Multiparticle Brown–Ravenhall Operators in External Fields

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Zusammenfassung

Das Modell von Brown und Ravenhall wird in der Quantenphysik und Quantenchemie verwendet, um relativistische Mehrteilchensysteme, insbesondere Atome und Moleküle, zu beschreiben. In dieser Dissertation untersuchen wir einige mathematischen Eigenschaften dieses Modells. Wir zeigen, dass unter sehr allgemeinen Annahmen über die Wechselwirkungspotentiale das wesentliche Spektrum von Mehrteilchen–Brown–Ravenhall–Operatoren die rechte Halbachse ist, deren Führungspunkt durch die minimale Energie bei Zerlegung des Systems in zwei Teilsysteme (Cluster) bestimmt ist. Dieses Resultat, das man oft in der Mehrteilchentheorie der HVZ–Satz nennt, ist von fundamentaler Bedeutung in der Spektralanalyse von Mehrteilchen–Hamilton–Operatoren mit abfallenden Potentialen.

Nehmen wir jetzt an, dass die Teilchen des Systems einander abstoßen, aber durch ein äußeres Potential gebunden sind, das am Unendlichen abfällt. Dann beweisen wir den exponentiellen Abfall der Eigenfunktionen zu Eigenwerten unterhalb des wesentlichen Spektrums.

Falls einige Teilchen des Systems identisch sind, verlangen die Gesetze der Quantemechanik oft eine Reduktion des Operators auf den Unterraum der Funktionen, die gemäß einer irreduziblen Darstellung der Permutationsgruppe identischer Teilchen transformiert werden. Andererseits sind die Wechselwirkungen oft invariant gegen Drehungen und Spiegelungen. Wir beweisen, dass sowohl der HVZ–Satz als auch der exponentielle Abfall der Eigenfunktionen für die Operatoren gelten, die auf irreduzible Darstellungen der oben genannten Gruppen reduziert sind.

Unsere Ergebnisse sind potentiell wichtig für die weitere Untersuchung des Spektrums von Brown–Ravenhall–Operatoren und deren Streutheorie.

Abstract

The Brown–Ravenhall model is used in quantum physics and chemistry to describe relativistic multiparticle systems, particularly atoms and molecules. In this dissertation we analyse some general properties of this model on the mathematically rigorous level. We show that under very general assumptions on the interaction potentials the essential spectrum of multiparticle Brown–Ravenhall operators is the right semiaxis starting from the minimal energy possible for the decompositions of the system into two clusters. This result, usually called HVZ theorem, is the fundamental starting point in the spectral analysis of multiparticle Hamiltonians with decaying potentials.

Suppose now that the particles constituting the system repel each other but are confined by an external field decaying at infinity. In this situation we prove that the eigenfunctions corresponding to the eigenvalues below the essential spectrum decay exponentially.

If some particles of the system are identical, the laws of quantum mechanics often require to reduce the operator to the subspace of functions which transform according to some irreducible representation of the group of permutation of identical particles. On the other hand, the interactions are often invariant under some rotations and reflections. We prove that both the HVZ theorem and the exponential decay of eigenfunctions hold true for operators reduced to the irreducible representations of the above groups.

Our results are potentially important in further studies of the spectrum and in the scattering theory of Brown–Ravenhall operators.

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0.1 Notation and Units

1. Throughout the text we use the conventional units $\hbar = c = 1$. We denote all auxiliary constants whose exact numeric values are not important by C, sometimes with indices. We often explicitly indicate in brackets the parameters on which such auxiliary constants can depend.

2. We use the following notation:

Symbol	Meaning
$\lvert \cdot \rvert$	euclidean norm for numbers, vectors or matrices;
$[A, B]$	commutator of operators A and B, $AB - BA$;
Ω	arbitrary C^1–regular domain in $\mathbb{R}^k$, $k \in \mathbb{N}$ with bounded boundary;
$C^k(\Omega)$	space of k times continuously differentiable functions on Ω;
$L_2(\Omega, \mathbb{C}^d)$	space of square integrable d–dimensional vector valued functions on Ω;
$H^s(\Omega, \mathbb{C}^d)$	Sobolev space $W^{s,2}(\Omega, \mathbb{C}^d)$ (see e. g. [1]);
$\langle \cdot, \cdot \rangle$, $\lVert \cdot \rVert$	inner product and norm in $L_2(\mathbb{R}^{3d}, \mathbb{C}^{4^d})$ with d being the dimension of the underliyng configuration space, if not otherwise specified by a subscript;
I_Ω	indicator function of the set Ω;
$\sigma(A)$	spectrum of a selfadjoint operator A;
$\langle A\cdot, \cdot \rangle = \langle \cdot, A\cdot \rangle$	sesquilinear form of a selfadjoint operator A;
$\widehat{\cdot}$	unitary Fourier transform;
B_R	ball in $\mathbb{R}^3$ of radius $R > 0$ centered at the origin.

Part 1
Introduction

1.1 Brown–Ravenhall Operators

It is well known that the eigenvalues of the one–particle Coulomb–Dirac operator are in better accordance with spectroscopic data then the eigenvalues of the Schrödinger operator. However, due to the presence of the negative continuum of positronic states the multiparticle Coulomb–Dirac operators have no eigenvalues and their essential spectrum is the whole real line. Coupling with the quantized electromagnetic field does not correct this situation [25]. This is why in the modern physics and chemistry literature the Dirac operator is often projected onto some subspace where it appears to be semi-bounded from below and allows for a spectral analysis along the same lines as for Schrödinger operators. Such models find their applications in numerical studies of heavy elements and cosmology, where relativistic effects cannot be ignored.

We now give a formal definition of multiparticle Brown–Ravenhall operators. In the Hilbert space $L_2(\mathbb{R}^3, \mathbb{C}^4)$ the Dirac operator describing a particle of mass $m > 0$ is given by

$$D_m = -i\boldsymbol{\alpha} \cdot \nabla + \beta m,$$

where $\boldsymbol{\alpha} := (\alpha_1, \alpha_2, \alpha_3)$ and β are the 4×4 Dirac matrices [26]. The form domain of D_m is the Sobolev space $H^{1/2}(\mathbb{R}^3, \mathbb{C}^4)$ and its spectrum is $(-\infty, -m] \cup [m, +\infty)$. Let Λ_m be the orthogonal projector onto the positive spectral subspace of D_m:

$$\Lambda_m := \frac{1}{2} + \frac{-i\boldsymbol{\alpha} \cdot \nabla + \beta m}{2\sqrt{-\Delta + m^2}}. \tag{1.1.1}$$

We consider a finite system of N particles with positive masses m_n, $n = 1, \dots, N$. To simplify the notation we write D_n and Λ_n for D_{m_n} and Λ_{m_n}, respectively. Let $\mathfrak{H}_N := \bigotimes_{n=1}^{N} \Lambda_n L_2(\mathbb{R}^3, \mathbb{C}^4)$ be the Hilbert space with the inner product induced by the one on $\bigotimes_{n=1}^{N} L_2(\mathbb{R}^3, \mathbb{C}^4) \cong L_2(\mathbb{R}^{3N}, \mathbb{C}^{4^N})$. In this space the N–particle Brown–Ravenhall operator is formally given by

$$\mathcal{H}_N = \Lambda^N \left(\sum_{n=1}^{N} (D_n + V_n) + \sum_{n<j}^{N} U_{nj} \right) \Lambda^N, \tag{1.1.2}$$

with

$$\Lambda^N := \prod_{n=1}^{N} \Lambda_n = \bigotimes_{n=1}^{N} \Lambda_n. \tag{1.1.3}$$

Here the indices n and j indicate the particle on whose coordinates the corresponding operator acts.

In (1.1.2) V_n and U_{nj} are the operators of multiplication by the potential energy of interactions of the particles of the system with an external field and between themselves, respectively.

In most applications to atomic and molecular physics Brown–Ravenhall operators are considered in the Born–Oppenheimer approximation. Then V_n is the potential energy of the n^{th} particle in the electrostatic field of static nuclei

$$V_n := e_n \sum_{k=1}^{K} \frac{z_k}{|\mathbf{x}_n - \mathbf{r}_k|},$$

where e_n is the electric charge of the particle, and z_k and $\mathbf{r}_k$ are the charges and positions of the nuclei. The interaction between the particles is given by the Coulomb potential energy

$$U_{nj} := \frac{e_n e_j}{|\mathbf{x}_n - \mathbf{x}_j|}.$$

In this dissertation we will consider a more general situation, where the interaction potentials are not necessarily Coulombic and can be matrix–valued. This, for example, allows to include the magnetic vector–potential into V_n (in the same manner as it is usually done for Dirac operators, see e. g. [26], Section 4.2) and thus study the system in external magnetic field.

We assume that V_n are the operators of multiplication by measurable hermitian 4×4 matrix valued functions $V_n(\mathbf{x}_n)$, $n = 1, \dots, N$, and U_{nj} are given by the operators of multiplication by a measurable hermitian 16×16 matrix valued function $U_{nj}(\mathbf{x}_n - \mathbf{x}_j)$, $n < j = 1, \dots, N$. More explicitly, if $s_j \in \{1, 2, 3, 4\}$ denotes the spinor index of the j^{th} particle, then

$$\begin{aligned}&(V_n\psi)(\mathbf{x}_1, s_1; \dots; \mathbf{x}_n, s_n; \dots; \mathbf{x}_N, s_N)\\ &:= \sum_{\widetilde{s}_n} V_n^{s_n, \widetilde{s}_n}(\mathbf{x}_n)\psi(\mathbf{x}_1, s_1; \dots; \mathbf{x}_n, \widetilde{s}_n; \dots; \mathbf{x}_N, s_N),\end{aligned}$$

and

$$\begin{aligned}&(U_{nj}\psi)(\mathbf{x}_1, s_1; \dots; \mathbf{x}_n, s_n; \dots; \mathbf{x}_j, s_j; \dots; \mathbf{x}_N, s_N)\\ &:= \sum_{\widetilde{s}_n, \widetilde{s}_j} U_{nj}^{s_n s_j, \widetilde{s}_n \widetilde{s}_j}(\mathbf{x}_n - \mathbf{x}_j)\psi(\mathbf{x}_1, s_1; \dots; \mathbf{x}_n, \widetilde{s}_n; \dots; \mathbf{x}_j, \widetilde{s}_j; \dots; \mathbf{x}_N, s_N).\end{aligned}$$

In the Brown–Ravenhall model (1.1.2) every particle is confined to the positive spectral subspace of the corresponding free Dirac operator. A discussion concerning other possible choices of the subspaces to which the particles can be constrained, which corresponds to the replacement of Λ^N by some different projectors, can be found in [25]. The benefit of Brown–Ravenhall operators is that the potentials describing the interactions between the particles of the system are treated in the same way as the external field potential, which is a physically reasonable assumption. On the other hand, the numeric values obtained for the eigenvalues of Brown–Ravenhall operators are not in perfect correspondence with spectroscopic data, which often motivates the choice of other models.

We now review some mathematically rigorous results about Brown–Ravenhall operators. In all these previous studies systems of identical electrons were considered in the Born–Oppenheimer approximation.

The mathematical study of the Brown–Ravenhall operators started with the article of Evans, Perry, and Siedentop [9]. These authors proved that the one–electron atomic Hamiltonian is semibounded from below if and only if the nuclear charge does not exceed $2\alpha^{-1}/(\pi/2+2/\pi) \approx 124$. This makes the Brown–Ravenhall model applicable to all existing elements. Note that this is not the case for another relativistic model often discussed in the literature, the Chandrasekhar operator, where the kinetic energy of the n^{th} particle is given by $\sqrt{-\Delta_n + m^2}$ (which coincides, in fact, with $\Lambda_n D_n \Lambda_n$ on the range of Λ_n), but the electrostatic potentials are unprojected (see Herbst [13]). It was also proved in [9] that for subcritical charges the essential spectrum of the one–particle atomic Brown–Ravenhall operator is $[m, \infty)$ with m being the mass of the particle, and that the singular continuous spectrum is empty.

Further results include the lower bounds by Tix [27, 28] (see also Burenkov and Evans [4]) in the atomic case, the proof that the eigenvalues of the Brown–Ravenhall operator are strictly bigger than those of the one–particle Dirac operator by Griesemer et al. [11], the proof of stability of one-electron molecules by Balinsky and Evans [3], and the proof of stability of matter by Hoever and Siedentop [14].

The essential spectrum of multiparticle atomic Hamiltonians was characterized in the articles of Jakubaßa–Amundsen [16, 17], and in our joint work with S. Vugalter [21] in terms of two–cluster decompositions (HVZ theorem). It is also proved in [21] that neutral atoms and positively charged atomic ions have infinitely many bound states.

In the recent preprint by Jakubaßa–Amundsen [15] the essential spectrum was characterized in presence of constant magnetic field. In the articles of Cassanas and Siedentop [7] the leading term of the asymptotics of the ground state energy of the multiparticle atomic Brown–Ravenhall operator for large atomic charges is found under the assumption that the ratio of the atomic charge and the speed of light is constant.

1.2 Outline of the Model and Main Results

Considering particles with different masses and interaction potentials, we will take into account that some of the particles of the system can be identical. As usual in quantum mechanics, this will require the restriction of the configuration space of the system to the subspace of functions which transform according to some proper representation of the group generated by transpositions of identical particles. The most physically motivated is the assumption that the wave–functions describing the state of the system should be antisymmetric with respect to such transpositions, since the Brown–Ravenhall operators describe particles with spin 1/2, thus fermions. On the other hand, if the interaction potentials have some rotation–reflection symmetry, it is very fruitful to consider the reductions to different irreducible representations of the symmetry group separately. Note that the spectrum of the whole operator is then the union of the spectra of all such reduced operators.

There are two main new results obtained in this dissertation. First, in Theorem 3.1.1 we characterize the essential spectrum of Brown–Ravenhall operators reduced to some irreducible representations of rotation–reflection and permutation symmetry groups in terms of two–cluster decompositions. An analogous result is well–known in the theory of multiparticle Schrödinger operators under the name "Hunzicker–van Winter–Zhislin theorem". The closest resemblance is the formulation of the HVZ theorem given in the book of Jörgens and Weidmann [18].

Historically the first proof of what is now known as the HVZ theorem for Schrödinger operators was obtained by Zhislin [30]. This result was since then generalized in many ways (see, e. g., [8] and references therein). For multiparticle Chandrasekhar operators the HVZ theorem was proved by Lewis, Siedentop and Vugalter [19]. The HVZ theorem for atomic Brown–Ravenhall operators in the Born–Oppenheimer approximation was obtained in the articles of Jakubaßa–Amundsen [16, 17] and our joint work with S. Vugalter [21]. In the recent preprint of Matte and Stockmeyer [20] the HVZ theorem is proved for a wide class of models which are obtained by projecting of multiparticle Dirac operators to subspaces dependent on the external electromagnetic field.

Our second main result is Theorem 4.2.1. We prove that for Brown–Ravenhall operators (reduced to any irreducible representations of rotation–reflection and permutation symmetry groups) the eigenfunctions corresponding to the eigenvalues below the essential spectrum decay exponentially. We also prove that the exponent characterizing the decay grows at least linearly with the distance between the eigenvalue and the essential spectrum. The assumptions of Theorem 4.2.1 are not as general as those of Theorem 3.1.1, see Section 4.1. The main difference is that the interparticle interaction potential is assumed to be nonnegative.

Note that the eigenvalues for which we prove the decay of eigenfunctions can be embedded in the essential spectrum of the whole operator, still being below the essential spectrum of a reduction to some irreducible representation of the symmetry group. Existence of such eigenvalues for some specific models including atoms and molecules in the Born–Oppenheimer approximation can be obtained along the same lines as in the proof of Theorem 2 of [21], where it is proved that atoms and positive ions have infinitely many eigenvalues below the essential spectrum.

The exponential decay of eigenfunctions has important implications for bound–state and scattering problems for multiparticle systems. There are many results on the decay of eigenfunctions of multiparticle Schrödinger operators, including anisotropic estimates and lower bounds, see e. g. [5] and references therein. A very detailed analysis of the non–isotropic exponential decay of eigenfunctions of Schrödinger operators in terms of a metric in configuration space is presented in the book of Agmon [2]. It is proved by Carmona and Simon [5] that the upper bound of [2] is exact at least for the ground state. Another very simple proof of the exponential decay, based on the approach of Agmon [2] can be found in [12], Lemma 6.2.

As for relativistic operators, Carmona, Masters and Simon [6] have proved the exponential decay and gave lower bounds for eigenfunctions of a wide class of models including one–particle Chandrasekhar operators. Exponential decay of eigenfunctions of some projected multiparticle Dirac operators is proved in [20].

Let us mention some features of Brown–Ravenhall Hamiltonians which make their analysis more complicated in comparison to Schrödinger operators. First, the operators we are considering are nonlocal due to the presence of the spectral projector Λ^N. Many times we will need to estimate the commutators of this projector with operators of multiplication by some functions. In order to obtain the desired estimates we will apply the method of [21], considering such commutators as singular integral operators. It also turns out that the separation of the center of mass motion, unlike for multiparticle Schrödinger operators, does not allow to decompose the multiparticle Brown–Ravenhall operator without external field as

$$\mathcal{H} = A \otimes I + I \otimes B,$$

where A would describe the free motion of the center of mass and B would be the internal Hamiltonian of the system (see e. g. [18], [8]). This makes many questions more thorny, especially in presence of rotation–reflection symmetries. For example, it is not obvious that the spectrum of the free cluster is a semiaxis, what we prove in Proposition 3.6.1. For the same reason we refrain to characterize the spectral structure of the internal Hamiltonian, since it will now depend on the momentum of the center of mass.

Note that the proof of the HVZ theorem for a system of particles described by the Chandrasekhar operator reduced to some nontrivial irreducible representation of the rotation–reflection symmetry group was till now not known (see the article of Lewis, Siedentop and Vugalter [19] for the proof without reductions). Such a proof can now be obtained as a simplified modification of the proof of Theorem 3.1.1.

Finally, we sketch the class of potentials for which our results are applicable. Whereas the exact assumptions are given in Sections 2.1 and 4.1, let us consider the case of purely electrostatic interactions. To satisfy the hypothesis of Theorem 3.1.1 it would suffice that the interaction potentials have the following properties:

- The operators describing the system and its subsystems are semibonded from below after multiplication of all potentials by $1 + \varepsilon$ with some $\varepsilon > 0$;
- All the interaction potentials decay at infinity in the L_∞ sense;
- The absolute value of each potential can be dominated by a sum of finite number of Coulomb "bumps"$C/|\cdot - \mathbf{x}_0|$ and a sufficiently big constant.

To satisfy the hypothesis of Theorem 4.2.1 it is enough to add the assumption

- The interaction potentials U_{nj}, $n < j = 1, \ldots, N$ are non–negative.

As for semiboundedness from below, it appears that attractive Coulombic singularities are only allowed up to some critical coupling constant dependent on the masses of the particles (and thus represent the borderline case), see [9]. It follows from the result of [3] that the Brown–Ravenhall operator is semibounded from below if the external field has a finite number of Coulombic wells of subcritical magnitude and the interparticle interaction potentials are non–negative.

1.3 Structure of the Dissertation

In Part 2 we will formulate the explicit assumptions on the interaction potentials, which will allow us to define the Brown–Ravenhall operator via a semibounded from below quadratic form. We also introduce the necessary reductions to the subspaces corresponding to irreducible representations of rotation–reflection and permutation symmetry groups.

