The second bound in (7.2.21) for $j = 2$ can be proven similarly; we leave the details to the reader. □

7.2.5 Definition of N_0 and proof of Proposition 7.2

From (7.2.20), we are led to the definition

$$
\Gamma_N = W_{N_0} e^{\mathcal{B}_1} T_c \Gamma T_c^* e^{-\mathcal{B}_1} W_{N_0}^* = W_{N_0} e^{\mathcal{B}_1} T_c e^{\mathcal{B}_2}\, \Gamma_0 \, e^{-\mathcal{B}_2} T_c^* e^{-\mathcal{B}_1} W_{N_0}^* \tag{7.2.26}
$$

as trial state for the Hamiltonian $\mathcal{H}_N$ on the small, rescaled box Λ. In the next proposition, we estimate the expected number of particles in the state Γ_N. Its proof is deferred to Section 7.4.7, because it makes use of some properties of T_c that will be discussed in Section 7.4.

Proposition 7.7. *Let Γ_N be given by (7.2.26). Then there exists a constant $C > 0$ such that for ε chosen as in (7.1.9) we have*

$$
N_0 + \mathrm{Tr}\, \mathcal{N}_S \Gamma \leqslant \mathrm{Tr}\, \mathcal{N} \Gamma_N \leqslant N_0 + \mathrm{Tr}\, \mathcal{N}_S \Gamma + CN^{3\kappa/2 - \varepsilon}. \tag{7.2.27}
$$

Prop. 7.7 motivates the following choice of $N_0 \in \mathbb{R}_+$

$$
N_0 := N - \mathrm{Tr}\, \mathcal{N}_S \Gamma + N^{3\kappa/2 - (\kappa - 1/2)}. \tag{7.2.28}
$$

From Lemma 7.6, we conclude that $cN^{3\kappa/2} \leqslant N - N_0 \leqslant CN^{3\kappa/2}$ for all $\kappa > 1/2$ and N large enough. The term $N^{3\kappa/2 - (\kappa - 1/2)}$, which is small compared with $\mathrm{Tr}\, \mathcal{N}_S \Gamma$ for $\kappa > 1/2$, will be used to make sure that the lower bound in (7.1.7) holds true. We are now set to show Prop. 7.2.

Proof of Prop. 7.2. Combining (7.2.28) with Prop. 7.7, we obtain constants $c_1, c_2 > 0$ such that

$$N + c_1 N^{3\kappa/2-(\kappa-1/2)} \leqslant \operatorname{Tr} \mathcal{N}\Gamma_N \leqslant N + c_2 N^{3\kappa/2-\varepsilon}. \tag{7.2.29}$$

Furthermore, we observe that with the definition (7.2.20) of the density matrix Γ and the choice (7.2.28) of N_0, all assumptions in Lemma 7.5 are satisfied. Thus, inserting (7.2.18) into Lemma 7.5 we find

$$\begin{aligned}
&\operatorname{Tr} \mathcal{H}_N\Gamma_N - TN^{2-2\kappa}S(\Gamma_N) \\
&\quad\leqslant 4\pi\mathfrak{a}N^{1+\kappa} + \frac{1}{2}\sum_{p\in S}\big[\sqrt{|p|^4 + 16\pi\mathfrak{a}N^\kappa p^2} - p^2 - 8\pi\mathfrak{a}N^\kappa + \frac{(8\pi\mathfrak{a}N^\kappa)^2}{2p^2}\big] \\
&\qquad + \operatorname{Tr}\sum_{p\in S}\sqrt{|p|^4 + 16\pi\mathfrak{a}N^\kappa p^2}\, a_p^* a_p \Gamma_0 - TN^{2-2\kappa}S(\Gamma_0) + 8\pi\mathfrak{a}N^{5\kappa/2-(\kappa-1/2)} + \delta(\Gamma).
\end{aligned} \tag{7.2.30}$$

Combining (7.2.16) and Lemma 7.6, we conclude that

$$\delta(\Gamma) \lesssim N^{5\kappa/2-\varepsilon/2}$$

if $1/2 < \kappa < 14/27$ and $\varepsilon > 0$ is small enough. As in the proof of Lemma 7.6, we scale $p \mapsto p/N^{\kappa/2}$ in the first sum on the r.h.s. of (7.2.30). We find

$$\begin{aligned}
&\frac{1}{2}\sum_{p\in S}\big[\sqrt{|p|^4 + 16\pi\mathfrak{a}N^\kappa p^2} - p^2 - 8\pi\mathfrak{a}N^\kappa + \frac{(8\pi\mathfrak{a}N^\kappa)^2}{2p^2}\big] \\
&\quad= \frac{N^{5\kappa/2}}{(2\pi)^3}\frac{(2\pi)^3}{N^{3\kappa/2}} \sum_{\substack{p\in N^{-\kappa/2}2\pi\mathbb{Z}^3: \\ N^{-\varepsilon}\leqslant|p|\leqslant N^\varepsilon}} \big[\sqrt{|p|^4 + 16\pi\mathfrak{a}p^2} - p^2 - 8\pi\mathfrak{a} + \frac{(8\pi\mathfrak{a})^2}{2p^2}\big] \\
&\quad\leqslant \frac{N^{5\kappa/2}}{(2\pi)^3}\int_{\mathbb{R}^3} \big[\sqrt{|p|^4 + 16\pi\mathfrak{a}p^2} - p^2 - 8\pi\mathfrak{a} + \frac{(8\pi\mathfrak{a})^2}{2p^2}\big]dp + CN^{2\kappa} \\
&\quad= 4\pi\mathfrak{a}N^{5\kappa/2}\frac{128\mathfrak{a}^{3/2}}{15\sqrt{\pi}} + CN^{2\kappa}.
\end{aligned} \tag{7.2.31}$$

Here, we could extend the sum to all of $\mathbb{Z}^3$ as an upper bound, since the term in the brackets is positive. We then approximated the Riemann sum by an integral, see [39, eq. (8.11)] with $n\ell^{-1} = N^\kappa$ for more details.

Next, we consider the term in the second line of (7.2.30). From the choice (7.2.19) of Γ_0 we conclude, by the Gibbs principle, that

$$\begin{aligned}
&\operatorname{Tr}\sum_{p\in S}\sqrt{|p|^4 + 16\pi\mathfrak{a}N^\kappa p^2}\, a_p^* a_p \Gamma_0 - TN^{2-2\kappa}S(\Gamma_0) \\
&\qquad = -TN^{2-2\kappa}\log Z = TN^{2-2\kappa}\sum_{p\in S}\log\Big[1 - \exp\Big(-\frac{1}{TN^{2-2\kappa}}\sqrt{|p|^4 + 16\pi\mathfrak{a}N^\kappa p^2}\Big)\Big],
\end{aligned}$$

where the last equality is a standard ideal gas computation as in (7.2.22). As before we rescale $p \mapsto p/N^{\kappa/2}$ and replace the resulting Riemann sum by an integral, while keeping in mind the condition $TN^{2-3\kappa} \leqslant C$. We obtain

$$\begin{aligned}
&TN^{2-2\kappa}\sum_{p\in S}\log\Big[1 - \exp\Big(-\frac{1}{TN^{2-2\kappa}}\sqrt{|p|^4 + 16\pi\mathfrak{a}N^\kappa p^2}\Big)\Big] \\
&\qquad\leqslant T^{5/2}N^{5-5\kappa}(2\pi)^{-3}\int_{\mathbb{R}^3}\log\Big[1 - \exp\Big(-\sqrt{|q|^4 + \frac{16\pi\mathfrak{a}q^2}{TN^{2-3\kappa}}}\Big)\Big]dq + CN^{5\kappa/2-\varepsilon},
\end{aligned} \tag{7.2.32}$$

see [39, eq. (9.13)] for more details. Inserting (7.2.32) and (7.2.31) into (7.2.30), we arrive at

$$\begin{aligned}&\operatorname{Tr}\mathcal{H}_N\Gamma_N - TN^{2-2\kappa}S(\Gamma_N)\\&\quad\leqslant\ 4\pi\mathfrak{a}N^{1+\kappa}\left(1+\frac{128}{15\sqrt{\pi}}(N^{-2+3\kappa}\mathfrak{a}^3)^{1/2}\right)\\&\qquad + T^{5/2}N^{5-5\kappa}(2\pi)^{-3}\int_{\mathbb{R}^3}\log\Big[1-\exp\Big(-\sqrt{|q|^4+\frac{16\pi\mathfrak{a}q^2}{TN^{2-3\kappa}}}\Big)\Big]dq + CN^{5\kappa/2-\varepsilon/2}.\end{aligned}\tag{7.2.33}$$

Next, we scale back to the box $\Lambda_L = [-L/2, L/2]^3$, with $L = \rho^{-\gamma}$, for some $\gamma > 1$. We recall the choice $N = \rho L^3 = \rho^{1-3\gamma}$ which translates into $L = N^{1-\kappa}$, with $\kappa = (2\gamma-1)/(3\gamma-1)$. We observe that the condition $\gamma > 1$ is equivalent to $\kappa > 1/2$. We define the unitary operator $\mathcal{U}_L : \mathcal{F}(\Lambda) \to \mathcal{F}(\Lambda_L)$, $(\mathcal{U}_L\psi)^{(n)}(x_1,\dots,x_n) = L^{-3n/2}\psi^{(n)}(x_1/L,\dots,x_n/L)$, for all $n \in \mathbb{N}$ and all $\Psi = \{\psi^{(n)}\}_{n\in\mathbb{N}} \in \mathcal{F}(\Lambda)$ and we remark that the Hamiltonian (7.1.6) satisfies $L^{-2}\mathcal{U}_L\mathcal{H}_N\mathcal{U}_L^* = \mathcal{H}$. Therefore, a good trial state for $\mathcal{H}$ is given by the density matrix $\Gamma_L = \mathcal{U}_L\Gamma_N\mathcal{U}_L^*$ on $\mathcal{F}(\Lambda_L)$. Since $\operatorname{Tr}\mathcal{N}\Gamma_L = \operatorname{Tr}\mathcal{N}\Gamma_N$, it follows from (7.2.29) that

$$c_1\rho^{(\gamma+2)/2} \leqslant \frac{1}{L^3}\operatorname{Tr}\mathcal{N}\Gamma_L - \rho \leqslant c_2\rho^{3/2}$$

in accordance with (7.1.4). Here we used the facts that $N^{\kappa/2}/L = \rho^{1/2}$, that $N^{-2+3\kappa} = \rho$ and that $\kappa = (2\gamma-1)/(3\gamma-1)$. Moreover, from (7.2.33) we obtain

$$\begin{aligned}&\frac{1}{L^3}\Big[\operatorname{Tr}\mathcal{H}\Gamma_L - TS(\Gamma_L)\Big] = L^{-5}\big[\operatorname{Tr}\mathcal{H}_N\Gamma_N - TN^{2-2\kappa}S(\Gamma_N)\big]\\&\leqslant\ 4\pi\mathfrak{a}\rho^2\Big(1+\frac{128}{15\sqrt{\pi}}(\rho\mathfrak{a}^3)^{1/2}\Big) + \frac{T^{5/2}}{(2\pi)^3}\int_{\mathbb{R}^3}\log\Big[1-\exp\big(-\sqrt{|q|^4+16\pi\mathfrak{a}\rho q^2/T}\big)\Big]dq + \rho^{5/2+\epsilon}\end{aligned}$$

for a sufficiently small $\epsilon > 0$ and for all $T \leqslant C\rho\mathfrak{a}$. This concludes the proof of Prop. 7.2. ☐

7.3 Quadratic Transformation on Large Momenta

The goal of this section is to prove Lemma 7.4. Throughout, we will assume $0 \leqslant N - N_0 \lesssim N^{3\kappa/2}$ as in Lemma 7.4. With this aim, we consider separately the action of the Bogoliubov transformation $e^{\mathcal{B}_1}$, determined by (7.2.6), on each term in the excitation Hamiltonian (7.2.2). We start with the diagonal term.

Lemma 7.8. *We have*

$$\begin{aligned}&e^{-\mathcal{B}_1}\sum_{p\in\Lambda^*}\Big(p^2+N_0\widehat{V}_N(0)+N_0\widehat{V}_N(p)\Big)a_p^*a_pe^{\mathcal{B}_1}\\&\qquad = 2\widehat{V}(0)N^\kappa\mathcal{N} + \sum_{p\in\Lambda^*}p^2a_p^*a_p + \sum_{p\in\Lambda^*}p^2s_p\big(a_p^*a_{-p}^*+\text{h.c.}\big) + \sum_{p\in\Lambda^*}p^2s_p^2 + \mathcal{E}_1^{(\text{diag})},\end{aligned}\tag{7.3.1}$$

with

$$\pm\mathcal{E}_1^{(\text{diag})} \lesssim N^{-2+3\kappa}\sum_{p\in\Lambda^*}p^2a_p^*a_p + N^{\kappa-\varepsilon/2}\mathcal{N} + N^{5\kappa/2-\varepsilon/2},$$

for all $0 < \kappa < 2/3$ *and with* $\varepsilon > 0$ *as introduced in* (7.1.9).

Proof. Denote $\beta_p = \Big(p^2+N_0\widehat{V}_N(0)+N_0\widehat{V}_N(p)\Big)$. With (7.2.6) and $c_p^2 - s_p^2 = 1$, we compute

$$e^{-\mathcal{B}_1}\sum_{p\in\Lambda^*}\beta_pa_p^*a_pe^{\mathcal{B}_1} - \sum_{p\in\Lambda^*}\beta_pa_p^*a_p = 2\sum_{p\in\Lambda^*}\beta_ps_p^2a_p^*a_p + \sum_{p\in\Lambda^*}\beta_pc_ps_p\big(a_p^*a_{-p}^*+\text{h.c.}\big) + \sum_{p\in\Lambda^*}\beta_ps_p^2$$

and we obtain

$$
\begin{aligned}
&e^{-\mathcal{B}_1} \sum_{p\in\Lambda^*} \beta_p a_p^* a_p e^{\mathcal{B}_1} - 2\widehat{V}(0)N^\kappa \mathcal{N} - \sum_{p\in\Lambda^*} p^2 a_p^* a_p - \sum_{p\in\Lambda^*} p^2 s_p (a_p^* a_{-p}^* + \mathrm{h.c.}) - \sum_{p\in\Lambda^*} p^2 s_p^2 \\
&= \sum_{p\in\Lambda^*} \Big(N_0 \widehat{V}_N(0) + N_0 \widehat{V}_N(p) - 2\widehat{V}(0)N^\kappa + 2\beta_p s_p^2 \Big) a_p^* a_p \qquad (7.3.2)\\
&+ \sum_{p\in\Lambda^*} \big((N_0 \widehat{V}_N(0) c_p + N_0 \widehat{V}_N(p) c_p + p^2 (c_p - 1) \big) s_p \big(a_p^* a_{-p}^* + \mathrm{h.c.}\big) + \sum_{p\in\Lambda^*} N_0 (\widehat{V}_N(0) + \widehat{V}_N(p)) s_p^2.
\end{aligned}
$$

Let us denote the term on the right-hand side of the previous equation by $\mathcal{E}_1^{(\mathrm{diag})}$. We obtain (7.3.1) and it remains to estimate the error term. In order to control the diagonal part of $\mathcal{E}_1^{(\mathrm{diag})}$, we use $|\widehat{V}_N(p) - \widehat{V}_N(0)| \lesssim p^2 N^{-3+3\kappa}$, which easily follows from the fact that V is even, the assumption of Lemma 7.4 that $0 \leqslant N - N_0 \lesssim N^{3\kappa/2}$, as well as the estimate $\beta_p s_p^2 \lesssim N^{\kappa - 2\varepsilon}$ from (7.2.7) and Lemma 7.3. We find

$$
\begin{aligned}
&\pm \sum_{p\in\Lambda^*} \Big(N_0 \widehat{V}_N(0) + N_0 \widehat{V}_N(p) - 2\widehat{V}(0)N^\kappa + 2\beta_p s_p^2 \Big) a_p^* a_p \\
&\qquad \lesssim N^{-2+3\kappa} \sum_{p\in\Lambda^*} p^2 a_p^* a_p + N^{\kappa-2\varepsilon}\mathcal{N} + N^{-1+5\kappa/2}\mathcal{N}. \qquad (7.3.3)
\end{aligned}
$$

As for the constant term in $\mathcal{E}_1^{(\mathrm{diag})}$, we have

$$
\pm \sum_{p\in\Lambda^*} N_0 (\widehat{V}_N(0) + \widehat{V}_N(p)) s_p^2 \lesssim N^\kappa \|s\|_2^2 \lesssim N^{5\kappa/2 - \varepsilon}. \qquad (7.3.4)
$$

Finally, we consider the off-diagonal part of $\mathcal{E}_1^{(\mathrm{diag})}$. From $0 \leqslant c_p - 1 \leqslant s_p^2$ we find the inequality $N_0 \widehat{V}_N(0) c_p + N_0 \widehat{V}_N(p) c_p + p^2 (c_p - 1) \lesssim N^\kappa$. Thus, Cauchy–Schwarz implies

$$
\begin{aligned}
&\pm \sum_{p\in\Lambda^*} \big((N_0 \widehat{V}_N(0) c_p + N_0 \widehat{V}_N(p) c_p + p^2 (c_p - 1) \big) s_p \big(a_p^* a_{-p}^* + \mathrm{h.c.}\big) \\
&\qquad \lesssim N^\kappa \Big(N^{-\varepsilon/2}\mathcal{N} + N^{\varepsilon/2} \|s\|_\infty^2 \mathcal{N} + N^{\varepsilon/2}\|s\|_2^2 \Big) \lesssim N^{\kappa - \varepsilon/2}\mathcal{N} + N^{5\kappa/2 - \varepsilon/2}.
\end{aligned}
$$

Inserting (7.3.3), (7.3.4) and the last estimate into (7.3.2) yields Lemma 7.8 (using also the assumption $-2 + 3\kappa + 4\varepsilon < 0$ from (7.1.9)). □

Next, we consider the action of $e^{\mathcal{B}_1}$ on the quadratic term Q_2, defined in (7.2.2).

Lemma 7.9. *We have*

$$
e^{-\mathcal{B}_1} Q_2 e^{\mathcal{B}_1} = Q_2 + N_0 \sum_{p\in\Lambda^*} \widehat{V}_N(p) s_p + \mathcal{E}_1^{(Q_2)} \qquad (7.3.5)
$$

with

$$
\pm \mathcal{E}_1^{(Q_2)} \lesssim N^{\kappa - 2\varepsilon}\mathcal{N} + N^{5\kappa/2 - 3\varepsilon},
$$

for all $0 < \kappa < 2/3$ *and with* $\varepsilon > 0$ *as introduced in* (7.1.9).

Proof. With (7.2.6), we compute

$$\begin{aligned}&e^{-\mathcal{B}_1} Q_2 e^{\mathcal{B}_1} - Q_2 \\ &\qquad = N_0 \sum_{p\in\Lambda^*} \widehat{V}_N(p) s_p^2 \,(a_p^* a_{-p}^* + \text{h.c.}) + N_0 \sum_{p\in\Lambda^*} \widehat{V}_N(p) c_p s_p \, a_p^* a_p + N_0 \sum_{p\in\Lambda^*} \widehat{V}_N(p) s_p c_p.\end{aligned}$$

We obtain

$$\mathcal{E}_1^{(Q_2)} = N_0 \sum_{p\in\Lambda^*} \widehat{V}_N(p) s_p^2 \,(a_p^* a_{-p}^* + \text{h.c.}) + N_0 \sum_{p\in\Lambda^*} \widehat{V}_N(p) c_p s_p a_p^* a_p + N_0 \sum_{p\in\Lambda^*} \widehat{V}_N(p) s_p (c_p - 1).$$

The bound for $\mathcal{E}_1^{(Q_2)}$ follows from Cauchy–Schwarz, $0 \leqslant c_p - 1 \leqslant s_p^2$ and Lemma 7.3. $\square$

Next, we consider the cubic term Q_3. Notice that here, and also in the next lemma which is devoted to Q_4, we only bound the restriction of the error term on the range of the projection Ξ; this is enough, since our trial state will be in the range of Ξ.

Lemma 7.10. *We have*

$$e^{-\mathcal{B}_1} Q_3 e^{\mathcal{B}_1} = Q_3 + \mathcal{E}_1^{(Q_3)}, \tag{7.3.6}$$

where, on the range of Ξ*,*

$$\pm \mathcal{E}_1^{(Q_3)} \lesssim N^{-2+4\kappa+5\varepsilon} \big(\mathcal{N}_H + 1\big)^2 + N^{\kappa - 4\varepsilon} \big(\mathcal{N} + N^{3\kappa/2+3\varepsilon}\big),$$

for all $0 < \kappa < 2/3$ *and with* $\varepsilon > 0$ *as introduced in* (7.1.9).

Proof. To compute $e^{-\mathcal{B}_1} Q_3 e^{\mathcal{B}_1}$, we apply (7.2.6). We find (7.3.6), with an error $\mathcal{E}_1^{(Q_3)}$ given, as a quadratic form on the range of Ξ, by

$$\begin{aligned}\mathcal{E}_1^{(Q_3)} = {}& N_0^{1/2} \sum_{p,r\in\Lambda^*} \widehat{V}_N(r) (c_r c_{r+p} c_p - 1)\, a_{-r}^* a_{r+p}^* a_p + N_0^{1/2} \sum_{p,r\in\Lambda^*} \widehat{V}_N(r) c_r c_{r+p} s_p \, a_{-r}^* a_{r+p}^* a_{-p}^* \\ &+ N_0^{1/2} \sum_{p,r\in\Lambda^*} \widehat{V}_N(r) c_r s_{r+p} c_p \, a_{-r}^* a_{-(r+p)} a_p + N_0^{1/2} \sum_{p,r\in\Lambda^*} \widehat{V}_N(r) c_r s_{r+p} s_p \, a_{-r}^* a_{-p}^* a_{-(r+p)} \\ &+ N_0^{1/2} \sum_{p,r\in\Lambda^*} \widehat{V}_N(r) s_r c_{r+p} c_p \, a_{r+p}^* a_r a_p + N_0^{1/2} \sum_{p,r\in\Lambda^*} \widehat{V}_N(r) s_r c_{r+p} s_p \, a_{r+p}^* a_{-p}^* a_r \\ &+ N_0^{1/2} \sum_{p,r\in\Lambda^*} \widehat{V}_N(r) s_r s_{r+p} c_p \, a_r a_{-(r+p)} a_p + \text{h.c.}\end{aligned} \tag{7.3.7}$$

Here we already used the fact that terms that annihilate or create particles with momenta in $(H \cup S)^c$, as well as terms that do not preserve the parity of $\mathcal{N}_H$ vanish on the range of Ξ. In particular, all contributions where two momenta contract in the canonical commutation relation must vanish since, by momentum conservation, these terms are either proportional to a_0 or to a_0^*. Additionally, the terms proportional to $s_r s_{r+p} s_p$ must vanish on the range of Ξ because, since s is zero on S, we would need $-r, p+r, p \in H$; this, however, breaks the parity of $\mathcal{N}_H$. To bound the contributions in (7.3.7), we argue again with the parity of $\mathcal{N}_H$ to conclude that among the three momenta $r, r+p, p$, two must be in H, one in S. Keeping this in mind, and moving around factors of $(\mathcal{N}_H+1)^{\pm 1}$, $(\mathcal{N}+1)^{\pm 1/2}$ as needed, we can estimate the terms on the right-hand side of (7.3.7) as follows. Let us consider the first term. We use $|c_r c_{r+p} c_p - 1| \leqslant s_r^2 + s_{r+p}^2 + s_p^2$ and the notation s_H for the restriction of the coefficients s_p to the set H. Then, for $\xi \in \operatorname{Ran}\Xi$, we obtain

$$\begin{aligned}&\Big| N_0^{1/2} \sum_{p,r\in\Lambda^*} \widehat{V}_N(r) (c_r c_{r+p} c_p - 1) \langle \xi, a_r^* a_{r+p}^* a_p \xi\rangle \Big| \\ &\qquad \lesssim N^{-1/2+\kappa} \big(\|s_H^2\|_2 + \|s_H^2\|_\infty N^{3\kappa/4+3\varepsilon/2}\big) \|(\mathcal{N}_H+1)\xi\| \|(\mathcal{N}+1)^{1/2}\xi\| \\ &\qquad \lesssim N^{-3+11\kappa/2+5\varepsilon/2} \|(\mathcal{N}_H+1)\xi\| \|(\mathcal{N}+1)^{1/2}\xi\|.\end{aligned}$$

Here we used that in the term proportional to s_p^2 we have $p \in H$ so that either $r \in S$ or $r+p \in S$; this allows us to sum up the second momentum after a Cauchy–Schwarz inequality (recall that $|S| \leqslant CN^{3\kappa/2+3\varepsilon}$). Moreover, we used Lemma 7.3 to bound $\|s_H^2\|_2 \leqslant CN^{-5/2+9\kappa/2+5\varepsilon/2}$, $\|s_H^2\|_\infty \leqslant CN^{-4+6\kappa+4\varepsilon}$ and the condition $4\varepsilon - 2 + 3\kappa < 0$ from (7.1.9).