In Part 3 we analyse the structure of the essential spectrum of multiparticle Brown–Ravenhall operators. The main result of this part is Theorem 3.1.1. In Section 3.2 we represent the orthogonal projector Λ_m on the positive spectral subspace of the Dirac operator as a singular integral operator. Section 3.3 contains useful tools for establishing the boundedness of integral operators. We will apply these tools to estimate some commutators of Λ_m with operators of multiplication by smooth functions in Section 3.4. In Sections 3.5—3.7 we give the proof of Theorem 3.1.1.

In Part 4 we prove that the eigenfunctions of multiparticle Brown–Ravenhall operators corresponding to the eigenvalues below the essential spectrum decay exponentially. Before we formulate the main result in Theorem 4.2.1, we will need to make some assumptions on the interaction potentials which are more restrictive than those of Part 3. This is done in Section 4.1. Theorem 4.2.1 is proved in Sections 4.3—4.6.

Part 5 contains two appendices. In Appendix A we overview some properties of modified Bessel functions which we often use throughout the text. Appendix B contains the proof of Lemma 3.5.2.

Part 2
Model

2.1 Assumptions and Definitions

Before we introduce our assumptions on the interaction potentials, let us consider possible decompositions of the system into two clusters. Let $Z = (Z_1, Z_2)$ be a decomposition of the index set $I := \{1, \ldots, N\}$ into two disjoint subsets:

$$I = Z_1 \cup Z_2, \quad Z_1 \cap Z_2 = \varnothing.$$

For $n = 1, \ldots, N$ we will say that the n^{th} particle belongs to the cluster j if $n \in Z_j$. Let

$$N_j := \#Z_j, \quad j = 1, 2 \tag{2.1.1}$$

be the number of particles in each cluster. We will write $n\#j$ if the particles with numbers n and j belong to different clusters. Let

$$\mathcal{H}_{Z,1} := \sum_{n \in Z_1} (D_n + V_n) + \sum_{\substack{n,j \in Z_1 \\ n<j}} U_{nj}, \tag{2.1.2}$$

$$\mathcal{H}_{Z,2} := \sum_{n \in Z_2} D_n + \sum_{\substack{n,j \in Z_2 \\ n<j}} U_{nj}. \tag{2.1.3}$$

We omit $\mathcal{H}_{Z,j}$ if $Z_j = \varnothing$, $j = 1, 2$. Let us introduce the operators corresponding to noninteracting clusters, with the second cluster transferred far away from the sources of the external field:

$$\widetilde{\mathcal{H}}_{Z,j} := \Lambda_{Z,j} \mathcal{H}_{Z,j} \Lambda_{Z,j}, \quad \text{in} \quad \mathfrak{H}_{Z,j} := \bigotimes_{n \in Z_j} \Lambda_n L_2(\mathbb{R}^3, \mathbb{C}^4), \quad j = 1, 2, \tag{2.1.4}$$

where

$$\Lambda_{Z,j} := \prod_{n \in Z_j} \Lambda_n.$$

We make the following assumptions:

Assumption 2.1.1 *There exists $C > 0$ such that for any Z and $j = 1, 2$*

$$\big|\langle \mathcal{H}_{Z,j} \varphi, \psi \rangle\big| \leqslant C \|\varphi\|_{H^{1/2}} \|\psi\|_{H^{1/2}}, \quad \textit{for any} \quad \varphi, \psi \in \bigotimes_{n \in Z_j} H^{1/2}(\mathbb{R}^3, \mathbb{C}^4). \tag{2.1.5}$$

For Coulomb interaction potentials (2.1.5) follows from Kato's inequality.

Assumption 2.1.2 *There exist $C_1 > 0$ and $C_2 \in \mathbb{R}$ such that for any Z*

$$\langle \widetilde{\mathcal{H}}_{Z,j}\psi, \psi\rangle \geqslant C_1 \langle \sum_{n\in Z_j} D_n\psi, \psi\rangle - C_2\|\psi\|^2, \quad \text{for any} \quad \psi \in \underset{n\in Z_j}{\otimes} \Lambda_n H^{1/2}(\mathbb{R}^3, \mathbb{C}^4), \quad j = 1, 2. \tag{2.1.6}$$

Remark 2.1.3 *Note that for $\psi \in \underset{n\in Z_j}{\otimes} \Lambda_n H^{1/2}(\mathbb{R}^3, \mathbb{C}^4)$ the metric*

$$\langle \sum_{n\in Z_j} D_n\psi, \psi\rangle^{1/2} = \Big\| \sum_{n\in Z_j} |D_n|^{1/2}\psi \Big\|$$

is equivalent to the norm of ψ in $\underset{n\in Z_j}{\otimes} H^{1/2}(\mathbb{R}^3, \mathbb{C}^4)$, since

$$\Lambda_n D_n \Lambda_n = \Lambda_n |D_n| \Lambda_n = \Lambda_n \sqrt{-\Delta + m_n^2}\,\Lambda_n. \tag{2.1.7}$$

An equivalent formulation of Assumption 2.1.2 is that the operator $\widetilde{\mathcal{H}}_{Z,j}$ is semibounded from below even if we multiply all the interaction potentials by $1+\varepsilon$ with $\varepsilon > 0$ small enough. This is only slightly more restrictive than the semiboundedness of $\widetilde{\mathcal{H}}_{Z,j}$.

Assumption 2.1.4 *For any $R > 0$ there exists a finite constant $C_R \geqslant 0$ such that*

$$\sum_{n=1}^{N} \Big(\int_{|\mathbf{x}|\leqslant R} \big|V_n(\mathbf{x})\big|^2 d\mathbf{x} \Big)^{1/2} + \sum_{n<j}^{N} \Big(\int_{|\mathbf{x}|\leqslant R} \big|U_{nj}(\mathbf{x})\big|^2 d\mathbf{x} \Big)^{1/2} \leqslant C_R. \tag{2.1.8}$$

This means that the interaction potentials are locally square integrable.

Assumption 2.1.5 *For any $\varepsilon > 0$ there exists $R > 0$ big enough such that for all $n = 1, \dots, N$*

$$\|V_n I_{\{|\mathbf{x}_n|>R\}}\psi\| \leqslant \varepsilon \big\| |D_n|^{1/2}\psi \big\|, \quad \text{for all} \quad \psi \in H^{1/2}(\mathbb{R}^3, \mathbb{C}^4), \tag{2.1.9}$$

and for all $n < j = 1, \dots, N$

$$\|U_{nj} I_{\{|\mathbf{x}_n-\mathbf{x}_j|>R\}}\varphi\| \leqslant \varepsilon \min\Big\{ \big\| |D_n|^{1/2}\varphi \big\|, \big\| |D_j|^{1/2}\varphi \big\| \Big\}, \quad \text{for all} \quad \varphi \in H^{1/2}(\mathbb{R}^6, \mathbb{C}^{16}). \tag{2.1.10}$$

By Remark 2.1.3 this assumption is *weaker* then the decay of L_∞ norms of the interaction potentials at infinity.

It follows from (2.1.6) and Remark 2.1.3 that for any Z there exists a constant $C > 0$ such that for any $\psi \in \bigotimes_{n \in Z_j} \Lambda_n H^{1/2}(\mathbb{R}^3, \mathbb{C}^4)$

$$\|\psi\|^2_{H^{1/2}} \leqslant C\big(\langle \widetilde{\mathcal{H}}_{Z,j}\psi, \psi\rangle + \|\psi\|^2\big), \quad j = 1, 2. \tag{2.1.11}$$

Hence by Assumptions 2.1.1 and 2.1.2, the quadratic forms of operators (2.1.4) (and, in particular, $\mathcal{H}_N$) are semibounded from below and closed on $\bigotimes_{n \in Z_j} \Lambda_n H^{1/2}(\mathbb{R}^3, \mathbb{C}^4)$. Thus these operators are well–defined in the form sense.

Some particles of the system (say, k^{th} and l^{th}) can be identical (in which case $m_k = m_l$, $V_k = V_l$, and $U_{kj} = U_{lj}$ for all j). Then the operator $\mathcal{H}_N$ can be reduced to the subspace of functions which transform in a certain way under permutations of identical particles. The most physically motivated assumption is that any transposition of two identical particles should change the sign of the wave function $\psi \in \mathfrak{H}_N$ describing the system. This is the Pauli principle applied to the identical fermions (the model describes spin 1/2 particles, thus fermions).

Let Π be the subgroup of the symmetric group $\mathcal{S}_N$ generated by transpositions of identical particles. We denote the number of elements of Π by h_Π. Let E be some irreducible representation of Π with dimension d_E and character ξ_E. For $\psi \in \mathfrak{H}_N$ let

$$P^E\psi := \frac{d_E}{h_\Pi} \sum_{\pi \in \Pi} \overline{\xi_E(\pi)}\pi\psi, \tag{2.1.12}$$

where π is the operator of permutation:

$$(\pi\psi)(\mathbf{x}_1, s_1; \ldots; \mathbf{x}_N, s_N) = \psi\big(\mathbf{x}_{\pi^{-1}(1)}, s_{\pi^{-1}(1)}; \ldots; \mathbf{x}_{\pi^{-1}(N)}, s_{\pi^{-1}(N)}\big).$$

Here $s_1, \ldots, s_N$ are the spinor coordinates of the particles. The operator P^E defined in (2.1.12) is the projector to the subspace of functions in $\mathfrak{H}_N$ which transform according to the representation E of Π. Since any $\pi \in \Pi$ commutes with $\mathcal{H}_N$, P^E reduces $\mathcal{H}_N$. Let $\mathcal{H}_N^E$ be the corresponding reduced selfadjoint operator in

$$\mathfrak{H}_N^E := P^E\mathfrak{H}_N.$$

For a decomposition $Z = (Z_1, Z_2)$ let Π_j^Z be the group generated by transpositions of identical particles inside Z_j, $j = 1, 2$. For any irreducible representation E_j of Π_j^Z with dimension d_{E_j} and character ξ_{E_j} the projection to the space of functions in $\mathfrak{H}_{Z,j}$ transforming according to E_j under the action of Π_j^Z is given by

$$P^{E_j}\psi := \frac{d_{E_j}}{h_{\Pi_j^Z}} \sum_{\pi\in\Pi_j^Z} \overline{\xi_{E_j}(\pi)}\pi\psi, \quad \psi \in \mathfrak{H}_{Z,j},$$

where $h_{\Pi_j^Z}$ is the cardinality of Π_j^Z. Projectors P^{E_j} reduce operators $\widetilde{\mathcal{H}}_{Z,j}$. We introduce the reduced operators $\widetilde{\mathcal{H}}_{Z,j}^{E_j}$ in

$$\mathfrak{H}_{Z,j}^{E_j} := P^{E_j}\mathfrak{H}_{Z,j}, \quad j = 1, 2.$$

Given an irreducible representation E of Π and a decomposition $Z = (Z_1, Z_2)$, we have

$$\mathfrak{H}_N^E \subset \bigoplus_{(E_1,E_2)} \big(\mathfrak{H}_{Z,1}^{E_1} \otimes \mathfrak{H}_{Z,2}^{E_2}\big), \tag{2.1.13}$$

where $E_{1,2}$ are some irreducible representations of $\Pi_{1,2}^Z$. We write

$$(E_1, E_2) \underset{Z}{\prec} E$$

if the corresponding term cannot be omitted on the r. h. s. of (2.1.13) without violation of the inclusion.

Apart from permutations of identical particles the operator $\mathcal{H}_N^E$ can have some rotation–reflection symmetries. Let γ be an orthogonal transform in $\mathbb{R}^3$: the rotation around the axis directed along a unit vector $\mathbf{n}_\gamma$ through an angle φ_γ, possibly combined with the reflection $\mathbf{x} \mapsto -\mathbf{x}$. The corresponding unitary operator O_γ acts on the functions $\psi \in \mathfrak{H}^N$ as (see [26], Chapter 2)

$$(O_\gamma\psi)(\mathbf{x}_1, \ldots, \mathbf{x}_N) = \prod_{n=1}^{N} e^{-i\varphi_\gamma \mathbf{n}_\gamma\cdot\mathbf{S}_n}\psi(\gamma^{-1}\mathbf{x}_1, \ldots, \gamma^{-1}\mathbf{x}_N).$$

Here $\mathbf{S}_n = -\frac{i}{4}\alpha_n \wedge \alpha_n$ is the spin operator acting on the spinor coordinates of the n^{th} particle. The compact group of orthogonal transformations γ such that O_γ commutes with V_n and U_{nj} for all n, $j = 1, \ldots, N$ (and thus with $\mathcal{H}_N^E$) we denote by Γ. Further, we decompose $\mathfrak{H}_N^E$ into the orthogonal sum

$$\mathfrak{H}_N^E = \bigoplus_{\alpha\in A} \mathfrak{H}_N^{D_\alpha,E}, \tag{2.1.14}$$

where $\mathfrak{H}_N^{D_\alpha,E}$ consists of functions which transform under O_γ according to some irreducible representation D_α of Γ, and A is the set indexing all such irreducible representations. The decomposition (2.1.14) reduces $\mathcal{H}_N^E$. We denote the selfadjoint restrictions of $\mathcal{H}_N^E$ to $\mathfrak{H}_N^{D_\alpha,E}$ by $\mathcal{H}_N^{D_\alpha,E}$. For any fixed irreducible representation D with dimension d_D and character ζ_D the orthogonal projector in $\mathfrak{H}_N$ onto the subspace of functions which transform according to D is

$$P^D := d_D \int_\Gamma \overline{\zeta_D(\gamma)} O_\gamma d\mu(\gamma),$$

where μ is the invariant probability measure on Γ.

For $j = 1, 2$ let D_j be some irreducible representations of Γ with dimensions d_{D_j} and characters ζ_{D_j}. The corresponding projectors in $\mathfrak{H}_{Z,j}$ are given by

$$P^{D_j} = d_{D_j} \int_\Gamma \overline{\zeta_{D_j}(\gamma)} O_{\gamma,j} d\mu(\gamma),$$

where $O_{\gamma,j}$ is the restriction of O_γ to $\mathfrak{H}_{Z,j}$:

$$(O_{\gamma,j}\psi)(\mathbf{x}_{n_1}, \ldots, \mathbf{x}_{n_{N_j}}) = \prod_{n \in Z_j} e^{-i\varphi_\gamma \mathbf{n}_\gamma \cdot \mathbf{S}_n} \psi(\gamma^{-1}\mathbf{x}_{n_1}, \ldots, \gamma^{-1}\mathbf{x}_{n_{N_j}}).$$

Given representations D_j and E_j, projector $P^{D_j}P^{E_j} = P^{E_j}P^{D_j}$ reduces $\widetilde{\mathcal{H}}_{Z,j}$. We denote the reduced operators in

$$\mathfrak{H}_{Z,j}^{D_j,E_j} := P^{D_j}P^{E_j}\mathfrak{H}_{Z,j}$$

by $\widetilde{\mathcal{H}}_{Z,j}^{D_j,E_j}$.

We write $(D_1, E_1; D_2, E_2) \underset{Z}{\prec} (D, E)$ if the corresponding term cannot be omitted on the r. h. s. of

$$\mathfrak{H}_N^{D,E} \subset \bigoplus_{\substack{(D_1,E_1)\\(D_2,E_2)}} \left(\mathfrak{H}_{Z,1}^{D_1,E_1} \otimes \mathfrak{H}_{Z,2}^{D_2,E_2}\right)$$

without violation of the inclusion.

Part 3
Essential Spectrum of Multiparticle Brown–Ravenhall Operators

3.1 Characterization of the Essential Spectrum

We now formulate the main theorem of this part of the dissertation, which is an analogue of the HVZ theorem for Schrödinger operators. We use the notation introduced in Section 2.1.

Theorem 3.1.1 *Suppose Assumptions 2.1.1, 2.1.2, 2.1.4, and 2.1.5 hold true. For $N \in \mathbb{N}$ let D be some irreducible representation of Γ, and E some irreducible representation of Π, such that $P^D P^E \neq 0$. Let*

$$\varkappa_j(Z, D_j, E_j) := \inf \sigma(\widetilde{\mathcal{H}}_{Z,j}^{D_j,E_j}). \tag{3.1.1}$$

For $Z_2 \neq \varnothing$ let

$$\varkappa(Z, D, E) := \begin{cases} \inf\limits_{(D_1,E_1;D_2,E_2) \underset{Z}{\prec} (D,E)} \big\{\varkappa_1(Z, D_1, E_1) + \varkappa_2(Z, D_2, E_2)\big\}, & Z_1 \neq \varnothing, \\ \varkappa_2(Z, D, E), & Z_1 = \varnothing. \end{cases} \tag{3.1.2}$$

Let

$$\varkappa(D, E) = \min\big\{\varkappa(Z, D, E) : Z = (Z_1, Z_2),\ Z_2 \neq \varnothing\big\}. \tag{3.1.3}$$

Then

$$\sigma_{\mathrm{ess}}(\mathcal{H}_N^{D,E}) = \big[\varkappa(D, E), \infty\big).$$

Remark 3.1.2 *We only need Assumption 2.1.2 for the operators $\widetilde{\mathcal{H}}_{Z,j}^{D_j,E_j}$ which appear in* (3.1.1), (3.1.2).

3.2 Projector to the Positive Spectral Subspace as an Integral Operator

In this section we calculate the integral kernel of the orthogonal projector Λ_m to the positive spectral subspace of the free Dirac operator with mass

$m > 0$ (see (1.1.1)). Note that for $n = 1, \ldots, N$ we write Λ_n instead of Λ_{m_n}.

Lemma 3.2.1 *Let $f \in C_0^1(\mathbb{R}^3, \mathbb{C}^4)$. Then for $m > 0$*

$$(\Lambda_m f)(\mathbf{x}) = \frac{f(\mathbf{x})}{2} + \frac{im}{2\pi^2} \lim_{\varepsilon \to +0} \int_{|\mathbf{y}-\mathbf{x}|>\varepsilon} \frac{\boldsymbol{\alpha} \cdot (\mathbf{x}-\mathbf{y})}{|\mathbf{x}-\mathbf{y}|^3} K_1\big(m|\mathbf{x}-\mathbf{y}|\big) f(\mathbf{y}) d\mathbf{y}$$
$$+ \frac{m^2}{4\pi^2} \int_{\mathbb{R}^3} \left(\beta \frac{K_1\big(m|\mathbf{x}-\mathbf{y}|\big)}{|\mathbf{x}-\mathbf{y}|} + \frac{i\boldsymbol{\alpha} \cdot (\mathbf{x}-\mathbf{y})}{|\mathbf{x}-\mathbf{y}|^2} K_0\big(m|\mathbf{x}-\mathbf{y}|\big) \right) f(\mathbf{y}) d\mathbf{y}. \tag{3.2.1}$$

Here K_0 and K_1 are modified Bessel functions. We recall some of their properties in Appendix A.