To estimate the second term on the right-hand side of (7.3.7), we assume for example that $r, p \in H$, $r+p \in S$ (the case $r+p, p \in H$, $r \in S$ can be treated similarly). Since c is bounded uniformly in N and with the estimate $\|s_H\|_2 \lesssim N^{(-1+3\kappa+\varepsilon)/2}$ we find

$$\begin{aligned}\Big|N_0^{1/2} \sum \widehat{V}_N(r) c_r c_{r+p} s_p \, \langle \xi, a^*_{-r} a^*_{r+p} a^*_{-p} \xi \rangle\Big| &\lesssim N^{-1/2+\kappa} \sum s_p \|a_{-r} a_{-p} \xi\| \left[\|a_{r+p}\xi\| + \|\xi\|\right] \\ &\lesssim N^{-1/2+\kappa} \|s_H\|_2 \|\mathcal{N}_H \xi\| \big(\|\mathcal{N}^{1/2}\xi\| + N^{3\kappa/4+3\varepsilon/2}\|\xi\|\big) \\ &\lesssim N^{\frac{-2+5\kappa+\varepsilon}{2}} \|\mathcal{N}_H \xi\| \big(\|\mathcal{N}^{1/2}\xi\| + N^{3\kappa/4+3\varepsilon/2}\|\xi\|\big).\end{aligned}$$

The next four terms on the right-hand side of (7.3.7) can all be estimated in the same way applying a Cauchy–Schwarz inequality. We obtain

$$\begin{aligned}&\Big|N_0^{1/2} \sum_{p,r\in\Lambda^*} \widehat{V}_N(r) c_r s_{r+p} c_p \, \langle \xi, a^*_{-r} a_{-(r+p)} a_p \xi\rangle\Big|, \; \Big|N_0^{1/2} \sum_{p,r\in\Lambda^*} \widehat{V}_N(r) c_r s_{r+p} s_p \, \langle \xi, a^*_{-r} a^*_{-p} a_{-(r+p)} \xi\rangle\Big|, \\ &\Big|N_0^{1/2} \sum_{p,r\in\Lambda^*} \widehat{V}_N(r) s_r c_{r+p} c_p \, \langle \xi, a^*_{r+p} a_r a_p \xi\rangle\Big|, \; \Big|N_0^{1/2} \sum_{p,r\in\Lambda^*} \widehat{V}_N(r) s_r c_{r+p} s_p \, \langle \xi, a^*_{r+p} a^*_{-p} a_r \xi\rangle\Big| \\ &\qquad \lesssim N^{-1/2+\kappa} \|s_H\|_2 \|(\mathcal{N}_H+1)\xi\| \|(\mathcal{N}+1)^{1/2}\xi\| \\ &\qquad \lesssim N^{\frac{-2+5\kappa+\varepsilon}{2}} \|(\mathcal{N}_H+1)\xi\| \|(\mathcal{N}+1)^{1/2}\xi\|.\end{aligned}$$

Finally, we control the last term on the right-hand side of (7.3.7). We find

$$\begin{aligned}&\Big|N_0^{1/2} \sum_{p,r\in\Lambda^*} \widehat{V}_N(r) s_r s_{r+p} c_p \, \langle \xi, a_r a_{-(r+p)} a_p \xi\rangle\Big| \\ &\qquad\qquad \lesssim N^{-1/2+\kappa} \sum s_r s_{r+p} \|a_r a_{-(r+p)}\xi\| \big(\|a_p\xi\| + \|\xi\|\big) \\ &\qquad\qquad \lesssim N^{-1/2+\kappa} \|\mathcal{N}_H\xi\| \big(\|s_H\|_2 \|s_H\|_\infty \|\mathcal{N}^{1/2}\xi\| + \|s_H\|_2^2 \|\xi\|\big) \\ &\qquad\qquad \lesssim N^{-3+11\kappa/2+5\varepsilon/2} \|\mathcal{N}_H\xi\| \|\mathcal{N}^{1/2}\xi\| + N^{-3/2+4\kappa+\varepsilon} \|\mathcal{N}_H\xi\| \|\xi\|.\end{aligned}$$

Putting all together, we conclude that, for any $0 < \kappa < 2/3$ and $\varepsilon > 0$ as in (7.1.9), we have

$$\begin{aligned}|\langle \xi, \mathcal{E}_1^{(Q_3)} \xi\rangle| &\lesssim N^{\frac{-2+5\kappa+\varepsilon}{2}} \|(\mathcal{N}_H+1)\xi\| \big(\|\mathcal{N}^{1/2}\xi\| + N^{3\kappa/4+3\varepsilon/2}\|\xi\|\big) \\ &\leqslant N^{-2+4\kappa+5\varepsilon} \|(\mathcal{N}_H+1)\xi\|^2 + N^{\kappa-4\varepsilon}\big(\|\mathcal{N}^{1/2}\xi\|^2 + N^{3\kappa/2+3\varepsilon}\|\xi\|^2\big).\end{aligned}$$

□

Finally, let us compute the action of $e^{\mathcal{B}_1}$ on the quartic term Q_4. Here, the restriction on κ and ε only serves to simplify the form of the error terms.

Lemma 7.11. *We have*

$$e^{-\mathcal{B}_1} Q_4 e^{\mathcal{B}_1} = Q_4 + \frac{1}{2} \sum_{p,r\in\Lambda^*} \widehat{V}_N(r-p) s_r \big(a^*_p a^*_{-p} + \text{h.c.}\big) + \frac{1}{2} \sum_{p,r\in\Lambda^*} \widehat{V}_N(p-r) s_p s_r + \mathcal{E}_1^{(Q_4)}, \quad (7.3.8)$$

where, on the range of Ξ*,*

$$\pm \mathcal{E}_1^{(Q_4)} \lesssim N^{-\kappa/2-\varepsilon} \mathcal{N}^2 + N^{-3+7\kappa+4\varepsilon} \mathcal{N}_H^2 + N^{2-2\kappa-2\varepsilon} \mathcal{N}_H + N^{\kappa-3\varepsilon} \mathcal{N} + N^{5\kappa/2-\varepsilon},$$

if $1/2 < \kappa < 8/15 - 2\varepsilon/3$ *and* $\varepsilon > 0$ *is chosen as in* (7.1.9).

Proof. With (7.2.6), we decompose

$$e^{-\mathcal{B}_1} Q_4 e^{\mathcal{B}_1} = \frac{1}{2}\sum_{j=0}^{4} A_j \tag{7.3.9}$$

where A_j collects all contributions with exactly j coefficients s_k, with $k \in \{p+r, q, q+r, p\}$. We will see that the contributing terms stem from A_0, A_1 and A_2. For $j = 0$, we clearly have

$$A_0 = \sum_{p,r,q\in\Lambda^*} \widehat{V}_N(r) c_{p+r} c_q c_{q+r} c_p a^*_{p+r} a^*_q a_{q+r} a_p.$$

We observe that

$$A_0 - 2Q_4 = \sum_{p,r,q\in\Lambda^*} \widehat{V}_N(r)\big[c_{p+r} c_q c_{q+r} c_p - 1\big] a^*_{p+r} a^*_q a_{q+r} a_p.$$

Estimating $|c_{p+r} c_q c_{q+r} c_p - 1| \leqslant s^2_{p+r} + s^2_q + s^2_{q+r} + s^2_p$, we find

$$\big|\langle \xi, (A_0 - 2Q_4)\xi\rangle\big| \leqslant 4\Big|\sum \widehat{V}_N(r) s^2_p \langle a_{p+r} a_q \xi, a_{q+r} a_p \xi\rangle\Big|.$$

For ξ in the range of Ξ, we must have $p+r, q, q+r, p \in H \cup S$. Since $s_p = 0$ for $p \in S$, we can assume $p \in H$. To preserve the parity of $\mathcal{N}_H$, there must be a second momentum in H. Assuming for example $q \in H$, we can estimate, using Lemma 7.3,

$$\begin{aligned}
\Big|&\sum_{p,q\in H, r\in\Lambda^*} \widehat{V}_N(r) s^2_p \langle a_{p+r} a_q \xi, a_p a_{q+r}\xi\rangle\Big| \\
&\lesssim \sum_{p,q\in H, r\in\Lambda^*} |\widehat{V}_N(r)||s_p| \|a_{p+r} a_q \xi\| \|a_p a_{q+r}\xi\| \\
&\lesssim \Big[\sum_{p,q\in H, r\in\Lambda^*} s^4_p \|a_{p+r} a_q \xi\|^2\Big]^{1/2} \Big[\sum_{p,q\in H, r\in\Lambda^*} \widehat{V}^2_N(r) \|a_p a_{q+r}\xi\|^2\Big]^{1/2} \\
&\lesssim N^{-2+4\kappa+5\varepsilon/2} \|\mathcal{N}^{1/2}\mathcal{N}_H^{1/2}\xi\|^2,
\end{aligned}$$

where we used $\|\widehat{V}_N\|_2 \lesssim N^{(1-\kappa)/2}$ and $s_p \lesssim N^\kappa p^{-2}$. Moving factors of $(\mathcal{N}+1)^{1/2}, (\mathcal{N}_H+1)^{1/2}$ around, we can similarly bound also contributions arising when $p+r \in H$ or $q+r \in H$. With the assumption $-2+3\kappa+4\varepsilon < 0$ from (7.1.9), we conclude that, on the range of Ξ,

$$\pm\Big(\frac{1}{2}A_0 - Q_4\Big) \lesssim N^{-2+4\kappa+5\varepsilon/2}(\mathcal{N}+1)(\mathcal{N}_H+1) \lesssim N^{-\kappa/2-\varepsilon}\mathcal{N}^2 + N^{-4+17\kappa/2+6\varepsilon}\mathcal{N}_H^2 + N^{5\kappa/2-\varepsilon}. \tag{7.3.10}$$

Next, we consider the term A_1 in (7.3.9). Arranging operators in normal order we find

$$A_1 = 2\sum_{p,q,r\in\Lambda^*} \widehat{V}_N(r) s_{p+r} c_q c_{q+r} c_p \big(a^*_q a_{-p-r} a_{q+r} a_p + \text{h.c.}\big) + \sum_{p,r\in\Lambda^*} \widehat{V}_N(r) s_{p+r} c_{p+r} c^2_p \left(a_p a_{-p} + \text{h.c.}\right).$$

Let us start to bound the first term. On the range of Ξ, all momenta must be in $H \cup S$. In particular, $p+r \in H$. To preserve parity of $\mathcal{N}_H$, there can be, in total, two or four momenta in H. Handling these two cases separately (if all momenta are in H, we need to use $\widehat{V}_N$ to perform one of the sum; if instead 2 momenta are in S, we can use $|S| \leqslant N^{3\kappa/2+3\varepsilon}$), we arrive at

$$\begin{aligned}
\Big|&\sum_{p,q,r} \widehat{V}_N(r) s_{p+r} c_q c_{q+r} c_p \langle \xi, a^*_q a_{-p-r} a_{q+r} a_p \xi\rangle\Big| \\
&\lesssim N^{\kappa+\varepsilon/2}\|(\mathcal{N}_H+1)\xi\|^2 + N^{\frac{-6+13\kappa+2\varepsilon}{4}}\|(\mathcal{N}+1)^{1/2}(\mathcal{N}_H+1)^{1/2}\xi\|^2.
\end{aligned}$$

As for the quadratic contribution to A_1, we observe that

$$\begin{aligned}
&\Big|\sum_{p,r}\widehat{V}_N(r)s_{p+r}(c_{p+r}c_p^2-1)\langle\xi,a_pa_{-p}\xi\rangle\Big| \\
&\lesssim \sum_{p,r}|\widehat{V}_N(r)|s_{p+r}\big(s_{p+r}^2+s_p^2\big)\left[\|a_p\xi\|^2+\|a_p\xi\|\|\xi\|\right] \\
&\lesssim \|s^2\|_\infty\||\widehat{V}_N|*s\|_\infty\|\mathcal{N}^{1/2}\xi\|^2+\||\widehat{V}_N|*s\|_\infty\|s^2\|_2\|\mathcal{N}^{1/2}\xi\|\|\xi\|+\sum_p\big(|\widehat{V}_N|*s^3\big)(p)\|a_p\xi\|\|\xi\|.
\end{aligned}$$

The first two terms are bounded with $\||\widehat{V}_N|*s\|_\infty\lesssim N^\kappa$. To bound the last term, we distinguish the cases $p\in H$ and $p\in S$ (on the range of Ξ, there is no other possibility). We find, with $\||\widehat{V}_N|*s^3\|_2\lesssim\|\widehat{V}_N\|_2\|s^3\|_1\lesssim N^{1/2+\kappa-3\varepsilon}$,

$$\begin{aligned}
\sum_p\big(|\widehat{V}_N|*s^3\big)(p)\|a_p\xi\|\|\xi\| &\lesssim \||\widehat{V}_N|*s^3\|_2\|\mathcal{N}_H^{1/2}\xi\|\|\xi\|+\||\widehat{V}_N|*s^3\|_\infty N^{3\kappa/4+3\varepsilon/2}\|\mathcal{N}^{1/2}\xi\|\|\xi\| \\
&\lesssim N^{1/2+\kappa-3\varepsilon}\|\mathcal{N}_H^{1/2}\xi\|\|\xi\|+N^{7\kappa/4-5\varepsilon/2}\|\mathcal{N}^{1/2}\xi\|\|\xi\|
\end{aligned}$$

We conclude that, on Ran Ξ,

$$\begin{aligned}
&\pm\Big[A_1-\sum_{p,r\in\Lambda^*}\widehat{V}(r)s_{p+r}\big(a_pa_{-p}+\text{h.c.}\big)\Big] \\
&\quad\lesssim N^{\kappa+\varepsilon/2}(\mathcal{N}_H^2+1)+N^{-\kappa/2-\varepsilon}\mathcal{N}^2+N^{-3+7\kappa+2\varepsilon}\mathcal{N}_H^2+N^{\kappa-4\varepsilon}\mathcal{N}+N^{1-\kappa/2-5\varepsilon}\mathcal{N}_H+N^{5\kappa/2-\varepsilon}
\end{aligned}\tag{7.3.11}$$

for any $0<\kappa<2/3$ and $\varepsilon>0$ as in (7.1.9).

We switch our attention to the term

$$\begin{aligned}
A_2=&\sum\widehat{V}_N(r)c_{p+r}c_qs_{q+r}s_p\big(a_{p+r}^*a_q^*a_{-q-r}^*a_{-p}^*+\text{h.c.}\big) \\
&+2\sum\widehat{V}_N(r)c_{p+r}s_qc_{q+r}s_pa_{p+r}^*a_{-p}^*a_{-q}a_{q+r} \\
&+2\sum\widehat{V}_N(r)c_{p+r}s_qs_{q+r}c_pa_{p+r}^*a_{-q-r}^*a_{-q}a_p \\
&+\sum\widehat{V}_N(r)c_qs_qc_{q+r}s_{q+r}\big(4a_q^*a_q+1\big) \\
&+2\sum\widehat{V}_N(r)c_p^2s_{p+r}^2a_p^*a_p+2\widehat{V}_N(0)\sum c_p^2s_q^2a_p^*a_p.
\end{aligned}\tag{7.3.12}$$

The only contributing term is the constant in the fourth line. We estimate the other terms. To control the term in the first line, we observe that, on the range of Ξ, the four momenta $p+r,q,-q-r,-p$ must be in $H\cup S$ and, more precisely, either 4 or 2 of them must be in H (to preserve parity). Let us assume, first, that all four momenta are in H. Denoting by $\sum^*$ the sum over all $p,q,r\in\Lambda^*$, with $p+r,q,-q-r,-p\in H$, we can bound

$$\begin{aligned}
&\Big|\sum^*\widehat{V}_N(r)c_{p+r}c_qs_{q+r}s_p\langle\xi,a_{p+r}^*a_q^*a_{-q-r}^*a_{-p}^*\xi\rangle\Big| \\
&\lesssim\sum^*|\widehat{V}_N(r)|s_{q+r}s_p\|a_{p+r}a_{-p}a_{-q-r}(\mathcal{N}_H+1)^{-1/2}\xi\|\left[\|a_q(\mathcal{N}_H+1)^{1/2}\xi\|+\|(\mathcal{N}_H+1)^{1/2}\xi\|\right] \\
&\lesssim\|(\mathcal{N}_H+1)\xi\|\Bigg(\|\widehat{V}_N\|_\infty\Big[\sum^*s_{q+r}^2s_p^2\|a_q(\mathcal{N}_H+1)^{1/2}\xi\|^2\Big]^{1/2} \\
&\qquad\qquad+\|(\mathcal{N}_H+1)^{1/2}\xi\|\Big[\sum^*|\widehat{V}_N(r)|^2s_{q+r}^2s_p^2\Big]^{1/2}\Bigg) \\
&\lesssim N^{-2+4\kappa+\varepsilon}\|(\mathcal{N}_H+1)\xi\|^2+N^{-1/2+5\kappa/2+\varepsilon}\|(\mathcal{N}_H+1)\xi\|\|(\mathcal{N}_H+1)^{1/2}\xi\| \\
&\lesssim\big(N^{-2+4\kappa+\varepsilon}+N^{-3+7\kappa+4\varepsilon}\big)\|(\mathcal{N}_H+1)\xi\|^2+N^{2-2\kappa-2\varepsilon}\|(\mathcal{N}_H+1)^{1/2}\xi\|^2
\end{aligned}$$

for $0 < \kappa < 2/3$ (we absorb the second contribution by a Cauchy–Schwarz inequality with appropriate weights). If two momenta are in H and two in S (in this case, we must have $p + r, q \in S$, $q + r, p \in H$, since $s = 0$ on S), we proceed similarly, but instead of using the potential $\widehat{V}_N$ to sum over the third momentum (as we did in the fourth line of the last equation), we use the restriction onto S, estimating $\widehat{V}_N$ in ℓ^∞. Indicating with $\sum^{**}$ the sum over $p + r, q \in S, q + r, p \in H$, we find

$$
\begin{aligned}
&\Big|\sum^{**}\widehat{V}_N(r)c_{p+r}c_q s_{q+r}s_p\langle\xi, a^*_{p+r}a^*_q a^*_{-q-r}a^*_{-p}\xi\rangle\Big| \\
&\quad\lesssim N^{-2+4\kappa+\varepsilon}\|(\mathcal{N}+1)^{1/2}(\mathcal{N}_H+1)^{1/2}\xi\|^2 + N^{-2+\frac{19\kappa}{4}+\frac{5\varepsilon}{2}}\|(\mathcal{N}+1)^{1/2}(\mathcal{N}_H+1)^{1/2}\xi\|\|(\mathcal{N}_H+1)^{1/2}\xi\| \\
&\quad\lesssim N^{-2+4\kappa+2\varepsilon}\|(\mathcal{N}+1)^{1/2}(\mathcal{N}_H+1)^{1/2}\xi\|^2 + N^{-2+11\kappa/2+3\varepsilon}\|(\mathcal{N}_H+1)^{1/2}\xi\|^2.
\end{aligned}
$$

The second and the third terms on the right-hand side of (7.3.12) can be bounded by a simple Cauchy–Schwarz inequality (remarking that, on the range of Ξ, the momenta associated with the coefficients s must lie in H). We find

$$
\begin{aligned}
\Big|\sum \widehat{V}_N(r)c_{p+r}s_q c_{q+r}s_p\langle\xi, a^*_{p+r}a^*_{-p}a_{-q}a_{q+r}\xi\rangle\Big| &\lesssim N^{-2+4\kappa+\varepsilon}\|\mathcal{N}_H^{1/2}\mathcal{N}^{1/2}\xi\|^2 \\
\Big|\sum \widehat{V}_N(r)c_{p+r}s_q s_{q+r}c_p\langle\xi, a^*_{p+r}a^*_{-q-r}a_{-q}a_p\xi\rangle\Big| &\lesssim N^{-2+4\kappa+\varepsilon}\|\mathcal{N}_H^{1/2}\mathcal{N}^{1/2}\xi\|^2.
\end{aligned}
$$

The quadratic part of the fourth term in (7.3.12) can be bounded, using that $\|\widehat{V}_N * s\|_\infty \lesssim N^\kappa$ and that $q \in H$ on the range of Ξ (because $s_q = 0$ for $|q| \leqslant N^{\kappa/2+\varepsilon}$). We find

$$
\Big|\sum \widehat{V}_N(r)c_q s_q c_{q+r}s_{q+r}\langle a_q\xi, a_q\xi\rangle\Big| \lesssim N^{-2+4\kappa+2\varepsilon}\|\mathcal{N}_H^{1/2}\xi\|^2.
$$

As for the constant term, we extract a contribution observing that

$$
\Big|\sum \widehat{V}_N(r)(c_q c_{q+r}-1)s_q s_{q+r}\Big| \leqslant \sum |\widehat{V}_N(r)|(s_q^3 s_{q+r} + s_q s_{q+r}^3) \lesssim \|\widehat{V}_N\|_\infty\|s\|_1\|s^3\|_1 \lesssim N^{5\kappa/2-3\varepsilon},
$$

where we used that $\|s\|_1 \lesssim N\|\varphi\|_1 \lesssim N$. The terms on the last line of (7.3.12) are simply estimated by

$$
\Big|\sum \widehat{V}_N(r)c_p^2 s_{p+r}^2\langle\xi, a^*_p a_p\xi\rangle\Big|,\ |\widehat{V}_N(0)|\Big|\sum c_p^2 s_q^2\langle\xi, a^*_p a_p\xi\rangle\Big| \lesssim N^{-1+5\kappa/2-\varepsilon}\|\mathcal{N}^{1/2}\xi\|^2.
$$

Thus, on Ran Ξ,

$$
\begin{aligned}
\pm\Big[A_2 - \sum_{q,r\in\Lambda^*}\widehat{V}_N(r)s_q s_{q+r}\Big] \lesssim\ & N^{-3+7\kappa+4\varepsilon}\mathcal{N}_H^2 + \big(N^{2-2\kappa-2\varepsilon} + N^{-2+11\kappa/2+3\varepsilon}\big)(\mathcal{N}_H+1) \\
&+ N^{-2+4\kappa+2\varepsilon}\mathcal{N}\mathcal{N}_H + N^{-1+5\kappa/2-\varepsilon}\mathcal{N} + N^{5\kappa/2-\varepsilon} \\
\leqslant\ & N^{-3+7\kappa+4\varepsilon}\mathcal{N}_H^2 + \big(N^{2-2\kappa-2\varepsilon} + N^{-2+11\kappa/2+3\varepsilon}\big)(\mathcal{N}_H+1) \\
&+ N^{-\kappa/2-\varepsilon}\mathcal{N}^2 + N^{-1+5\kappa/2-\varepsilon}\mathcal{N} + N^{5\kappa/2-\varepsilon} \qquad (7.3.13)
\end{aligned}
$$

for all $0 < \kappa < 2/3$ and for $\varepsilon > 0$ as in (7.1.9).

Next, we consider

$$
\begin{aligned}
A_3 = &\ 2\sum \widehat{V}_N(r)c_{p+r}s_q s_{q+r}s_p\big(a^*_{p+r}a^*_{-q-r}a^*_{-p}a_{-q} + \text{h.c.}\big) \\
&+ 2\sum \widehat{V}_N(r)s_q c_q s_{q+r}^2\big(a^*_q a^*_{-q} + \text{h.c.}\big) \\
&+ \sum \widehat{V}_N(r)s_q c_q s_{q+r}^2\big(a^*_{q+r}a^*_{-q-r} + \text{h.c.}\big) \\
&+ 2\widehat{V}_N(0)\sum s_q^2 s_p c_p\big(a^*_p a^*_{-p} + \text{h.c.}\big).
\end{aligned}
$$

We can control the quartic term noticing that, on the range of Ξ, all momenta $p+r, q, q+r, p$ must be in H (because $s=0$ on S and because of parity). With $\|s_H\|_\infty \lesssim N^{3\kappa-2+2\varepsilon}$, we find, for $\xi \in \operatorname{Ran} \Xi$,

$$\begin{aligned}\Big|\sum \widehat{V}_N(r) c_{p+r} s_q s_{q+r} s_p \langle \xi, a^*_{p+r} a^*_{-q-r} a^*_{-p} a_{-q} \xi\rangle\Big| &\lesssim \|\widehat{V}_N\|_\infty \|s_H\|_\infty \|s_H\|_2^2 \|(\mathcal{N}_H+1)\xi\|^2 \\ &\lesssim N^{-4+7\kappa+3\varepsilon} \|(\mathcal{N}_H+1)\xi\|^2.\end{aligned}$$

The quadratic terms can be estimated, for $\xi \in \operatorname{Ran} \Xi$, by

$$\begin{aligned}&\Big|\sum \widehat{V}_N(r) s_q c_q s^2_{q+r} \langle \xi, a^*_q a^*_{-q} \xi\rangle\Big|, \Big|\widehat{V}_N(0) \sum s_q^2 s_p c_p \langle \xi, a^*_p a^*_{-p} \xi\rangle\Big| \\ &\qquad \lesssim \|\widehat{V}_N\|_\infty \|s\|_2^2 \|s_H\|_2 \|(\mathcal{N}_H+1)^{1/2}\xi\|^2 \lesssim N^{-3/2+4\kappa-\varepsilon/2} \|(\mathcal{N}_H+1)^{1/2}\xi\|^2\end{aligned}$$

and by

$$\begin{aligned}\Big|\sum \widehat{V}_N(r) s_{q+r} c_{q+r} s_q^2 \langle \xi, a^*_q a^*_{-q} \xi\rangle\Big| &\lesssim \|\widehat{V}_N * s\|_\infty \|s_H^2\|_2 \|(\mathcal{N}_H+1)^{1/2}\xi\|^2 \\ &\lesssim N^{-5/2+11\kappa/2+5\varepsilon/2} \|(\mathcal{N}_H+1)^{1/2}\xi\|^2\end{aligned}$$

We conclude that, on the range of Ξ,

$$\pm A_3 \lesssim N^{-4+7\kappa+3\varepsilon} \mathcal{N}_H^2 + N^{-3/2+4\kappa+\varepsilon/2} \mathcal{N}_H + N^{5\kappa/2-\varepsilon} \tag{7.3.14}$$

for all $0<\kappa<2/3$ and for $\varepsilon>0$ as in (7.1.9).