Proof. We start with the operator $2\Lambda_m - 1$, which is the multiplication by the matrix valued function $\dfrac{\boldsymbol{\alpha} \cdot \mathbf{p} + \beta m}{\sqrt{|\mathbf{p}|^2 + m^2}}$ in the momentum space (see (1.1.1)). It can be factorized as $A \cdot B$ with

$$A := (\boldsymbol{\alpha} \cdot \mathbf{p} + \beta m)\big(|\mathbf{p}|^2 + m^2\big), \quad B := \big(|\mathbf{p}|^2 + m^2\big)^{-3/2}.$$

In the coordinate representation $B : L_2(\mathbb{R}^3, \mathbb{C}^4) \to H^3(\mathbb{R}^3, \mathbb{C}^4)$ is a bounded integral operator. Its kernel is given by the convergent integral

$$B(\mathbf{x}, \mathbf{y}) = \frac{1}{(2\pi)^3} \int_{\mathbb{R}^3} \frac{e^{i\mathbf{p}\cdot(\mathbf{x}-\mathbf{y})}}{\big(|\mathbf{p}|^2 + m^2\big)^{3/2}} d\mathbf{p}$$
$$= \frac{1}{2\pi^2} \int_0^\infty \frac{p \sin\big(p|\mathbf{x}-\mathbf{y}|\big)}{|\mathbf{x}-\mathbf{y}|(p^2+m^2)^{3/2}} dp = \frac{1}{2\pi^2} K_0\big(m|\mathbf{x}-\mathbf{y}|\big).$$

In the configuration space A is the differential operator $(-i\boldsymbol{\alpha}\cdot\nabla + \beta m)(-\Delta + m^2)$ mapping $H^3(\mathbb{R}^3, \mathbb{C}^4)$ onto $L_2(\mathbb{R}^3, \mathbb{C}^4)$. Thus with the help of (5.1.2) for any $f \in C_0^1(\mathbb{R}^3, \mathbb{C}^4)$ we get

$$\begin{aligned}
&\big((2\Lambda_m - 1)f\big)(\mathbf{x}) \\
&= (-i\boldsymbol{\alpha} \cdot \nabla + \beta m)(-\Delta + m^2) \frac{1}{2\pi^2} \int_{\mathbb{R}^3} K_0\big(m|\mathbf{x}-\mathbf{y}|\big) f(\mathbf{y}) d\mathbf{y} \\
&= (-i\boldsymbol{\alpha} \cdot \nabla + \beta m) \frac{m}{2\pi^2} \int_{\mathbb{R}^3} \frac{K_1\big(m|\mathbf{x}-\mathbf{y}|\big)}{|\mathbf{x}-\mathbf{y}|} f(\mathbf{y}) d\mathbf{y} \\
&= (-i\boldsymbol{\alpha} \cdot \nabla + \beta m) \frac{m}{2\pi^2} \int_{\mathbb{R}^3} \frac{K_1\big(m|\mathbf{y}|\big)}{|\mathbf{y}|} f(\mathbf{x}-\mathbf{y}) d\mathbf{y}.
\end{aligned} \tag{3.2.2}$$

The term with β defines a function from $L_2(\mathbb{R}^3, \mathbb{C}^4)$, because $|\cdot|^{-1}K_1\big(|\cdot|\big) \in L_1(\mathbb{R}^3)$. We rewrite the gradient term on the r. h. s. of (3.2.2) as

$$\begin{aligned} & - i\boldsymbol{\alpha}\cdot\nabla_{\mathbf{x}}\frac{m}{2\pi^2}\int_{\mathbb{R}^3}\frac{K_1\big(m|\mathbf{y}|\big)}{|\mathbf{y}|}f(\mathbf{x}-\mathbf{y})d\mathbf{y} \\ & = \frac{im}{2\pi^2}\Big(\int_{\mathbb{R}^3\setminus B_\varepsilon} + \int_{B_\varepsilon}\Big)\frac{K_1\big(m|\mathbf{y}|\big)}{|\mathbf{y}|}\boldsymbol{\alpha}\cdot\nabla_{\mathbf{y}}\big(f(\mathbf{x}-\mathbf{y})\big)d\mathbf{y}. \end{aligned} \tag{3.2.3}$$

The second integral on the r. h. s. of (3.2.3) can be estimated as

$$\left|\frac{im}{2\pi^2}\int_{B_\varepsilon}\frac{K_1\big(m|\mathbf{y}|\big)}{|\mathbf{y}|}\boldsymbol{\alpha}\cdot\nabla_{\mathbf{y}}\big(f(\mathbf{x}-\mathbf{y})\big)d\mathbf{y}\right| \leqslant \frac{3m}{2\pi^2}\|\nabla f\|_{L_\infty}\int_{B_\varepsilon}\frac{K_1\big(m|\mathbf{y}|\big)}{|\mathbf{y}|}d\mathbf{y}, \tag{3.2.4}$$

where the r. h. s. of (3.2.4) tends to zero as $\varepsilon \to 0$. For the first integral on the r. h. s. of (3.2.3) the integration by parts gives

$$\begin{aligned} & \frac{im}{2\pi^2}\int_{\mathbb{R}^3\setminus B_\varepsilon}\frac{K_1\big(m|\mathbf{y}|\big)}{|\mathbf{y}|}\boldsymbol{\alpha}\cdot\nabla_{\mathbf{y}}\big(f(\mathbf{x}-\mathbf{y})\big)d\mathbf{y} \\ & = -\frac{im}{2\pi^2}\int_{\mathbb{R}^3\setminus B_\varepsilon}\boldsymbol{\alpha}\cdot\nabla_{\mathbf{y}}\Big(\frac{K_1\big(m|\mathbf{y}|\big)}{|\mathbf{y}|}\Big)f(\mathbf{x}-\mathbf{y})d\mathbf{y} \\ & + \frac{imK_1(m\varepsilon)}{2\pi^2\varepsilon}\int_{\partial B_\varepsilon}\boldsymbol{\alpha}\cdot\frac{\mathbf{y}}{|\mathbf{y}|}f(\mathbf{x}-\mathbf{y})d\mathbf{y}. \end{aligned} \tag{3.2.5}$$

We can rewrite the last integral on the r. h. s. of (3.2.5) as the sum of two integrals, using the Taylor expansion $f(\mathbf{x}-\mathbf{y}) = f(\mathbf{x}) - \nabla f(\mathbf{z})\cdot\mathbf{y}$ with $\mathbf{z}$ lying on the segment connecting $\mathbf{x}$ and $\mathbf{y}$. The integral containing $f(\mathbf{x})$ vanishes, because the function $\mathbf{y}|\mathbf{y}|^{-1}$ is odd. The integral with $\nabla f(\mathbf{z})\mathbf{y}$ is different from zero only for $\mathbf{x}$ in the compact region

$$\Theta := \big\{\mathbf{x}\big|\mathbf{x}\in\mathbb{R}^3,\ \mathrm{dist}\,\{\mathbf{x},\,\mathrm{supp}\,f\} \leqslant \varepsilon\big\}.$$

For $\mathbf{x} \in \Theta$ we have

$$\left|\frac{imK_1(m\varepsilon)}{2\pi^2\varepsilon}\int_{\partial B_\varepsilon}\Big(\boldsymbol{\alpha}\cdot\frac{\mathbf{y}}{|\mathbf{y}|}\Big)\big(\nabla f(\mathbf{z})\cdot\mathbf{y}\big)d\mathbf{y}\right| \leqslant \frac{3mK_1(m\varepsilon)}{2\pi^2}\|\nabla f\|_{L_\infty}4\pi\varepsilon^2. \tag{3.2.6}$$

Hence by (5.1.1) the last term on the r. h. s. of (3.2.5) converges to zero in the L_2–norm. Together with (3.2.2) — (3.2.5) and (5.1.2) this proves Lemma 3.2.1. •

3.3 Boundedness of Integral Operators

It is clear from (1.1.1) that for any $m > 0$ and any $s \geqslant 0$ the operator Λ_m is bounded in the Sobolev space $H^s(\mathbb{R}^3, \mathbb{C}^4)$. This fact is much less evident from the formula (3.2.1). On the other hand, it is easy to calculate the integral kernels for products and commutators of Λ_m with multiplication operators once the integral kernel of Λ_m is known.

In order to be able to extract the information on the boundedness of (singular) integral operators with given integral kernels we will need the following two theorems:

Theorem 3.3.1 (Stein [24], Chapter 2, Section 3.2) *Let $K : \mathbb{R}^n \to \mathbb{C}$ be measurable such that for some $B > 0$*

$$\big|K(\mathbf{x})\big| \leqslant B|\mathbf{x}|^{-n}, \quad \mathbf{x} \neq \mathbf{0}, \tag{3.3.1}$$

$$\big|\nabla K(\mathbf{x})\big| \leqslant B|\mathbf{x}|^{-n-1}, \tag{3.3.2}$$

and

$$\int_{R_1<|\mathbf{x}|<R_2} K(\mathbf{x}) d^n\mathbf{x} = 0, \quad \textit{for all} \quad 0 < R_1 < R_2 < \infty. \tag{3.3.3}$$

For $g \in L_p(\mathbb{R}^n)$, $1 < p < \infty$, let

$$T_\varepsilon(g)(\mathbf{x}) = \int_{|\mathbf{y}|\geqslant\varepsilon} g(\mathbf{x}-\mathbf{y})K(\mathbf{y})d^n\mathbf{y}, \quad \varepsilon > 0. \tag{3.3.4}$$

Then

$$\big\|T_\varepsilon(g)\big\|_p \leqslant A_p\|g\|_p \tag{3.3.5}$$

with A_p independent of g and ε.

Remark 3.3.2 *Inequality* (3.3.5) *shows that the operator $T = \lim\limits_{\varepsilon\to+0} T_\varepsilon$ exists as a bounded operator in $L_p(\mathbb{R}^n)$ and its norm satisfies $\|T\|_p \leqslant A_p$.*

The second theorem is known as Schur's test:

Theorem 3.3.3 *Let Ω_1 and Ω_2 be two spaces with measures. Let $A(\cdot,\cdot)$ be a measurable (matrix) function on $\Omega_1 \times \Omega_2$ satisfying*

$$Q_1 := \sup_{\mathbf{y}\in\Omega_2} \int_{\Omega_1} \big|A(\mathbf{x},\mathbf{y})\big| d\mathbf{x} < \infty, \quad Q_2 := \sup_{\mathbf{x}\in\Omega_1} \int_{\Omega_2} \big|A(\mathbf{x},\mathbf{y})\big| d\mathbf{y} < \infty. \tag{3.3.6}$$

Then the integral operator

$$(A\psi)(\mathbf{x}) := \int_{\Omega_2} A(\mathbf{x},\mathbf{y})\psi(\mathbf{y})d\mathbf{y} \tag{3.3.7}$$

is bounded from $L_2(\Omega_2)$ to $L_2(\Omega_1)$ and $\|A\| \leqslant \sqrt{Q_1 Q_2}$.

We will only use Theorem 3.3.3 in the case $\Omega_1 = \Omega_2 = \mathbb{R}^3$ with Lebesgue measure.

Note that in the case of convolution (i. e. for $A(\mathbf{x},\mathbf{y}) = A(\mathbf{x}-\mathbf{y})$, $\Omega_1 = \Omega_2 = \mathbb{R}^d$) Theorem 3.3.3 reduces to Young's inequality for convolution with L_1–function (see e. g. [22]).

For a 4×4 measurable matrix function A on $\mathbb{R}^3 \times \mathbb{R}^3$ we define the corresponding integral operator by

$$(Ag)(\mathbf{x}) := \lim_{\varepsilon \to +0} \int_{|\mathbf{x}-\mathbf{y}|>\varepsilon} A(\mathbf{x},\mathbf{y})g(\mathbf{y})d\mathbf{y}, \quad g \in C_0^1(\mathbb{R}^3,\mathbb{C}^4). \tag{3.3.8}$$

We will only work with such A that (3.3.8) makes sense and extends to a bounded operator in $L_2(\mathbb{R}^3,\mathbb{C}^4)$ either by Theorem 3.3.1, in which case $A(\mathbf{x},\mathbf{y})$ has to depend only on $(\mathbf{x}-\mathbf{y})$, or by Theorem 3.3.3.

In particular, according to the definition given above and (3.2.1), the integral kernel of $(\Lambda_m - 1/2)$ is

$$\begin{aligned}\mathcal{K}(\mathbf{x},\mathbf{y}) := {}& \frac{im}{2\pi^2}\frac{\boldsymbol{\alpha}\cdot(\mathbf{x}-\mathbf{y})}{|\mathbf{x}-\mathbf{y}|^3} K_1\big(m|\mathbf{x}-\mathbf{y}|\big) \\ &+ \frac{m^2}{4\pi^2}\Big(\beta\frac{K_1\big(m|\mathbf{x}-\mathbf{y}|\big)}{|\mathbf{x}-\mathbf{y}|} + \frac{i\boldsymbol{\alpha}\cdot(\mathbf{x}-\mathbf{y})}{|\mathbf{x}-\mathbf{y}|^2}K_0\big(m|\mathbf{x}-\mathbf{y}|\big)\Big).\end{aligned} \tag{3.3.9}$$

The boundedness follows from Theorem 3.3.1 and (5.1.2) since $\mathcal{K}(\mathbf{x},\mathbf{y})$ depends only on $(\mathbf{x}-\mathbf{y})$.

Note that the function (3.3.9) rapidly decays together with the derivative if $|\mathbf{x}-\mathbf{y}|$ becomes big. Namely, if for $r > 0$ we let

$$G(r) := \sup_{|\mathbf{x}-\mathbf{y}|>r} \big|\mathcal{K}(\mathbf{x},\mathbf{y})\big| + \sup_{|\mathbf{x}-\mathbf{y}|>r} \big|\nabla_{\mathbf{x}}\mathcal{K}(\mathbf{x},\mathbf{y})\big|, \tag{3.3.10}$$

then by (5.1.2) and the first asymptotic in (5.1.1) for any $R > 0$ there exists $C(R) > 0$ such that

$$G(r) \leqslant C(R) r^{-3/2} e^{-r}, \quad \text{for all} \quad r \geqslant R. \tag{3.3.11}$$

3.4 Commutator Estimates

3.4.1 One Particle Commutator Estimate

Lemma 3.4.1 *Let χ be a bounded twice–differentiable function on $\mathbb{R}^3$ with bounded derivatives. Then for $m > 0$ the commutator $[\chi, \Lambda_m]$ is a bounded operator from $L_2(\mathbb{R}^3, \mathbb{C}^4)$ to $H^1(\mathbb{R}^3, \mathbb{C}^4)$. There exists $C(m) > 0$ such that*

$$\big\|[\chi, \Lambda_m]\big\|_{L_2(\mathbb{R}^3,\mathbb{C}^4)\to H^1(\mathbb{R}^3,\mathbb{C}^4)} \leqslant C(m)\big(\|\nabla\chi\|_{L_\infty} + \|\partial^2\chi\|_{L_\infty}\big). \tag{3.4.1}$$

Here $\|\partial^2\chi\|_{L_\infty} = \max_{\substack{\mathbf{z}\in\mathbb{R}^3\\ k,l\in\{1,2,3\}}} \big|\partial^2_{kl}\chi(\mathbf{z})\big|.$

Proof. Let us first prove that $[\chi, \Lambda_m]$ is a bounded operator in $L_2(\mathbb{R}^3, \mathbb{C}^4)$. For $f \in C^1_0(\mathbb{R}^3, \mathbb{C}^4)$ formula (3.2.1) implies

$$\begin{aligned}
&\big([\chi, \Lambda_m]f\big)(\mathbf{x})\\
&= \frac{m^2}{4\pi^2}\int_{\mathbb{R}^3}\Big(\beta\frac{K_1\big(m|\mathbf{x}-\mathbf{y}|\big)}{|\mathbf{x}-\mathbf{y}|} + \frac{i\boldsymbol{\alpha}\cdot(\mathbf{x}-\mathbf{y})}{|\mathbf{x}-\mathbf{y}|^2}K_0\big(m|\mathbf{x}-\mathbf{y}|\big)\Big)\\
&\times\big(\chi(\mathbf{x}) - \chi(\mathbf{y})\big)f(\mathbf{y})d\mathbf{y}\\
&+ \frac{im}{2\pi^2}\lim_{\varepsilon\to+0}\int_{|\mathbf{y}-\mathbf{x}|>\varepsilon}\frac{\boldsymbol{\alpha}\cdot(\mathbf{x}-\mathbf{y})}{|\mathbf{x}-\mathbf{y}|^3}K_1\big(m|\mathbf{x}-\mathbf{y}|\big)\big(\chi(\mathbf{x}) - \chi(\mathbf{y})\big)f(\mathbf{y})d\mathbf{y}.
\end{aligned} \tag{3.4.2}$$

Estimating $\big|\chi(\mathbf{x}) - \chi(\mathbf{y})\big|$ by $|\mathbf{x}-\mathbf{y}|\|\nabla\chi\|_{L_\infty}$, using the density of $C^1_0(\mathbb{R}^3, \mathbb{C}^4)$ in $L_2(\mathbb{R}^3, \mathbb{C}^4)$ and applying Young's inequality for the convolution with a kernel from $L_1(\mathbb{R}^3)$, we arrive at

$$\begin{aligned}
&\big\|[\chi, \Lambda_m]\big\|_{L_2(\mathbb{R}^3,\mathbb{C}^4)\to L_2(\mathbb{R}^3,\mathbb{C}^4)}\\
&\leqslant \|\nabla\chi\|_{L_\infty}\frac{m^2}{4\pi^2}\int_{\mathbb{R}^3}\Big(K_1\big(m|\mathbf{x}|\big) + 3K_0\big(m|\mathbf{x}|\big) + 6\frac{K_1\big(m|\mathbf{x}|\big)}{m|\mathbf{x}|}\Big)d\mathbf{x}\\
&\leqslant Cm^{-1}\|\nabla\chi\|_{L_\infty}.
\end{aligned} \tag{3.4.3}$$

To complete the proof it remains to show that

$$\big\|\nabla[\chi, \Lambda_m]f\big\|_{L_2(\mathbb{R}^3,\mathbb{C}^4)} \leqslant C(m)\big(\|\nabla\chi\|_{L_\infty} + \|\partial^2\chi\|_{L_\infty}\big)\|f\|_{L_2(\mathbb{R}^3,\mathbb{C}^4)}.$$

The differentiation of the first term on the r. h. s. of (3.4.2) according to (5.1.2) gives absolutely convergent integrals with L_2–norms bounded by $\|\nabla\chi\|_{L_\infty}\|f\|$ by Young's inequality. The differentiation of the second integral on the r. h. s. of (3.4.2) in the j^{th} component of $\mathbf{x}$ gives for $f \in C_0^1(\mathbb{R}^3, \mathbb{C}^4)$ (cf. (5.1.2))

$$\begin{aligned}&\frac{im}{2\pi^2}\lim_{\varepsilon\to+0}\int_{|\mathbf{x}-\mathbf{y}|>\varepsilon}\Big(\alpha_j\frac{K_1\big(m|\mathbf{x}-\mathbf{y}|\big)}{|\mathbf{x}-\mathbf{y}|^3}-\frac{m\boldsymbol{\alpha}\cdot(\mathbf{x}-\mathbf{y})(x_j-y_j)K_0\big(m|\mathbf{x}-\mathbf{y}|\big)}{|\mathbf{x}-\mathbf{y}|^4}\\&-\frac{4\boldsymbol{\alpha}\cdot(\mathbf{x}-\mathbf{y})(x_j-y_j)K_1\big(m|\mathbf{x}-\mathbf{y}|\big)}{|\mathbf{x}-\mathbf{y}|^5}\Big)\big(\chi(\mathbf{x})-\chi(\mathbf{y})\big)f(\mathbf{y})d\mathbf{y}\\&+\frac{im}{2\pi^2}\lim_{\varepsilon\to+0}\int_{|\mathbf{x}-\mathbf{y}|>\varepsilon}\frac{\boldsymbol{\alpha}\cdot(\mathbf{x}-\mathbf{y})K_1\big(m|\mathbf{x}-\mathbf{y}|\big)}{|\mathbf{x}-\mathbf{y}|^3}\partial_j\chi(\mathbf{x})f(\mathbf{y})d\mathbf{y}.\end{aligned} \tag{3.4.4}$$

The term

$$-\frac{im^2}{2\pi^2}\int_{\mathbb{R}^3}\frac{\boldsymbol{\alpha}\cdot(\mathbf{x}-\mathbf{y})(x_j-y_j)K_0\big(m|\mathbf{x}-\mathbf{y}|\big)}{|\mathbf{x}-\mathbf{y}|^4}\big(\chi(\mathbf{x})-\chi(\mathbf{y})\big)f(\mathbf{y})d\mathbf{y}$$

is bounded by $C\|\nabla\chi\|_{L_\infty}\|f\|$.