Finally, we bound the contribution

$$\begin{aligned}A_4 = &\sum \widehat{V}_N(r) s_{p+r} s_q s_{q+r} s_p a^*_{-q-r} a^*_{-p} a_{-p-r} a_{-q} \\ &+ \sum \widehat{V}_N(r) s^2_{p+r} s_p^2 \big(2a^*_{-p} a_{-p} + 1\big) + \widehat{V}_N(0) \sum s_p^2 s_q^2 \big(2a^*_{-q} a_{-q} + 1\big).\end{aligned}$$

Proceeding similarly as we did for A_3, we easily find that, on $\operatorname{Ran} \Xi$,

$$\begin{aligned}A_4 &\lesssim \|\widehat{V}_N\|_\infty \|s_H^2\|_\infty \|s_H\|_2^2 \mathcal{N}_H^2 + \|\widehat{V}_N\|_\infty \|s_H^2\|_\infty \|s^2\|_1 \mathcal{N}_H + \|\widehat{V}_N\|_\infty \|s^2\|_1^2 \\ &\lesssim N^{-6+10\kappa+5\varepsilon} \mathcal{N}_H^2 + N^{-5+17\kappa/2+3\varepsilon} \mathcal{N}_H + N^{-1+4\kappa-2\varepsilon}.\end{aligned}$$

Combining the last equation with (7.3.10), (7.3.11), (7.3.13), (7.3.14), we obtain (7.3.8), with an error $\mathcal{E}_1^{(Q_4)}$ satisfying, on $\operatorname{Ran} \Xi$,

$$\pm \mathcal{E}_1^{(Q_4)} \lesssim N^{-\kappa/2-\varepsilon} \mathcal{N}^2 + N^{-3+7\kappa+4\varepsilon} \mathcal{N}_H^2 + N^{2-2\kappa-2\varepsilon} \mathcal{N}_H + N^{\kappa-3\varepsilon} \mathcal{N} + N^{5\kappa/2-\varepsilon},$$

where we used the assumption $1/2 < \kappa < 8/15 - 2\varepsilon/3$ (in particular $\varepsilon < 1/20$). □

7.3.1 Proof of Lemma 7.4

We are now ready to show Lemma 7.4. Combining the statements of Lemmas 7.8, 7.9, 7.10 and 7.11, we find

$$\begin{aligned}&e^{-\mathcal{B}_1} W^*_{N_0} \mathcal{H}_N W_{N_0} e^{\mathcal{B}_1} \\ &\quad = \frac{N_0^2}{2} \widehat{V}_N(0) + \sum_{p \in \Lambda^*} p^2 a^*_p a_p + 2N^\kappa \widehat{V}(0) \mathcal{N} + Q_3 + Q_4 \\ &\qquad + \sum_{p \in \Lambda^*} \Big[p^2 s_p + \frac{1}{2} N_0 \widehat{V}_N(p) + \frac{1}{2} \sum_{r \in \Lambda^*} \widehat{V}_N(r-p) s_r\Big] (a^*_p a^*_{-p} + \text{h.c.}) \\ &\qquad + \sum_{p \in \Lambda^*} \Big[p^2 s_p^2 + N_0 \widehat{V}_N(p) s_p + \frac{1}{2} \sum_{r \in \Lambda^*} \widehat{V}_N(p-r) s_p s_r\Big] + \widetilde{\mathcal{E}}_1\end{aligned} \tag{7.3.15}$$

where, on the range of Ξ,

$$\widetilde{\mathcal{E}}_1 \lesssim N^{-3\varepsilon} \sum_{p\in\Lambda^*} p^2 a_p^* a_p + N^{-\kappa/2-\varepsilon}\mathcal{N}^2 + N^{-3+7\kappa+4\varepsilon}\mathcal{N}_H^2 \\ + N^{2-2\kappa-2\varepsilon}\mathcal{N}_H + N^{\kappa-\varepsilon/2}\mathcal{N} + N^{5\kappa/2-\varepsilon/2}, \tag{7.3.16}$$

if $1/2 < \kappa < 8/15 - 2\varepsilon/3$. Here we also used the fact that the contribution $e^{-\mathcal{B}_1} Q_1 e^{\mathcal{B}_1}$, with Q_1 as in (7.2.2), vanishes on the range of Ξ. With a slight abuse of notation that is only used in this subsection, we introduce the following momentum sets

$$L = \{p \in \Lambda^*\backslash\{0\} : |p| \leqslant N^{\kappa/2+\varepsilon}\}, \quad L^c = \{p \in \Lambda^* : |p| > N^{\kappa/2+\varepsilon}\}.$$

The constant term on the last line of (7.3.15) can be rewritten, using (7.2.7), (7.2.3) and (7.2.4). We find

$$\begin{aligned}
&\sum_{p\in\Lambda^*}\Big[p^2 s_p^2 + N_0 \widehat{V}_N(p) s_p + \frac{1}{2}\sum_{r\in\Lambda^*}\widehat{V}_N(p-r) s_p s_r\Big] \\
&\quad = \frac{N_0^2}{2}\sum_{p\in L^c}\widehat{V}_N(p)\varphi_p - \frac{N_0^2}{2}\sum_{\substack{r\in L\\ p\in L^c}}\widehat{V}_N(p-r)\varphi_p\varphi_r \\
&\quad = \frac{N_0^2}{2N^{1-\kappa}}(8\pi\mathfrak{a}_N - \widehat{V}(0)) - N_0^2\sum_{p\in L}\varphi_p\left[\frac{\widehat{V}_N(p)}{2} + \frac{1}{2}\sum_{r\in L^c}\widehat{V}_N(p-r)\varphi_r\right] \\
&\quad = \frac{N_0^2}{2N}N^\kappa(8\pi\mathfrak{a}_N - \widehat{V}(0)) + N_0^2\sum_{p\in L}p^2\varphi_p^2 + \frac{N_0^2}{2}\sum_{p,r\in L}\widehat{V}_N(p-r)\varphi_p\varphi_r.
\end{aligned}$$

The last term is bounded by $CN^{-1+4\kappa+2\varepsilon}$. We write

$$\frac{N_0^2}{2}\sum_{p,r\in L}\widehat{V}_N(p-r)\varphi_p\varphi_r = \mathcal{O}\left(N^{-1+4\kappa+2\varepsilon}\right).$$

As for the second term, we observe that

$$N_0^2\sum_{p\in L}p^2\varphi_p^2 = N_0^2\sum_{p\in S}p^2\varphi_p^2 + \mathcal{O}\big(N^{5\kappa/2-\varepsilon}\big).$$

Estimating $|\widehat{V}_N(p-r) - \widehat{V}_N(r)| \lesssim N^{-2+2\kappa}|p|$ and using again equations (7.2.3), (7.2.4), we deduce that

$$\Big|p^2\varphi_p + \frac{4\pi\mathfrak{a}_N N^\kappa}{N}\Big| \lesssim N^{-2+2\kappa}|p|. \tag{7.3.17}$$

Together with the bound $|\mathfrak{a}_N - \mathfrak{a}| \lesssim N^{-1+\kappa}$ from Lemma 7.3, this yields

$$\begin{aligned}
&\sum_{p\in\Lambda^*}\Big[p^2 s_p^2 + N_0 \widehat{V}_N(p) s_p + \frac{1}{2}\sum_{r\in\Lambda^*}\widehat{V}_N(p-r) s_p s_r\Big] \\
&\quad = \frac{N_0^2}{2N}N^\kappa(8\pi\mathfrak{a} - \widehat{V}(0)) + \frac{N_0^2}{N^2}\sum_{p\in S}\frac{(4\pi\mathfrak{a}N^\kappa)^2}{p^2} + \mathcal{O}\big(N^{5\kappa/2-\varepsilon}\big),
\end{aligned}$$

if $-2 + 3\kappa + 6\varepsilon < 0$. Combining this with the first term on the right-hand side of (7.3.15), we conclude that

$$\begin{aligned}
&\frac{N_0^2}{2}\widehat{V}_N(0) + \sum_{p\in\Lambda^*}\Big[p^2 s_p^2 + N_0 \widehat{V}_N(p) s_p + \frac{1}{2}\sum_{r\in\Lambda^*}\widehat{V}_N(p-r) s_p s_r\Big] \\
&\quad = 4\pi\mathfrak{a}N^{1+\kappa} - 8\pi\mathfrak{a}N^\kappa(N - N_0) + \sum_{p\in S}\frac{(4\pi\mathfrak{a}N^\kappa)^2}{p^2} + \mathcal{O}\big(N^{5\kappa/2-\varepsilon}\big),
\end{aligned} \tag{7.3.18}$$

where we used the assumption $0 \leqslant N - N_0 \lesssim N^{3\kappa/2}$.

To deal with the off-diagonal quadratic term in (7.3.15), we use again (7.2.3), (7.2.7) and (7.2.4). As a form on the range of the projection $\Xi = \mathbb{1}_{\{\mathcal{N}_{(S\cup H)^c}=0\}}\mathbb{1}_{\{\mathcal{N}_H \in 2\mathbb{N}_0\}}$, we find

$$\begin{aligned}\sum_{p\in\Lambda^*}\Big[p^2 s_p + \frac{1}{2}N_0\widehat{V}_N(p) + \frac{1}{2}\sum_{r\in\Lambda^*}\widehat{V}_N(r-p)s_r\Big](a_p^*a_{-p}^* + \text{h.c.})\\ = -N_0\sum_{p\in S}p^2\varphi_p\,(a_p^*a_{-p}^* + \text{h.c.}) - \frac{N_0}{2}\sum_{\substack{p\in\Lambda^*\\ r\in L}}\widehat{V}_N(r-p)\varphi_r\,(a_p^*a_{-p}^* + \text{h.c.}).\end{aligned} \tag{7.3.19}$$

Recalling (7.3.17), we can estimate

$$\pm\Big[-N_0\sum_{p\in S}p^2\varphi_p\,(a_p^*a_{-p}^* + \text{h.c.}) - 4\pi\mathfrak{a}N^\kappa\sum_{p\in S}(a_p^*a_{-p}^* + \text{h.c.})\Big] \lesssim N^{-1+5\kappa/2+5\varepsilon/2}(\mathcal{N} + N^{3\kappa/2}).$$

As for the last term on the right-hand side of (7.3.19), we can bound it switching to position space. For $\xi \in \mathcal{F}(\Lambda)$ we find

$$\begin{aligned}&\Big|\frac{N_0}{2}\sum_{\substack{p\in\Lambda^*\\ r\in L}}\widehat{V}_N(r-p)\varphi_r\langle\xi, a_p^*a_{-p}^*\xi\rangle\Big| = \Big|\frac{N_0}{2}\int_{\Lambda^2}V_N(x-y)\sum_{r\in L}e^{i(x-y)r}\varphi_r\langle a_xa_y\xi,\xi\rangle\,\mathrm{d}x\mathrm{d}y\Big|\\ &\leqslant N_0\sum_{r\in L}|\varphi_r|\left(\delta\langle\xi, Q_4\xi\rangle + C\delta^{-1}N^{-1+\kappa}\|\xi\|^2\right) \lesssim N^{-1/2+3\kappa/4}\Big(\langle\xi, Q_4\xi\rangle + N^{5\kappa/2+2\varepsilon}\|\xi\|^2\Big),\end{aligned}$$

choosing $\delta = N^{-1/2-3\kappa/4-\varepsilon}$. We conclude that

$$\sum_{p\in\Lambda^*}\Big[p^2 s_p + \frac{1}{2}N_0\widehat{V}_N(p) + \frac{1}{2}\sum_{r\in\Lambda^*}\widehat{V}_N(r-p)s_r\Big](a_p^*a_{-p}^* + \text{h.c.}) = 4\pi\mathfrak{a}N^\kappa\sum_{p\in S}(a_p^*a_{-p}^* + \text{h.c.}) + \mathcal{E}_1'$$

where, on the range of Ξ,

$$\pm\mathcal{E}_1' \lesssim N^{-5\varepsilon/2}Q_4 + N^{-1+5\kappa/2+5\varepsilon/2}\mathcal{N} + N^{5\kappa/2-\varepsilon/2},$$

if $-2+3\kappa+10\varepsilon < 0$. Combining this estimate with (7.3.16), and simplifying the absorbing the term proportional to $\mathcal{N}$ by a Cauchy–Schwarz inequality, we arrive at (7.2.8), (7.2.9) given that $1/2 < \kappa < 8/15 - 2\varepsilon/3$ (note that this implies the previous inequality on ε and κ). $\square$

7.4 Cubic transformation

The goal of this section is to show Lemma 7.5 and Proposition 7.7. All lemmas in this section hold for all $0 < \kappa < 2/3$ and $\varepsilon > 0$ as introduced in (7.1.9).

7.4.1 Properties of the cubic transformation

We start by observing that the action of the transformation $T_k = e^{\mathcal{B}_k}$, defined in (7.2.12), can be computed explicitly. To this end, we define, for $k \in S$,

$$X_k = \sqrt{\mathcal{B}_k^\circ\mathcal{B}_k^\sharp}.$$

Lemma 7.12. *Let $k \in S$. We have*

$$X_k^2 = \mathcal{B}_k^\circ\mathcal{B}_k^\sharp = \sum_{r\in H_k}N\varphi_r(\varphi_r + \varphi_{r+k})a_k^*a_k\Theta_{k,r}. \tag{7.4.1}$$

Furthermore, recalling the notation $\mathcal{N}_k = a_k^*a_k$,

$$X_k^2 \leqslant 2N\|\varphi_H\|_2^2\mathcal{N}_k \lesssim N^{-2+3\kappa+\varepsilon}\mathcal{N}_k. \tag{7.4.2}$$

Proof. Let us compute

$$\begin{aligned}
\mathcal{B}_k^\circ \mathcal{B}_k^\sharp &= \sum_{r,t\in H_k} N\varphi_r\varphi_t \Theta_{k,r} a_k^* a_{r+k} a_{-r} a_{-t}^* a_{t+k}^* a_k \Theta_{k,t} \\
&= \sum_{r,t\in H_k} N\varphi_r\varphi_t \Theta_{k,r} a_k^* [a_{k+r} a_{-r}, a_{-t}^* a_{t+k}^*] a_k \Theta_{k,t} \\
&= \sum_{r,t\in H_k} N\varphi_r\varphi_t \Theta_{k,r} a_k^* \left(\delta_{t,r} + \delta_{k+r+t,0}\right)\left(1 + a_{-r}^* a_{-r} + a_{r+k}^* a_{r+k}\right) a_k \Theta_{k,t} \\
&= \sum_{r\in H_k} N\varphi_r(\varphi_r + \varphi_{r+k}) a_k^* a_k \Theta_{k,r}.
\end{aligned} \tag{7.4.3}$$

To obtain the second equality, we used that $a_{r+k}a_{-r}\Theta_{k,t} = 0$ (since the cutoff imposes that there is no k-connection). In the last identity, we used $\Theta_{k,r}a_{-r}^* = \Theta_{k,r}a_{r+k}^* = 0$ (because the cutoff imposes that the shell-neighborhood of $-(k+r)$ and r are empty) and $\Theta_{k,-(r+k)} = \Theta_{k,r}$. The bound (7.4.2) then follows from Lemma 7.3. $\square$

Lemma 7.13. *For $k \in S$ we have*

$$T_k = \cos X_k + \mathcal{B}_k^\sharp \frac{\sin X_k}{X_k} - \frac{\sin X_k}{X_k}\mathcal{B}_k^\circ + \mathcal{B}_k^\sharp \frac{\cos X_k - 1}{X_k^2}\mathcal{B}_k^\circ$$

Proof. Due to the cutoff, $\mathcal{B}_k^\sharp$ cannot create a k-connection if there is one already. That is,

$$(\mathcal{B}_k^\sharp)^2 = (\mathcal{B}_k^\circ)^2 = 0.$$

Recall that $T_k = e^{\mathcal{B}_k}$ and that $i\mathcal{B}_k$ is essentially self-adjoint on any core domain of $\mathcal{N}$ [81, Theorem X.36]. Together with the nilpotent property, we can expand the exponential explicitly on any state with finite particle number to obtain

$$\begin{aligned}
T_k = e^{\mathcal{B}_k} &= \sum_{m\geqslant 0} \frac{(\mathcal{B}_k^\sharp - \mathcal{B}_k^\circ)^m}{m!} = \sum_{m\geqslant 0} \frac{(\mathcal{B}_k^\sharp - \mathcal{B}_k^\circ)^{2m}}{(2m)!} + \frac{(\mathcal{B}_k^\sharp - \mathcal{B}_k^\circ)^{2m+1}}{(2m+1)!} \\
&= \sum_{m\geqslant 1} \frac{(-1)^m}{(2m)!} \mathcal{B}_k^\sharp \left(\mathcal{B}_k^\circ \mathcal{B}_k^\sharp\right)^{m-1} \mathcal{B}_k^\circ + \sum_{m\geqslant 0} \frac{(-1)^m}{(2m!)} \left(\mathcal{B}_k^\circ \mathcal{B}_k^\sharp\right)^m \\
&\quad + \sum_{m\geqslant 0} \frac{(-1)^m}{(2m+1)!} \mathcal{B}_k^\sharp \left(\mathcal{B}_k^\circ \mathcal{B}_k^\sharp\right)^m - \sum_{m\geqslant 0} \frac{(-1)^m}{(2m+1)!} \left(\mathcal{B}_k^\circ \mathcal{B}_k^\sharp\right)^m \mathcal{B}_k^\circ.
\end{aligned}$$

With Lemma 7.12, we find

$$\begin{aligned}
T_k &= \mathcal{B}_k^\sharp \left(\sum_{m\geqslant 1} \frac{(-1)^m}{(2m)!} X_k^{2m-2}\right) \mathcal{B}_k^\circ + \sum_{m\geqslant 0} \frac{(-1)^m}{(2m!)} X_k^{2m} \\
&\quad + \mathcal{B}_k^\sharp \sum_{m\geqslant 0} \frac{(-1)^m}{(2m+1)!} X_k^{2m} - \sum_{m\geqslant 0} \frac{(-1)^m}{(2m+1)!} X_k^{2m} \mathcal{B}_k^\circ \\
&= \mathcal{B}_k^\sharp \frac{\cos X_k - 1}{X_k^2} \mathcal{B}_k^\circ + \cos X_k + \mathcal{B}_k^\sharp \frac{\sin X_k}{X_k} - \frac{\sin X_k}{X_k} \mathcal{B}_k^\circ.
\end{aligned}$$

$\square$

For $k \in S$, we introduce the notation

$$\Lambda_k := \Theta_k^{(1)} \mathbb{1}_{\{\mathcal{N}_{(S\cup H)^c}=0\}} \mathbb{1}_{\{\mathcal{N}_H \in 2\mathbb{N}_0\}}.$$

We observe that

$$\prod_{k\in S} \Lambda_k \mathbb{1}_{\{\mathcal{N}_{S^c}=0\}} = \mathbb{1}_{\{\mathcal{N}_{S^c}=0\}}.$$

Thus, on the range of $\mathbb{1}_{\{\mathcal{N}_{S^c}=0\}}$, we have

$$T_k = T_k \Lambda_k = \Big(\cos X_k + \mathcal{B}_k^\sharp \frac{\sin X_k}{X_k} \Big) \Lambda_k =: \widetilde{T}_k. \tag{7.4.4}$$

Moreover, since Λ_k commutes with $T_{k'}$ for all $k' \neq k$, we obtain, on the range of $\mathbb{1}_{\{\mathcal{N}_{S^c}=0\}}$,

$$T_c = \prod_{k\in S} T_k = \prod_{k\in S} \widetilde{T}_k. \tag{7.4.5}$$

In the next lemma, we control moments of the number operator with respect to the action of the cubic transformation.

Lemma 7.14. *For $S' \subset S$, let $T_{c,S'} := \prod_{p\in S'} T_p$. There is a constant $C > 0$ such that, for all $S' \subset S$ and all $j \geqslant 1$, we have, on the range of $\mathbb{1}_{\{\mathcal{N}_{S^c}=0\}}$,*

$$\pm \Big(T_{c,S'}^* \mathcal{N}_S^j T_{c,S'} - \mathcal{N}_S^j \Big) \leqslant C j N^{-2+3\kappa+\varepsilon} \mathcal{N}_S^j, \tag{7.4.6}$$

$$T_{c,S'}^* \mathcal{N}_S^j T_{c,S'} \leqslant \mathcal{N}_S^j. \tag{7.4.7}$$

Moreover, for all $j \geqslant 1$, there is a constant $C_j > 0$ such that, for all $S' \subset S$, we have, on the range of $\mathbb{1}_{\{\mathcal{N}_{S^c}=0\}}$,

$$T_{c,S'}^* \mathcal{N}_H^j T_{c,S'} \leqslant C_j N^{-2+3\kappa+\varepsilon} \mathcal{N}_S \left(N^{-2+3\kappa+\varepsilon} \mathcal{N}_S + 1 \right)^{j-1}. \tag{7.4.8}$$

Proof. We start by proving (7.4.6) and (7.4.7). First of all, we observe that $[\mathcal{B}_k, \mathcal{N}_S + \mathcal{N}_H/2] = 0$, for all $k \in S$. This implies that

$$T_{c,S'}^* \big(\mathcal{N}_S + \mathcal{N}_H/2 \big)^j T_{c,S'} = \big(\mathcal{N}_S + \mathcal{N}_H/2 \big)^j \tag{7.4.9}$$

for all $j \in \mathbb{N}$ and all $S' \subset S$. We immediately obtain

$$T_{c,S'}^* \mathcal{N}_S^j T_{c,S'} \leqslant \big(\mathcal{N}_S + \mathcal{N}_H/2 \big)^j = \mathcal{N}_S^j \tag{7.4.10}$$

on the range of $\mathbb{1}_{\{\mathcal{N}_{S^c}=0\}}$. To prove the lower bound we choose k as the "first" element in $S' \subset S$ (according to the order used to define T_c) and we compute

$$\begin{aligned}
\widetilde{T}_k^* \mathcal{N}_S^j \widetilde{T}_k &= \Lambda_k \Big(\cos X_k + \frac{\sin X_k}{X_k} \mathcal{B}_k^\circ \Big) \mathcal{N}_S^j \Big(\cos X_k + \mathcal{B}_k^\sharp \frac{\sin X_k}{X_k} \Big) \Lambda_k \\
&= \Lambda_k \Big(\cos^2 X_k \mathcal{N}_S^j + \frac{\sin X_k}{X_k} \mathcal{B}_k^\circ \mathcal{N}_S^j \mathcal{B}_k^\sharp \frac{\sin X_k}{X_k} \Big) \Lambda_k \\
&= \Lambda_k \Big(\cos^2 X_k \mathcal{N}_S^j + \frac{\sin X_k}{X_k} (\mathcal{N}_S - 1)^j X_k^2 \frac{\sin X_k}{X_k} \Big) \Lambda_k \\
&= \Lambda_k \Big(\mathcal{N}_S^j + ((\mathcal{N}_S - 1)^j - \mathcal{N}_S^j) \sin^2 X_k \Big) \Lambda_k.
\end{aligned} \tag{7.4.11}$$

On the range of Λ_k, we find (with φ_H the restriction of φ on H)

$$T_k^* \mathcal{N}_S^j T_k \geqslant \mathcal{N}_S^j - j2N\|\varphi_H\|_2^2 \mathcal{N}_k \mathcal{N}_S^{j-1} \geqslant \mathcal{N}_S^j - CjN^{-2+3\kappa+\varepsilon}\mathcal{N}_S^{j-1}\mathcal{N}_k$$

Conjugating with $T_{c,S'\setminus\{k\}}$ and using (7.4.10) we obtain, on the range of $\mathbb{1}_{\{\mathcal{N}_{S^c}=0\}}$,

$$\begin{aligned} T_{c,S'}^* \mathcal{N}_S^j T_{c,S} &\geqslant T_{c,S'\setminus\{k\}}^* \mathcal{N}_S^j T_{c,S'\setminus\{k\}} - CjN^{-2+3\kappa+\varepsilon}\mathcal{N}_k^{1/2} T_{c,S'\setminus\{k\}}^* \mathcal{N}_S^{j-1} T_{c,S'\setminus\{k\}} \mathcal{N}_k^{1/2} \\ &\geqslant T_{c,S'\setminus\{k\}}^* \mathcal{N}_S^j T_{c,S'\setminus\{k\}} - CjN^{-2+3\kappa+\varepsilon}\mathcal{N}_S^{j-1}\mathcal{N}_k. \end{aligned}$$

Iterating to cover all $k \in S'$, we obtain

$$T_{c,S'}^* \mathcal{N}_S^j T_{c,S} \geqslant \mathcal{N}_S^j - CjN^{-2+3\kappa+\varepsilon}\mathcal{N}_S^{j-1}\sum_{k\in S'}\mathcal{N}_k \geqslant \mathcal{N}_S^j - CjN^{-2+3\kappa+\varepsilon}\mathcal{N}_S^j.$$

Let us now show (7.4.8). Similarly as in (7.4.11), we find

$$\widetilde{T}_k^* \mathcal{N}_H^j \widetilde{T}_k = \Lambda_k\big(\mathcal{N}_H^j + ((\mathcal{N}_H+2)^j - \mathcal{N}_H^j)\sin^2 X_k\big)\Lambda_k.$$

Thus, there exists $C > 0$ depending on j such that, on the range of Λ_k,

$$\widetilde{T}_k^* \mathcal{N}_H^j \widetilde{T}_k \leqslant \mathcal{N}_H^j + CN^{-2+3\kappa+\varepsilon}(\mathcal{N}_H^{j-1}+1)\mathcal{N}_k.$$

Conjugating with $T_{c,S'\setminus\{k\}}$ we obtain, on the range of $\mathbb{1}_{\{\mathcal{N}_{S^c}=0\}}$,

$$T_{c,S'}^* \mathcal{N}_H^j T_{c,S'} \leqslant T_{c,S'\setminus\{k\}}^* \mathcal{N}_H^j T_{c,S'\setminus\{k\}} + CN^{-2+3\kappa+\varepsilon}\mathcal{N}_k^{1/2}(T_{c,S'\setminus\{k\}}^* \mathcal{N}_H^{j-1} T_{c,S'\setminus\{k\}} + 1)\mathcal{N}_k^{1/2}. \tag{7.4.12}$$