The Taylor expansion of χ gives

$$\chi(\mathbf{x})-\chi(\mathbf{y})=(x_k-y_k)\partial_k\chi(\mathbf{x})-\frac{1}{2}(x_k-y_k)(x_l-y_l)\partial^2_{kl}\chi(\mathbf{z_{xy}}). \tag{3.4.5}$$

Here $\mathbf{z_{xy}}$ is some point on the line segment connecting $\mathbf{x}$ and $\mathbf{y}$ and summations in k and l from 1 to 3 are assumed. Substituting (3.4.5) into (3.4.4) we arrive at

$$\begin{aligned}&\frac{im\partial_k\chi(\mathbf{x})}{2\pi^2}\lim_{\varepsilon\to+0}\int_{|\mathbf{x}-\mathbf{y}|>\varepsilon}\Big(\alpha_j-\frac{4\boldsymbol{\alpha}\cdot(\mathbf{x}-\mathbf{y})(x_j-y_j)}{|\mathbf{x}-\mathbf{y}|^2}\Big)\\&\times\frac{K_1\big(m|\mathbf{x}-\mathbf{y}|\big)(x_k-y_k)}{|\mathbf{x}-\mathbf{y}|^3}f(\mathbf{y})d\mathbf{y}\\&+\frac{im\partial_j\chi(\mathbf{x})}{2\pi^2}\lim_{\varepsilon\to+0}\int_{|\mathbf{x}-\mathbf{y}|>\varepsilon}\frac{\boldsymbol{\alpha}\cdot(\mathbf{x}-\mathbf{y})K_1\big(m|\mathbf{x}-\mathbf{y}|\big)}{|\mathbf{x}-\mathbf{y}|^3}f(\mathbf{y})d\mathbf{y}\\&-\frac{im}{4\pi^2}\int_{\mathbb{R}^3}\Big(\alpha_j-\frac{4\boldsymbol{\alpha}\cdot(\mathbf{x}-\mathbf{y})(x_j-y_j)}{|\mathbf{x}-\mathbf{y}|^2}\Big)\frac{K_1\big(m|\mathbf{x}-\mathbf{y}|\big)}{|\mathbf{x}-\mathbf{y}|^3}\\&\times(x_k-y_k)(x_l-y_l)\partial^2_{kl}\chi(\mathbf{z_{xy}})f(\mathbf{y})d\mathbf{y}.\end{aligned} \tag{3.4.6}$$

According to Theorem 3.3.1 (see (5.1.1) for the asymptotics of Bessel functions) the L_2–norms of the first two integrals in (3.4.6) are bounded by $C\|f\|_{L_2(\mathbb{R}^3,\mathbb{C}^4)}$. For the last term in (3.4.6) Theorem 3.3.3 gives the bound

$$Cm^{-1}\|\partial^2\chi\|_{L_\infty}\|f\|_{L_2(\mathbb{R}^3,\mathbb{C}^4)}.$$

This completes the proof of Lemma 3.4.1. •

Remark 3.4.2 *Since we only deal with a finite number of particles with positive masses, we will not trace the m-dependence of the constant in* (3.4.1) *any longer.*

3.4.2 Multiparticle Commutator Estimate

Lemma 3.4.3 *For any $d, k \in \mathbb{N}$ there exists $C > 0$ such that for any bounded differentiable function χ on $\mathbb{R}^d$ with bounded gradient and $u \in H^{1/2}(\mathbb{R}^d, \mathbb{C}^k)$*

$$\|\chi u\|_{H^{1/2}(\mathbb{R}^d,\mathbb{C}^k)} \leqslant C\big(\|\chi\|_{L_\infty(\mathbb{R}^d)} + \|\nabla\chi\|_{L_\infty(\mathbb{R}^d)}\big)\|u\|_{H^{1/2}(\mathbb{R}^d,\mathbb{C}^k)}. \tag{3.4.7}$$

Proof of Lemma 3.4.3. We can choose the norm in $H^{1/2}(\mathbb{R}^d, \mathbb{C}^k)$ as (see [1], Theorem 7.48)

$$\|u\|^2_{H^{1/2}(\mathbb{R}^d,\mathbb{C}^k)} := \|u\|^2_{L_2(\mathbb{R}^d,\mathbb{C}^k)} + \iint \frac{\big|u(\mathbf{x}) - u(\mathbf{y})\big|^2}{|\mathbf{x}-\mathbf{y}|^{d+1}} d\mathbf{x} d\mathbf{y}.$$

Then

$$\begin{aligned} \|\chi u\|^2_{H^{1/2}(\mathbb{R}^d,\mathbb{C}^k)} &= \|\chi u\|^2_{L_2(\mathbb{R}^d,\mathbb{C}^k)} + \iint \frac{\big|\chi(\mathbf{x})u(\mathbf{x}) - \chi(\mathbf{y})u(\mathbf{y})\big|^2}{|\mathbf{x}-\mathbf{y}|^{d+1}} d\mathbf{x} d\mathbf{y} \\ &\leqslant \|\chi\|^2_{L_\infty}\|u\|^2_{L_2} \\ &+ \iint \left(\frac{\big|\chi(\mathbf{x})\big|^2\big|u(\mathbf{x}) - u(\mathbf{y})\big|^2}{|\mathbf{x}-\mathbf{y}|^{d+1}} + \frac{\big|\chi(\mathbf{x}) - \chi(\mathbf{y})\big|^2\big|u(\mathbf{y})\big|^2}{|\mathbf{x}-\mathbf{y}|^{d+1}}\right) d\mathbf{x} d\mathbf{y} \\ &\leqslant \|\chi\|^2_{L_\infty}\|u\|^2_{H^{1/2}} + \sup_{\mathbf{y}\in\mathbb{R}^d} \int \frac{\big|\chi(\mathbf{x}) - \chi(\mathbf{y})\big|^2}{|\mathbf{x}-\mathbf{y}|^{d+1}} d\mathbf{x}\|u\|^2_{L_2}. \end{aligned} \tag{3.4.8}$$

The supremum on the r. h. s. of (3.4.8) can be estimated as

$$\begin{aligned} \sup_{\mathbf{y}\in\mathbb{R}^d} \int \frac{\big|\chi(\mathbf{x}) - \chi(\mathbf{y})\big|^2}{|\mathbf{x}-\mathbf{y}|^{d+1}} d\mathbf{x} &\leqslant \sup_{\mathbf{y}\in\mathbb{R}^d} \int_{|\mathbf{x}-\mathbf{y}|\leqslant 1} \frac{\big|\chi(\mathbf{x}) - \chi(\mathbf{y})\big|^2}{|\mathbf{x}-\mathbf{y}|^{d+1}} d\mathbf{x} \\ &+ \sup_{\mathbf{y}\in\mathbb{R}^d} \int_{|\mathbf{x}-\mathbf{y}|>1} \frac{\big|\chi(\mathbf{x}) - \chi(\mathbf{y})\big|^2}{|\mathbf{x}-\mathbf{y}|^{d+1}} d\mathbf{x} \leqslant |\mathbb{S}^{d-1}|\big(\|\nabla\chi\|^2_{L_\infty} + 4\|\chi\|^2_{L_\infty}\big), \end{aligned} \tag{3.4.9}$$

where $|\mathbb{S}^{d-1}|$ is the area of $(d-1)$–dimensional unit sphere. Substituting (3.4.9) into (3.4.8) we obtain (3.4.7). •

Lemma 3.4.4 *For any bounded twice differentiable function χ on $\mathbb{R}^{3N}$ with bounded derivatives the operator $[\chi, \Lambda^N]$ is bounded in $H^{1/2}(\mathbb{R}^{3N}, \mathbb{C}^{4^N})$, and for any $\psi \in H^{1/2}(\mathbb{R}^{3N}, \mathbb{C}^{4^N})$ we have*

$$\big\|[\chi, \Lambda^N]\psi\big\|_{H^{1/2}} \leqslant C\big(\|\nabla\chi\|_{L_\infty} + \|\partial^2\chi\|_{L_\infty}\big)\big(\|\chi\|_{L_\infty} + \|\nabla\chi\|_{L_\infty}\big)\|\psi\|_{H^{1/2}} \tag{3.4.10}$$

with C depending only on N and the masses of the particles.

Proof. Successively commuting χ with Λ_n, $n = 1, \dots, N$ (see (1.1.3)) we obtain

$$[\chi, \Lambda^N] = \sum_{n=1}^{N} \prod_{k=1}^{n-1} \Lambda_k [\chi, \Lambda_n] \prod_{l=n+1}^{N} \Lambda_l, \tag{3.4.11}$$

where the empty products should be replaced by identity operators. By (1.1.1) the operators Λ_n are bounded in $H^{1/2}$ for any $n = 1, \dots, N$. This, together with (3.4.11) and Lemmata 3.4.1 and 3.4.3, implies (3.4.10). •

3.5 Lower Bound of the Essential Spectrum

In this section we prove that

$$\inf \sigma_{\text{ess}}(\mathcal{H}_N^{D,E}) \geqslant \varkappa(D, E). \tag{3.5.1}$$

3.5.1 Partition of Unity

Lemma 3.5.1 *There exists a set of nonnegative functions $\{\chi_Z\}$ indexed by possible 2–cluster decompositions $Z = (Z_1, Z_2)$ satisfying*

1. $\chi_Z \in C^\infty(\mathbb{R}^{3N})$ *for all* Z;
2. $\chi_Z(\kappa \mathbf{X}) = \chi_Z(\mathbf{X})$ *for all* $|\mathbf{X}| = 1,\ \kappa > 1,\ Z_2 \neq \varnothing$;
3. $\sum_Z \chi_Z^2(\mathbf{X}) = 1,$ *for all* $\mathbf{X} \in \mathbb{R}^{3N}$; (3.5.2)
4. *There exists $C > 0$ such that for any $\mathbf{X} \in \operatorname{supp} \chi_Z$* $\min\{|\mathbf{x}_j - \mathbf{x}_n| : \mathbf{x}_j \in Z_1,\ \mathbf{x}_n \in Z_2;\ |\mathbf{x}_n| : \mathbf{x}_n \in Z_2\} \geqslant C|\mathbf{X}|$; (3.5.3)
5. $\chi_Z(\gamma \mathbf{x}_1, \dots, \gamma \mathbf{x}_N) = \chi_Z(\mathbf{x}_1, \dots, \mathbf{x}_N)$ *for any orthogonal transformation γ*;
6. χ_Z *is invariant under permutations of variables preserving $Z_{1,2}$.*

Proof of Lemma 3.5.1. The proof is essentially based on the modification of the argument given in [23], Lemma 2.4.

1. We first prove that for any $\mathbf{X} = (\mathbf{x}_1, \dots, \mathbf{x}_N) \in \mathbb{R}^{3N}$ with $|\mathbf{X}| = 1$ there exists a 2–cluster decomposition $Z = (Z_1, Z_2)$ such that

$$\min\{|\mathbf{x}_j - \mathbf{x}_n| : \mathbf{x}_j \in Z_1,\ \mathbf{x}_n \in Z_2;\ |\mathbf{x}_n| : \mathbf{x}_n \in Z_2\} > N^{-3/2}. \tag{3.5.4}$$

Indeed, let k be such that $|\mathbf{x}_k| \geqslant |\mathbf{x}_j|$ for all $j = 1, \dots, N$. Then, since $|\mathbf{X}| = 1$,

$$|\mathbf{x}_k| \geqslant N^{-\frac{1}{2}}. \tag{3.5.5}$$

Choose Cartesian coordinates in $\mathbb{R}^3$ with the first axis passing through the origin and $\mathbf{x}_k$, so that $\mathbf{x}_k = \big(|\mathbf{x}_k|, 0, 0\big)$. Consider N regions

$$R_1 := \big\{\mathbf{x} \in \mathbb{R}^3 : x^1 \leqslant |\mathbf{x}_k|/N\big\},$$
$$R_l := \Big\{\mathbf{x} \in \mathbb{R}^3 : x^1 \in \big((l-1)|\mathbf{x}_k|/N,\ l|\mathbf{x}_k|/N\big]\Big\}, \quad l = 2, \dots, N.$$

At least one of these regions does not contain $\mathbf{x}_j$ with $j \neq k$. Let l_0 be the maximal index of such regions. Let Z_2 be the set of indices n such that $\mathbf{x}_n \in \bigcup_{l > l_0} R_l$. Z_2 is nonempty since $\mathbf{x}_k \in Z_2$. Setting $Z_1 := I \setminus Z_2$ we observe that

$$\min\big\{|\mathbf{x}_j - \mathbf{x}_n| : \mathbf{x}_j \in Z_1,\ \mathbf{x}_n \in Z_2;\ |\mathbf{x}_n| : \mathbf{x}_n \in Z_2\big\} > |\mathbf{x}_k|/N,$$

which together with (3.5.5) implies (3.5.4).

2. Choose $\eta \in C^\infty\big(\mathbb{R}_+, [0,1]\big)$ so that

$$\eta(t) \equiv \begin{cases} 0, & t \in [0,1], \\ 1, & t \in [2, \infty). \end{cases}$$

Let

$$\zeta_Z(\mathbf{X}) := \begin{cases} \eta\big(2|\mathbf{X}|\big) \displaystyle\prod_{n \in Z_2} \eta\bigg(\frac{2|\mathbf{x}_n|}{|\mathbf{X}|N^{-3/2}}\bigg) \prod_{j \in Z_1} \eta\bigg(\frac{2|\mathbf{x}_j - \mathbf{x}_n|}{|\mathbf{X}|N^{-3/2}}\bigg), & Z_2 \neq \varnothing, \\ 1 - \eta\big(2|\mathbf{X}|\big), & Z_2 = \varnothing. \end{cases} \tag{3.5.6}$$

Functions (3.5.6) satisfy conditions 1, 2, 4 (with $C = N^{-3/2}/2$), 5, and 6 of Lemma 3.5.1. Moreover, by the first part of the proof

$$\sum_Z \zeta_Z(\mathbf{X}) \geqslant 1, \quad \text{for all} \quad \mathbf{X} \in \mathbb{R}^{3N}.$$

Hence all the conditions are satisfied by the functions

$$\chi_Z := \zeta_Z^{1/2}\Big(\sum_Z \zeta_Z\Big)^{-1/2}.$$

•

Let

$$\chi_Z^R(\mathbf{X}) := \chi_Z(\mathbf{X}/R), \tag{3.5.7}$$

where the functions χ_Z are defined in Lemma 3.5.1. The derivatives of χ_Z^R decay as R tends to infinity:

$$\|\nabla\chi_Z^R\|_\infty \leqslant CR^{-1}, \quad \|\partial^2\chi_Z^R\|_\infty \leqslant CR^{-2}. \tag{3.5.8}$$

To simplify the notation we omit the superscript R further on.

3.5.2 Cluster Decomposition and Lower Bound

We now estimate from below the quadratic form of $\mathcal{H}_N^{D,E}$ on a function ψ from $\mathfrak{H}_N^{D,E} \cap \Lambda^N \bigotimes_{n=1}^N H^{1/2}(\mathbb{R}^3, \mathbb{C}^4)$, which is the form domain of $\mathcal{H}_N^{D,E}$.

$$\begin{aligned}\langle \mathcal{H}_N^{D,E}\psi, \psi\rangle &= \langle \Big(\sum_{n=1}^N (D_n + V_n) + \sum_{n<j}^N U_{nj} \Big) \sum_Z \chi_Z^2 \psi, \psi\rangle \\ &= \sum_Z \langle \Big(\sum_{n=1}^N (D_n + V_n) + \sum_{n<j}^N U_{nj} \Big) \chi_Z\psi, \chi_Z\psi\rangle.\end{aligned}$$

Here we have used (3.5.2) and the relation

$$\sum_Z \langle f, \sum_{n=1}^N \nabla_n(\chi_Z^2 g)\rangle = \sum_Z \langle \chi_Z f, \sum_{n=1}^N \nabla_n(\chi_Z g)\rangle + \sum_Z \langle f, \sum_{n=1}^N \nabla_n\Big(\frac{\chi_Z^2}{2}\Big) g\rangle \tag{3.5.9}$$

which holds for any $f, g \in \bigotimes_{n=1}^N H^{1/2}(\mathbb{R}^3, \mathbb{C}^4)$. The last term on the r. h. s. of (3.5.9) is equal to zero due to (3.5.2). Thus

$$\begin{aligned}\langle \mathcal{H}_N^{D,E}\psi, \psi\rangle = \sum_{Z=(Z_1,Z_2)} \Big(&\langle (\mathcal{H}_{Z,1} + \mathcal{H}_{Z,2})\Lambda^N \chi_Z\psi, \Lambda^N\chi_Z\psi\rangle \\ &+ \langle (\mathcal{H}_{Z,1} + \mathcal{H}_{Z,2})[\chi_Z, \Lambda^N]\psi, \Lambda^N\chi_Z\psi\rangle \\ &+ \langle (\mathcal{H}_{Z,1} + \mathcal{H}_{Z,2})\chi_Z\psi, [\chi_Z, \Lambda^N]\psi\rangle \\ &+ \langle \sum_{n\in Z_2} V_n\chi_Z^2\psi, \psi\rangle + \langle \sum_{\substack{n<j \\ n\# j}} U_{nj}\chi_Z^2\psi, \psi\rangle \Big).\end{aligned} \tag{3.5.10}$$