Next, we claim that for all $j \in \mathbb{N}$ there exists $C_j > 0$ independent of S' such that, on the range of $\mathbb{1}_{\{\mathcal{N}_{S^c}=0\}}$,

$$T_{c,S'}^* \mathcal{N}_H^j T_{c,S'} \leqslant C_j N^{-2+3\kappa+\varepsilon}\mathcal{N}_S\big(N^{-2+3\kappa+\varepsilon}\mathcal{N}_S+1\big)^{j-1}. \tag{7.4.13}$$

For $j = 1$, the claim follows (7.4.12), iterating to cover all $k \in S'$. Assuming (7.4.13), we use (7.4.12) to estimate

$$\begin{aligned} T_{c,S'}^* \mathcal{N}_H^{j+1} T_{c,S'} &\leqslant T_{c,S'\setminus\{k\}}^* \mathcal{N}_H^{j+1} T_{c,S'\setminus\{k\}} + CN^{-2+3\kappa+\varepsilon}\mathcal{N}_k^{1/2}(T_{c,S'\setminus\{k\}}^* \mathcal{N}_H^j T_{c,S'\setminus\{k\}} + 1)\mathcal{N}_k^{1/2} \\ &\leqslant T_{c,S'\setminus\{k\}}^* \mathcal{N}_H^{j+1} T_{c,S'\setminus\{k\}} + C_jCN^{-2+3\kappa+\varepsilon}(N^{-2+3\kappa+\varepsilon}\mathcal{N}_S+1)^j\mathcal{N}_k. \end{aligned}$$

Iterating over all $k \in S'$ we conclude that, on the range of $\mathbb{1}_{\{\mathcal{N}_{S^c}=0\}}$,

$$\begin{aligned} T_{c,S'}^* \mathcal{N}_H^{j+1} T_{c,S'} &\leqslant \mathcal{N}_H^{j+1} + C_{j+1}N^{-2+3\kappa+\varepsilon}(N^{-2+3\kappa+\varepsilon}\mathcal{N}_S+1)^j\sum_{k\in S'}\mathcal{N}_k \\ &\leqslant C_{j+1}N^{-2+3\kappa+\varepsilon}\mathcal{N}_S(N^{-2+3\kappa+\varepsilon}\mathcal{N}_S+1)^j. \end{aligned}$$

By induction, we obtain (7.4.8). □

7.4.2 Action on the off-diagonal quadratic term

Next, we control the action of T_c on the quadratic off-diagonal term on the right-hand side of (7.2.8). We introduce the notation

$$\widetilde{Q}_2^\sharp = 4\pi\mathfrak{a}N^\kappa \sum_{p\in S} a_p^* a_{-p}^* = (\widetilde{Q}_2^\circ)^*.$$

Lemma 7.15. *On the range of* $\mathbb{1}_{\{\mathcal{N}_{S^c}=0\}}$*, we have*

$$\pm\left[T_c^*(\widetilde{Q}_2^\sharp+\widetilde{Q}_2^\circ)T_c-(\widetilde{Q}_2^\sharp+\widetilde{Q}_2^\circ)\right]\lesssim N^{-2+4\kappa+\varepsilon}(\mathcal{N}_S+N^{3\kappa/2+3\varepsilon}).$$

Proof. Let $p,k\in S$. If $p\notin\{\pm k\}$, then clearly

$$\widetilde{T}_k^*a_p^*a_{-p}^*\widetilde{T}_k=\Lambda_k a_p^*a_{-p}^*\Lambda_k. \tag{7.4.14}$$

Let us now consider the case $p\in\{\pm k\}$, say $p=k$. Since $\Theta_k^{(1)}$ only depends on operators $\mathcal{N}_t$, with $t\in H$, we have $[a_p^*a_{-p}^*,\Theta_k^{(1)}]=0$ and therefore $\Lambda_k a_p^*a_{-p}^*\mathcal{B}_c^\sharp=\mathcal{B}_c^\circ a_p^*a_{-p}^*\Lambda_k=0$. We find

$$\begin{aligned}\widetilde{T}_k^*a_k^*a_{-k}^*\widetilde{T}_k&=\Lambda_k\Big(\cos X_k a_k^*a_{-k}^*\cos X_k+\frac{\sin X_k}{X_k}\mathcal{B}_k^\circ a_k^*a_{-k}^*\mathcal{B}_k^*\frac{\sin X_k}{X_k}\Big)\Lambda_k\\&=\Lambda_k\Big(\cos X_k a_k^*a_{-k}^*\cos X_k+\frac{\sin X_k}{X_k}a_k^*a_{-k}^*X_k\sin X_k\Big)\Lambda_k,\end{aligned}$$

where we used that $[\mathcal{B}_k^\circ,a_k^*a_{-k}^*]=0$. With the formula (7.4.1) for X_k^2 and since $\mathcal{N}_k a_k^*a_{-k}^*=a_k^*a_{-k}^*(\mathcal{N}_k+1)$, we obtain

$$X_k^2a_k^*a_{-k}^*=a_k^*a_{-k}^*Y_k^2,$$

with Y_k being defined as the square root of the positive operator

$$Y_k^2:=X_k^2+\sum_{t\in H_k}N\varphi_t(\varphi_t+\varphi_{t+k})\Theta_{k,t}.$$

Since (with $\Theta_{k,t}=\Theta_{k,-t-k}$)

$$Y_k^2-X_k^2=\sum_{t\in H_k}N\varphi_t(\varphi_t+\varphi_{t+k})\Theta_{k,t}=\frac{N}{2}\sum_{t\in H_k}(\varphi_t+\varphi_{t+k})^2\Theta_{k,t} \tag{7.4.15}$$

we conclude that $Y_k^2\geqslant X_k^2$. Since X_k and Y_k commute, we arrive at

$$\begin{aligned}\widetilde{T}_k^*a_k^*a_{-k}^*\widetilde{T}_k&=\Lambda_k a_k^*a_{-k}^*\Big(\cos Y_k\cos X_k+X_k\sin X_k\frac{\sin Y_k}{Y_k}\Big)\Lambda_k\\&=\Lambda_k a_k^*a_{-k}^*\Big(\cos(Y_k-X_k)+(X_k-Y_k)\sin X_k\frac{\sin Y_k}{Y_k}\Big)\Lambda_k\\&=:\Lambda_k a_k^*a_{-k}^*\big(1+R_k\big)\Lambda_k.\end{aligned} \tag{7.4.16}$$

From $|\cos(y-x)-1+(x-y)\sin(x)\sin(y)/y|\leqslant C(y^2-x^2)$ for all $0\leqslant x\leqslant y$ and from Lemma 7.3, we obtain

$$\pm R_k\lesssim N\|\varphi_H\|_2^2\lesssim N^{-2+3\kappa+\varepsilon}.$$

With (7.4.16), we conclude that

$$\pm\,\Lambda_k\left(T_k^*a_k^*a_{-k}^*T_k-a_k^*a_{-k}^*\right)\Lambda_k+\text{h.c.}\lesssim N^{-2+3\kappa+\varepsilon}(\mathcal{N}_k+\mathcal{N}_{-k}+1).$$

Conjugation with T_{-k} can be handled similarly. Since moreover the error term is invariant w.r.t. T_p, for $p\in S\backslash\{\pm k\}$, we find

$$\pm\big(T_c^*a_k^*a_{-k}^*T_c-a_k^*a_{-k}^*\big)+\text{h.c.}\lesssim N^{-2+3\kappa+\varepsilon}(\mathcal{N}_k+\mathcal{N}_{-k}+1)$$

on the range of $\mathbb{1}_{\{\mathcal{N}_{S^c}=0\}}$. The claim follows by summing over $k\in S$ (recall that $|S|\lesssim N^{3\kappa/2+3\varepsilon}$). $\square$

7.4.3 Action on the kinetic energy operator

In this subsection, we control the action of a single cubic transformation T_k, for a fixed $k \in S$, on the kinetic energy operator. In the next subsections, we show similar statements for the action of T_k on the cubic term Q_3 and on the quartic term Q_4, appearing in Lemma 7.4 on the right hand side of (7.2.8). Eventually, we will obtain the action of the full transformation T_c by iteration.

Lemma 7.16. *For $k \in S$ we have, on the range of Λ_k,*

$$\pm\Big[T_k^* \sum_{p\in\Lambda^*} p^2 a_p^* a_p T_k - \sum_{p\in\Lambda^*} p^2 a_p^* a_p - 2\sum_{r\in H_k} N r^2 \varphi_r(\varphi_r + \varphi_{k+r}) a_k^* a_k \Theta_{k,r}\Big] \lesssim N^{-1+5\kappa/2+3\varepsilon/2}\mathcal{N}_k^2. \tag{7.4.17}$$

Proof. Using that $\mathcal{B}_k^\circ \Lambda_k = 0$ and that $[X_k^2, \Lambda_k] = 0$, we obtain

$$\begin{aligned}
\Lambda_k T_k^* \sum_{q\in\Lambda^*} q^2 a_q^* a_q T_k \Lambda_k &= \Lambda_k\Big(\cos X_k + \frac{\sin X_k}{X_k}\mathcal{B}_k^\circ\Big) \sum_{q\in\Lambda^*} q^2 a_q^* a_q \Big(\cos X_k + \mathcal{B}_k^\sharp \frac{\sin X_k}{X_k}\Big)\Lambda_k \\
&= \Lambda_k\Big(\cos^2 X_k \sum_{p\in\Lambda^*} p^2 a_p^* a_p + \frac{\sin X_k}{X_k}\mathcal{B}_k^\circ \sum_{p\in\Lambda^*} p^2 a_p^* a_p \mathcal{B}_k^\sharp \frac{\sin X_k}{X_k}\Big)\Lambda_k \\
&= \Lambda_k\Big(\sum_{p\in\Lambda^*} p^2 a_p^* a_p + \frac{\sin X_k}{X_k}\big[\mathcal{B}_k^\circ, \sum_{p\in\Lambda^*} p^2 a_p^* a_p\big]\mathcal{B}_k^\sharp \frac{\sin X_k}{X_k}\Big)\Lambda_k.
\end{aligned}$$

Let us now compute

$$\begin{aligned}
\big[\mathcal{B}_k^\circ, \sum_{p\in\Lambda^*} p^2 a_p^* a_p\big]\mathcal{B}_k^\sharp &= \sum_{r\in H_k} N^{1/2}\varphi_r \left((r^2 + (k+r)^2 - k^2\right)\Theta_{k,r} a_k^* a_{-r} a_{k+r} \mathcal{B}_k^\sharp \\
&= 2\sum_{r\in H_k} N\varphi_r(\varphi_r + \varphi_{k+r})\left(r^2 + k\cdot r\right) a_k^* a_k \Theta_{k,r},
\end{aligned}$$

where we used that, similarly as in the proof of Lemma 7.12,

$$a_{-r} a_{k+r} \mathcal{B}_k^\sharp = (\varphi_r + \varphi_{r+k}) a_k \Theta_{k,r}.$$

We therefore obtain

$$\begin{aligned}
&\Lambda_k\Big(T_k^* \sum_{p\in\Lambda^*} p^2 a_p^* a_p T_k - \sum_{p\in\Lambda^*} p^2 a_p^* a_p - 2\sum_{r\in H_k} N r^2 \varphi_r(\varphi_r + \varphi_{k+r}) a_k^* a_k \Theta_{k,r}\Big)\Lambda_k \\
&= \Lambda_k\Big(2\sum_{r\in H_k} N\varphi_r(\varphi_r + \varphi_{k+r}) a_k^* a_k \Theta_{k,r}\Big[r^2\Big(\frac{\sin^2 X_k}{X_k^2} - 1\Big) + r\cdot k\,\frac{\sin^2 X_k}{X_k^2}\Big]\Big)\Lambda_k.
\end{aligned}$$

From Lemma 7.3 we find that

$$\sum_{r\in H_k} N r^2 |\varphi_r(\varphi_r + \varphi_{k+r})| \lesssim N^\kappa \|\varphi\|_1 \lesssim N^\kappa$$

and that

$$\sum_{r\in H_k} N|r||k||\varphi_r||\varphi_r + \varphi_{k+r}| \lesssim N|k|\|p\varphi\|_2\|\varphi_H\|_2 \lesssim N^{-1+5\kappa/2+3\varepsilon/2},$$

since $|k| \leqslant N^{\kappa/2+\varepsilon}$. Moreover, (7.4.2) implies that

$$\Big(1 - \frac{\sin^2 X_k}{X_k^2}\Big) \lesssim N^{-2+3\kappa+\varepsilon}\mathcal{N}_k.$$

Since $N^\kappa N^{-2+3\kappa+\varepsilon} = N^{-2+4\kappa+\varepsilon} \leqslant N^{-1+5\kappa/2+3\varepsilon/2}$ for all $\kappa < 2/3$, we obtain (7.4.17). $\square$

7.4.4 Action on the cubic term

Next, we proceed with the conjugation of the cubic term Q_3 appearing on the right-hand side of (7.2.8). On the range of the projection $\Xi = \mathbb{1}_{\{\mathcal{N}_{(H\cup S)^c}=0\}}\mathbb{1}_{\{\mathcal{N}_H\in 2\mathbb{N}_0\}}$, we can decompose

$$Q_3 = \sqrt{\frac{N_0}{N}}\left(Q_3^H + Q_3^M + Q_3^S\right) \tag{7.4.18}$$

with

$$\begin{aligned}
Q_3^H &= \sum_{r\in H_p, p\in S} N^{1/2}\widehat{V}_N(r)a^*_{-r}a^*_{r+p}a_p + \text{h.c.}\\
Q_3^M &= \sum_{\substack{r,p\in H:\\ r+p\in S}} N^{1/2}\widehat{V}_N(r)a^*_{-r}a^*_{r+p}a_p + \sum_{p\in H_r, r\in S} N^{1/2}\widehat{V}_N(r)a^*_{-r}a^*_{r+p}a_p + \text{h.c.}\\
Q_3^S &= \sum_{\substack{r,p\in S:\\ r+p\in S}} N^{1/2}\widehat{V}_N(r)a^*_{-r}a^*_{r+p}a_p + \text{h.c.}
\end{aligned}$$

Note that since $0 \leqslant N - N_0 \lesssim N^{3\kappa/2}$, we have $\sqrt{N_0/N} = 1 + \mathcal{O}(N^{-1+3\kappa/2})$.

In the next lemma we conjugate the operator Q_3^H.

Lemma 7.17. *Let $k \in S$. On the range of Λ_k, we have*

$$\begin{aligned}
&\pm\Big(T_k^* Q_3^H T_k - Q_3^H - 2\sum_{r\in H_k} N\widehat{V}_N(r)(\varphi_r + \varphi_{r+k})\mathcal{N}_k\Theta_{k,r}\Big)\\
&\lesssim N^{-2+4\kappa+\varepsilon}\mathcal{N}_k^2 + N^{-5+15\kappa/2+7\varepsilon}\Big(N^{2-2\kappa}\sum_{r,q\in H}\mathbb{1}_S(r+q)a^*_r a^*_q a_q a_r + N^\kappa \mathcal{N}_S\Big)(\mathcal{N}_k+1)
\end{aligned} \tag{7.4.19}$$

Proof. Let us write $Q_3^H = \sum_{p\in S} Q_{3,p}^{H,\sharp} + Q_{3,p}^{H,\circ}$ with $Q_{3,p}^{H,\circ} = (Q_{3,p}^{H,\sharp})^*$ and

$$Q_{3,p}^{H,\sharp} := \sum_{r\in H_p} N^{1/2}\widehat{V}_N(r)a^*_{-r}a^*_{r+p}a_p.$$

Let $k,p \in S$. With (7.4.4) and using that $\Lambda_k Q_{3,p}^{H,\sharp}\mathcal{B}_k^\sharp = 0$ (since $Q_{3,p}^{H,\sharp}$ cannot annihilate a k-connection), we find

$$\begin{aligned}
\Lambda_k T_k^* Q_{3,p}^{H,\sharp} T_k \Lambda_k = \Lambda_k \cos X_k Q_{3,p}^{H,\sharp} \cos X_k \Lambda_k + \Lambda_k \frac{\sin X_k}{X_k}\mathcal{B}_k^\circ Q_{3,p}^{H,\sharp}\mathcal{B}_k^\sharp \frac{\sin X_k}{X_k}\Lambda_k\\
+ \Lambda_k \frac{\sin X_k}{X_k}\mathcal{B}_k^\circ Q_{3,p}^{H,\sharp}\cos X_k \Lambda_k.
\end{aligned} \tag{7.4.20}$$

We compute

$$\begin{aligned}
\mathcal{B}_k^\circ Q_{3,p}^{H,\sharp} &= \sum_{t\in H_k, r\in H_p} N\varphi_t \widehat{V}_N(r)\Theta_{k,t} a_k^* a_{k+t}a_{-t}a^*_{-r}a^*_{r+p}a_p\\
&= \sum_{t\in H_k, r\in H_p} N\varphi_t \widehat{V}_N(r)\Theta_{k,t}\Big(a^*_{-r}a^*_{r+p}a_{k+t}a_{-t} + \delta_{k,p}(\delta_{t,r} + \delta_{t,-(p+r)})\\
&\qquad + a^*_{p+r}a_{r+k}(\delta_{t,r} + \delta_{t,-r-k}) + a^*_{-r}a_{-p-r+k}(\delta_{t,-p-r} + \delta_{t,p+r-k})\Big)\, a_k^* a_p\\
&= \sum_{t\in H_k, r\in H_p} N\varphi_t \widehat{V}_N(r)\Theta_{k,t}\Big(a^*_{-r}a^*_{r+p}a_{k+t}a_{-t} + \delta_{k,p}(\delta_{t,r} + \delta_{t,-(p+r)})\Big)a_k^* a_p,
\end{aligned} \tag{7.4.21}$$

where, in the last step, we used the definition of $\Theta_{k,t}$ (which implies for example that $\Theta_{k,r} a^*_{p+r} = 0$ and similarly for the other terms on the third line).

Next, we distinguish the cases $k = p$ and $k \neq p$. Let us first assume that $k = p$. Since $\Lambda_k Q^{H,\sharp}_{3,k} = 0$, the first term on the right-hand side of (7.4.20) vanishes. Using (7.4.21) and $\Theta_{k,t} a^*_{-r} a^*_{r+k} = 0$, we conclude that also the second term on the right-hand side of (7.4.20) is zero (because Λ_k can be moved through $\mathcal{B}^\circ_k Q^{H,\sharp}_{3,p}$ and $\Lambda_k \mathcal{B}^\sharp_k = 0$). Thus, we have

$$\Lambda_k T^*_k Q^{H,\sharp}_{3,k} T_k \Lambda_k = \Lambda_k \frac{\sin X_k \cos X_k}{X_k} \sum_{r \in H_k} N \widehat{V}_N(r)(\varphi_r + \varphi_{r+k}) a^*_k a_k \Theta_{k,r} \Lambda_k.$$

With the elementary inequality

$$0 \leqslant 1 - \frac{\sin x \cos x}{x} \leqslant \frac{2}{3} x^2,$$

using Lemma 7.3 to estimate

$$\Big| \sum_{r \in H_k} N \widehat{V}_N(r)(\varphi_r + \varphi_{r+k}) \Big| \lesssim N^\kappa$$

and applying the bound (7.4.2), we obtain

$$\pm \Lambda_k \Big(T^*_k Q^{H,\sharp}_{3,k} T_k - \sum_{r \in H_k} N \widehat{V}_N(r)(\varphi_r + \varphi_{r+k}) a^*_k a_k \Theta_{k,r} \Big) \Lambda_k \lesssim N^{-2+4\kappa+\varepsilon} \mathcal{N}_k^2. \tag{7.4.22}$$

We now consider the case $p \neq k$. We will prove that

$$\begin{aligned} &\pm \Lambda_k \Big(T^*_k \sum_{p \in S \setminus \{k\}} Q^{H,\sharp}_{3,p} T_k - \sum_{p \in S \setminus \{k\}} Q^{H,\sharp}_{3,p} \Big) \Lambda_k + \text{h.c.} \\ &\quad \lesssim N^{-5+15\kappa/2+7\varepsilon} \Big(N^{2-2\kappa} \sum_{r,q \in H} \mathbb{1}_S(r+q) a^*_r a^*_q a_q a_r + N^\kappa \mathcal{N}_S \Big) (\mathcal{N}_k + 1). \end{aligned} \tag{7.4.23}$$

Together with (7.4.22) and $\Lambda_k \big(Q^{H,\sharp}_{3,k} + Q^{H,\circ}_{3,k} \big) \Lambda_k = 0$ this implies (7.4.19).

To show (7.4.23), we observe that, from (7.4.21), $\mathcal{B}^\circ_k Q^{H,\sharp}_{3,p} \Lambda_k = 0$ since $a_{k+t} a_{-t} \Lambda_k = 0$ for $t \in H_k$. Therefore, the last term in (7.4.20) vanishes. Using (7.4.21) to rewrite the second term on the right-hand side of (7.4.20), we find

$$\begin{aligned} \Lambda_k T^*_k Q^{H,\sharp}_{3,p} T_k \Lambda_k &= \Lambda_k \cos X_k Q^{H,\sharp}_{3,p} \cos X_k \Lambda_k \\ &\quad + \Lambda_k \frac{\sin X_k}{X_k} \sum_{t \in H_k, r \in H_p} N \varphi_t \widehat{V}_N(r) \Theta^{(2)}_{k,t} a^*_{-r} a^*_{r+p} a_{k+t} a_{-t} a^*_k a_p \mathcal{B}^\sharp_k \frac{\sin X_k}{X_k} \Lambda_k \end{aligned} \tag{7.4.24}$$

In the second term, we move the cutoff $\Theta^{(2)}_{k,t}$ to the right to reconstruct the operator $\mathcal{B}^\circ_k$. To this end, we use the identity

$$\Theta^{(2)}_{k,t} a^*_r = a^*_r \Theta^{(2)}_{k,t} \left(1 - \mathbb{1}_{(t+S) \cup (-(t+k)+S)}(r) \right) \quad \forall k \in S, t \in H_k, r \in \Lambda^* \tag{7.4.25}$$

We find

$$\begin{aligned} &\sum_{t \in H_k, r \in H_p} N \varphi_t \widehat{V}_N(r) \Theta^{(2)}_{k,t} a^*_{-r} a^*_{r+p} a_{k+t} a_{-t} a^*_k a_p \mathcal{B}^\sharp_k \\ &\quad = \sum_{t \in H_k, r \in H_p} N \varphi_t \widehat{V}_N(r) a^*_{-r} a^*_{r+p} a_p \Theta^{(2)}_{k,t} a_{k+t} a_{-t} a^*_k \mathcal{B}^\sharp_k \big(1 - \mathbb{1}(-r, r+p \sim_{\mathrm{S}} -(t+k), t) \big) \end{aligned}$$

with the notation

$$\mathbb{1}(-r, r+p \sim_{\mathrm{S}} -(t+k), t) := \begin{cases} 1 & \text{if } \{-r, r+p\} \cap \big((t+S) \cup (-(t+k)+S)\big) \neq \emptyset \\ 0 & \text{otherwise.} \end{cases}$$

Proceeding as in the proof of Lemma 7.12, we find

$$\sum_{t \in H_k, r \in H_p} N\varphi_t \widehat{V}_N(r)\Theta^{(2)}_{k,t} a^*_{-r} a^*_{r+p} a_{k+t} a_{-t} a^*_k a_p \mathcal{B}^\sharp_k = \sum_{r \in H_p} N^{1/2}\widehat{V}_N(r) a^*_{-r} a^*_{r+p} a_p (X_k^{(-r,r+p)})^2$$

where we defined

$$\big(X_k^{(-r,r+p)}\big)^2 = \sum_{t \in H_k} \left(1 - \mathbb{1}(-r, r+p \sim_{\mathrm{S}} -(t+k), t)\right) \Theta_{k,t} N\varphi_t(\varphi_t + \varphi_{t+k}) a^*_k a_k \tag{7.4.26}$$

We can decompose $\big(X_k^{(-r,r+p)}\big)^2 = X_k^2 - \delta_k^{(-r,r+p)}$ with

$$\delta_k^{(-r,r+p)} = \sum_{t \in H_k} \mathbb{1}(-r, r+p \sim_{\mathrm{S}} -(t+k), t)\Theta_{k,t} N\varphi_t(\varphi_t + \varphi_{t+k})\mathcal{N}_k \tag{7.4.27}$$

Notice that $(X_k^{(-r,r+p)})^2$ and $\delta_k^{(-r,r+p)}$ are both non-negative operators (this can be shown similarly as in (7.4.15)). Moreover, with Lemma 7.3, we find

$$\delta_k^{(-r,r+p)} \lesssim N|S|\|\varphi_H\|_\infty^2 \mathcal{N}_k \lesssim N^{-5+15\kappa/2+7\varepsilon}\mathcal{N}_k.$$

Hence, after summing over $p \in S\backslash\{k\}$, the contribution of $\delta_k^{(-r,r+p)}$ can be bounded with Cauchy–Schwarz on the range of Λ_k by

$$\begin{aligned} &\pm \sum_{p \in S\backslash\{k\}, r \in H_p} N^{1/2}\widehat{V}_N(r) a^*_{-r} a^*_{r+p} a_p \delta_k^{(-r,r+p)} + \text{h.c.} \\ &\qquad \lesssim N^{-5+15\kappa/2+7\varepsilon}\Big(N^{2-2\kappa}\sum_{r,q \in H} \mathbb{1}_S(r+q) a^*_r a^*_q a_q a_r + N^\kappa \mathcal{N}_S\Big)(\mathcal{N}_k + 1). \end{aligned} \tag{7.4.28}$$