By (2.1.9), (2.1.10), (3.5.3), (3.5.7), and (2.1.11) the terms at the last line of (3.5.10) can be estimated as

$$\langle \sum_{n\in Z_2} V_n\chi_Z^2\psi, \psi\rangle + \langle \sum_{\substack{n<j \\ n\# j}} U_{nj}\chi_Z^2\psi, \psi\rangle \geqslant -\varepsilon_1(R)\big(\langle \mathcal{H}_N^{D,E}\psi, \psi\rangle + \|\psi\|^2\big) \tag{3.5.11}$$

with $\varepsilon_1(R) \to 0$ as $R \to \infty$. The terms at the second and third lines of (3.5.10) can also be estimated as

$$\begin{aligned}&\langle(\mathcal{H}_{Z,1}+\mathcal{H}_{Z,2})[\chi_Z,\Lambda^N]\psi,\Lambda^N\chi_Z\psi\rangle+\langle(\mathcal{H}_{Z,1}+\mathcal{H}_{Z,2})\chi_Z\psi,[\chi_Z,\Lambda^N]\psi\rangle\\&\geqslant -\varepsilon_2(R)\big(\langle\mathcal{H}_N^{D,E}\psi,\psi\rangle+\|\psi\|^2\big),\quad \varepsilon_2(R)\underset{R\to\infty}{\longrightarrow}0,\end{aligned}$$

according to (2.1.5), (3.4.7), (3.4.10), (3.5.8), and (2.1.11). For $Z_2 \neq \varnothing$ we estimate the terms at the first line of (3.5.10) in the following way (recall the definitions (3.1.1)—(3.1.3)):

$$\begin{aligned}&\langle(\mathcal{H}_{Z,1}+\mathcal{H}_{Z,2})\Lambda^N\chi_Z\psi,\Lambda^N\chi_Z\psi\rangle\\&=\sum_{(D_1,E_1;D_2,E_2)\underset{Z}{\prec}(D,E)}\langle(\mathcal{H}_{Z,1}P^{D_1}P^{E_1}+\mathcal{H}_{Z,2}P^{D_2}P^{E_2})\Lambda^N\chi_Z\psi,\Lambda^N\chi_Z\psi\rangle\\&\geqslant\sum_{(D_1,E_1;D_2,E_2)\underset{Z}{\prec}(D,E)}\langle\big(\varkappa_1(Z,D_1,E_1)P^{D_1}P^{E_1}\\&+\varkappa_2(Z,D_2,E_2)P^{D_2}P^{E_2}\big)\Lambda^N\chi_Z\psi,\Lambda^N\chi_Z\psi\rangle\\&\geqslant\varkappa(D,E)\langle\Lambda^N\chi_Z\psi,\Lambda^N\chi_Z\psi\rangle\\&=\varkappa(D,E)\langle\chi_Z^2\psi,\psi\rangle+\varkappa(D,E)\langle[\Lambda^N,\chi_Z]\psi,\chi_Z\psi\rangle.\end{aligned}\tag{3.5.12}$$

By (3.4.7), (3.4.10), (3.5.8), and (2.1.11) the last term on the r. h. s. of (3.5.12) can be estimated as

$$\varkappa(D,E)\langle[\Lambda^N,\chi_Z]\psi,\chi_Z\psi\rangle\geqslant-\varepsilon_3(R)\big(\langle\mathcal{H}_N^{D,E}\psi,\psi\rangle+\|\psi\|^2\big),\quad\varepsilon_3(R)\underset{R\to\infty}{\longrightarrow}0.\tag{3.5.13}$$

Substituting the estimates (3.5.11) — (3.5.13) into (3.5.10) we obtain

$$\begin{aligned}\langle\mathcal{H}_N^{D,E}\psi,\psi\rangle\geqslant\varkappa(D,E)\langle\sum_{\substack{Z=(Z_1,Z_2)\\Z_2\neq\varnothing}}\chi_Z^2\psi,\psi\rangle+\langle\mathcal{H}_N^{D,E}\Lambda^N\chi_{(I,\varnothing)}\psi,\Lambda^N\chi_{(I,\varnothing)}\psi\rangle\\-\varepsilon_4(R)\big(\langle\mathcal{H}_N^{D,E}\psi,\psi\rangle+\|\psi\|^2\big),\quad\varepsilon_4(R)\underset{R\to\infty}{\longrightarrow}0.\end{aligned}\tag{3.5.14}$$

3.5.3 Estimate Inside of the Compact Region

It remains to estimate from below the quadratic form of $\mathcal{H}_N^{D,E}$ on $\Lambda^N\chi_{(I,\varnothing)}\psi$. Note that according to Lemma 3.5.1 and (3.5.7) $\operatorname{supp}\chi_{(I,\varnothing)}\subset[-R,R]^{3N}$. To simplify the notation let

$$\chi_0:=\chi_{(I,\varnothing)}.$$

Lemma 3.5.2 *For $M > 0$ let*

$$W_M := \big\{\mathbf{p} \in \mathbb{R}^{3N} : |p_i| \leqslant M, i = 1, \ldots, 3N\big\},\ \widetilde{W}_M := \mathbb{R}^{3N} \setminus W_M.$$

There exists a finite set $Q_M \subset L_2(\mathbb{R}^{3N})$ such that for any $f \in L_2(\mathbb{R}^{3N})$ with $\mathrm{supp} f \subset [-R, R]^{3N}$, $f \perp Q_M$ *holds*

$$\|\hat{f}\|_{L_2(\widetilde{W}_M)} \geqslant \frac{1}{2}\|\hat{f}\|_{L_2(\mathbb{R}^{3N})}.$$

The proof of Lemma 3.5.2 is analogous to the proof of Theorem 7 of [29] and is given in Appendix B.

It follows from (2.1.6) that for any $M > 0$

$$\langle \mathcal{H}_N^{D,E} \Lambda^N \chi_0 \psi, \Lambda^N \chi_0 \psi\rangle \geqslant C_1 \langle \sum_{n=1}^{N} D_n I_{\widetilde{W}_M} \Lambda^N \chi_0 \psi, \Lambda^N \chi_0 \psi\rangle - C_2 \|\chi_0 \psi\|^2. \tag{3.5.15}$$

Here $I_{\widetilde{W}_M}$ is the operator of multiplication by the characteristic function of $\widetilde{W}_M$ in momentum space.

We choose

$$M := 8\big(\varkappa(D, E) + C_2\big) C_1^{-1} \tag{3.5.16}$$

and assume henceforth that $f := \chi_0 \psi$ is orthogonal to the set Q_M defined in Lemma 3.5.2. Since in momentum space the operator D_n acts on functions from $\Lambda_n L_2(\mathbb{R}^3, \mathbb{C}^4)$ as multiplication by $\sqrt{|\mathbf{p}|^2 + m_n^2}$, by construction of $\widetilde{W}_M$ we have

$$\langle \sum_{n=1}^{N} D_n I_{\widetilde{W}_M} \Lambda^N \chi_0 \psi, \Lambda^N \chi_0 \psi\rangle \geqslant M \|I_{\widetilde{W}_M} \Lambda^N \chi_0 \psi\|^2. \tag{3.5.17}$$

Inequalities (3.5.15) and (3.5.17) imply

$$\begin{aligned}
&\langle \mathcal{H}_N^{D,E} \Lambda^N \chi_0 \psi, \Lambda^N \chi_0 \psi\rangle \geqslant C_1 M \|I_{\widetilde{W}_M} \Lambda^N \chi_0 \psi\|^2 - C_2 \|\chi_0 \psi\|^2 \\
&\geqslant C_1 M \Big(\|I_{\widetilde{W}_M} \chi_0 \psi\| - \big\|I_{\widetilde{W}_M} [\Lambda^N, \chi_0] \psi\big\|\Big)^2 - C_2 \|\chi_0 \psi\|^2 \\
&\geqslant C_1 M \Big(\frac{1}{2}\|I_{\widetilde{W}_M} \chi_0 \psi\|^2 - \big\|I_{\widetilde{W}_M} [\Lambda^N, \chi_0] \psi\big\|^2\Big) - C_2 \|\chi_0 \psi\|^2 \\
&\geqslant 4\big(\varkappa(D, E) + C_2\big) \|I_{\widetilde{W}_M} \chi_0 \psi\|^2 \\
&- 8\big(\varkappa(D, E) + C_2\big) \big\|[\Lambda^N, \chi_0] \psi\big\|^2 - C_2 \|\chi_0 \psi\|^2.
\end{aligned} \tag{3.5.18}$$

At the last step we have used (3.5.16). The second term on the r. h. s. of (3.5.18) can be estimated analogously to (3.5.13) as

$$-8\big(\varkappa(D,E)+C_2\big)\big\|[\Lambda^N,\chi_0]\psi\big\|^2 \geqslant -\varepsilon_5(R)\big(\langle\mathcal{H}_N^{D,E}\psi,\psi\rangle+\|\psi\|^2\big),\ \varepsilon_5(R) \underset{R\to\infty}{\longrightarrow} 0.$$

For the first term on the r. h. s. of (3.5.18) Lemma 3.5.2 implies

$$4\|I_{\widetilde{W}_M}\chi_0\psi\|^2 \geqslant \|\chi_0\psi\|^2. \tag{3.5.19}$$

As a consequence of (3.5.18) — (3.5.19), we have

$$\langle\mathcal{H}_N^{D,E}\Lambda^N\chi_0\psi,\Lambda^N\chi_0\psi\rangle \geqslant \varkappa(D,E)\|\chi_0\psi\|^2 - \varepsilon_5(R)\big(\langle\mathcal{H}_N^{D,E}\psi,\psi\rangle + \|\psi\|^2\big),$$
$$\varepsilon_5(R) \underset{R\to\infty}{\longrightarrow} 0. \tag{3.5.20}$$

3.5.4 Completion of the Proof

By (3.5.14), (3.5.20), and (3.5.2)

$$\langle\mathcal{H}_N^{D,E}\psi,\psi\rangle \geqslant \varkappa(D,E)\|\psi\|^2 - \varepsilon_6(R)\big(\langle\mathcal{H}_N^{D,E}\psi,\psi\rangle + \|\psi\|^2\big), \quad \varepsilon_6(R) \underset{R\to\infty}{\longrightarrow} 0.$$

for any ψ in the form domain of $\mathcal{H}_N^{D,E}$ orthogonal to the finite set of functions (cardinality of this set depends on R). This implies the discreteness of the spectrum of $\mathcal{H}_N^{D,E}$ below $\varkappa(D,E)$ and thus (3.5.1).

3.6 Spectrum of the Free Cluster

In this section we characterize the spectrum of the cluster 2 which does not interact with the external field.

Proposition 3.6.1 *For any irreducible representations D_2, E_2 of rotation–reflection and permutation groups the spectrum of $\widetilde{\mathcal{H}}_{Z,2}^{D_2,E_2}$ is*

$$\sigma(\widetilde{\mathcal{H}}_{Z,2}^{D_2,E_2}) = \sigma_{\text{ess}}(\widetilde{\mathcal{H}}_{Z,2}^{D_2,E_2}) = \big[\varkappa_2(Z,D_2,E_2),\infty\big),$$

with some $\varkappa_2(Z,D_2,E_2) \in \mathbb{R}$.

Proof. Let us introduce the new coordinates in the configuration space $\mathbb{R}^{3N_2}$, in the same manner as it is done in [19]. Let $M := \sum_{n\in Z_2} m_n$ be the total mass of the particles constituting the cluster. We introduce

$$\mathbf{y}_0 := \frac{1}{M}\sum_{n\in Z_2} m_n\mathbf{x}_n,$$
$$\mathbf{y}_k := \mathbf{x}_{n_{k+1}} - \mathbf{x}_{n_1}, \quad k = 1,\dots,N_2-1. \tag{3.6.1}$$

The Jacobian of this variable change is one. Here $\mathbf{y}_0$ is the coordinate of the center of mass, whereby $\mathbf{y}_k$, $k = 1, \dots, N_2 - 1$ are the internal coordinates of the cluster. Accordingly,

$$\begin{aligned} \mathbf{x}_{n_1} &= \mathbf{y}_0 - \frac{1}{M} \sum_{k=1}^{N_2-1} m_{n_{k+1}} \mathbf{y}_k, \\ \mathbf{x}_{n_{l+1}} &= \mathbf{y}_0 + \mathbf{y}_l - \frac{1}{M} \sum_{k=1}^{N_2-1} m_{n_{k+1}} \mathbf{y}_k, \quad l = 1, \dots, N_2 - 1. \end{aligned} \tag{3.6.2}$$

The momentum operators in the new coordinates are

$$\begin{aligned} \mathbf{p}_{n_1} &:= -i\nabla_{\mathbf{x}_{n_1}} = \frac{m_{n_1}}{M} \mathbf{P} - \sum_{k=1}^{N_2-1} (-i\nabla_{\mathbf{y}_k}), \\ \mathbf{p}_{n_k} &:= -i\nabla_{\mathbf{x}_{n_k}} = \frac{m_{n_k}}{M} \mathbf{P} + (-i\nabla_{\mathbf{y}_{k-1}}), \quad k = 2, \dots, N_2, \end{aligned} \tag{3.6.3}$$

where $\mathbf{P}$ is the total momentum of the cluster:

$$\mathbf{P} := \sum_{n \in Z_2} -i\nabla_{\mathbf{x}_n} = -i\nabla_{\mathbf{y}_0}.$$

Let $\mathcal{F}_0$ be the partial Forurier transform on $\mathfrak{H}_{Z,2}^{D_2,E_2}$ defined by

$$(\mathcal{F}_0 f)(\mathbf{P}, \mathbf{y}_1, \dots, \mathbf{y}_{N_2-1}) := \frac{1}{(2\pi)^{3/2}} \int_{\mathbb{R}^3} f(\mathbf{y}_0, \mathbf{y}_1, \dots, \mathbf{y}_{N_2-1}) e^{-i\mathbf{P}\mathbf{y}_0} d\mathbf{y}_0.$$

By (2.1.3) and (2.1.4) we have

$$\widetilde{\mathcal{H}}_{Z,2}^{D_2,E_2} = \mathcal{F}_0^{-1} \widehat{\Lambda}_{Z,2} \widehat{\mathcal{H}}_{Z,2}^{D_2,E_2} \widehat{\Lambda}_{Z,2} \mathcal{F}_0,$$

where in the new coordinates

$$\widehat{\mathcal{H}}_{Z,2}^{D_2,E_2} := \sum_{n \in Z_2} (\boldsymbol{\alpha}_n \cdot \mathbf{p}_n + \beta_n m_n) + \sum_{k=2}^{N_2-1} U_{n_1 n_k}(\mathbf{y}_k) + \sum_{1<k<l\leqslant N_2-1} U_{n_k n_l}(\mathbf{y}_k - \mathbf{y}_l), \tag{3.6.4}$$

$$\widehat{\Lambda}_{Z,2} := \prod_{n \in Z_2} \widehat{\Lambda}_n, \tag{3.6.5}$$

$$\widehat{\Lambda}_n := \frac{1}{2} + \frac{\boldsymbol{\alpha}_n \cdot \mathbf{p}_n + \beta_n m_n}{2\sqrt{\mathbf{p}_n^2 + m_n^2}},$$

$\mathbf{p}_n$ are given by (3.6.3), and $\mathbf{P}$ should now be interpreted as multiplication by the vector–function. The operators (3.6.4) and (3.6.5) obviously commute with $\mathfrak{P} := |\mathbf{P}|$. The operator $\mathcal{F}_0^{-1}\mathfrak{P}\mathcal{F}_0$ (unlike $\mathcal{F}_0^{-1}\mathbf{P}\mathcal{F}_0$) is well–defined in $\mathfrak{H}_{Z,2}^{D_2,E_2}$, since it commutes with P^{D_2} an P^{E_2} in $\mathfrak{H}_{Z,2}$. This implies that $\widetilde{\mathcal{H}}_{Z,2}^{D_2,E_2}$ commutes with $\mathcal{F}_0^{-1}\mathfrak{P}\mathcal{F}_0$.

Let $\omega := \mathbf{P}/\mathfrak{P} \in S^2$. We decompose the Hilbert space $\mathfrak{H}_{Z,2}^{D_2,E_2}$ into the direct integral

$$\mathfrak{H}_{Z,2}^{D_2,E_2} = \int_0^\infty \oplus \mathfrak{H}_{Z,2}^{D_2,E_2,\mathfrak{P}} \mathfrak{P}^2 d\mathfrak{P}. \tag{3.6.6}$$

The fibre space $\mathfrak{H}_{Z,2}^{D_2,E_2,\mathfrak{P}}$ can be considered as a subspace of $L_2(\mathbb{R}^{3N_2-3} \times S^2, \mathbb{C}^{4^{N_2}})$ with the inner product

$$\langle f, g\rangle_* := \int_{\mathbb{R}^{3(N_2-1)}\times S^2} \langle f, g\rangle_{\mathbb{C}^{4^{N_2}}} d\mathbf{y}_1 \cdots d\mathbf{y}_{N_2-1} d\omega.$$

For $f \in \mathfrak{H}_{Z,2}^{D_2,E_2}$ the corresponding element of $\mathfrak{H}_{Z,2}^{D_2,E_2,\mathfrak{P}}$ is given by

$$f_{\mathfrak{P}} := \mathcal{F}_0 f|_{|\mathbf{P}|=\mathfrak{P}}.$$

We have

$$\|f\|^2 = \int_0^\infty \|f_{\mathfrak{P}}\|_*^2 \mathfrak{P}^2 d\mathfrak{P} \tag{3.6.7}$$

in compliance with (3.6.6). The form domain of $\widetilde{\mathcal{H}}_{Z,2}^{D_2,E_2,\mathfrak{P}}$ is

$$\mathfrak{D}^{\mathfrak{P}} := \Lambda_{Z,2}^{\mathfrak{P}} P^{D_2} P^{E_2} H^{1/2}(\mathbb{R}^{3(N_2-1)} \times S^2, \mathbb{C}^{4^{N_2}}),$$

where $\Lambda_{Z,2}^{\mathfrak{P}}$ is given by (3.6.5) with the only difference that we should replace $\mathbf{P}$ by $\omega\mathfrak{P}$ in (3.6.3). The operators on fibres of the direct integral (3.6.6) are

$$\widetilde{\mathcal{H}}_{Z,2}^{D_2,E_2,\mathfrak{P}} := \Lambda_{Z,2}^{\mathfrak{P}} \mathcal{H}_{Z,2}^{D_2,E_2,\mathfrak{P}} \Lambda_{Z,2}^{\mathfrak{P}},$$

where $\mathcal{H}_{Z,2}^{D_2,E_2,\mathfrak{P}}$ is given by the r. h. s. of (3.6.4) with $\mathbf{P}$ replaced by $\omega\mathfrak{P}$ in (3.6.3). We thus have

$$\widetilde{\mathcal{H}}_{Z,2}^{D_2,E_2} = \int_0^\infty \oplus \widetilde{\mathcal{H}}_{Z,2}^{D_2,E_2,\mathfrak{P}} \mathfrak{P}^2 d\mathfrak{P}. \tag{3.6.8}$$

The spectrum of $\widetilde{\mathcal{H}}_{Z,2}^{D_2,E_2}$ can be represented as

$$\sigma(\widetilde{\mathcal{H}}_{Z,2}^{D_2,E_2}) = \overline{\text{ess} \bigcup_{\mathfrak{P}\in\mathbb{R}_+} \sigma(\widetilde{\mathcal{H}}_{Z,2}^{D_2,E_2,\mathfrak{P}})}, \tag{3.6.9}$$

where the essential union is taken with respect to the Lebesgue measure in $\mathbb{R}_+$. The bottom of the spectrum of $\widetilde{\mathcal{H}}_{Z,2}^{D_2,E_2,\mathfrak{P}}$ is given by

$$\mu(\mathfrak{P}) := \inf_{\psi\in\mathfrak{D}^{\mathfrak{P}}} \frac{\langle \widetilde{\mathcal{H}}_{Z,2}^{D_2,E_2,\mathfrak{P}}\psi, \psi\rangle_*}{\|\psi\|_*^2}. \tag{3.6.10}$$

Lemma 3.6.2 *Function* (3.6.10) *is continuous on* $\mathbb{R}_+$.