Therefore

$$\begin{aligned} &\pm \sum_{p \in S\backslash\{k\}} \Lambda_k \Big[T_k^* Q^{H,\sharp}_{3,p} T_k - \cos X_k Q^{H,\sharp}_{3,p} \cos X_k - \frac{\sin X_k}{X_k} Q^{H,\sharp}_{3,p} X_k \sin X_k + \text{h.c.}\Big]\Lambda_k \\ &\qquad \lesssim N^{-5+15\kappa/2+7\varepsilon}\Big(N^{2-2\kappa}\sum_{r,q \in H} \mathbb{1}_S(r+q) a^*_r a^*_q a_q a_r + N^\kappa \mathcal{N}_S\Big)(\mathcal{N}_k + 1). \end{aligned} \tag{7.4.29}$$

Arguing as in (7.4.25), we also obtain

$$\Lambda_k X_k^2 a^*_{-r} a^*_{r+p} a_p \Lambda_k = \Lambda_k a^*_{-r} a^*_{r+p} a_p \big(X_k^{(-r,r+p)}\big)^2 \Lambda_k. \tag{7.4.30}$$

Since moreover X_k and $X_k^{(-r,r+p)}$ commute, we find

$$\begin{aligned} &\Lambda_k \cos X_k a^*_{-r} a^*_{r+p} a_p \cos X_k \Lambda_k + \Lambda_k \frac{\sin X_k}{X_k} a^*_{-r} a^*_{r+p} a_p X_k \sin X_k \Lambda_k \\ &= \Lambda_k a^*_{-r} a^*_{r+p} a_p \left(\cos X_k^{(-r,r+p)} \cos X_k + \frac{\sin X_k^{(-r,r+p)}}{X_k^{(-r,r+p)}} X_k \sin X_k\right)\Lambda_k \\ &= \Lambda_k a^*_{-r} a^*_{r+p} a_p \left(\cos(X_k - X_k^{(-r,r+p)}) + (X_k - X_k^{(-r,r+p)}) \sin X_k \frac{\sin X_k^{(-r,r+p)}}{X_k^{(-r,r+p)}}\right)\Lambda_k \\ &=: \Lambda_k a^*_{-r} a^*_{r+p} a_p \left(1 + R_k^{(-r,r+p)}\right)\Lambda_k \end{aligned}$$

With $|\cos(x-y)-1+(x-y)\sin(x)\sin(y)/y| \leqslant C(x^2-y^2)$ for all $0 \leqslant y \leqslant x$, we conclude that

$$\pm R_k^{(-r,r+p)} \leqslant C\delta_k^{(-r,r+p)}.$$

Thus, proceeding as in (7.4.28), we arrive, on the range of Λ_k, at

$$\begin{aligned}\pm \sum_{p\in S\setminus\{k\}, r\in H_p} & N^{1/2}\widehat{V}_N(r)a^*_{-r}a^*_{r+p}a_pR_k^{(-r,r+p)} + \text{h.c.} \\ & \lesssim N^{-5+15\kappa/2+7\varepsilon}\left(N^{2-2\kappa}\sum_{r,q\in H}\mathbb{1}_S(r+q)a^*_ra^*_qa_qa_r + N^\kappa\mathcal{N}_S\right)(\mathcal{N}_k+1).\end{aligned}$$

Inserting this bound into (7.4.29), we arrive at (7.4.23). $\square$

As for the observables Q_3^M, Q_3^S, we employ the parity operators $\mathbb{P}_k$ defined in (7.2.14) and the assumption $[\mathbb{P}_k,\Gamma]=0$ for all $k\in S$ to show that their expectation vanishes in the state described by the density matrix Γ. Here, we will make use of the following property stating that, for $p\in H$, the density matrix $T_c\Gamma T_c^*$ can only have either zero or one particle with momentum p and that, in the second case, there must be exactly one particle with momentum in the set $-p+S$, forming an S-connection with the particle with momentum p.

Lemma 7.18. *Let $\Gamma = \mathbb{1}_{\{\mathcal{N}_{S^c}=0\}}\Gamma\mathbb{1}_{\{\mathcal{N}_{S^c}=0\}}$. For $p\in H$, define*

$$\begin{aligned}\chi_p &= \mathbb{1}_{\{\mathcal{N}_p=0\}} + \mathbb{1}_{\{\mathcal{N}_p=1\}}\sum_{x\in S}\mathbb{1}_{\{\mathcal{N}_{-p+x}=1\}}\prod_{y\in S\setminus\{x\}}\mathbb{1}_{\{\mathcal{N}_{-p+y}=0\}} \\ \widetilde{\chi}_p &= \mathbb{1}_{\{\mathcal{N}_p=0\}} + \mathbb{1}_{\{\mathcal{N}_p=1\}}\sum_{x\in S}\mathbb{1}_{\{\mathcal{N}_{-p+x}=1\}}\end{aligned} \tag{7.4.31}$$

Then we have

$$T_c\Gamma T_c^* = \chi_pT_c\Gamma T_c^*\chi_p = \widetilde{\chi}_pT_c\Gamma T_c^*\widetilde{\chi}_p. \tag{7.4.32}$$

Proof. Let $p\in H$. Note that $\Gamma=\chi_p\Gamma\chi_p$. We now show that $[a^*_{-r}a^*_{r+k}a_k\Theta_{k,r},\chi_p]=0$ for all $k\in S, r\in H_k$, which implies $[T_c,\chi_p]=0$ and thus the first identity in (7.4.32).

We start by observing that from the definition of $\Theta_{k,r}$ in (7.2.11) we have

$$a^*_{-r}a^*_{r+k}a_k\Theta_{k,r} = \mathbb{1}_{\{\mathcal{N}_{-r}=1\}}\mathbb{1}_{\{\mathcal{N}_{r+k}=1\}}\prod_{y\in S\setminus\{k\}}\mathbb{1}_{\{\mathcal{N}_{r+y}=0\}}a^*_{-r}a^*_{r+k}a_k\Theta_{k,r}. \tag{7.4.33}$$

This implies

$$\begin{aligned}&\big[a^*_{-r}a^*_{r+k}a_k\Theta_{k,r}, \mathbb{1}_{\{\mathcal{N}_p=0\}}\big] \\ &\qquad = a^*_{-r}a^*_{r+k}a_k\Theta_{k,r}\mathbb{1}_{\{\mathcal{N}_p=0\}}\big(\delta_{-r,p}+\delta_{r+k,p}\big) \\ &\qquad = \mathbb{1}_{\{\mathcal{N}_p=1\}}\mathbb{1}_{\{\mathcal{N}_{-p+k}=1\}}\prod_{y\in S\setminus\{k\}}\mathbb{1}_{\{\mathcal{N}_{-p+y}=0\}}a^*_pa^*_{-p+k}a_k\Theta_{k,-p}\left(\delta_{-r,p}+\delta_{r+k,p}\right).\end{aligned} \tag{7.4.34}$$

To compute the commutator with the second summand in the definition (7.4.31) of the projection χ_p, we distinguish four cases.

Case 1: $p=-r$ or $p=r+k$. This implies that $p\in-(r+k)+S$ or $p\in r+S$, which by definition of $\Theta^{(2)}_{k,r}$ gives $\Theta_{k,r}\mathbb{1}_{\{\mathcal{N}_p=1\}}=0$. Thus

$$\begin{aligned}\Big[a^*_{-r}a^*_{r+k}a_k\Theta_{k,r},\mathbb{1}_{\{\mathcal{N}_p=1\}}\sum_{x\in S}\mathbb{1}_{\{\mathcal{N}_{-p+x}=1\}}\prod_{y\in S\setminus\{x\}}\mathbb{1}_{\{\mathcal{N}_{-p+y}=0\}}\Big]&\\ =-\mathbb{1}_{\{\mathcal{N}_p=1\}}\sum_{x\in S}\mathbb{1}_{\{\mathcal{N}_{-p+x}=1\}}\prod_{y\in S\setminus\{x\}}\mathbb{1}_{\{\mathcal{N}_{-p+y}=0\}}a^*_pa^*_{-p+k}a_k\Theta_{k,-p}&\\ =-\mathbb{1}_{\{\mathcal{N}_p=1\}}\mathbb{1}_{\{\mathcal{N}_{-p+k}=1\}}\prod_{y\in S\setminus\{k\}}\mathbb{1}_{\{\mathcal{N}_{-p+y}=0\}}a^*_pa^*_{-p+k}a_k\Theta_{k,-p},&\end{aligned}$$

where the last equality follows from (7.4.33). With (7.4.34), this proves $[a^*_{-r}a^*_{r+k}a_k\Theta_{k,r},\chi_p]=0$.

Case 2: $p=r+z$ for some $z\in S\setminus\{k\}$. Then $p\notin\{-r,r+k\}$ and also $\Theta_{k,r}\mathbb{1}_{\{\mathcal{N}_p=1\}}=0$, which implies

$$\Big[a^*_{-r}a^*_{r+k}a_k\Theta_{k,r},\mathbb{1}_{\{\mathcal{N}_p=1\}}\sum_{x\in S}\mathbb{1}_{\{\mathcal{N}_{-p+x}=1\}}\prod_{y\in S\setminus\{x\}}\mathbb{1}_{\{\mathcal{N}_{-p+y}=0\}}\Big]=0$$

Since, in this case, we find from (7.4.34) that $[a^*_{-r}a^*_{r+k}a_k\Theta_{k,r},\mathbb{1}_{\{\mathcal{N}_p=0\}}]=0$, we conclude again that $[a^*_{-r}a^*_{r+k}a_k\Theta_{k,r},\chi_p]=0$.

Case 3: $p=-(r+k)+z$ for some $z\in S\setminus\{k\}$. Then $p\notin\{-r,r+k\}$ and $\Theta_{k,r}\mathbb{1}_{\{\mathcal{N}_p=1\}}=0$. Again, we find $[a^*_{-r}a^*_{r+k}a_k\Theta_{k,r},\chi_p]=0$.

Case 4: If none of the conditions apply, terms commute and $[a^*_{-r}a^*_{r+k}a_k\Theta_{k,r},\chi_p]=0$.

This shows that $\chi_pT_c\Gamma T^*_c\chi_p=T_c\Gamma T^*_c$. The second identity in (7.4.32) can be shown similarly. □

With Lemma 7.18, we can now show that the expectation of Q^S_3 and Q^M_3 vanish in the state $T^*_c\Gamma T_c$.

Lemma 7.19. *Let Γ be a density matrix on $\mathcal{F}(\Lambda)$ satisfying $\Gamma=\mathbb{1}_{\{\mathcal{N}_{S^c}=0\}}\Gamma\mathbb{1}_{\{\mathcal{N}_{S^c}=0\}}$ as well as $[\Gamma,\mathbb{P}_k]=0$ for all $k\in S$. Then*

$$\mathrm{Tr}\ T^*_cQ^S_3T_c\,\Gamma=\mathrm{Tr}\ T^*_cQ^M_3T_c\,\Gamma=0. \tag{7.4.35}$$

Proof. As noticed below (7.2.14), we have $[\mathbb{P}_k,T_c]=0$ for all $k\in S$. By assumption, we consider density matrices Γ such that $[\Gamma,\mathbb{P}_k]=0$ for all $k\in S$. It follows that

$$T_c\Gamma T^*_c=\mathbb{P}_kT_c\Gamma T^*_c\mathbb{P}_k+\mathbb{Q}_kT_c\Gamma T^*_c\mathbb{Q}_k \tag{7.4.36}$$

for all $k\in S$. On the other hand, from the definition of $\mathcal{M}_x$ in (7.2.13) and $\mathcal{N}_ia^*_j=a^*_j(\mathcal{N}_i+\delta_{i,j})$ we find

$$\mathcal{M}_xa^*_{-r}a^*_{r+p}a_p=a^*_{-r}a^*_{r+p}a_p\left(\mathcal{M}_x+\delta_{x,-r}+\delta_{x,r+p}-\delta_{x,p}\right). \tag{7.4.37}$$

The analogous statement holds for $\mathcal{M}_{-x}$. Distinguishing different cases, we readily show that the parity has to be violated for some $x\in S$, i.e. for every $r,p\in S$ with $r+p\in S$ there exists a $x\in S$ such that

$$\mathbb{P}_xa^*_{-r}a^*_{r+p}a_p=a^*_{-r}a^*_{r+p}a_p\mathbb{Q}_x.$$

Thus we find that Tr $a^*_{-r}a^*_{r+p}a_pT_c\Gamma T^*_c=0$ for all $r,p\in S$ with $r+p\in S$. Hence $\mathrm{Tr}\,Q^S_3T_c\Gamma T^*_c=0$.

To show the second equality in (7.4.35), we derive an identity similar to (7.4.37). Here this task is more subtle than above, because the second term in the definition (7.2.13) of $\mathcal{M}_x$, measuring the number of x-connections, does not commute with Q_3^M. We are going to use Lemma 7.18. We decompose

$$Q_3^M = \sum_{\substack{r,p\in H:\\ r+p\in S}} N^{1/2}\widehat{V}_N(r)a_{-r}^* a_{r+p}^* a_p + \text{h.c.} + \sum_{p\in H_r, r\in S} N^{1/2}\widehat{V}_N(r)a_{-r}^* a_{r+p}^* a_p + \text{h.c.} =: Q_3^{M,1} + Q_3^{M,2}.$$

First, we consider $Q_3^{M,1}$. From (7.4.32), we find

$$\begin{aligned}\text{Tr } T_c^* Q_3^{M,1} T_c\Gamma &= \sum_{\substack{r,p\in H:\\ r+p\in S}} N^{1/2}\widehat{V}_N(r)\text{Tr } a_{-r}^* a_{r+p}^* a_p T_c\Gamma T_c^* \\ &= \sum_{\substack{r,p\in H:\\ r+p\in S}} N^{1/2}\widehat{V}_N(r)\text{Tr } \chi_{-r} a_{-r}^* a_{r+p}^* a_p \chi_p T_c\Gamma T_c^*.\end{aligned}$$

Using that $a_{-r}^* = \mathbb{1}_{\{\mathcal{N}_{-r}\geqslant 1\}}a_{-r}^*$ and $a_p = a_p\mathbb{1}_{\{\mathcal{N}_p\geqslant 1\}}$, we may equivalently consider the expectation, in the state $T_c\Gamma T_c^*$, of the observable

$$\sum_{y,z\in S}\mathbb{1}_{\{\mathcal{N}_{-r}=1\}}\mathbb{1}_{\{\mathcal{N}_{r+y}=1\}}\prod_{y'\in S\setminus\{y\}}\mathbb{1}_{\{\mathcal{N}_{r+y'}=0\}}a_{-r}^* a_{r+p}^* a_p\mathbb{1}_{\{\mathcal{N}_p=1\}}\mathbb{1}_{\{\mathcal{N}_{-p+z}=1\}}\prod_{z'\in S\setminus\{z\}}\mathbb{1}_{\{\mathcal{N}_{-p+z'}=0\}} \tag{7.4.38}$$

for $r,p\in H$ such that $r+p\in S$. To show that the expectation of each summand in the previous line vanishes, we apply the parity argument as we did for Q_3^S. For $x\in S$, using the definition of $\mathcal{M}_x$ in (7.2.13) and $\mathcal{N}_i a_j^* = a_j^*(\mathcal{N}_i + \delta_{i,j})$, we find

$$\begin{aligned}\mathcal{M}_x a_{-r}^* a_{r+p}^* a_p &= a_{-r}^* a_{r+p}^*\left(\mathcal{M}_x + \delta_{x,r+p} + \frac{1}{2}\sum_{t\in H_x}(\delta_{t,r}\mathcal{N}_{t+x} + \delta_{t+x,-r}\mathcal{N}_{-t})\right)a_p \\ &= a_{-r}^* a_{r+p}^* a_p\big(\mathcal{M}_x + \delta_{x,r+p}\big) + \mathcal{N}_{r+x}\mathbb{1}_{H_x}(r)a_{-r}^* a_{r+p}^* a_p - a_{-r}^* a_{r+p}^* a_p\mathcal{N}_{-p+x}\mathbb{1}_{H_x}(-p).\end{aligned}$$

Thus, we obtain, for $y,z\in S$ such that $r+y,-p+z\in H$ (note that otherwise the expectation in (7.4.38) vanishes as $r+y,-p+z$ cannot be in S and there is no particle in $(H\cup S)^c$)

$$\begin{aligned}&\mathcal{M}_x\mathbb{1}_{\{\mathcal{N}_{r+y}=1\}}\prod_{y'\in S\setminus\{y\}}\mathbb{1}_{\{\mathcal{N}_{r+y'}=0\}}a_{-r}^* a_{r+p}^* a_p\mathbb{1}_{\{\mathcal{N}_{-p+z}=1\}}\prod_{z'\in S\setminus\{z\}}\mathbb{1}_{\{\mathcal{N}_{-p+z'}=0\}} \\ &\quad= \mathbb{1}_{\{\mathcal{N}_{r+y}=1\}}\prod_{y'\in S\setminus\{y\}}\mathbb{1}_{\{\mathcal{N}_{r+y'}=0\}}a_{-r}^* a_{r+p}^* a_p\mathbb{1}_{\{\mathcal{N}_{-p+z}=1\}}\prod_{z'\in S\setminus\{z\}}\mathbb{1}_{\{\mathcal{N}_{-p+z'}=0\}} \\ &\qquad\times(\mathcal{M}_x + \delta_{x,r+p} + \delta_{x,y} - \delta_{x,z})\end{aligned}$$

(compare this to (7.4.37)). The same calculation for $\mathcal{M}_{-x}$ and a case distinction shows that the parity is violated for some $x\in S$, i.e. for every $p,r\in H$ such that $r+p\in S$ and for every $y,z\in S$, there exists $x\in S$ such that

$$\begin{aligned}&\mathbb{P}_x\mathbb{1}_{\{\mathcal{N}_{r+y}=1\}}\prod_{y'\in S\setminus\{y\}}\mathbb{1}_{\{\mathcal{N}_{r+y'}=0\}}a_{-r}^* a_{r+p}^* a_p\mathbb{1}_{\{\mathcal{N}_{-p+z}=1\}}\prod_{z'\in S\setminus\{y\}}\mathbb{1}_{\{\mathcal{N}_{r+z'}=0\}} \\ &\quad= \mathbb{1}_{\{\mathcal{N}_{r+y}=1\}}\prod_{y'\in S\setminus\{y\}}\mathbb{1}_{\{\mathcal{N}_{r+y'}=0\}}a_{-r}^* a_{r+p}^* a_p\mathbb{1}_{\{\mathcal{N}_{-p+z}=1\}}\prod_{z'\in S\setminus\{y\}}\mathbb{1}_{\{\mathcal{N}_{r+z'}=0\}}\mathbb{Q}_x.\end{aligned} \tag{7.4.39}$$

With (7.4.36) this implies that the expectation of each term in (7.4.38) vanishes. By linearity, we conclude that Tr $T_c^* Q_3^{M,1}T_c\Gamma = 0$. Similarly, swapping the roles of $-r$ and $r+p$, we also obtain Tr $T_c^* Q_3^{M,2}T_c\Gamma = 0$. □

7.4.5 Action on the quartic potential energy operator

Finally, we study the conjugation of the quartic term Q_4 in (7.2.8). On the range of the projection $\Xi = \mathbb{1}_{\{\mathcal{N}_{(H\cup S)^c}=0\}}\mathbb{1}_{\{\mathcal{N}_H\in 2\mathbb{N}_0\}}$, we can decompose

$$Q_4 = Q_4^H + Q_4^M + Q_4^S$$

with

$$\begin{aligned}
Q_4^H &= \frac{1}{2}\sum_{\substack{r\in\Lambda^*\\ p,q\in H_r}} \widehat{V}_N(r)a^*_{p+r}a^*_q a_{q+r}a_p\\
Q_4^M &= \frac{1}{2}\sum_{\substack{q\in H,p\in S,r\in\Lambda^*:\\ p+r\in H,q+r\in S}} \widehat{V}_N(r)a^*_{p+r}a^*_q a_{q+r}a_p + \text{h.c.} + \frac{1}{2}\sum_{\substack{p,q\in S,r\in\Lambda^*:\\ p+r,q+r\in H}} \widehat{V}_N(r)a^*_{p+r}a^*_q a_{q+r}a_p + \text{h.c.}\\
&\quad + \frac{1}{2}\sum_{\substack{p\in H,q\in S,r\in\Lambda^*:\\ p+r\in H,q+r\in S}} \widehat{V}_N(r)a^*_{p+r}a^*_q a_{q+r}a_p + \text{h.c.} =: Q_4^{M,1} + Q_4^{M,2} + Q_4^{M,3}\\
Q_4^S &= \frac{1}{2}\sum_{\substack{q,p\in S,r\in\Lambda^*:\\ p+r,q+r\in S}} \widehat{V}_N(r)a^*_{p+r}a^*_q a_{q+r}a_p.
\end{aligned} \tag{7.4.40}$$

Let us first consider the term Q_4^H. It is convenient to define

$$\widetilde{Q}_4^H = \frac{1}{2}\sum_{\substack{r\in\Lambda^*\\ p,q\in H_r}} \widehat{V}_N(r)\mathbb{1}_S(p+q+r)a^*_{p+r}a^*_q a_{q+r}a_p.$$

In the next lemma we show that the difference $Q_4^H - \widetilde{Q}_4^H$ is small on an appropriate class of trial states.

Lemma 7.20. *Suppose that Γ is a density matrix on $\mathcal{F}(\Lambda)$ satisfying $\Gamma = \mathbb{1}_{\{\mathcal{N}_{S^c}=0\}}\Gamma\mathbb{1}_{\{\mathcal{N}_{S^c}=0\}}$. Then we have*

$$\pm\text{Tr}\ T_c^*(Q_4^H - \widetilde{Q}_4^H)T_c\Gamma \lesssim N^{-1+5\kappa/2+3\varepsilon}\text{Tr}\ T_c^*\mathcal{N}_H^2 T_c\Gamma,$$

Proof. Let us first explain the idea of the proof, heuristically. Consider the expectation of $a^*_{p+r}a^*_q a_{q+r}a_p$ in the state $T_c\Gamma T_c^*$. The operator a_p annihilates a particle with momentum p which, by (7.4.32), has to be connected to exactly one other particle with momentum $-p+x, x\in S$. After the annihilation and application of the remaining $a^*_{p+r}a^*_q a_{q+r}$ this particle again needs to be connected. So either $q+r=-p+x$, which is the main term of $\widetilde{Q}_4^H$, or $-p+x\in -(p+r)+S\cup -q+S$. This leads to the condition $r\in S+S$ or $q-p\in S+S$. Either constraint is enough to show that these contributions are negligible.

We will now make this argument rigorous. First, let us assume that $r\notin S+S$ and $q-p\notin S+S$. Then from Lemma 7.18, we find

$$\begin{aligned}
&\text{Tr}\left(a^*_{p+r}a^*_q a_{q+r}a_p T_c\Gamma T_c^*\right)\\
&\quad= \text{Tr}\left(a^*_{p+r}a^*_q a_{q+r}a_p\mathbb{1}_{\{\mathcal{N}_p=1\}}\sum_{x\in S}\mathbb{1}_{\{\mathcal{N}_{-p+x}=1\}}T_c\Gamma T_c^*\right)\\
&\quad= \sum_{x\in S}\text{Tr}\left(\mathbb{1}_{\{\mathcal{N}_{-p+x}=1\}}a^*_{p+r}a^*_q a_{q+r}a_p\mathbb{1}_{\{\mathcal{N}_p=1\}}T_c\Gamma T_c^*\right)\mathbb{1}(q,p+r\neq -p+x)
\end{aligned}$$

because, on the one hand, $-p+x \neq q+r$ (from the assumption $p+q+r \notin S$) and, on the other hand, the contributions from $-p+x=q$ and $-p+x=p+r$ vanish, since there cannot be two H-particles in the same momentum state on the range of $T_c\Gamma T_c^*$, i.e. $\mathbb{1}_{\{\mathcal{N}_k \geqslant 2\}} T_c \Gamma T_c^* = 0$ for all $k \in H$, which follows from (7.4.32). Applying again (7.4.32), we obtain

$$\begin{aligned}
&\operatorname{Tr}\left(a_{p+r}^* a_q^* a_{q+r} a_p T_c \Gamma T_c^*\right) \\
&\quad = \sum_{x,y \in S} \operatorname{Tr}\left(\mathbb{1}_{\{\mathcal{N}_{-p+x}=1\}} \mathbb{1}_{\{\mathcal{N}_{p-x+y}=1\}} a_{p+r}^* a_q^* a_{q+r} a_p \mathbb{1}_{\{\mathcal{N}_p=1\}} T_c \Gamma T_c^*\right) \mathbb{1}(q, p+r \neq -p+x) \\
&\quad = \sum_{x,y \in S} \operatorname{Tr}\left(a_{p+r}^* a_q^* a_{q+r} a_p \mathbb{1}_{\{\mathcal{N}_{-p+x}=1\}} \mathbb{1}_{\{\mathcal{N}_{p-x+y}=1\}} \mathbb{1}_{\{\mathcal{N}_p=1\}} T_c \Gamma T_c^*\right) \\
&\qquad\qquad\qquad\qquad \times \mathbb{1}(q, p+r \neq -p+x) \mathbb{1}(q+r, p \neq p-x+y)
\end{aligned}$$

since $p-x+y \neq p+r, q$ from the assumption $r, q-p \notin S+S$ and the contribution from $p-x+y = q+r, p$ can be excluded as above, using that $\mathbb{1}_{\{\mathcal{N}_k \geqslant 2\}} T_c \Gamma T_c^* = 0$ for all $k \in H$. Since the particle with momentum $-p+x$ is S-connected both with the particle with momentum p and the particle with momentum $p-x+y$, we conclude that

$$\operatorname{Tr}\left(a_{p+r}^* a_q^* a_{q+r} a_p T_c \Gamma T_c^*\right) = 0 \tag{7.4.41}$$

To handle the case $r \in S+S$ or $q-p \in S+S$, we observe that, by the Cauchy–Schwarz inequality, we find

$$\begin{aligned}
\pm \sum_{\substack{r \in \Lambda^* \\ p,q \in H_r}} \widehat{V}_N(r) a_{p+r}^* a_q^* a_{q+r} a_p \mathbb{1}_{S^c}(p+q+r) \left(\mathbb{1}_{S+S}(r) + \mathbb{1}_{(S+S)^c}(r) \mathbb{1}_{S+S}(q-p)\right)& \\
\lesssim N^{-1+5\kappa/2+3\varepsilon} \mathcal{N}_H^2&,
\end{aligned}$$

where we used that $\|\widehat{V}\|_\infty \lesssim N^{-1+\kappa}$ and $|S| \lesssim N^{3\kappa/2+3\varepsilon}$. □

Next, we conjugate $\widetilde{Q}_4^H$ with T_k, for a $k \in S$.

Lemma 7.21. *On the range of Λ_k, we have, in the sense of quadratic forms,*

$$\begin{aligned}
\pm\Bigg(T_k^* \widetilde{Q}_4^H T_k - \widetilde{Q}_4^H - \sum_{r,p \in H_k} \widehat{V}_N(r-p) N \varphi_r (\varphi_p + \varphi_{p+k}) \Theta_{k,r}^{(2)} \Theta_{k,p}^{(2)} a_k^* a_k\Bigg)& \\
\lesssim N^{-5+15\kappa/2+9\varepsilon} (\mathcal{N}_k + 1) \sum_{p,q \in H} \mathbb{1}_S(p+q) |q|^2 a_p^* a_q^* a_q a_p + N^{-2+4\kappa+\varepsilon} \mathcal{N}_k^2&.
\end{aligned}$$

Proof. Let us fix $k \in S$, $r \in \Lambda^*$, $p, q \in H_r$ with $p+q+r \in S$. Using (7.4.4), we obtain, on $\operatorname{Ran}\Lambda_k$,

$$\begin{aligned}
T_k^* a_{p+r}^* a_q^* a_{q+r} a_p T_k = \cos(X_k) a_{p+r}^* a_q^* a_{q+r} a_p \cos(X_k) + \frac{\sin(X_k)}{X_k} \mathcal{B}_k^\circ a_{p+r}^* a_q^* a_{q+r} a_p \mathcal{B}_k^\sharp \frac{\sin(X_k)}{X_k}& \\
+ \left[\cos(X_k) a_{p+r}^* a_q^* a_{q+r} a_p \mathcal{B}_k^\sharp \frac{\sin(X_k)}{X_k} + \text{h.c.}\right]&
\end{aligned} \tag{7.4.42}$$

Let us first show that the cross terms on the second line vanish. We have

$$\begin{aligned}
a_{p+r}^* a_q^* a_{q+r} a_p \mathcal{B}_k^\sharp &= \sum_{t \in H_k} a_{p+r}^* a_q^* a_{q+r} a_p a_{-t}^* a_{k+t}^* a_k N^{1/2} \varphi_t \Theta_{k,t} \\
&= \sum_{t \in H_k} \left(a_{-t}^* a_{k+t}^* a_{p+r}^* a_q^* a_{q+r} a_p + a_{p+r}^* a_q^* \left[a_{q+r} a_p, a_{-t}^* a_{k+t}^*\right]\right) a_k N^{1/2} \varphi_t \Theta_{k,t}
\end{aligned}$$

Using

$$\begin{aligned}\left[a_{q+r}a_p, a^*_{-t}a^*_{k+t}\right] &= a^*_{k+t}a_{q+r}\delta_{p,-t} + a^*_{-t}a_{q+r}\delta_{p,k+t} + \delta_{q+r,-t}a^*_{k+t}a_p + \delta_{q+r,k+t}a^*_{-t}a_p \\ &\quad + \delta_{q+r,k+t}\delta_{p,-t} + \delta_{p,k+t}\delta_{q+r,-t}\end{aligned} \tag{7.4.43}$$

and noticing that, since the cutoff $\Theta_{k,t}$ imposes that the S-neighborhoods of t and of $-(t+k)$ are empty and since $p+q+r \in S$, the contribution of the quadratic terms on the right-hand side of (7.4.43) vanishes, we obtain

$$\begin{aligned}&a^*_{p+r}a^*_q a_{q+r}a_p \mathcal{B}^\sharp_k \\ &\quad= \sum_{t\in H_k} \left(a^*_{-t}a^*_{k+t}a^*_{p+r}a^*_q a_{q+r}a_p + a^*_{p+r}a^*_q(\delta_{q+r,-t}\delta_{p,k+t} + \delta_{q+r,k+t}\delta_{p,-t})\right) a_k N^{1/2}\varphi_t\Theta_{k,t}.\end{aligned} \tag{7.4.44}$$

Observing now that all terms in the sum on the right-hand side create a k-connection, we conclude that $\Lambda_k a^*_{p+r}a^*_q a_{q+r}a_p\mathcal{B}^\sharp_k = 0$. Thus, the cross terms vanish on $\mathrm{Ran}\Lambda_k$.

Let us now consider the second term on the right-hand side of (7.4.42). From (7.4.44) and using, similarly to (7.4.3), the fact that $\Theta_{k,t}$ excludes k-connections and particles in the S-neighborhoods of t and $-(t+k)$, we find, on the range of Λ_k,

$$\begin{aligned}&\mathcal{B}^\circ_k a^*_{p+r}a^*_q a_{q+r}a_p \mathcal{B}^\sharp_k \\ &= \sum_{t\in H_k} \mathcal{B}^\circ_k \left(a^*_{-t}a^*_{k+t}a^*_{p+r}a^*_q a_{q+r}a_p + a^*_{p+r}a^*_q(\delta_{q+r,-t}\delta_{p,k+t} + \delta_{q+r,k+t}\delta_{p,-t})\right) a_k N^{1/2}\varphi_t\Theta_{k,t} \\ &= \sum_{t\in H_k} \Theta_{k,t}N\varphi_t(\varphi_t + \varphi_{k+t})a^*_k a_k a^*_{p+r}a^*_q a_{q+r}a_p\Theta_{k,t} \\ &\quad + \sum_{t,t'\in H_k} N\varphi_t\varphi_{t'}(\delta_{p+r,-t'}\delta_{q,k+t'} + \delta_{p+r,k+t'}\delta_{q,-t'})(\delta_{q+r,k+t}\delta_{p,-t} + \delta_{q+r,-t}\delta_{p,k+t})\Theta_{k,t'}a^*_k a_k\Theta_{k,t} \\ &= a^*_{p+r}a^*_q(X_k^{(p+r,q,q+r,p)})^2 a_{q+r}a_p + N(\varphi_p + \varphi_{p-k})(\varphi_q + \varphi_{q-k})\Theta_{k,-p}\Theta_{k,-q}\delta_{p+q+r,k}\mathcal{N}_k\end{aligned}$$

with

$$\begin{aligned}(X_k^{(p+r,q,q+r,p)})^2 &= \sum_{t\in H_k} N\varphi_t(\varphi_t+\varphi_{k+t})\Theta_{k,t}a^*_k a_k\big(1 - \mathbb{1}(p+r,q,q+r,p \sim_{\mathrm{S}} -(t+k),t)\big) \\ &=: X_k^2 - \delta_k^{(p+r,q,q+r,p)}.\end{aligned} \tag{7.4.45}$$

Here, similarly to the analysis of Q_3^H, we used (7.4.25) to commute $\Theta_{k,t}$ (on the range of Λ_k, we have $\Theta_{k,t} = \Theta^{(2)}_{k,t}$) and we defined

$$\mathbb{1}(p+r,q,q+r,p \sim_{\mathrm{S}} -(t+k),t) := \begin{cases} 1 & \text{if } \{p+r,q,q+r,p\} \cap \big((-(t+k)+S)\cup(t+S)\big) \neq \emptyset \\ 0 & \text{otherwise,}\end{cases}$$

which checks if at least one of the momenta $p+r, q, q, +r$ or p is in the shell-neighborhood of $-(t+k)$ or t. Notice that $\delta_k^{(p+r,q,q+r,p)}$ is a non-negative operator, which can be shown as in (7.4.15). Moreover, Lemma 7.3 implies that

$$\delta_k^{(p+r,q,q+r,p)} \leqslant 8|S|N\|\varphi_H\|^2_\infty\mathcal{N}_k \lesssim N^{-5+15\kappa/2+7\varepsilon}\mathcal{N}_k. \tag{7.4.46}$$

Recalling the definition (7.4.26) and using (7.4.30) we have, from (7.4.42), on $\mathrm{Ran}\Lambda_k$,

$$
\begin{aligned}
&T_k^* a_{p+r}^* a_q^* a_{q+r} a_p T_k \\
&= a_{p+r}^* a_q^* \Big(\cos(X_k^{(p+r,q)}) \cos(X_k^{(p,q+r)}) + \frac{\sin(X_k^{(p+r,q)})}{X_k^{(p+r,q)}} (X_k^{(p+r,q,q+r,p)})^2 \frac{\sin(X_k^{(p,q+r)})}{X_k^{(p,q+r)}} \Big) a_{q+r} a_p \\
&\quad + N(\varphi_p + \varphi_{p-k})(\varphi_q + \varphi_{q-k}) \Theta_{k,-p} \Theta_{k,-q} \delta_{p+q+r,k} \mathcal{N}_k \frac{\sin^2 X_k}{X_k^2}. \qquad (7.4.47)
\end{aligned}
$$

Using trigonometric identities and the fact that the operators $X_k^{(p+r,q)}, X_k^{(q,p+r)}, X_k^{(p+r,q,q+r,p)}$ commute with each other, we can write

$$
\begin{aligned}
&\cos(X_k^{(p+r,q)}) \cos(X_k^{(p,q+r)}) + \frac{\sin(X_k^{(p+r,q)})}{X_k^{(p+r,q)}} (X_k^{(p+r,q,q+r,p)})^2 \frac{\sin(X_k^{(p,q+r)})}{X_k^{(p,q+r)}} \\
&= \cos(X_k^{(p+r,q)} - X_k^{(p,q+r)}) + \frac{\sin(X_k^{(p+r,q)})}{X_k^{(p+r,q)}} \frac{\sin(X_k^{(p,q+r)})}{X_k^{(p,q+r)}} \Big((X_k^{(p+r,q,q+r,p)})^2 - X_k^{(p+r,q)} X_k^{(p,q+r)} \Big) \\
&= 1 + R_k^{(p+r,q,q+r,p)}.
\end{aligned}
$$

We can estimate

$$
\pm R_k^{(p+r,q,q+r,p)} \leqslant \delta_k^{(p+r,q,q+r,p)} + 3\delta_k^{(p+r,q)} + 2\delta_k^{(p,q+r)} \lesssim N^{-5+15\kappa/2+7\varepsilon} \mathcal{N}_k
$$

as follows from the inequality

$$
\Big| \cos(x-y) + \frac{\sin x}{x} \frac{\sin y}{y} (z^2 - xy) - 1 \Big| \leqslant (v^2 - z^2) + 3(v^2 - x^2) + 2(v^2 - y^2)
$$

for all $0 \leqslant x, y, z \leqslant v$ (with v playing the role of X_k). The contribution of the remainder terms $R_k^{(p+r,q,q+r,p)}$ to $T_k \widetilde{Q}_4^H T_k$ can therefore be estimated, using the Cauchy-Schwarz inequality, by

$$
\begin{aligned}
&\pm \sum_{\substack{r \in \Lambda^* \\ p,q \in H_r}} \widehat{V}_N(r) \mathbb{1}_S(p+q+r) a_{p+r}^* a_q^* R_k^{(p+r,q,q+r,p)} a_{q+r} a_p \\
&\quad \leqslant \sum_{\substack{r \in \Lambda^* \\ p,q \in H_r}} \eta \frac{|\widehat{V}_N(r)|}{p^2} \mathbb{1}_S(p+q+r) q^2 a_{p+r}^* a_q^* R_k^{(p+r,q,q+r,p)} (\mathcal{N}_k + 1)^{-1} R_k^{(p+r,q,q+r,p)} a_q a_{p+r} \\
&\qquad + \eta^{-1} \sum_{\substack{r \in \Lambda^* \\ p,q \in H_r}} \frac{|\widehat{V}_N(r)|}{q^2} p^2 \mathbb{1}_S(p+q+r) a_p^* a_{q+r}^* (\mathcal{N}_k + 1) a_{q+r} a_p
\end{aligned}
$$

for every $\eta > 0$. Choosing $\eta^{-1} = N^{-5+15\kappa/2+7\varepsilon}$, we obtain

$$
\begin{aligned}
&\pm \sum_{\substack{r \in \Lambda^* \\ p,q \in H_r}} \widehat{V}_N(r) \mathbb{1}_S(p+q+r) a_{p+r}^* a_q^* R_k^{(p+r,q,q+r,p)} a_{q+r} a_p \\
&\qquad \lesssim N^{-5+15\kappa/2+7\varepsilon} \sum_{\substack{r \in \Lambda^* \\ q \in H}} \frac{|\widehat{V}_N(r)|}{|p-r|^2} \mathbb{1}_S(p+q) |p|^2 a_p^* a_q^* a_p a_q (\mathcal{N}_k + 1) \\
&\qquad \lesssim N^{-5+15\kappa/2+9\varepsilon} \sum_{\substack{r \in \Lambda^* \\ q \in H}} \mathbb{1}_S(p+q) |p|^2 a_p^* a_q^* a_p a_q (\mathcal{N}_k + 1). \qquad (7.4.48)
\end{aligned}
$$

In the last inequality, we applied Hölder's inequality and the bound $\|V_N\|_{L^{3/2+\varepsilon}} \lesssim N^{2\varepsilon}$.

Let us now consider the last term on the right-hand side of (7.4.47). To evaluate its contribution to $T_k^* \widetilde{Q}_4^H T_k$, we observe that

$$\begin{aligned} &\frac{1}{2} \sum_{\substack{r \in \Lambda^* \\ p,q \in H_r}} \widehat{V}_N(r) N(\varphi_p + \varphi_{p-k})(\varphi_q + \varphi_{q-k}) \Theta_{k,-p} \Theta_{k,-q} \delta_{p+q+r,k} \mathcal{N}_k \\ &\qquad\qquad = \sum_{r,p \in H_k} N \widehat{V}_N(r-p) \varphi_r (\varphi_p + \varphi_{p+k}) \Theta_{k,p} \Theta_{k,r} \mathcal{N}_k. \end{aligned} \tag{7.4.49}$$

By Young's inequality and estimating $\|\varphi\|_1 \lesssim C$ with Lemma 7.3, we find

$$\Big| \sum_{r,p \in H_k} N \widehat{V}_N(r-p) \varphi_r (\varphi_p + \varphi_{p+k}) \Big| \lesssim N^\kappa.$$

With the bound

$$\Big| \frac{\sin^2 x}{x^2} - 1 \Big| \leqslant C x^2$$

valid for all $x > 0$ and with the estimate (7.4.2) for X_k, we conclude that

$$\begin{aligned} \pm \Big[&\sum_{\substack{r \in \Lambda^* \\ p,q \in H_r}} \widehat{V}_N(r) \mathbb{1}_S(p+q+r) N(\varphi_p + \varphi_{p-k})(\varphi_q + \varphi_{q-k}) \Theta_{k,-p} \Theta_{k,-q} \delta_{p+q+r,k} \mathcal{N}_k \frac{\sin^2 X_k}{X_k^2} \\ &\qquad - \sum_{r,p \in H_k} N \widehat{V}_N(r-p) \varphi_r (\varphi_p + \varphi_{p+k}) \Theta_{k,p} \Theta_{k,r} \mathcal{N}_k \Big] \lesssim N^{-2+4\kappa+\varepsilon} \mathcal{N}_k^2. \end{aligned}$$

Together with (7.4.48), we obtain the statement of the lemma. □

Next, we consider the term Q_4^S, where the four momenta are in the shell. We show that its contribution is negligible.

Lemma 7.22. *Let Γ be a density matrix on $\mathcal{F}(\Lambda)$ satisfying $\Gamma = \mathbb{1}_{\{\mathcal{N}_{S^c}=0\}} \Gamma \mathbb{1}_{\{\mathcal{N}_{S^c}=0\}}$ as well as $[\Gamma, \mathbb{P}_k] = 0$ for all $k \in S$ (with $\mathbb{P}_k$ the parity operator defined in (7.2.14)). Then we have*

$$\operatorname{Tr} T_c^* Q_4^S T_c \Gamma \lesssim N^{-1+\kappa} \operatorname{Tr} T_c^* \mathcal{N}_S (\mathcal{N}_S + N^{3\kappa/2+3\varepsilon}) T_c \Gamma.$$

Proof. Let us once again use the parity argument: Recall (7.2.13), where, for $k \in S$, we defined

$$\mathcal{M}_k = \mathcal{N}_k + \sum_{t \in H_k} \mathcal{N}_{-t} \mathcal{N}_{t+k},$$

counting the number of particles with momenta k and the number of k-connections. From the assumption $\Gamma = \mathbb{1}_{\{\mathcal{N}_{S^c}=0\}} \Gamma \mathbb{1}_{\{\mathcal{N}_{S^c}=0\}}$ with $[\Gamma, \mathbb{P}_k] = 0$, and from the observation that $[T_c, \mathbb{P}_k] = 0$, we have $T_c \Gamma T_c^* = \mathbb{P}_k T_c \Gamma T_c^* \mathbb{P}_k + \mathbb{Q}_k T_c \Gamma T_c^* \mathbb{Q}_k$, for all $k \in S$. After computing the commutator of $\mathcal{M}_k$ and $\mathcal{M}_{-k}$ with $a_{p+r}^* a_q^* a_{q+r} a_p$ we find that the contribution of $a_{p+r}^* a_q^* a_{q+r} a_p$ vanishes unless one of the following conditions holds true:

- $p + r = \pm q$ and $q + r = \pm p$
- $p + r = \pm q + r$ and $q = \pm p$
- $p + r = \pm p$ and $q = \pm q + r$,

This implies that, necessarily, $-r = p+q$, $p = q$ or $r = 0$ must hold true. Therefore, we find that

$$\begin{aligned}
&\mathrm{Tr}\ T_c^* Q_4^S T_c \Gamma T_c^* \\
&\lesssim \mathrm{Tr}\ \Big(\sum_{p,q\in S} \widehat{V}_N(p+q) a^*_{-q} a^*_q a_{-p} a_p + \sum_{p,r\in S} \widehat{V}_N(r) a^*_{p+r} a^*_p a_{p+r} a_p \quad + \sum_{p,q\in S} \widehat{V}_N(0) a^*_p a^*_q a_q a_p \Big) T_c \Gamma T_c^*.
\end{aligned}$$

Thus

$$\mathrm{Tr}\ T_c^* Q_4^S T_c \Gamma \lesssim \|\widehat{V}_N\|_{L^\infty} \mathrm{Tr}\ \mathcal{N}_S (\mathcal{N}_S + N^{3\kappa/2+3\varepsilon}) T_c \Gamma T_c^*.$$

Here we used that

$$\begin{aligned}
\sum_{p,q\in S} \widehat{V}_N(p+q) a^*_{-q} a^*_q a_{-p} a_p &= \sum_{p\in S} \widehat{V}_N(0) \mathcal{N}_p (\mathcal{N}_p - 1) + \sum_{\substack{p,q\in S\\ p\neq q}} \widehat{V}_N(p+q) (a^*_{-q} a_{-p})(a^*_q a_p) \\
&\lesssim \|\widehat{V}_N\|_{L^\infty} \mathcal{N}_S (\mathcal{N}_S + N^{3\kappa/2+3\varepsilon}).
\end{aligned}$$

□

As for the term Q_4^M, we decompose it as in (7.4.40), writing $Q_4^M = Q_4^{M,1} + Q_4^{M,2} + Q_4^{M,3}$. First, we handle $Q_4^{M,1}$.

Lemma 7.23. *Let Γ be a density matrix on $\mathcal{F}(\Lambda)$ satisfying $\Gamma = \mathbb{1}_{\{\mathcal{N}_{S^c}=0\}} \Gamma \mathbb{1}_{\{\mathcal{N}_{S^c}=0\}}$ as well as $[\Gamma, \mathbb{P}_k] = 0$ for all $k \in S$. Then we have*

$$\mathrm{Tr}\ T_c^* Q_4^{M,1} T_c \Gamma = 0.$$

Proof. Recall that

$$Q_4^{M,1} = \frac{1}{2} \sum_{\substack{q\in H, p\in S, r\in\Lambda^*:\\ p+r\in H, q+r\in S}} \widehat{V}_N(r) a^*_{p+r} a^*_q a_{q+r} a_p + \text{h.c.}.$$

From $q \in H, q+r \in S$, we find $r \notin S+S$. Similarly, from $p+r \in H, q+r \in S$, we obtain $q-p \notin S+S$. With the analysis at the beginning of the proof of Lemma 7.20, in particular (7.4.41), we conclude that, unless $p+q+r \in S$, the expectation of $a^*_{p+r} a^*_q a_{q+r} a_p$ in the state $T_c \Gamma T_c^*$ vanishes. For $p+q+r \in S$, the operator $a^*_{p+r} a^*_q a_{q+r} a_p$ creates a $(p+q+r)$-connection, annihilates a particle with momentum $p \in S$ and a particle with momentum $q+r \in S$. Consequently, also this term vanishes in expectation due to the same parity argument that was used in the previous lemmata. □

Finally, we estimate the expectation of the terms $Q_4^{M,2}$ and $Q_4^{M,3}$.

Lemma 7.24. *Let Γ be a density matrix on $\mathcal{F}(\Lambda)$ satisfying $\Gamma = \mathbb{1}_{\{\mathcal{N}_{S^c}=0\}} \Gamma \mathbb{1}_{\{\mathcal{N}_{S^c}=0\}}$ as well as $[\Gamma, \mathbb{P}_k] = 0$ for all $k \in S$. Then we have*

$$\pm \mathrm{Tr}\ T_c^* (Q_4^{M,2} + Q_4^{M,3}) T_c \Gamma \lesssim N^{-1+\kappa} \mathrm{Tr}\ T_c^* \mathcal{N}_H (\mathcal{N}_S + N^{3\kappa/2+3\varepsilon}) T_c \Gamma.$$

Proof. Let us focus on the contribution of $Q_4^{M,2}$, the one of $Q_4^{M,3}$ can be handled analogously. Recall that

$$Q_4^{M,2} = \frac{1}{2} \sum_{\substack{p,q\in S, r\in\Lambda^*:\\ p+r, q+r\in H}} \widehat{V}_N(r) a^*_{p+r} a^*_q a_{q+r} a_p + \text{h.c.}$$

Using Lemma 7.18, we write

$$\begin{aligned}&\mathrm{Tr}\ a_{p+r}^* a_q^* a_{q+r} a_p T_c \Gamma T_c^*\\&= \mathrm{Tr} \sum_{x,y\in S} \mathbb{1}_{\{\mathcal{N}_{p+r}=1\}} \mathbb{1}_{\{N_{y-(p+r)}=1\}} a_{p+r}^* a_q^* a_{q+r} a_p \mathbb{1}_{\{\mathcal{N}_{q+r}=1\}} \mathbb{1}_{\{\mathcal{N}_{x-(q+r)}=1\}} T_c \Gamma T_c^*\end{aligned}$$

The term annihilates a x-connection and a particle with momentum p, and creates a y-connection and a particle with momentum q. Thus, by our standard parity argument, we find that one of the following conditions must be fulfilled:

(1) $x = \pm p$ and $y = \pm q$,

(2) $x = \pm q$ and $y = \pm p$,

(3) $x = \pm y$ and $p = \pm q$.

Case (1)*:* With Cauchy–Schwarz we obtain

$$\begin{aligned}&\pm \mathbb{1}_{\{\mathcal{N}_{p+r}=1\}} \mathbb{1}_{\{N_{y-(p+r)}=1\}} a_{p+r}^* a_q^* a_{q+r} a_p \mathbb{1}_{\{\mathcal{N}_{q+r}=1\}} \mathbb{1}_{\{\mathcal{N}_{x-(q+r)}=1\}}\\&= \pm \mathbb{1}_{\{\mathcal{N}_{p+r}=1\}} \mathbb{1}_{\{N_{y-(p+r)}=1\}} a_{p+r}^* (a_p a_q^* - \delta_{p,q}) a_{q+r} \mathbb{1}_{\{\mathcal{N}_{q+r}=1\}} \mathbb{1}_{\{\mathcal{N}_{x-(q+r)}=1\}}\\&\leqslant a_{p+r}^* (a_p^* a_p + 1) a_{p+r} \mathbb{1}_{\{\mathcal{N}_{p+r}=1\}} \mathbb{1}_{\{N_{y-(p+r)}=1\}} + a_{q+r}^* (a_q^* a_q + 1) a_{q+r} \mathbb{1}_{\{\mathcal{N}_{q+r}=1\}} \mathbb{1}_{\{\mathcal{N}_{x-(q+r)}=1\}}\\&\qquad - \delta_{p,q}\, a_{p+r}^* a_{p+r} \mathbb{1}_{\{\mathcal{N}_{p+r}=1\}} \mathbb{1}_{\{N_{y-(p+r)}=1\}} \mathbb{1}_{\{\mathcal{N}_{x-(p+r)}=1\}}. \qquad (7.4.50)\end{aligned}$$

We sum over x and y and write $\pm p, \pm q$ for either value that x respectively y could take. The contribution of the first two terms on the right-hand side of the previous equation can be bounded by

$$\begin{aligned}&\sum_{\substack{p,q\in S, r\in\Lambda^*:\\ p+r,q+r\in H}} \widehat{V}_N(r) \mathrm{Tr}\ a_{p+r}^* (a_p^* a_p + 1) a_{p+r} \mathbb{1}_{\{\mathcal{N}_{p+r}=1\}} \mathbb{1}_{\{N_{\pm q-(p+r)}=1\}} T_c \Gamma T_c^*\\&\qquad \leqslant \|\widehat{V}_N\|_\infty \mathrm{Tr} \sum_{p\in S} (a_p^* a_p + 1) \sum_{r\in H} a_r^* a_r \mathbb{1}_{\{\mathcal{N}_r=1\}} \sum_{q\in S} \mathbb{1}_{\{N_{\pm q-r}=1\}} T_c \Gamma T_c^*\\&\qquad = \|\widehat{V}_N\|_\infty \mathrm{Tr} \Big(T_c^* (\mathcal{N}_S + |S|) \mathcal{N}_H T_c \Gamma \Big),\end{aligned}$$

where we first shifted $r \to r - p$ and then we used Lemma 7.18 to replace the $q-$sum by 1. For the third term on the right-hand side of (7.4.50) we readily find

$$\sum_{\substack{p,q\in S, r\in\Lambda^*:\\ p+r,q+r\in H}} \widehat{V}_N(r) \delta_{p,q}\, a_{p+r}^* a_{p+r} \mathbb{1}_{\{\mathcal{N}_{p+r}=1\}} \mathbb{1}_{\{N_{\pm q-(p+r)}=1\}} \mathbb{1}_{\{\mathcal{N}_{\pm p-(p+r)}=1\}} \leqslant \|\widehat{V}_N\|_\infty \mathcal{N}_H |S|.$$

Case (2)*:* This can be handled like Case (1) but without interchanging a_q^* and a_p.