Proof of Lemma 3.6.2. Let us fix $\mathfrak{P} \in \mathbb{R}_+$ and $\varepsilon > 0$. We will prove that $\big|\mu(\mathfrak{P}+\mathfrak{p}) - \mu(\mathfrak{P})\big| < \varepsilon$ if $|\mathfrak{p}|$ is small enough. Choose $\psi \in \mathfrak{D}^{\mathfrak{P}}$ such that

$$\left|\frac{\langle \widetilde{\mathcal{H}}_{Z,2}^{D_2,E_2,\mathfrak{P}}\psi, \psi\rangle_*}{\|\psi\|_*^2} - \mu(\mathfrak{P})\right| \leqslant \frac{\varepsilon}{2}. \tag{3.6.11}$$

Let

$$\phi := \Lambda_{Z,2}^{\mathfrak{P}+\mathfrak{p}}\psi \in \mathfrak{D}^{\mathfrak{P}+\mathfrak{p}}.$$

We have

$$\phi - \psi = (\Lambda_{Z,2}^{\mathfrak{P}+\mathfrak{p}} - \Lambda_{Z,2}^{\mathfrak{P}})\psi = \sum_{k=1}^{N_2}\prod_{i<k}\Lambda_{n_i}^{\mathfrak{P}+\mathfrak{p}}(\Lambda_{n_k}^{\mathfrak{P}+\mathfrak{p}} - \Lambda_{n_k}^{\mathfrak{P}})\prod_{j>k}\Lambda_{n_j}^{\mathfrak{P}}\psi. \tag{3.6.12}$$

Let $\mathcal{F}$ be the unitary Fourier transform in $L_2(\mathbb{R}^{3(N_2-1)} \times S^2, \mathbb{C}^{4^{N_2}})$ defined by

$$(\mathcal{F}\xi)(\omega, \mathbf{q}_1, \ldots, \mathbf{q}_{N_2-1})$$
$$:= (2\pi)^{3(1-N_2)/2} \int\limits_{\mathbb{R}^{3(N_2-1)}} \xi(\omega, \mathbf{y}_1, \ldots, \mathbf{y}_{N_2-1}) e^{-i\sum\limits_{k=1}^{N_2-1}\mathbf{q}_k\cdot\mathbf{y}_k} d\mathbf{y}_1 \cdots d\mathbf{y}_{N_2-1}.$$

We can rewrite (3.6.12) as

$$\phi - \psi = \mathcal{F}^{-1}\sum_{k=1}^{N_2}\prod_{i<k}\widehat{\Lambda}_{n_i}^{\mathfrak{P}+\mathfrak{p}}(\widehat{\Lambda}_{n_k}^{\mathfrak{P}+\mathfrak{p}} - \widehat{\Lambda}_{n_k}^{\mathfrak{P}})\prod_{j>k}\widehat{\Lambda}_{n_j}^{\mathfrak{P}}\mathcal{F}\psi, \tag{3.6.13}$$

where $\widehat{\Lambda}_n^{\mathfrak{P}}$, $n \in Z_2$ are the operators of multiplication by the symbols

$$\widehat{\Lambda}_n^{\mathfrak{P}} := \frac{1}{2} + \frac{\boldsymbol{\alpha}_n \cdot \widehat{\mathbf{p}}_n + \beta_n m_n}{2\sqrt{\widehat{\mathbf{p}}_n^2 + m_n^2}}, \tag{3.6.14}$$

$$\begin{aligned} \widehat{\mathbf{p}}_{n_1} &:= \frac{m_{n_1}}{M}\omega\mathfrak{P} - \sum_{k=1}^{N_2-1}\mathbf{q}_k, \\ \widehat{\mathbf{p}}_{n_k} &:= \frac{m_{n_k}}{M}\omega\mathfrak{P} + \mathbf{q}_{k-1}, \quad k = 2, \ldots, N_2. \end{aligned} \tag{3.6.15}$$

The matrix–functions (3.6.14) are uniformly continuous in $\mathfrak{P}$. Thus by (3.6.13)

$$\|\phi - \psi\|_{H^{1/2}(\mathbb{R}^{3(N_2-1)}\times S^2, \mathbb{C}^{4^{N_2}})} \leqslant C\sum_{k=1}^{N_2}\|\widehat{\Lambda}_{n_k}^{\mathfrak{P}+\mathfrak{p}} - \widehat{\Lambda}_{n_k}^{\mathfrak{P}}\|_{L_\infty}\|\psi\|_{H^{1/2}} \underset{|\mathfrak{p}|\to 0}{\longrightarrow} 0. \tag{3.6.16}$$

We write

$$\begin{aligned}\langle \widetilde{\mathcal{H}}_{Z,2}^{D_2,E_2,\mathfrak{P}+\mathfrak{p}}\phi,\phi\rangle_* &= \langle \widetilde{\mathcal{H}}_{Z,2}^{D_2,E_2,\mathfrak{P}}\psi,\psi\rangle_* + \langle \mathcal{H}_{Z,2}^{D_2,E_2,\mathfrak{P}}(\phi-\psi),\psi\rangle_* \\ &+ \langle \mathcal{H}_{Z,2}^{D_2,E_2,\mathfrak{P}}\phi,(\phi-\psi)\rangle_* + \langle (\widetilde{\mathcal{H}}_{Z,2}^{D_2,E_2,\mathfrak{P}+\mathfrak{p}} - \mathcal{H}_{Z,2}^{D_2,E_2,\mathfrak{P}})\phi,\phi\rangle_*.\end{aligned} \tag{3.6.17}$$

The second and third terms on the r. h. s. of (3.6.17) tend to zero as $|\mathfrak{p}| \to 0$ according to (3.6.16) and (2.1.5). The last term also tends to zero for small $|\mathfrak{p}|$, since the symbol of the difference is

$$\mathcal{F}(\widetilde{\mathcal{H}}_{Z,2}^{D_2,E_2,\mathfrak{P}+\mathfrak{p}} - \mathcal{H}_{Z,2}^{D_2,E_2,\mathfrak{P}})\mathcal{F}^{-1} = \sum_{n\in Z_2} \frac{m_n}{M}\boldsymbol{\alpha}_n \cdot \omega\mathfrak{p}.$$

From (3.6.16) and (3.6.17) follows that

$$\left| \frac{\langle \widetilde{\mathcal{H}}_{Z,2}^{D_2,E_2,\mathfrak{P}}\psi,\psi\rangle_*}{\|\psi\|_*^2} - \frac{\langle \widetilde{\mathcal{H}}_{Z,2}^{D_2,E_2,\mathfrak{P}+\mathfrak{p}}\phi,\phi\rangle_*}{\|\phi\|_*^2} \right| \leqslant \frac{\varepsilon}{2}, \tag{3.6.18}$$

if $|\mathfrak{p}|$ is small enough. Hence by (3.6.11) and (3.6.18) for any $\varepsilon > 0$

$$\big|\mu(\mathfrak{P}+\mathfrak{p}) - \mu(\mathfrak{P})\big| < \varepsilon$$

for $|\mathfrak{p}|$ small enough. •

Now we prove that μ is semibounded from below and tends to infinity as $|\mathfrak{P}| \to \infty$. This, together with (3.6.9) and Lemma 3.6.2, implies that the spectrum of $\widetilde{\mathcal{H}}_{Z,2}^{D_2,E_2}$ is purely essential and is concentrated on a semi–axis. Proposition 3.6.1 will be thus proved.

According to (2.1.6) for $j = 2$ and (2.1.7) we have

$$\begin{aligned}\langle \widetilde{\mathcal{H}}_{Z,2}^{D_2,E_2}\psi,\psi\rangle &\geqslant C_1\langle \sum_{n\in Z_2} \sqrt{-\Delta_n + m_n^2}\,\psi,\psi\rangle - C_2\|\psi\|^2, \\ &\text{for any} \quad \psi \in P^D P^E \bigotimes_{n\in Z_2} \Lambda_n H^{1/2}(\mathbb{R}^3,\mathbb{C}^4).\end{aligned} \tag{3.6.19}$$

Since all the operators corresponding to the quadratic forms involved in (3.6.19) commute with $\mathcal{F}_0^{-1}\mathfrak{P}\mathcal{F}_0$, it follows from (3.6.8) that for almost all $\mathfrak{P}$ the inequality

$$\langle \widetilde{\mathcal{H}}_{Z,2}^{D_2,E_2,\mathfrak{P}}\psi,\psi\rangle_* \geqslant C_1\langle \sum_{n\in Z_2} \sqrt{\widehat{\mathbf{p}}_n^2 + m_n^2}\,\mathcal{F}\psi,\mathcal{F}\psi\rangle_* - C_2\|\psi\|_*^2 \tag{3.6.20}$$

holds for every $\psi \in \mathfrak{D}^{\mathfrak{P}}$, where $\widehat{\mathbf{p}}_n$ are defined in (3.6.15). Thus μ is semibounded from below. Since by (3.6.15)

$$\mathfrak{P} = \Big| \sum_{n\in Z_2} \widehat{\mathbf{p}}_n \Big|,$$

there exists $n \in Z_2$ such that

$$|\widehat{\mathbf{p}}_n| \geqslant \frac{\mathfrak{P}}{N_2}$$

and hence

$$\sum_{n \in Z_2} \sqrt{\widehat{\mathbf{p}}_n^2 + m_n^2} \geqslant \frac{\mathfrak{P}}{N_2}.$$

Thus the r. h. s. of (3.6.20) tends to infinity as $\mathfrak{P} \to \infty$. •

3.7 Absence of Gaps

We are now ready to finish the proof of Theorem 3.1.1 by proving that

$$\big[\varkappa(D,E), \infty\big) \subseteq \sigma(\mathcal{H}_N^{D,E}). \tag{3.7.1}$$

Let us first fix a decomposition Z on which the minimum is attained in (3.1.3).

Following the general strategy of [18], we will prove that for any irreducible representations $(D_1, E_1; D_2, E_2) \underset{Z}{\prec} (D, E)$ any

$$\lambda \geqslant \varkappa_1(Z, D_1, E_1) + \varkappa_2(Z, D_2, E_2)$$

belongs to $\sigma(\mathcal{H}_N^{D,E})$. This will imply (3.7.1) according to the definition (3.1.2). Let

$$\lambda_1 := \lambda - \varkappa_1(Z, D_1, E_1) \geqslant \varkappa_2(Z, D_2, E_2). \tag{3.7.2}$$

We will use the notation and results of Section 3.6. The following lemma is a slight modification of Theorem 8.11 of [18] and is proved along the same lines:

Lemma 3.7.1 *Let A be a selfadjoint operator in a Hilbert space $\mathfrak{H}$ and $U(\gamma)$ be a continuous representation of a compact group Γ by unitary operators in $\mathfrak{H}$ such that $U(\gamma)\operatorname{Dom} A \subset \operatorname{Dom} A$ and $U(\gamma)A = AU(\gamma)$ for any $\gamma \in \Gamma$. Then for any irreducible (matrix) representation D of Γ the corresponding subspace $P^D\mathfrak{H}$ reduces A. For every $\lambda \in \sigma(A^D)$ where A^D is the reduced operator and every $\varepsilon > 0$ there exists a D–generating subspace G of* $\operatorname{Dom} A$ *such that*

$$\|Au - \lambda u\| \leqslant \varepsilon \|u\|, \text{ for all } u \in G.$$

Remark 3.7.2 *Recall that a subspace G of $\mathfrak{H}$ is called D–*generating *if the operator $U(\gamma)|G$ is unitary in G for all $\gamma \in \Gamma$ and there exists an orthonormal base in G such that for every $\gamma \in \Gamma$ the operator $U(\gamma)|G$ is represented by the matrix $D(\gamma)$.*

Proof of Lemma 3.7.1. Let r be the dimension of the representation $D : \gamma \mapsto \big(D_{lk}(\gamma)\big)_{l,k=1}^{r}$. Let us introduce in $\mathfrak{H}$ the bounded operators P_{lk} by

$$P_{lk} := r \int_{\Gamma} \overline{D_{lk}(\gamma)} U(\gamma) d\mu(\gamma), \quad l,k = 1,\dots,r,$$

where μ is the invariant probability measure on Γ. It is shown in the proof of Theorem 8.11 of [18] that P_{ll} are orthogonal projections onto mutually orthogonal subspaces of $\mathfrak{H}$ and that

$$P^D = \sum_{l=1}^{r} P_{ll}. \tag{3.7.3}$$

In fact, P_{ll} is the projection on the subspace of function which belong to the l^{th} row of the representation D. Moreover, P_{lk} is a partial isometry between $P_{kk}\mathfrak{H}$ and $P_{ll}\mathfrak{H}$. Since $\lambda \in \sigma(A^D)$, there exists a vector $u_0 \in \operatorname{Dom} A^D$ such that

$$\|A^D u_0 - \lambda u_0\| \leqslant \varepsilon \|u_0\|.$$

It follows from (3.7.3) that there exists $l \in \{1,\dots,r\}$ such that $\|P_{ll}u_0\| \geqslant r^{-1}$. We can thus define $u_l := P_{ll}u_0 / \|P_{ll}u_0\|$ and then $u_k := P_{kl}u_l$ for $k = 1,\dots,r$. The subspace G spanned by $\{u_k\}_{k=1}^{r}$ satisfies the statement of the lemma. •

Let

$$r_j := \dim(D_j \otimes E_j), \quad j = 1,2. \tag{3.7.4}$$

Since $\varkappa_1(Z, D_1, E_1)$ belongs to the spectrum of $\widetilde{\mathcal{H}}_{Z,1}^{D_1,E_1}$ (see definition (3.1.1)), by Lemma 3.7.1 we can choose a sequence of $(D_1 \otimes E_1)$–generating subspaces $\{G_q\}_{q=1}^{\infty}$ of $\operatorname{Dom}(\widetilde{\mathcal{H}}_{Z,1}^{D_1,E_1})$ such that for all $q \in \mathbb{N}$

$$\big\|\widetilde{\mathcal{H}}_{Z,1}^{D_1,E_1}\phi_q - \varkappa_1(Z, D_1, E_1)\phi_q\big\|_{\mathfrak{H}_{Z,1}} \leqslant q^{-1}\|\phi_q\|_{\mathfrak{H}_{Z,1}}, \text{ for all } \phi_q \in G_q. \tag{3.7.5}$$

Analogously, for any $\mathfrak{P} \geqslant 0$ we can find a sequence $\{G_q^{\mathfrak{P}}\}_{q=1}^{\infty}$ of $(D_2 \otimes E_2)$–generating subspaces of $\operatorname{Dom} \widetilde{\mathcal{H}}_{Z,2}^{D_2,E_2,\mathfrak{P}}$ such that

$$\big\|\widetilde{\mathcal{H}}_{Z,2}^{D_2,E_2,\mathfrak{P}}\psi_q^{\mathfrak{P}} - \mu(\mathfrak{P})\psi_q^{\mathfrak{P}}\big\|_* \leqslant q^{-1}\|\psi_q^{\mathfrak{P}}\|_*, \text{ for all } \psi_q^{\mathfrak{P}} \in G_q^{\mathfrak{P}}. \tag{3.7.6}$$

Moreover, we can choose an orthonormal base $\{\psi_{q,l}^{\mathfrak{P}}\}_{l=1}^{r_2}$ in $G_q^{\mathfrak{P}}$ in such a way that for every $q \in \mathbb{N}$ and $l = 1,\dots,r_2$ $\psi_{q,l}$ belongs to the l^{th} row of the representation $(D_2 \otimes E_2)$ and satisfies (3.7.6). By Proposition 3.6.1, Lemma 3.6.2, and (3.7.2) we can choose $\mathfrak{P}_0$ in such a way that

$$\mu(\mathfrak{P}_0) = \lambda_1. \tag{3.7.7}$$

We choose $R_q > q$ so that (2.1.9) and (2.1.10) hold true for all $n, j = 1, \dots, N$, $n < j$ with

$$\varepsilon := q^{-1}(N_1+1)^{-1}N_2^{-1/2}C_1^{1/2}\big(C_2 + |\lambda_1| + 2\big)^{-1/2}, \tag{3.7.8}$$

where $N_{1,2}$ are the numbers of elements in $Z_{1,2}$, and $C_{1,2}$ are the constants in (2.1.6) for $j = 2$, and so that for some orthonormal base $\{\phi_{q,k}\}_{k=1}^{r_1}$ of G_q

$$\Big\|\Big(1 - \prod_{j\in Z_1} I_{\{|\mathbf{x}_j|<R_q\}}\Big)\phi_{q,k}\Big\|_{L_2(\mathbb{R}^{3N_1},\mathbb{C}^{4^{N_1}})} \leqslant \frac{\nu_0}{4d_E^2 r_1 r_2}, \tag{3.7.9}$$

where d_E is the dimension of E, $r_{1,2}$ are defined in (3.7.4), and the constant $\nu_0 > 0$ depending only on E, E_1, E_2 will be specified later in the proof of Lemma 3.7.6.

By Assumption 2.1.4 and Lemma 3.6.2, we can choose a sequence of positive numbers $\{\delta_q\}_{q=1}^{\infty}$ tending to zero in such a way that

$$\big|\mu(\mathfrak{P}) - \lambda_1\big| \leqslant q^{-1} \quad \text{for all} \quad \mathfrak{P} \in [\mathfrak{P}_0, \mathfrak{P}_0 + \delta_q], \tag{3.7.10}$$

$$\frac{1}{2\pi^2}(\mathfrak{P}_0 + \delta_q)^2\delta_q C_{R_q} < q^{-2}, \tag{3.7.11}$$

where C_{R_q} is the constant in (2.1.8), and

$$\frac{1}{2\pi^2}(\mathfrak{P}_0 + \delta_q)^2\delta_q \cdot \frac{4}{3}\pi R_q^3 < \frac{\nu_0^2}{16 d_E^4 r_1^2 r_2^2}. \tag{3.7.12}$$

Let us choose a function $f_q \in L_2(\mathbb{R}_+)$ with $\operatorname{supp} f_q \subset [\mathfrak{P}_0, \mathfrak{P}_0 + \delta_q]$ so that

$$\int_{\mathfrak{P}_0}^{\mathfrak{P}_0+\delta_q} \big|f_q(\mathfrak{P})\big|^2 \mathfrak{P}^2 d\mathfrak{P} = 1. \tag{3.7.13}$$

Let

$$\begin{aligned} &\psi_{q,l}(\mathbf{y}_0, \dots, \mathbf{y}_{N_2-1}) \\ &:= \frac{1}{(2\pi)^{\frac{3}{2}}} \int_{\mathfrak{P}_0}^{\mathfrak{P}_0+\delta_q} \int_{S^2} e^{i\mathfrak{P}\omega\mathbf{y}_0} f_q(\mathfrak{P})\psi_{q,l}^{\mathfrak{P}}(\omega, \mathbf{y}_1, \dots, \mathbf{y}_{N_2-1})\mathfrak{P}^2 d\omega d\mathfrak{P}, \end{aligned} \tag{3.7.14}$$

where $\{\mathbf{y}_0, \dots, \mathbf{y}_{N_2-1}\}$ and $\{\mathbf{x}_n\}_{n\in Z_2}$ are related by (3.6.1) and (3.6.2). It follows from (3.7.13) and the choice of $\psi_{q,l}^{\mathfrak{P}}$ that

$$\|\psi_{q,l}\|_{\mathfrak{H}_{Z,2}} = 1, \quad l = 1, \dots, N_2, \tag{3.7.15}$$

and that $\psi_{q,l}$ belongs to the l^{th} row of $(D_2 \otimes E_2)$. Clearly the linear subspace $\widetilde{G}_q$ spanned by $\{\psi_{q,l}\}_{l=1}^{r_2}$ is a $(D_2 \otimes E_2)$–generating subspace of $\operatorname{Dom} \widetilde{\mathcal{H}}_{Z,2}^{D_2,E_2}$.