Case (3)*:* With Cauchy-Schwarz, we obtain

$$\begin{aligned}&\pm \mathbb{1}_{\{\mathcal{N}_{p+r}=1\}} \mathbb{1}_{\{N_{y-(p+r)}=1\}} a_{p+r}^* a_q^* a_{q+r} a_p \mathbb{1}_{\{\mathcal{N}_{q+r}=1\}} \mathbb{1}_{\{\mathcal{N}_{x-(q+r)}=1\}}\\&\qquad \leqslant a_{p+r}^* a_q^* a_q a_{p+r} \mathbb{1}_{\{\mathcal{N}_{p+r}=1\}} \mathbb{1}_{\{N_{y-(p+r)}=1\}} + a_{q+r}^* a_p^* a_p a_{q+r} \mathbb{1}_{\{\mathcal{N}_{q+r}=1\}} \mathbb{1}_{\{\mathcal{N}_{x-(q+r)}=1\}}.\end{aligned}$$

The contribution of the first term (the second term can be handled analogously) can be estimated, after summing over p and x, by

$$\begin{aligned}&\sum_{\substack{q\in S, r\in\Lambda^*:\\ p+r,q+r\in H}} \sum_{y\in S} \widehat{V}_N(r) \mathrm{Tr}\ a_{p+r}^* a_q^* a_q a_{p+r} \mathbb{1}_{\{\mathcal{N}_{p+r}=1\}} \mathbb{1}_{\{N_{y-(p+r)}=1\}} \delta_{p,\pm q} T_c \Gamma T_c^*\\&\qquad \leqslant \|\widehat{V}_N\|_\infty \mathrm{Tr} \sum_{q\in S} a_q^* a_q \sum_{r\in H} a_r^* a_r \mathbb{1}_{\{\mathcal{N}_r=1\}} \sum_{y\in S} \mathbb{1}_{\{N_{y-r}=1\}} T_c \Gamma T_c^*\\&\qquad \leqslant \|\widehat{V}_N\|_\infty \mathrm{Tr}\ \mathcal{N}_S \mathcal{N}_H T_c \Gamma T_c^*\,.\end{aligned}$$

$\square$

7.4.6 Proof of Lemma 7.5

First of all, we combine the statements of Lemma 7.16, Lemma 7.17 and Lemma 7.21 to estimate the expectation of kinetic energy, cubic and quartic terms on the right hand side of (7.2.8).

Lemma 7.25. *Let Γ be a density matrix on $\mathcal{F}(\Lambda)$ satisfying $\Gamma = \mathbb{1}_{\{\mathcal{N}_{S^c}=0\}}\Gamma\mathbb{1}_{\{\mathcal{N}_{S^c}=0\}}$ as well as $[\Gamma, \mathbb{P}_k] = 0$ for all $k \in S$. Then we have*

$$\mathrm{Tr}\ T_c^*\Big[\sum_{p\in\Lambda^*} p^2 a_p^* a_p + Q_3^H + \widetilde{Q}_4^H\Big]T_c\Gamma \leqslant \mathrm{Tr}\ \sum_{p\in S} p^2 a_p^* a_p\Gamma + 2N^\kappa\big(8\pi\mathfrak{a} - \widehat{V}(0)\big)\mathrm{Tr}\ \mathcal{N}_S\Gamma + \delta_1(\Gamma) \tag{7.4.51}$$

with

$$\delta_1(\Gamma) \lesssim N^{-1+5\kappa/2+3\varepsilon/2}\mathrm{Tr}\sum_{p\in S}\mathcal{N}_p^2\Gamma + N^{-5+17\kappa/2+11\varepsilon}\mathrm{Tr}\sum_{p\in S}\mathcal{N}_p^2(\mathcal{N}_S + N^{3\kappa/2+3\varepsilon})\Gamma + N^{\kappa-\varepsilon}\mathrm{Tr}\ \mathcal{N}_S\Gamma. \tag{7.4.52}$$

Moreover, we have the bounds

$$\mathrm{Tr}\ T_c^*\sum_{p\in\Lambda^*} p^2 a_p^* a_p T_c\Gamma,\ \pm\mathrm{Tr}\ T_c^* Q_3^H T_c\Gamma,\ \mathrm{Tr}\ T_c^* Q_4^H T_c\Gamma \lesssim N^{\kappa+2\varepsilon}\mathrm{Tr}\mathcal{N}_S\Gamma + \delta_1(\Gamma). \tag{7.4.53}$$

Proof. We start with the proof of (7.4.51). As a first step, we derive a rough upper bound on the kinetic operator. Let $k \in S' \subset S$. From Lemma 7.16 and Lemma 7.3 we obtain, on the range of Λ_k,

$$T_k^*\sum_{p\in\Lambda^*} p^2 a_p^* a_p T_k \lesssim \sum_{p\in\Lambda^*} p^2 a_p^* a_p + N^\kappa\mathcal{N}_k + N^{-1+5\kappa/2+3\varepsilon/2}\mathcal{N}_k^2 \lesssim \sum_{p\in\Lambda^*} p^2 a_p^* a_p + N^\kappa\mathcal{N}_k^2.$$

Since $[\mathcal{N}_k, T_q] = 0$ for $k \neq q$, conjugating with $T_{c,S'\setminus\{k\}} = \prod_{p\in S'\setminus\{k\}} T_p$ yields

$$T_{c,S'}^*\sum_{p\in\Lambda^*} p^2 a_p^* a_p T_{c,S'} \lesssim T_{c,S'\setminus\{k\}}^*\sum_{p\in\Lambda^*} p^2 a_p^* a_p T_{c,S'\setminus\{k\}} + N^\kappa\mathcal{N}_k^2.$$

Iterating, we arrive, on the range of $\mathbb{1}_{\{\mathcal{N}_{S^c}=0\}}$, at

$$T_{c,S'}^*\sum_{p\in\Lambda^*} p^2 a_p^* a_p T_{c,S'} \lesssim \sum_{p\in S} p^2 a_p^* a_p + N^\kappa\sum_{k\in S}\mathcal{N}_k^2 \lesssim N^{\kappa+2\varepsilon}\sum_{k\in S}\mathcal{N}_k^2. \tag{7.4.54}$$

Next, we show (7.4.51). Let $k \in S$. By Lemmas 7.16, 7.17 and 7.21 we have

$$\begin{aligned}&\pm\Lambda_k\Big[T_k^*\big(\sum_{p\in\Lambda^*} p^2 a_p^* a_p + Q_3^H + \widetilde{Q}_4^H\big)T_k - \sum_{p\in\Lambda^*} p^2 a_p^* a_p - Q_3^H - \widetilde{Q}_4^H - Z^{(k)}\Big]\Lambda_k \\ &\quad\lesssim N^{-1+5\kappa/2+3\varepsilon/2}\mathcal{N}_k^2 + N^{-5+15\kappa/2+7\varepsilon}\Big(\sum_{\substack{p,r\in H\\ p+r\in S}} N^{2\varepsilon}|p|^2 a_r^* a_p^* a_p a_r + N^\kappa\mathcal{N}_S\Big)(\mathcal{N}_k + 1),\end{aligned} \tag{7.4.55}$$

where we denoted

$$Z^{(k)} = \sum_{r\in H_k} N\Big[2\widehat{V}_N(r) + 2r^2\varphi_r + \sum_{t\in H_k}\widehat{V}_N(r-t)\varphi_t\Theta_{k,t}^{(2)}\Big](\varphi_r + \varphi_{r+k})\mathcal{N}_k\Theta_{k,r}^{(2)}. \tag{7.4.56}$$

Conjugating with $T_{c,S\setminus\{k\}}$, we obtain, on the range of $\mathbb{1}_{\{\mathcal{N}_{S^c}=0\}}$,

$$\begin{aligned}
&\pm\Big[T_c^*\big(\sum_{p\in\Lambda^*} p^2 a_p^* a_p + Q_3^H + \widetilde{Q}_4^H\big)T_c \\
&\qquad\qquad - T_{c,S\setminus\{k\}}^*\big(\sum_{p\in\Lambda^*} p^2 a_p^* a_p + Q_3^H + \widetilde{Q}_4^H\big)T_{c,S\setminus\{k\}} - T_{c,S\setminus\{k\}}^* Z^{(k)} T_{c,S\setminus\{k\}}\Big] \\
&\quad\lesssim N^{-1+5\kappa/2+3\varepsilon/2}\mathcal{N}_k^2 \\
&\qquad + N^{-5+15\kappa/2+7\varepsilon} T_{c,S\setminus\{k\}}^*\Big[\sum_{\substack{p,r\in H\\ p+r\in S}} N^{2\varepsilon}|p|^2 a_r^* a_p^* a_p a_r + N^\kappa \mathcal{N}_S\Big](\mathcal{N}_k+1)T_{c,S\setminus\{k\}}. \qquad (7.4.57)
\end{aligned}$$

Using Lemma 7.18 (note that the r-sum runs over the shell-neighborhood of $-p$) we find

$$\begin{aligned}
&\mathrm{Tr}\,\Big(T_{c,S\setminus\{k\}}^* \sum_{p,r\in H} N^{2\varepsilon}|p|^2 \mathbb{1}_S(p+r) a_r^* a_p^* a_p a_r \mathcal{N}_k T_{c,S\setminus\{k\}}\Gamma\Big) \\
&\qquad\qquad \leqslant \mathrm{Tr}\, T_{c,S\setminus\{k\}}^* N^{2\varepsilon} \sum_{p\in H} |p|^2 a_p^* a_p \mathcal{N}_k T_{c,S\setminus\{k\}}\Gamma \\
&\qquad\qquad \leqslant N^{\kappa+4\varepsilon}\mathrm{Tr}\sum_{p\in S}\mathcal{N}_p^2\,\mathcal{N}_k\Gamma, \qquad (7.4.58)
\end{aligned}$$

where we used (7.4.54) in the last inequality.

Let us return to (7.4.57) and consider the term $T_{c,S\setminus\{k\}}^* Z^{(k)} T_{c,S\setminus\{k\}}$. We claim that

$$\pm\Lambda_q\big(T_q^* Z^{(k)} T_q - Z^{(k)}\big)\Lambda_q \lesssim N^{-5+17\kappa/2+7\varepsilon}\mathcal{N}_q\mathcal{N}_k, \qquad (7.4.59)$$

for all $q\in S\setminus\{k\}$. Since $T_\ell^*\mathcal{N}_q\mathcal{N}_k T_\ell = \mathcal{N}_q\mathcal{N}_k$ for all $\ell\in S\setminus\{k,q\}$, (7.4.59) immediately implies that

$$\pm\mathrm{Tr}\,\big(T_{c,S\setminus\{k\}}^* Z^{(k)} T_{c,S\setminus\{k\}} - Z^{(k)}\big)\Gamma \lesssim N^{-5+17\kappa/2+7\varepsilon}\mathrm{Tr}\,\mathcal{N}_S\mathcal{N}_k\Gamma. \qquad (7.4.60)$$

Inserting (7.4.58) and (7.4.60) in (7.4.57) yields

$$\begin{aligned}
&\mathrm{Tr}\ T_c^*\big(\sum_{p\in\Lambda^*} p^2 a_p^* a_p + Q_3^H + \widetilde{Q}_4^H\big)T_c\Gamma \\
&\qquad \leqslant \mathrm{Tr}\ T_{c,S\setminus\{k\}}^*\big(\sum_{p\in\Lambda^*} p^2 a_p^* a_p + Q_3^H + \widetilde{Q}_4^H\big)T_{c,S\setminus\{k\}}\Gamma + \mathrm{Tr}\ Z^{(k)}\Gamma \\
&\qquad\quad + CN^{-1+5\kappa/2+3\varepsilon/2}\mathrm{Tr}\,\mathcal{N}_k^2\Gamma + CN^{-5+17\kappa/2+11\varepsilon}\,\mathrm{Tr}\sum_{p\in S}\mathcal{N}_p^2(\mathcal{N}_k+1)\Gamma
\end{aligned}$$

Iterating (and using the assumption $\Gamma = \mathbb{1}_{\{\mathcal{N}_{S^c}=0\}}\Gamma\mathbb{1}_{\{\mathcal{N}_{S^c}=0\}}$), we conclude that

$$\begin{aligned}
&\mathrm{Tr}\ T_c^*\big(\sum_{p\in\Lambda^*} p^2 a_p^* a_p + Q_3^H + \widetilde{Q}_4^H\big)T_c\Gamma \\
&\quad\leqslant\ \mathrm{Tr}\Big[\sum_{p\in S} p^2 a_p^* a_p + \sum_{k\in S} Z^{(k)}\Big]\Gamma + CN^{-1+5\kappa/2+3\varepsilon/2}\mathrm{Tr}\sum_{p\in S}\mathcal{N}_p^2\Gamma \qquad (7.4.61)\\
&\qquad + CN^{-5+17\kappa/2+11\varepsilon}\,\mathrm{Tr}\sum_{p\in S}\mathcal{N}_p^2(\mathcal{N}_S + N^{3\kappa/2+3\varepsilon})\Gamma.
\end{aligned}$$

In the definition (7.4.56) of $Z^{(k)}$, we apply the scattering equation (7.2.3). With (7.2.4), Lemma 7.3 and $|\widehat{V}_N(r-k) - \widehat{V}_N(r)| \lesssim |k| N^{-2+2\kappa} \leqslant N^{-2+5\kappa/2+\varepsilon}$, we find

$$\begin{aligned}\sum_{r\in H_k} N\Big[2\widehat{V}_N(r)+2r^2\varphi_r + \sum_{t\in H_k} \widehat{V}_N(r-t)\varphi_t\Big](\varphi_r+\varphi_{r+k}) \\ = \sum_{r\in H_k} N\widehat{V}_N(r)(\varphi_r+\varphi_{r+k}) + \mathcal{O}(N^{\kappa-\varepsilon}) = 2N^\kappa\big(8\pi\mathfrak{a} - \widehat{V}(0)\big) + \mathcal{O}(N^{\kappa-\varepsilon}).\end{aligned}$$

With (7.4.61), this implies (7.4.51).

It remains to show (7.4.59). With (7.4.25), we obtain

$$\begin{aligned}\Lambda_q T_q^* \Theta^{(2)}_{k,r}\Theta^{(2)}_{k,t} T_q \Lambda_q &= \Lambda_q\left(\cos(X_q)\Theta^{(2)}_{k,r}\Theta^{(2)}_{k,t}\cos(X_q) + \frac{\sin(X_q)}{X_q}\mathcal{B}_q^\circ \Theta^{(2)}_{k,r}\Theta^{(2)}_{k,t}\mathcal{B}_q^\sharp \frac{\sin(X_q)}{X_q}\right)\Lambda_q \\ &= \Theta^{(2)}_{k,r}\Theta^{(2)}_{k,t}\Lambda_q\left(\cos(X_q)^2 + \left(\frac{\sin(X_q)}{X_q}\right)^2 (X_q^{(r,-(k+r),-(k+t),t)})^2\right)\Lambda_q \\ &= \Theta^{(2)}_{k,r}\Theta^{(2)}_{k,t}\Lambda_q\left(1 - \left(\frac{\sin(X_q)}{X_q}\right)^2 \delta_q^{(r,-(k+r),-(k+t),t)}\right)\Lambda_q,\end{aligned}$$

where $\delta_q^{(r,-(k+r),-(k+t),t)}$ and $X_q^{(r,-(k+r),-(k+t),t)}$ were defined in (7.4.45). Using (7.4.46) we find

$$\pm\Lambda_q\left(T_q^*\Theta^{(2)}_{k,r}\Theta^{(2)}_{k,t}T_q - \Theta^{(2)}_{k,r}\Theta^{(2)}_{k,t}\right)\Lambda_q \lesssim N^{-5+15\kappa/2+7\varepsilon}\mathcal{N}_q. \tag{7.4.62}$$

From this and

$$\sum_{r\in H_k} N\Big[2\widehat{V}_N(r) + 2r^2\varphi_r + \sum_{t\in H_k}\widehat{V}_N(r-t)\varphi_t\Big](\varphi_r+\varphi_{r+k}) \lesssim N^\kappa,$$

which follows from Lemma 7.3, we find (7.4.59).

Finally, let us show (7.4.53). The bound on the kinetic term $\sum p^2 a_p^* a_p$ was shown in (7.4.54). By Cauchy–Schwarz we find

$$\pm Q_3^H \leqslant \frac{1}{2}Q_4^H + CN^\kappa\mathcal{N}_S, \tag{7.4.63}$$

which implies

$$Q_4^H = Q_4^H + 2Q_3^H - 2Q_3^H \leqslant 2(Q_4^H + Q_3^H) + CN^\kappa\mathcal{N}_S.$$

This, together with (7.4.51), Lemma 7.20 and Lemma 7.14, implies the bound on the quartic term Q_4^H. The bound on the cubic term then follows again by (7.4.63). □

We are now set to conclude the proof of Lemma 7.5. Recalling the assumptions on Γ and the decomposition (7.4.18) and collecting the bounds from Lemma 7.4, Lemma 7.15, Lemma 7.19, Lemma 7.20, Lemma 7.22, Lemma 7.23, Lemma 7.24 and Lemma 7.25 , we have

$$\begin{aligned}&\mathrm{Tr}\ T_c^* e^{-\mathcal{B}_1} W_{N_0}^* \mathcal{H}_N W_{N_0} e^{\mathcal{B}_1} T_c \Gamma \\ &\qquad\leqslant 4\pi\mathfrak{a}N^{1+\kappa} - 8\pi\mathfrak{a}N^\kappa(N-N_0) + \sum_{p\in S}\frac{(4\pi\mathfrak{a}N^\kappa)^2}{p^2} \\ &\qquad\quad + \mathrm{Tr}\Big[\sum_{p\in S} p^2 a_p^* a_p + 16\pi\mathfrak{a}N^\kappa\mathcal{N}_S + 4\pi\mathfrak{a}N^\kappa\sum_{p\in S}\mathrm{Tr}\ \big(a_p^* a_{-p}^* + \mathrm{h.c.}\big)\Big]\Gamma + \delta(\Gamma)\end{aligned} \tag{7.4.64}$$

where

$$\begin{aligned}\delta(\Gamma) \lesssim\ &\mathrm{Tr}\ T_c^*\mathcal{E}_1 T_c\Gamma + (\sqrt{N_0/N}-1)\mathrm{Tr}\, T_c^* Q_3^H T_c\Gamma + N^{-2+4\kappa+\varepsilon}\mathrm{Tr}\ \big(\mathcal{N}_S + N^{3\kappa/2+3\varepsilon}\big)\Gamma \\ &+ N^{-1+5\kappa/2+3\varepsilon}\mathrm{Tr}\, T_c^*\mathcal{N}_H^2 T_c\Gamma + N^{-1+\kappa}\mathrm{Tr}\, T_c^*\mathcal{N}(\mathcal{N}_S + N^{3\kappa/2+3\varepsilon})T_c\Gamma + \delta_1(\Gamma).\end{aligned} \tag{7.4.65}$$

With (7.2.9), (7.4.52) and with Lemma 7.14, we find

$$\begin{aligned}
&\delta(\Gamma)\\
&\lesssim N^{-3\varepsilon}\mathrm{Tr}\ T_c^* \sum_{p\in\Lambda^*} p^2 a_p^* a_p T_c\Gamma + N^{-5\varepsilon/2}\mathrm{Tr}\ T_c^* Q_4 T_c\Gamma + (\sqrt{N_0/N}-1)\mathrm{Tr}\, T_c^* Q_3^H T_c\Gamma\\
&\quad + \big(N^{-\kappa/2-\varepsilon/2} + N^{-7+13\kappa+6\varepsilon}\big)\mathrm{Tr}\ \mathcal{N}_S^2\Gamma + N^{-1+\kappa+6\varepsilon}\mathrm{Tr}\,\big(\mathcal{N}_S + N^{3\kappa/2+3\varepsilon}\big)\sum_{p\in S}\mathcal{N}_p^2\Gamma + N^{5\kappa/2-\varepsilon/2},
\end{aligned}$$

if $1/2 < \kappa < 8/15 - 2\varepsilon/3$ (note again that in particular $\varepsilon < 1/20$). For the first three terms on the right hand side we use (7.4.53) and find that they can be absorbed in the error terms that are already present.

□

7.4.7 Proof of Proposition 7.7

From (7.2.1) and (7.2.6), we find

$$\begin{aligned}
e^{-\mathcal{B}_1} W_{N_0}^* \mathcal{N} W_{N_0} e^{\mathcal{B}_1} &= e^{-\mathcal{B}_1}\big(N_0 + \mathcal{N} + \sqrt{N_0}(a_0^* + a_0)\big)e^{\mathcal{B}_1}\\
&= N_0 + \sum_{p\in\Lambda^*}\big[(c_p^2+s_p^2)a_p^* a_p + c_p s_p(a_p^* a_{-p}^* + a_p a_{-p}) + s_p^2\big] + \sqrt{N_0}(a_0^*+a_0). \qquad (7.4.66)
\end{aligned}$$

From (7.2.7) and (7.4.35), we find that on the range of $T_c\Gamma$, the second term in (7.4.66) simplifies to

$$\sum_{p\in\Lambda^*}\big[(c_p^2+s_p^2)a_p^* a_p + c_p s_p(a_p^* a_{-p}^* + a_p a_{-p}) + s_p^2\big] = \mathcal{N} + 2\sum_{p\in H} N_0^2\varphi_p^2 a_p^* a_p + \sum_{|p|>N^{\kappa/2+\varepsilon}} N_0^2\varphi_p^2. \qquad (7.4.67)$$

Here we used Lemma 7.18 to argue that Tr $T_c^* a_p^* a_{-p}^* T_c\,\Gamma = 0$ for $p\in H$ as $a_p^* a_{-p}^*$ would leave two excitations in H which are no longer connected. Also, from the definition of Γ in (7.2.20), we clearly have

$$\mathrm{Tr}\ (T_c^* a_0^* T_c\Gamma) = \mathrm{Tr}\ (a_0^*\Gamma) = 0.$$

Recall from (7.4.9) that on the range of Γ we have

$$T_c^*\mathcal{N}T_c \geqslant T_c^*(\mathcal{N}_S + \frac{\mathcal{N}_H}{2})T_c = \mathcal{N}_S + \frac{\mathcal{N}_H}{2} = \mathcal{N}_S.$$

Then we obtain that

$$\mathrm{Tr}\,\mathcal{N}\Gamma_N \geqslant \mathrm{Tr}\,\mathcal{N}_S\Gamma + N_0.$$

To prove the upper bound, we combine the above identities (7.4.66) and (7.4.67) with Lemma 7.14 and $\varphi_p \lesssim p^{-2}N^{-1+\kappa}$ from Lemma 7.3, as well as $N_0 \lesssim N$, which follows directly from the definition (7.2.28) and Lemma 7.6. We find that on the range of Γ

$$T_c^* e^{-\mathcal{B}_1} W_{N_0}^* \mathcal{N} W_{N_0} e^{\mathcal{B}_1} T_c - \mathcal{N}_S - N_0 \lesssim N^{-2+3\kappa+\varepsilon}\mathcal{N}_S + N^{3\kappa/2-\varepsilon},$$

and from $\mathrm{Tr}\,\mathcal{N}_S\Gamma \lesssim N^{3\kappa/2}$, see Lemma 7.6, we obtain Proposition 7.7.

□

7.A Proof of Lemma 7.3

We begin by showing that (7.2.3) has a solution. Recall that $V_N(x) = N^{2-2\kappa}V(N^{1-\kappa}x)$. For N large enough, V_N is supported in Λ so that we may consider it as a function on the torus, i.e. $V_N \in L^2(\Lambda)$. Since $V_N \geqslant 0$ we may invert $-\Delta + \frac{1}{2}V_N$ on $P^\perp L^2(\Lambda)$, where $P^\perp = 1 - |\mathbb{1}_\Lambda\rangle\langle\mathbb{1}_\Lambda|$ is the projection onto the orthogonal complement of the zero mode. We define

$$\check{\varphi} = -\frac{1}{2}\frac{1}{P^\perp(-\Delta + \frac{1}{2}V_N)P^\perp}P^\perp V_N \in P^\perp L^2(\Lambda) \tag{7.A.1}$$

and readily find that in momentum space φ satisfies (7.2.3). Then, (7.2.3) and the positivity of V yield

$$\sum_{p\neq 0} p^2\varphi_p^2 = -\frac{1}{2}\sum_{p\neq 0}\varphi_p\widehat{V}_N(p) - \frac{1}{2}\sum_{p,q\neq 0}\varphi_p\widehat{V}_N(p-q)\varphi_q \leqslant -\frac{1}{2}\sum_{p\neq 0}\varphi_p\widehat{V}_N(p). \tag{7.A.2}$$

We will now show, that this inequality implies $\|p\varphi\|_2^2 \leqslant CN^{-1+\kappa}$ by a bootstrap argument. First, using $\varphi, V_N \in L^2$ and a simple Cauchy–Schwarz inequality in (7.A.2) implies $\sum_{p\neq 0} p^2\varphi_p^2 < \infty$. Next, using a weighted Cauchy–Schwarz inequality in (7.A.2) implies

$$\begin{aligned}\sum_{p\neq 0} p^2\varphi_p^2 \leqslant \sum_{p\neq 0}\frac{\widehat{V_N}(p)^2}{p^2} &= \sum_{0<|p|<N^{1-\kappa}}\frac{\widehat{V_N}(p)^2}{p^2} + \sum_{|p|\geqslant N^{1-\kappa}}\frac{\widehat{V_N}(p)^2}{p^2}\\ &\leqslant C\|\widehat{V}_N\|_\infty^2 N^{1-\kappa} + CN^{-2+2\kappa}\|V_N\|_2^2 \leqslant CN^{-1+\kappa}.\end{aligned}$$

Moreover, by using (7.2.3) again we deduce the pointwise bound $p^2\varphi_p \leqslant CN^{-1+\kappa}$. This readily implies the bounds $\|\varphi\|_\infty, \|\varphi_2\| \leqslant CN^{-1+\kappa}$ and the bounds for the cutoff version of φ.

It remains to estimate the ℓ^1-norm of φ. As before, we first show that it is finite and then show that it is bounded independently of N. Let $q \in [1,6)$, then with (7.2.3) as well as Hölder respectively Young inequalities we find

$$\begin{aligned}\|\varphi\|_q &\leqslant \frac{1}{2}\|p^{-2}\widehat{V}_N\|_q + \frac{1}{2}\|p^{-2}(\widehat{V}_N * \varphi)\|_q \leqslant \frac{1}{2}\|p^{-2}\widehat{V}_N\|_\infty^{(q-1)/q}\|p^{-2}\widehat{V}_N\|_1 + \frac{1}{2}\|p^{-2}\|_r\|\widehat{V}_N\|_2\|\varphi\|_s\\ &\leqslant C + C_N\|\varphi\|_s,\end{aligned}$$

where $\frac{1}{s} = \frac{1}{q} + \frac{1}{2} - \frac{1}{r}$ and we chose r larger than $3/2$, which implies $s < \frac{6q}{6-q}$. Here we used that $\|p^{-2}\widehat{V}_N\|_1 \leqslant C$, which can be shown as before by splitting the sum into a momenta below and above $N^{1-\kappa}$. By a bootstrap argument, choosing first $q = 1$, then $q = 6/5 - \varepsilon_1$ and finally $q = 3/2 - \varepsilon_2$ for $0 < \varepsilon_1, \varepsilon_2$ small enough we find a $\varepsilon_3 > 0$ small such that

$$\|\varphi\|_1 \leqslant C + C_N\|\varphi\|_{6/5-\varepsilon_1} \leqslant C_N + C_N\|\varphi\|_{3/2-\varepsilon_2} \leqslant C_N + C_N\|\varphi\|_{2-\varepsilon_3} < \infty.$$

Now we show that $\|\varphi\|_1$ is bounded independently of N. We split the sum at $DN^{1-\kappa}$ with a large but constant parameter D and obtain together with (7.2.3) and $p^2\varphi_p \leqslant CN^{-1+\kappa}$

$$\begin{aligned}\|\varphi\|_1 &= \|\varphi\mathbb{1}_{|p|<DN^{1-\kappa}}\|_1 + \|\varphi\mathbb{1}_{|p|\geqslant DN^{1-\kappa}}\|_1\\ &\leqslant C_D + \frac{1}{2}\|p^{-2}\widehat{V}_N\mathbb{1}_{|p|\geqslant DN^{1-\kappa}}\|_1 + \frac{1}{2}\|p^{-2}\widehat{V}_N * \varphi\mathbb{1}_{|p|\geqslant DN^{1-\kappa}}\|_1\\ &\leqslant C_D + C + \frac{1}{2}\|p^{-2}\mathbb{1}_{|p|\geqslant DN^{1-\kappa}}\|_2\|\widehat{V}_N\|_2\|\varphi\|_1\\ &\leqslant C_D + C + CD^{-1/2}\|\varphi\|_1\end{aligned}$$

Thus, choosing D large enough, we obtain $\|\varphi\|_1 \leqslant C$.

Next, we want to show (7.2.5). We want to compare the scattering solution φ on the torus to the one on $\mathbb{R}^3$. From Section 2.3 we know that the optimization problem

$$\inf\left\{\int_{\mathbb{R}^3}|\nabla w|^2+\frac{1}{2}\int_{\mathbb{R}^3}V|1+w|^2 : w\in H^1(\mathbb{R}^3)\right\}$$

has a unique minimizer ω and that the minimal value is given by $4\pi\mathfrak{a}$, see [58]. Moreover, ω solves the scattering equation

$$-\Delta\omega+\frac{1}{2}V(1+\omega)=0$$

and it holds that $|\omega|\leqslant\frac{C}{1+|\cdot|}$, as well as $|\nabla\omega|\leqslant\frac{C}{1+|\cdot|^2}$. In order to compare φ and ω we rescale and truncate the full space scattering solution. Let $\omega_N(x)=\omega(N^{1-\kappa}x)\chi(x)$, with $0\leqslant\chi\leqslant 1$ a smooth and radial function such that $\chi\equiv 1$ for $|x|\leqslant 1/2$ as well as $\chi\equiv 0$ for $|x|\geqslant 1$. We obtain that ω_N solves the following equation

$$(-\Delta+\frac{1}{2}V_N)\omega_N=-\frac{1}{2}V_N-2N^{1-\kappa}(\nabla\omega)(N^{1-\kappa}\cdot)\nabla\chi-\omega(N^{1-\kappa}\cdot)\Delta\chi=:-\frac{1}{2}V_N+\frac{1}{2}\epsilon_N. \quad (7.A.3)$$

From the estimate on ω we find $\|\omega_N\|_1\leqslant CN^{-1+\kappa}$ and $\|\epsilon_N\|_1\leqslant CN^{-1+\kappa}$. Observe that $8\pi\mathfrak{a}=\int_{\mathbb{R}^3}V(1+\omega)=N^{1-\kappa}\int_\Lambda V_N(1+\omega_N)$ and $8\pi\mathfrak{a}_N=N^{1-\kappa}\int_\Lambda V_N(1+\check{\varphi})$. Then with (7.A.3) and (7.A.1) we conclude that

$$\begin{aligned}
8\pi|\mathfrak{a}-\mathfrak{a}_N| &= N^{1-\kappa}|\langle V_N,\omega_N-\check{\varphi}\rangle_{L^2(\Lambda)}|\leqslant N^{1-\kappa}|\langle P^\perp V_N,\omega_N-\check{\varphi}\rangle|+N^{1-\kappa}\|V_N\|_1\|\omega_N\|_1\\
&\leqslant N^{1-\kappa}|\langle 2P^\perp(-\Delta+\frac{1}{2}V_N)\check{\varphi},\omega_N-\check{\varphi}\rangle|+CN^{-1+\kappa}\\
&\leqslant N^{1-\kappa}|\langle 2\check{\varphi},(-\Delta+\frac{1}{2}V_N)(\omega_N-\check{\varphi})\rangle|+N^{1-\kappa}|\langle\check{\varphi},V_NP\omega_N\rangle|+CN^{-1+\kappa}\\
&\leqslant N^{1-\kappa}|\langle\check{\varphi},\epsilon_N\rangle|+N^{1-\kappa}\|\check{\varphi}\|_\infty\|V_N\|_1\|\omega_N\|_1+CN^{-1+\kappa}\\
&\leqslant N^{1-\kappa}\|\check{\varphi}\|_\infty\|\epsilon_N\|_1+CN^{-1+\kappa}\\
&\leqslant CN^{-1+\kappa}.
\end{aligned}$$

7.B Proof of Proposition 7.1

We follow partly [6] and [83].

7.B.1 Dirichlet localization

Let Γ_L be a density matrix over $\mathcal{F}(\Lambda_L)$, satisfying periodic boundary conditions such that (7.1.2) holds true. By the spectral theorem, we can decompose

$$\Gamma_L=\sum_{j\in J}\lambda_j|\Psi_j\rangle\langle\Psi_j|$$

where $\lambda_j\geqslant 0$ for all $j\in J$, $\sum_{j\in J}\lambda_j=1$ and where $\Psi_j\in\mathcal{F}(\Lambda_L)$ is an orthonormal family on $\mathcal{F}(\Lambda_L)$. We have $\Psi_j=\{\Psi_j^{(n)}\}_{n\geqslant 0}$ where $\Psi_j^{(n)}$ is L-periodic in all its coordinates (we think of $\Psi_j^{(n)}$ as a periodic function defined on $\mathbb{R}^{3n}$). For fixed $j\in J$ and $u\in\Lambda_L$, we define now $\Psi_{j,u}^D=\{(\Psi_{j,u}^D)^{(n)}\}_{n\in\mathbb{N}}\in\mathcal{F}(\Lambda_{L+2\ell}^u)$, where $\Lambda_{L+2\ell}^u=u+\Lambda_{L+2\ell}$ is a box of side length $L+2\ell$, with center at u, setting

$$(\Psi_{j,u}^D)^{(n)}(x_1,\dots,x_n)=\Psi_j^{(n)}(x_1,\dots,x_n)\prod_{i=1}^n Q_{L,n}(x_i-u)$$

with $Q_{L,\ell}(x) = \prod_{j=1}^3 q_{L,\ell}(x^{(j)})$ for all $x = (x^{(1)}, x^{(2)}, x^{(3)}) \in \mathbb{R}^3$, with $q_{L,\ell} : \mathbb{R} \to [0;1]$ defined through

$$q_{L,\ell}(t) = \begin{cases} \cos\left(\frac{\pi(t+L/2-\ell)}{4\ell}\right) & \text{if } |t+L/2| \leqslant \ell \\ 1 & \text{if } |t| < L/2-\ell \\ \cos\left(\frac{\pi(t-L/2+\ell)}{4\ell}\right) & \text{if } |t-L/2| \leqslant \ell \\ 0 & \text{otherwise} \end{cases}$$

By construction $\Psi^D_{j,u}$ satisfies Dirichlet boundary conditions on the box $\Lambda^u_{L+2\ell}$.

Lemma 7.26 (Dirichlet localization). *We have*

$$\langle \Psi^D_{j,u}, \Psi^D_{i,u} \rangle_{\mathcal{F}(\Lambda^u_{L+2\ell})} = \langle \Psi_j, \Psi_i \rangle = \delta_{ij} \tag{7.B.1}$$

Thus, $\Gamma^D_{L+2\ell,u} := \sum_{j\in J} \lambda_j |\Psi^D_{j,u}\rangle\langle\Psi^D_{j,u}|$ *is a non-negative operator on* $\mathcal{F}(\Lambda^u_{L+2\ell})$*, with* $\operatorname{Tr}\Gamma^D_{L+2\ell,u} = 1$*, with* $S(\Gamma^D_{L+2\ell,u}) = S(\Gamma_L)$ *and*

$$\operatorname{Tr}\mathcal{N}^j\Gamma^D_{L+2\ell,u} = \operatorname{Tr}\mathcal{N}^j\Gamma_L \tag{7.B.2}$$

for all $j \in \mathbb{N}$ *and all* $u \in \Lambda_L$*. Moreover, there exists* $\bar{u} \in \Lambda_L$ *such that*

$$\operatorname{Tr}\,\mathcal{H}\Gamma^D_{L+2\ell,\bar{u}} \leqslant \operatorname{Tr}\mathcal{H}\Gamma_L + \frac{C}{L\ell}\operatorname{Tr}\mathcal{N}\Gamma_L \tag{7.B.3}$$

Proof. The proof is an adaptation of [6, Lemma A.1] to the mixed state setting. It is based on the observation that, for arbitrary L-periodic functions $\Phi \in L^1_{\text{loc}}(\mathbb{R})$,

$$\int_{-L/2-\ell}^{L/2+\ell} \Phi(t)|q_{L,\ell}(t)|^2 dt = \int_{-L/2}^{L/2} \Phi(t)dt\,.$$

This shows that in particular that

$$\langle (\Psi^D_{j,u})^{(n)}, (\Psi^D_{i,u})^{(n)} \rangle = \langle \Psi^{(n)}_j, \Psi^{(n)}_i \rangle$$
$$\left\langle (\Psi^D_{j,u})^{(n)}, \sum_{1\leqslant i<j\leqslant n} V(x_i-x_j)(\Psi^D_{i,u})^{(n)} \right\rangle = \left\langle \Psi^{(n)}_j, \sum_{1\leqslant i<j\leqslant n} V(x_i-x_j)\Psi^{(n)}_i \right\rangle$$

and thus implies (7.B.1) and (7.B.2). The fact that $S(\Gamma^D_{L+2\ell,u}) = S(\Gamma_L)$ is clear, since the operators $\Gamma^D_{L+2\ell,u}$ and Γ_L have the same eigenvalues. As for (7.B.3), we proceed as in the proof of Lemma [6, Lemma A.1] to show that, for all $j \in J$ and all $u \in \Lambda_L$,

$$\langle \psi^D_{j,u}, \mathcal{H}\psi^D_{j,u} \rangle \leqslant \langle \psi_j, \mathcal{H}\psi_j \rangle + \frac{C}{\ell^2}\sum_{n\in\mathbb{N}} n \int dx_1\, \widetilde{\chi}_{L,\ell}(x_1-u) \int_{\Lambda_L^{n-1}} dx_2 \dots dx_n\, |\Psi^{(n)}_j(x_1,\dots,x_n)|^2$$

where we set $\widetilde{\chi}_{L,\ell}(x) = \sum_{k=1}^3 \chi_{L,\ell}(x^{(k)}) \prod_{j\neq k} \chi_{[-L/2;L/2]}(x^{(j)})$ and we used the notation

$$\chi_{L,\ell} = \chi_{[-L/2-\ell;-L/2+\ell]} + \chi_{[L/2-\ell;L/2+\ell]}.$$

In particular, we replaced the potential V by its $L-$periodic extension V_L; this is justified by the pointwise inequality $V(x) \leqslant V_L(x)$. Summing over $j \in J$ with the weights λ_j, we obtain

$$\operatorname{Tr}\,\mathcal{H}\Gamma^D_{L+2\ell,u} \leqslant \operatorname{Tr}\mathcal{H}\Gamma_L + \frac{C}{\ell^2}\sum_{j\in J}\lambda_j \sum_{n\in\mathbb{N}} n \int dx_1\, \widetilde{\chi}_{L,\ell}(x_1-u) \int_{\Lambda_L^{n-1}} dx_2 \dots dx_n |\Psi^{(n)}_j(x_1,\dots,x_n)|^2$$

for all $u \in \Lambda_L$. Averaging over u, using $\|\widetilde{\chi}_{L,\ell}\|_1 \leqslant CL^2\ell$, we conclude that there exists $\bar{u} \in \Lambda_L$ such that

$$\operatorname{Tr}\,\mathcal{H}\Gamma^D_{L+2\ell,\bar{u}} \leqslant \operatorname{Tr}\mathcal{H}\Gamma_L + \frac{C}{L\ell}\operatorname{Tr}\mathcal{N}\Gamma_L$$

as claimed. □

7.B.2 Patching up the boxes

For $j \in J$, we define now $\Psi^D_{j,L+2\ell} \in \mathcal{F}(\Lambda_{L+2\ell})$ setting $(\Psi^D_{j,L+2\ell})^{(n)}(x_1, \dots, x_n) = (\Psi^D_{j,\bar{u}})^{(n)}(x_1 + \bar{u}, x_2 + \bar{u}, \dots, x_n + \bar{u})$, with $\bar{u}$ chosen as in Lemma 7.26. Correspondingly, we introduce the density matrix $\Gamma^D_{L+2\ell} \in \mathcal{F}(\Lambda_{L+2\ell})$ on the box $\Lambda_{L+2\ell} = [-L/2 - \ell; L/2 + \ell]^3$, satisfying Dirichlet boundary conditions. This allows us to replicate $\Gamma^D_{L+2\ell}$ into several adjacent copies of $\Lambda_{L+2\ell}$, separated by corridors of size $R > 0$ (to avoid interactions between particles in different boxes). For $t \in \mathbb{N}$, let

$$\widetilde{L} = t(L + 2\ell + R).$$

We think of the thermodynamic box $\Lambda_{\widetilde{L}}$ as the (almost) disjoint union of t^3 shifted copies of the small box $\Lambda_{L+2\ell+R}$, centered at

$$(-\widetilde{L}/2, -\widetilde{L}/2, -\widetilde{L}/2) + (L + 2\ell + R)(i_1 - 1/2, i_2 - 1/2, i_3 - 1/2)$$

for $i_1, i_2, i_3 \in \{1, \dots, t\}$. Let $(c_i)_{i=1,\dots,t^3}$ denote an enumeration of the centers of the boxes. Using $L^2(\Lambda_{\widetilde{L}}) = \oplus_{i=1}^{t^3} L^2(\Lambda^{c_i}_{L+2\ell+R})$ and the canonical identification (see, e.g., [28, Theorem 16])

$$\mathcal{F}(\Lambda_{\widetilde{L}}) \simeq \bigotimes_{i=1}^{t^3} \mathcal{F}(\Lambda^{c_i}_{L+2\ell+R}),$$

we can define on $\mathcal{F}(\Lambda_{\widetilde{L}})$ the state

$$\Gamma^D_{\widetilde{L}} \simeq \Gamma^D_{L+2\ell+R,c_1} \otimes \cdots \otimes \Gamma^D_{L+2\ell+R,c_{t^3}}. \tag{7.B.4}$$

Here the tensor products are symmetric. Then we have $\mathrm{Tr}\,\Gamma^D_{\widetilde{L}} = 1$,

$$\mathrm{Tr}\,\mathcal{N}\Gamma^D_{\widetilde{L}} = t^3 \mathrm{Tr}\,\mathcal{N}\Gamma^D_{L+2\ell+R}$$

as can be seen decomposing $\mathcal{N} = \sum_{i=1}^{t^3} \mathcal{N}_i$, where $\mathcal{N}_i$ measures the number of particles in the box with side length $(L + 2\ell + R)$ centered at c_i Moreover,

$$\mathrm{Tr}\,\mathcal{H}\Gamma^D_{\widetilde{L}} = t^3 \mathrm{Tr}\,\mathcal{H}\Gamma^D_{L+2\ell+R}$$

and $S(\Gamma^D_{\widetilde{L}}) = t^3 S(\Gamma^D_{L+2\ell+R})$, as follows by noticing that, if $(\lambda_j)_{j\in J}$ are the eigenvalues of $\Gamma_{L+2\ell+R}$, then the products $\lambda_{j_1} \dots \lambda_{j_{t^3}}$ are the eigenvalues of $\Gamma^D_{\widetilde{L}}$. In particular, we obtain

$$\mathrm{Tr}\,\mathcal{H}\Gamma^D_{\widetilde{L}} - TS(\Gamma^D_{\widetilde{L}}) = t^3 \left[\mathrm{Tr}\,\mathcal{H}\Gamma^D_{L+2\ell+R} - TS(\Gamma^D_{L+2\ell+r})\right]$$

The state $\Gamma^D_{\widetilde{L}}$ is a good trial state for the free energy in the grand canonical ensemble.

7.B.3 From grand canonical to canonical ensemble

As a last step, infer a bound on the canonical free energy, with a fixed number of particles, from the energy of a grand-canonical state.

Lemma 7.27. *Suppose there exists a sequence $\Gamma^D_{\widetilde{L}}$ of density matrices on $\mathcal{F}(\Lambda_{\widetilde{L}})$, parametrized by $\widetilde{L} > 0$ and satisfying Dirichlet boundary conditions and such that*

$$\lim_{\widetilde{L}\to\infty} \frac{1}{\widetilde{L}^3} \mathrm{Tr}\,\mathcal{N}\Gamma^D_{\widetilde{L}} = \widetilde{\rho}. \tag{7.B.5}$$

Then

$$f(\widetilde{\rho}, T) \leqslant \liminf_{\widetilde{L}\to\infty} \frac{1}{\widetilde{L}^3} \left[\mathrm{Tr}\,\mathcal{H}\Gamma^D_{\widetilde{L}} - TS(\Gamma^D_{L})\right].$$

Proof. We use the equivalence of ensembles: the free energy $\widetilde{\rho} \mapsto f(\widetilde{\rho}, T)$ is convex and is given by the Legendre transform of the pressure, see for example [84]

$$f(\widetilde{\rho}, T) = \sup_{\mu \in \mathbb{R}} \{\mu\widetilde{\rho} + f_{GC}(\mu, T)\} \tag{7.B.6}$$

with

$$f_{GC}(\mu, T) = \lim_{\widetilde{L}\to\infty} -\frac{T}{\widetilde{L}^3} \log \operatorname{Tr} e^{-\frac{1}{T}(\mathcal{H}-\mu\mathcal{N})}.$$

Then, for all $\mu \in \mathbb{R}$, using Gibbs' variational principle, we obtain

$$f_{GC}(\mu, T) \leqslant \liminf_{\widetilde{L}\to\infty} \frac{1}{\widetilde{L}^3} \left[\operatorname{Tr}(\mathcal{H} - \mu\mathcal{N})\Gamma^D_{\widetilde{L}} - TS(\Gamma^D_{\widetilde{L}})\right] = \liminf_{\widetilde{L}\to\infty} \frac{1}{\widetilde{L}^3} \left[\operatorname{Tr}\mathcal{H}\Gamma^D_{\widetilde{L}} - TS(\Gamma^D_{\widetilde{L}})\right] - \mu\widetilde{\rho}.$$

The above inequality being valid for all μ, we deduce the claim using (7.B.6). □

7.B.4 Proof of Proposition 7.1

We can now conclude the proof of Prop. 7.1.

Let Γ_L be a density matrix on $\mathcal{F}(\Lambda_L)$, satisfying periodic boundary conditions and

$$\operatorname{Tr}\mathcal{N}\Gamma_L < \infty.$$

With Lemma 7.26, we find a density matrix $\Gamma^D_{L+2\ell}$ on $\mathcal{F}(\Lambda_{L+2\ell})$ satisfying Dirichlet boundary conditions, with

$$\operatorname{Tr}\mathcal{N}\Gamma^D_{L+2\ell} = \operatorname{Tr}\mathcal{N}\Gamma_L$$

and

$$\operatorname{Tr}\mathcal{H}\Gamma^D_{L+2\ell} - TS(\Gamma^D_{L+2\ell}) \leqslant \operatorname{Tr}\mathcal{H}\Gamma_L - TS(\Gamma_L) + \frac{C}{L\ell}\operatorname{Tr}\mathcal{N}\Gamma_L.$$

From (7.B.4), we find, for any $t \in \mathbb{N}$, a density matrix $\Gamma^D_{\widetilde{L}}$ on $\mathcal{F}(\Lambda_{\widetilde{L}})$, with $\widetilde{L} = t(L + 2\ell + R)$, satisfying Dirichlet boundary conditions, with

$$\frac{1}{\widetilde{L}^3}\left(\operatorname{Tr}\mathcal{H}\Gamma^D_{\widetilde{L}} - TS(\Gamma^D_{\widetilde{L}})\right) \leqslant \frac{1}{(L+2\ell+R)^3}\left(\operatorname{Tr}\mathcal{H}\Gamma_L - TS(\Gamma_L)\right) + \frac{C}{(L\ell)(L+2\ell+R)^3}\operatorname{Tr}\mathcal{N}\Gamma_L.$$

Denoting

$$\widetilde{\rho} := \frac{1}{\widetilde{L}^3}\operatorname{Tr}\mathcal{N}\Gamma^D_{\widetilde{L}} = \frac{1}{(L+2\ell+R)^3}\operatorname{Tr}\mathcal{N}\Gamma_L,$$

which is independent of t, we obtain by Lemma 7.27, letting $\widetilde{L} \to \infty$ (i.e. $t \to \infty$), that

$$\begin{aligned} f(\widetilde{\rho}, T) &\leqslant \lim_{\widetilde{L}\to\infty} \frac{1}{\widetilde{L}^3}\left[\operatorname{Tr}\mathcal{H}\Gamma^D_{\widetilde{L}} - TS(\Gamma^D_{\widetilde{L}})\right] \\ &\leqslant \frac{1}{(L+2\ell+R)^3}\left[\operatorname{Tr}\mathcal{H}\Gamma_L - TS(\Gamma_L)\right] + \frac{C\widetilde{\rho}}{L\ell}. \end{aligned}$$

□

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Versicherung an Eides statt

(gemäß § 8 Abs. 2 Nr. 5 der Promotionsordnung vom 12. Juli 2011)

Hiermit erkläre ich, Florian Michael Haberberger, an Eides statt, dass die Dissertation mit dem Titel ,,The Free Energy of Dilute Bose Gases at Low Temperature“ von mir selbstständig und ohne unerlaubte Beihilfe angefertigt wurde.

München	09.03.2026	
Ort	Datum	Florian Michael Haberberger