Lemma 3.7.3 *For any $n \in Z_2$ and $\psi \in \widetilde{G}_q$ with $\|\psi\| = 1$ the one–particle density*

$$\rho_{\psi,n}(\mathbf{x}_n) := \int_{\mathbb{R}^{3N_2-3}} \big|\psi(\mathbf{x}_{n_1}, \ldots, \mathbf{x}_{n_{N_2}})\big|^2 (d\mathbf{x}_{n_1} \cdots d\mathbf{x}_{n_{N_2}})/d\mathbf{x}_n$$

satisfies

$$\|\rho_{\psi,n}\|_{L_\infty(\mathbb{R}^3)} \leqslant \frac{1}{2\pi^2}(\mathfrak{P}_0 + \delta_q)^2 \delta_q.$$

Proof. By (3.7.14)

$$\begin{aligned}
&\|\rho_{\psi,n}\|_{L_\infty(\mathbb{R}^3)} \leqslant (2\pi)^{-3/2} \|\widehat{\rho}_{\psi,n}\|_{L_1(\mathbb{R}^3)} \\
&= \frac{1}{(2\pi)^6} \int_{\mathbb{R}^3} \bigg| \int_{\mathbb{R}^{3N_2}} \int_{\mathfrak{P}_0}^{\mathfrak{P}_0+\delta_q} \int_{S^2} \int_{\mathfrak{P}_0}^{\mathfrak{P}_0+\delta_q} \int_{S^2} e^{-i\mathbf{p}(\mathbf{y}_0+\mathbf{r}_n)} e^{-i\mathfrak{P}\omega\mathbf{y}_0} \overline{f_q(\mathfrak{P})} \\
&\times \psi_q^{\mathfrak{P}*}(\omega, \mathbf{y}_1, \ldots, \mathbf{y}_{N_2-1}) e^{i\widetilde{\mathfrak{P}}\widetilde{\omega}\mathbf{y}_0} f_q(\widetilde{\mathfrak{P}}) \psi_q^{\widetilde{\mathfrak{P}}}(\widetilde{\omega}, \mathbf{y}_1, \ldots, \mathbf{y}_{N_2-1}) \mathfrak{P}^2 \widetilde{\mathfrak{P}}^2 \\
&\times d\widetilde{\omega}\, d\widetilde{\mathfrak{P}}\, d\omega\, d\mathfrak{P}\, d\mathbf{y}_0\, d\mathbf{y}_1 \cdots d\mathbf{y}_{N_2-1} \bigg| d\mathbf{p},
\end{aligned} \tag{3.7.16}$$

where $\mathbf{r}_n := \mathbf{x}_n - \mathbf{y}_0$, see (3.6.2). Integrating the r. h. s. of (3.7.16) in $\mathbf{y}_0$ we obtain $(2\pi)^3 \delta(\mathbf{p} + \mathfrak{P}\omega - \widetilde{\mathfrak{P}}\widetilde{\omega})$ from all the factors involving $\mathbf{y}_0$. Estimating the absolute value of the integral by the integral of absolute value and taking into account that $\int \delta(\mathbf{p} + \ldots) d\mathbf{p} = 1$ we get

$$\begin{aligned}
&\|\rho_{\psi,n}\|_{L_\infty(\mathbb{R}^3)} \leqslant \frac{1}{(2\pi)^3} \int_{\mathbb{R}^{3N_2-3}} \int_{\mathfrak{P}_0}^{\mathfrak{P}_0+\delta_q} \int_{S^2} \int_{\mathfrak{P}_0}^{\mathfrak{P}_0+\delta_q} \int_{S^2} \big|f_q(\mathfrak{P})\big| \big|f_q(\widetilde{\mathfrak{P}})\big| \\
&\times \big|\psi_q^{\mathfrak{P}}(\omega, \mathbf{y}_1, \ldots, \mathbf{y}_{N_2-1})\big| \big|\psi_q^{\widetilde{\mathfrak{P}}}(\widetilde{\omega}, \mathbf{y}_1, \ldots, \mathbf{y}_{N_2-1})\big| \mathfrak{P}^2 \widetilde{\mathfrak{P}}^2 \\
&\times d\widetilde{\omega}\, d\widetilde{\mathfrak{P}}\, d\omega\, d\mathfrak{P}\, d\mathbf{y}_1 \cdots d\mathbf{y}_{N_2-1} \leqslant \frac{1}{(2\pi)^3} 4\pi (\mathfrak{P}_0 + \delta_q)^2 \delta_q,
\end{aligned} \tag{3.7.17}$$

where at the last step we have used Schwarz inequality and $\|\psi\| = 1$. The formal calculation (3.7.16) — (3.7.17) is justified by the fact that the integral over $\mathbb{R}^{3N_2}$ can be considered as a limit of integrals over expanding finite volumes, since $\psi \in L_2(\mathbb{R}^{3N_2})$. •

Corollary 3.7.4 *For any $W \in L_2(\mathbb{R}^3)$, $n \in Z_2$, and $\psi \in \widetilde{G}_q$ with $\|\psi\| = 1$ we have*

$$\int_{\mathbb{R}^{3N_2}} \big|W(\mathbf{x}_n) \psi(\mathbf{x}_{n_1}, \ldots, \mathbf{x}_{n_{N_2}})\big|^2 d\mathbf{x}_{n_1} \cdots d\mathbf{x}_{n_{N_2}} \leqslant \frac{1}{2\pi^2} (\mathfrak{P}_0 + \delta_q)^2 \delta_q \|W\|^2.$$

Let F_q be the subspace of $\mathfrak{H}_N$ spanned by the functions

$$\varphi_{q,k,l}(\mathbf{x}_1,\dots,\mathbf{x}_N) := \phi_{q,k}(\mathbf{x}_j : j\in Z_1)\otimes\psi_{q,l}(\mathbf{x}_n : n\in Z_2),\qquad k=1,\dots,r_1,\quad l=1,\dots,r_2, \tag{3.7.18}$$

where $\{\phi_{q,k}\}_{k=1}^{r_1}$ and $\{\psi_{q,l}\}_{l=1}^{r_2}$ are orthonormal bases of G_q and $\widetilde{G}_q$, respectively. We obviously have $\|\varphi_{q,k,l}\|_{L_2(\mathbb{R}^{3N},\mathbb{C}^{4^N})}=1$.

Lemma 3.7.5 *For any $q\in\mathbb{N}$ $F_q\subset\operatorname{Dom}\mathcal{H}_N$. For any $\varphi\in F_q$*

$$\big\|(\mathcal{H}_N-\lambda)\varphi\big\|\leqslant 5q^{-1}r_1^{1/2}r_2^{1/2}\|\varphi\|.$$

Proof. It is enough to show that the functions (3.7.18) belong to $\operatorname{Dom}\mathcal{H}_N$ and satisfy

$$\big\|(\mathcal{H}_N-\lambda)\varphi_{q,k,l}\big\|_{L_2(\mathbb{R}^{3N},\mathbb{C}^{4^N})}\leqslant 5q^{-1}. \tag{3.7.19}$$

Indeed, by triangle and Cauchy inequalities for

$$\varphi=\sum_{k=1}^{r_1}\sum_{l=1}^{r_2}c_{kl}\varphi_{q,k,l} \tag{3.7.20}$$

we have

$$\begin{aligned}\big\|(\mathcal{H}_N-\lambda)\varphi\big\| &\leqslant \sum_{k=1}^{r_1}\sum_{l=1}^{r_2}|c_{kl}|\big\|(\mathcal{H}_N-\lambda)\varphi_{q,k,l}\big\|\\ &\leqslant \sup_{k,l}\big\|(\mathcal{H}_N-\lambda)\varphi_{q,k,l}\big\|r_1^{1/2}r_2^{1/2}\|\varphi\|.\end{aligned}$$

The operator domain of $\mathcal{H}_N$ can be characterized as the set of functions ξ from the form domain $\overset{N}{\underset{n=1}{\otimes}}\Lambda_n H^{1/2}(\mathbb{R}^3,\mathbb{C}^4)$ on which the sesquilinear form $\langle\mathcal{H}_N\xi,\cdot\rangle$ is a bounded linear functional in $\mathfrak{H}_N$. Functions (3.7.18) belong to $\overset{N}{\underset{n=1}{\otimes}}\Lambda_n H^{1/2}(\mathbb{R}^3,\mathbb{C}^4)$ by construction. By (1.1.2), (2.1.2), and (2.1.3) we have

$$\mathcal{H}_N=\mathcal{H}_{Z,1}+\mathcal{H}_{Z,2}+\Lambda^N\Bigg(\sum_{n\in Z_2}V_n+\sum_{\substack{n<j\\ n\# j}}U_{nj}\Bigg)\Lambda^N. \tag{3.7.21}$$

The sesquilinear forms $\langle(\mathcal{H}_{Z,1}+\mathcal{H}_{Z,2})\varphi_{q,k,l},\cdot\rangle$ are bounded linear functionals over $L_2(\mathbb{R}^{3N},\mathbb{C}^{4^N})$, since $\phi_{q,k}\in\operatorname{Dom}(\widetilde{\mathcal{H}}_{Z,1}^{D_1,E_1})$ and $\psi_{q,l}\in\operatorname{Dom}\widetilde{H}_{Z,2}^{D_2,E_2}$. Moreover, by (3.7.5)

$$\Big\|\big(\mathcal{H}_{Z,1}-\varkappa_1(Z,D_1,E_1)\big)\varphi_{q,k,l}\Big\|=\Big\|\big(\widetilde{\mathcal{H}}_{Z,1}^{D_1,E_1}-\varkappa_1(Z,D_1,E_1)\big)\phi_{q,k}\Big\|\leqslant q^{-1},$$

and by (3.7.6), (3.7.7), (3.7.10), (3.7.14), and (3.7.15)

$$\big\|(\mathcal{H}_{Z,2}-\lambda_1)\varphi_{q,k,l}\big\| = \big\|(\widetilde{\mathcal{H}}_{Z,2}^{D_2,E_2}-\lambda_1)\psi_{q,l}\big\| \leqslant 2q^{-1}. \tag{3.7.22}$$

In view of (3.7.21)—(3.7.22) and (3.7.2), to prove that $\varphi_{q,k,l} \in \operatorname{Dom}\mathcal{H}_N$ and that (3.7.19) holds true it is enough to obtain that

$$\Bigg\|\Bigg(\sum_{n\in Z_2} V_n + \sum_{\substack{n<j\\ n\#j}} U_{nj}\Bigg)\varphi_{q,k,l}\Bigg\| \leqslant 2q^{-1}. \tag{3.7.23}$$

To do this, we first note that by (2.1.9), (2.1.10), and Cauchy inequality

$$\begin{aligned}&\Bigg\|\Bigg(\sum_{n\in Z_2} V_n I_{\{|\mathbf{x}_n|>R_q\}} + \sum_{\substack{n<j\\ n\#j}} U_{nj} I_{\{|\mathbf{x}_n-\mathbf{x}_j|>R_q\}}\Bigg)\varphi_{q,k,l}\Bigg\| \\ &\leqslant \varepsilon(N_1+1)\sum_{n\in Z_2}\big\||D_n|^{\frac12}\psi_{q,l}\big\| \leqslant \varepsilon(N_1+1)N_2^{\frac12}\Bigg(\sum_{n\in Z_2}\big\||D_n|^{\frac12}\psi_{q,l}\big\|^2\Bigg)^{\frac12}.\end{aligned} \tag{3.7.24}$$

By (2.1.6), (3.7.15), and (3.7.22),

$$\begin{aligned}\sum_{n\in Z_2}\|D_n^{1/2}\psi_{q,l}\|^2 &\leqslant C_1^{-1}\Big(\big\|(\widetilde{\mathcal{H}}_{Z,2}^{D_2,E_2}-\lambda_1)\psi_{q,l}\big\| + C_2 + |\lambda_1|\Big) \\ &\leqslant C_1^{-1}\big(C_2+|\lambda_1|+2q^{-1}\big).\end{aligned} \tag{3.7.25}$$

Thus by (3.7.24), (3.7.25) and (3.7.8) for $q \geqslant 1$ we obtain

$$\Bigg\|\Bigg(\sum_{n\in Z_2} V_n I_{\{|\mathbf{x}_n|>R_q\}} + \sum_{\substack{n<j\\ n\#j}} U_{nj} I_{\{|\mathbf{x}_n-\mathbf{x}_j|>R_q\}}\Bigg)\varphi_{q,k,l}\Bigg\| \leqslant q^{-1}. \tag{3.7.26}$$

Now the scalar functions

$$V_{n,q}(\mathbf{x}) := \big|V_n(\mathbf{x})\big| I_{\{|\mathbf{x}|\leqslant R_q\}}(\mathbf{x}) \quad \text{and} \quad U_{nj,q}(\mathbf{x}) := \big|U_{nj}(\mathbf{x})\big| I_{\{|\mathbf{x}|\leqslant R_q\}}(\mathbf{x}) \tag{3.7.27}$$

are square integrable by (2.1.8). By Corollary 3.7.4, for $n \in Z_2$

$$\|V_{n,q}\varphi_{q,k,l}\|^2 = \|V_{n,q}\psi_{q,l}\|^2 \leqslant \frac{1}{2\pi^2}\delta_q(\mathfrak{P}_0+\delta_q)^2\|V_{n,q}\|^2_{L_2(\mathbb{R}^3)} \tag{3.7.28}$$

and for $n < j$, $n\#j$

$$\|U_{nj,q}\varphi_{q,k,l}\|^2 \leqslant \sup_{\mathbf{z}\in\mathbb{R}^3}\big\|U_{nj,q}(\cdot-\mathbf{z})\psi_{q,l}\big\|^2 \leqslant \frac{1}{2\pi^2}\delta_q(\mathfrak{P}_0+\delta_q)^2\|U_{nj,q}\|^2_{L_2(\mathbb{R}^3)}. \tag{3.7.29}$$

Hence by (3.7.27), (3.7.28), (3.7.29), (2.1.8), and (3.7.11)

$$\left\| \left(\sum_{n \in Z_2} V_n I_{\{|\mathbf{x}_n| \leqslant R_q\}} + \sum_{\substack{n<j \\ n \# j}} U_{nj} I_{\{|\mathbf{x}_n - \mathbf{x}_j| \leqslant R_q\}} \right) \varphi_{q,k,l} \right\| \leqslant q^{-1}. \tag{3.7.30}$$

It remains to add (3.7.26) and (3.7.30) to obtain (3.7.23), finishing the proof of the lemma. •

The subspace F_q spanned by the functions (3.7.18) is $D_1 \otimes E_1 \otimes D_2 \otimes E_2$–generating. Since $(D_1, E_1; D_2, E_2) \underset{Z}{\prec} (D, E)$, F_q contains some nontrivial D–generating subspace. Hence the subspace $K_q := P^D F_q$ is not equal to $\{0\}$ and is contained in F_q.

Lemma 3.7.6 *There exists a constant $C_E > 0$ such that for every $q \in \mathbb{N}$*

$$\|P^E \varphi\| \geqslant C_E \|\varphi\|, \quad \textit{for all} \quad \varphi \in F_q. \tag{3.7.31}$$

Proof. Projector (2.1.12) can be written as

$$P^E = \frac{d_E}{h_\Pi} \sum_{\pi \in \Pi_1^Z \times \Pi_2^Z} \overline{\xi_E(\pi)} \pi + \frac{d_E}{h_\Pi} \sum_{\pi \in \Pi \setminus (\Pi_1^Z \times \Pi_2^Z)} \overline{\xi_E(\pi)} \pi. \tag{3.7.32}$$

We will denote the first term in (3.7.32) by Q^E, and the second by R^E. Then

$$\|P^E \varphi\|^2 = \langle \varphi, P^E \varphi \rangle = \langle \varphi, Q^E \varphi \rangle + \langle \varphi, R^E \varphi \rangle. \tag{3.7.33}$$

Relation $(D_1, E_1; D_2, E_2) \underset{Z}{\prec} (D, E)$ implies that the representation $E|\Pi_1^Z \times \Pi_2^Z$ is unitarily equivalent to a sum $\overset{k}{\underset{i=0}{\oplus}} n_i E^{(i)}$, where $n_i > 0$ are multiplicities of the irreducible representations $E^{(i)}$ of the group $\Pi_1^Z \times \Pi_2^Z$ with $E^{(0)} = E_1 \otimes E_2$. For the corresponding characters this gives

$$\xi_E(\pi) = \sum_{i=0}^{k} n_i \xi^{(i)}(\pi), \quad \text{for all} \quad \pi \in \Pi_1^Z \times \Pi_2^Z.$$

Hence

$$Q^E = \sum_{i=0}^{k} \nu_i P_i,$$

where $\nu_i > 0$ and P_i is the projector corresponding to the representation $E^{(i)}$. By construction, $P_0 \varphi = \varphi$ for any $\varphi \in F_q$, hence $P_i \varphi = 0$ for $i = 1, \ldots, k$. Thus for any $\varphi \in F_q$

$$\langle \varphi, Q^E \varphi \rangle = \nu_0 \|\varphi\|^2, \quad \nu_0 > 0. \tag{3.7.34}$$

We will now estimate the second term on the r. h. s. of (3.7.33). For any $n \in Z_2$ and any $\psi \in \widetilde{G}_q$ with $\|\psi\| = 1$ by Corollary 3.7.4 and (3.7.12) we have

$$\|I_{\{|\mathbf{x}_j|<R_q\}}\psi\|^2 \leqslant \frac{\nu_0^2}{16d_E^4 r_1^2 r_2^2}. \tag{3.7.35}$$

For any functions (3.7.18) and any $\pi \in \Pi$ inequality (3.7.9) implies that

$$\big|\langle\varphi_{q,k,l}, \pi\varphi_{q,\widetilde{k},\widetilde{l}}\rangle\big| \leqslant \langle \prod_{j\in Z_1} I_{\{|\mathbf{x}_j|<R_q\}}|\varphi_{q,k,l}|, \pi|\varphi_{q,\widetilde{k},\widetilde{l}}|\rangle_{L_2(\mathbb{R}^{3N})} + \frac{\nu_0}{4d_E^2 r_1 r_2}.$$

Now if $\pi \in \Pi \setminus (\Pi_1^Z \times \Pi_2^Z)$, then there exists $j_0 \in Z_1$ such that $\pi j_0 \in Z_2$. Hence by (3.7.35)

$$\langle \prod_{j\in Z_1} I_{\{|\mathbf{x}_j|<R_q\}}|\varphi_{q,k,l}|, \pi|\varphi_{q,\widetilde{k},\widetilde{l}}|\rangle \leqslant \langle|\varphi_{q,k,l}|, I_{\{|\mathbf{x}_{j_0}|<R_q\}}\pi|\varphi_{q,\widetilde{k},\widetilde{l}}|\rangle \leqslant \frac{\nu_0}{4d_E^2 r_1 r_2}.$$

Thus

$$\big|\langle\varphi_{q,k,l}, \pi\varphi_{q,\widetilde{k},\widetilde{l}}\rangle\big| \leqslant \frac{\nu_0}{2d_E^2 r_1 r_2}, \quad \pi \in \Pi \setminus (\Pi_1^Z \times \Pi_2^Z). \tag{3.7.36}$$

Any $\varphi \in F_q$ can be written as (3.7.20). By (3.7.36) and Cauchy inequality for any $\pi \in \Pi \setminus (\Pi_1^Z \times \Pi_2^Z)$

$$\big|\langle\varphi, \pi\varphi\rangle\big| \leqslant \sum_{k,l,\widetilde{k},\widetilde{l}} |c_{kl}||c_{\widetilde{k}\widetilde{l}}|\big|\langle\varphi_{q,k,l}, \pi\varphi_{q,\widetilde{k},\widetilde{l}}\rangle\big| \leqslant \frac{\nu_0}{2d_E^2}\|\varphi\|^2. \tag{3.7.37}$$

Since the number of elements of $\Pi \setminus (\Pi_1^Z \times \Pi_2^Z)$ does not exceed d_Π and for any π $\big|\xi_E(\pi)\big| \leqslant d_E$ as a trace of unitary matrix of dimension d_E, (3.7.37) implies that

$$\big|\langle\varphi, R^E\varphi\rangle\big| \leqslant \nu_0\|\varphi\|^2/2.$$

By (3.7.33) and (3.7.34) we conclude that (3.7.31) holds with $C_E = \sqrt{\nu_0/2}$. •

Lemmata 3.7.5 and 3.7.6 imply that $L_q := P^E K_q$ is a nontrivial subspace of $\operatorname{Dom}\mathcal{H}_N^{D,E}$ and for every $f = P^E\varphi \in L_q$

$$\big\|(\mathcal{H}_N^{D,E}-\lambda)f\big\| \leqslant \big\|(\mathcal{H}_N-\lambda)\varphi\big\| \leqslant 5q^{-1}r_1^{\frac12}r_2^{\frac12}\|\varphi\| \leqslant 5q^{-1}r_1^{\frac12}r_2^{\frac12}C_E^{-1}\|f\|, \quad q \in \mathbb{N}.$$

This implies that $\lambda \in \sigma(\mathcal{H}_N^{D,E})$, and thus finishes the proof of Theorem 3.1.1.

Part 4
Exponential Decay of Eigenfunctions

4.1 Modified Assumptions

In this part we will prove that the eigenvalues of multiparticle Brown–Ravenhall operators decay exponentially if the corresponding eigenvalue is below the essential spectrum, which is characterized in Theorem 3.1.1.

Let $\{\Omega_j\}_{j=1}^N$ be a collection of uniformly C^1-regular domains with bounded boundaries. For $n = 1, \dots, N$ and $\Omega = \bigtimes_{j=1}^{N} \Omega_j$ let us introduce the spaces

$$H_n^s(\Omega, \mathbb{C}^{4^N}) := \big(\bigotimes_{j=1}^{n-1} L_2(\Omega_j, \mathbb{C}^4)\big) \otimes H^s(\Omega_n, \mathbb{C}^4) \otimes \big(\bigotimes_{j=n+1}^{N} L_2(\Omega_j, \mathbb{C}^4)\big). \quad (4.1.1)$$

We make the following assumptions, which are more restrictive than those of Section 2.1:

Assumption 4.1.1 *There exists $C > 0$ such that for any $n = 1, \dots, N$*

$$\big|\langle V_n\varphi, \psi\rangle\big| \leqslant C\|\varphi\|_{H_n^{1/2}}\|\psi\|_{H_n^{1/2}}, \quad \textit{for any} \quad \varphi, \psi \in H_n^{1/2}(\mathbb{R}^{3N}, \mathbb{C}^{4^N}), \quad (4.1.2)$$

and for any $n < j = 1, \dots, N$

$$\big|\langle U_{nj}\varphi, \psi\rangle\big| \leqslant C\|\varphi\|_{H^{1/2}}\|\psi\|_{H^{1/2}}, \quad \textit{for any} \quad \varphi, \psi \in H^{1/2}(\mathbb{R}^{3N}, \mathbb{C}^{4^N}). \quad (4.1.3)$$

For Coulomb interaction potentials (4.1.2) and (4.1.3) follow from Kato's inequality.

Assumption 4.1.2 *The interparticle interaction potentials are nonnegative:*

$$U_{nj} \geqslant 0, \quad \textit{for all} \quad n < j = 1, \dots, N. \quad (4.1.4)$$

This assumption together with Assumption 4.1.7 below restrict our result to the systems of particles with purely repulsive interaction in external field. Important examples of such systems are molecules with fixed positions of nuclei (Born–Oppenheimer approximation).

Assumption 4.1.3 *There exists $C > 0$ such that for any $n = 1, \dots, N$ and any $\psi \in H^1(\mathbb{R}^{3N}, \mathbb{C}^{4^N})$*

$$\|U_{nj}\psi\| \leqslant C \min_{k=n,j} \|\psi\|_{H^1_k}. \tag{4.1.5}$$

It is not surprising to have the minimum on the r. h. s. of (4.1.5), since U_{nj} only depends on the difference $\mathbf{x}_n - \mathbf{x}_j$. Note that (4.1.5) can be applied even if ψ is only known to belong either to $H^1_n(\mathbb{R}^{3N}, \mathbb{C}^{4^N})$ or to $H^1_j(\mathbb{R}^{3N}, \mathbb{C}^{4^N})$. For Coulomb interaction potentials Assumption 4.1.3 follows from Hardy's inequality.

Assumption 4.1.4 *There exist $C_1 > 0$ and $C_2 \in \mathbb{R}$ such that for any Z*

$$\begin{gathered}\langle \widetilde{\mathcal{H}}_{Z,j}\psi, \psi\rangle \geqslant C_1 \langle \sum_{n\in Z_j} D_n\psi, \psi\rangle - C_2\|\psi\|^2, \\ \textit{for any} \quad \psi \in \bigotimes_{n\in Z_j} \Lambda_n H^{1/2}(\mathbb{R}^3, \mathbb{C}^4), \quad j = 1, 2.\end{gathered} \tag{4.1.6}$$

An equivalent formulation of Assumption 4.1.4 is that the operator $\widetilde{\mathcal{H}}_{Z,j}$ is semibounded from below even if we multiply all the interaction potentials by $1 + \varepsilon$ with $\varepsilon > 0$ small enough. This is only slightly more restrictive than the semiboundedness of $\widetilde{\mathcal{H}}_{Z,j}$.

Assumption 4.1.5 *For any $R > 0$ there exists a finite constant $C_R \geqslant 0$ such that*

$$\sum_{n=1}^N \left(\int_{|\mathbf{x}|\leqslant R} \left|V_n(\mathbf{x})\right|^2 d\mathbf{x}\right)^{1/2} + \sum_{n<j}^N \left(\int_{|\mathbf{x}|\leqslant R} \left|U_{nj}(\mathbf{x})\right|^2 d\mathbf{x}\right)^{1/2} \leqslant C_R. \tag{4.1.7}$$

This means that the interaction potentials are locally square integrable.

Assumption 4.1.6 *The external field potentials decay at infinity in the L_∞–norm:*

$$\lim_{R\to\infty} \operatorname*{ess\,sup}_{|\mathbf{x}|>R} \left|V_n(\mathbf{x})\right| = 0, \quad n = 1, \dots, N. \tag{4.1.8}$$

Assumption 4.1.7 *For any $\varepsilon > 0$ there exists $R > 0$ big enough such that for all $n < j = 1, \dots, N$*

$$\|U_{nj} I_{\{|\mathbf{x}_n - \mathbf{x}_j| > R\}}\psi\| \leqslant \varepsilon \min_{k=n,j} \|\psi\|_{H^{1/2}_k}, \quad \textit{for all} \quad \psi \in H^{1/2}(\mathbb{R}^{3N}, \mathbb{C}^{4^N}). \tag{4.1.9}$$

4.2 Exponential Decay

The main result of Part 4 is the following theorem.

Theorem 4.2.1 *For $N \in \mathbb{N}$ let D be some irreducible representation of Γ, and E some irreducible representation of Π, such that $P^D P^E \neq 0$. Suppose that Assumptions 4.1.1— 4.1.7 hold true. Let ϕ be an eigenfunction of $\mathcal{H}_N^{D,E}$ corresponding to an eigenvalue λ below the essential spectrum, i.e.*

$$\mathcal{H}_N^{D,E}\phi = \lambda\phi, \tag{4.2.1}$$

$$\lambda < \varkappa(D,E). \tag{4.2.2}$$

Then there exists $S > 0$ independent of λ and ϕ such that for

$$s := \min\left\{\frac{1}{2\sqrt{N}}, \big(\varkappa(D,E) - \lambda\big)S\right\}$$

$$\int_{\mathbb{R}^{3N}} e^{2s|\mathbf{X}|}\big|\phi(\mathbf{X})\big|^2 d\mathbf{X} < \infty. \tag{4.2.3}$$

Note that as an eigenfunction ϕ belongs to the form domain of $\mathcal{H}_N^{D,E}$, which is $P^D P^E \bigotimes_{n=1}^{N} \Lambda_n H^{1/2}(\mathbb{R}^3, \mathbb{C}^4) \subset H^{1/2}(\mathbb{R}^{3N}, \mathbb{C}^{4^N})$.

4.3 Proof of Theorem 4.2.1

Some constants in the proof can depend on the masses of the particles. Since we only deal with a finite number of particles with positive masses, such dependence will not be indicated explicitly.

Lemma 4.3.1 *Suppose that for some $a > 0$*

$$\int_{\mathbb{R}^{3N}} e^{2a|\mathbf{x}_n|}\big|\phi(\mathbf{X})\big|^2 d\mathbf{X} < \infty, \quad n = 1, \dots, N. \tag{4.3.1}$$

Then (4.2.3) *hold with $s = N^{-1/2}a$.*

Proof of Lemma 4.3.1.

$$e^{2s|\mathbf{X}|} \leqslant e^{2\sqrt{N}s \max\limits_{n=1,\dots,N}|\mathbf{x}_n|} \leqslant \sum_{n=1}^{N} e^{2\sqrt{N}s|\mathbf{x}_n|} = \sum_{n=1}^{N} e^{2a|\mathbf{x}_n|}. \tag{4.3.2}$$

Thus (4.3.1) implies (4.2.3) after summation in n. •

It remains to prove that (4.3.1) holds for some suitable $a > 0$. Without loss of generality we will consider the case $n = 1$.

Let $\rho \in C^2\big([0,\infty),[0,\infty)\big)$ be given by

$$\rho(z) := \begin{cases} z^2 - \dfrac{z^3}{3}, & z \in [0,1), \\[2ex] z - \dfrac{1}{3}, & z \in [1,\infty). \end{cases} \tag{4.3.3}$$

For $\epsilon > 0$ let

$$f(\mathbf{X}) := f(\mathbf{x}_1) := \frac{\rho\big(|\mathbf{x}_1|\big)}{1 + \epsilon\rho\big(|\mathbf{x}_1|\big)}. \tag{4.3.4}$$

Since $\phi \in L_2(\mathbb{R}^{3N}, \mathbb{C}^{4^N})$, for $n = 1$ (4.3.1) is equivalent to

$$\|e^{af}\phi\|_{L_2(\mathbb{R}^{3N},\mathbb{C}^{4^N})} \leqslant C \tag{4.3.5}$$

with C independent of ϵ. Note that for any $\epsilon > 0$ e^{af} is a twice differentiable function with bounded derivatives. Hence multiplication by e^{af} is a bounded operator in the Sobolev spaces $H^s(\mathbb{R}^3, \mathbb{C}^4)$ with $s \in [0,2]$.

Lemma 4.3.2 *For any $a_0 \in [0,1)$ there exists $C(a_0) > 0$ such that for any $a \in [0,a_0]$ and $\psi \in L_2(\mathbb{R}^3, \mathbb{C}^4)$*

$$\big\|[\Lambda_1, e^{af}]\psi\big\|_{H^1(\mathbb{R}^3,\mathbb{C}^4)} \leqslant C(a_0)a\|e^{af}\psi\|, \tag{4.3.6}$$

and

$$\big\|e^{-af}[\Lambda_1, e^{af}]\psi\big\|_{H^1(\mathbb{R}^3,\mathbb{C}^4)} \leqslant C(a_0)a\|\psi\|. \tag{4.3.7}$$

Lemma 4.3.2 is proved in Section 4.4.

Lemma 4.3.3 *For any $a_0 \in [0,1)$ there exists $C(a_0) > 0$ such that for any $a \in [0,a_0]$ and $\psi \in L_2(\mathbb{R}^3, \mathbb{C}^4)$*

$$\|e^{-af}\Lambda_1 e^{af}\psi\| \leqslant C(a_0)\|\psi\|. \tag{4.3.8}$$

Proof of Lemma 4.3.3.

$$e^{-af}\Lambda_1 e^{af} = \Lambda_1 + e^{-af}[\Lambda_1, e^{af}],$$

and (4.3.7) implies the statement of the lemma. •

Lemma 4.3.4 *Let B_R be the ball of radius $R > 0$ in $\mathbb{R}^3$ centred at the origin. For any $a \in [0, 1/2)$ there exist $C(R) > 0$ and $C(a, R) > 0$ such that for any $\psi \in H^{1/2}(\mathbb{R}^3, \mathbb{C}^4)$*

$$\|\Lambda_1 \psi\|_{H^{1/2}(B_R,\mathbb{C}^4)} \leqslant C(R)\|\psi\|_{H^{1/2}(B_{3R},\mathbb{C}^4)} + C(a, R)\|e^{-2af}\psi\|_{L_2(\mathbb{R}^3,\mathbb{C}^4)}. \quad (4.3.9)$$

We prove Lemma 4.3.4 in Section 4.5.

In order to be able to apply Lemma 4.3.4 we will only consider $a \in [0, 1/2)$. We can thus fix $a_0 \in [1/2, 1)$ and no longer trace the dependence of the constants in Lemmata 4.3.2 and 4.3.3 on this parameter.

Let us fix a cluster decomposition

$$Z_0 := \big(\{2, \dots, N\}, \{1\}\big). \quad (4.3.10)$$

Then

$$\Lambda_1 e^{af}\phi = P^D P^E \Lambda_1 e^{af}\phi = \sum_{(D_1,E_1;D_2,1) \underset{Z_0}{\prec} (D,E)} (P^{D_1}P^{E_1} \otimes P^{D_2})\Lambda_1 e^{af}\phi. \quad (4.3.11)$$

Hence by (3.1.1), (3.1.2), and (3.1.3)

$$\begin{aligned} &\langle \Lambda_1 e^{af}\phi, (\widetilde{\mathcal{H}}_{Z_0,1} + \widetilde{\mathcal{H}}_{Z_0,2})\Lambda_1 e^{af}\phi\rangle \\ &\geqslant \langle \Lambda_1 e^{af}\phi, \sum_{(D_1,E_1;D_2) \underset{Z_0}{\prec} (D,E)} \big(\varkappa_1(Z_0, D_1, E_1) \\ &+ \varkappa_2(Z_0, D_2, 1)\big)(P^{D_1}P^{E_1} \otimes P^{D_2})\Lambda_1 e^{af}\phi\rangle \\ &\geqslant \varkappa(D, E)\|\Lambda_1 e^{af}\phi\|^2. \end{aligned} \quad (4.3.12)$$

Let us introduce

$$A_1 := \varkappa(D, E)\langle e^{af}\phi, [e^{af}, \Lambda_1]\phi\rangle, \quad (4.3.13)$$

$$A_2 := \langle \Lambda_1 e^{af}\phi, \Big(\sum_{n=2}^{N}(D_n + V_n) + \sum_{1<n<j}^{N} U_{nj} + D_1\Big)[\Lambda_1, e^{af}]\phi\rangle, \quad (4.3.14)$$

$$A_3 := \langle \Lambda_1 e^{af}\phi, [D_1, e^{af}]\phi\rangle, \quad (4.3.15)$$

$$A_4 := -\langle \Lambda_1 e^{af}\Lambda_1 e^{af}\phi, \Big(V_1 + \sum_{j=2}^{N} U_{1j}\Big)\phi\rangle. \quad (4.3.16)$$

Then by (4.3.12) (recall the definitions (2.1.2), (2.1.3), (2.1.4), and (1.1.2))

$$
\begin{aligned}
&\varkappa(D,E)\|e^{af}\phi\|^2 = \langle \Lambda_1 e^{af}\phi, \varkappa(D,E)\Lambda_1 e^{af}\phi\rangle + A_1 \\
&\leqslant \langle \Lambda_1 e^{af}\phi, (\widetilde{\mathcal{H}}_{Z_0,1} + \widetilde{\mathcal{H}}_{Z_0,2})\Lambda_1 e^{af}\phi\rangle + A_1 \\
&= \langle \Lambda_1 e^{af}\phi, \Big(\sum_{n=2}^{N}(D_n+V_n) + \sum_{1<n<j}^{N} U_{nj} + D_1\Big) e^{af}\phi\rangle + A_1 + A_2 \\
&= \langle \Lambda_1 e^{af}\phi, e^{af}\Big(\sum_{n=2}^{N}(D_n+V_n) + \sum_{1<n<j}^{N} U_{nj} + D_1\Big)\phi\rangle + \sum_{l=1}^{3} A_l \qquad (4.3.17)\\
&= \langle \Lambda_1 e^{af}\phi, e^{af}\mathcal{H}_N^{D,E}\phi\rangle + \sum_{l=1}^{4} A_l = \lambda\|\Lambda_1 e^{af}\phi\|^2 + \sum_{l=1}^{4} A_l \\
&\leqslant \lambda\|e^{af}\phi\|^2 + \sum_{l=1}^{4} A_l.
\end{aligned}
$$

Thus

$$\big(\varkappa(D,E) - \lambda\big)\|e^{af}\phi\|^2 \leqslant \sum_{l=1}^{4} A_l, \qquad (4.3.18)$$

and it remains to estimate $A_1, \ldots, A_4$. This will be done in the next 4 lemmata.

Lemma 4.3.5 *There exist a positive constant C_1 such that*

$$|A_1| \leqslant C_1 a\|e^{af}\phi\|^2. \qquad (4.3.19)$$

Proof. By (4.3.13) and Lemma 4.3.2 we have

$$|A_1| \leqslant \big|\varkappa(D,E)\big|\|e^{af}\phi\|\big\|[e^{af},\Lambda_1]\phi\big\| \leqslant Ca\big|\varkappa(D,E)\big|\|e^{af}\phi\|^2. \qquad (4.3.20)$$

•

Lemma 4.3.6 *There exist a positive constant C_2 such that*

$$|A_2| \leqslant C_2 a\|e^{af}\phi\|^2. \qquad (4.3.21)$$

Proof. Since Λ_1 commutes with $\sum_{n=2}^{N}(D_n+V_n) + \sum_{1<n<j}^{N} U_{nj}$, $\phi = \Lambda_1\phi$, and $\Lambda_1[\Lambda_1, e^{af}]\Lambda_1 = 0$, we have

$$\langle \Lambda_1 e^{af}\phi, \Big(\sum_{n=2}^{N}(D_n+V_n) + \sum_{1<n<j}^{N} U_{nj}\Big)[\Lambda_1, e^{af}]\phi\rangle = 0. \qquad (4.3.22)$$

According to Lemma 4.3.2

$$\big|\langle \Lambda_1 e^{af}\phi, D_1[\Lambda_1, e^{af}]\phi\rangle\big| \leqslant \|\Lambda_1 e^{af}\phi\|\big\||D_1|[\Lambda_1, e^{af}]\phi\big\| \leqslant Ca\|e^{af}\phi\|^2. \quad (4.3.23)$$

By (4.3.14) and (4.3.22) this implies (4.3.21). •

Lemma 4.3.7 *There exist a positive constant C_3 such that*

$$|A_3| \leqslant C_3 a\|e^{af}\phi\|^2. \quad (4.3.24)$$

Proof. We have $[D_1, e^{af}] = [-i\boldsymbol{\alpha}\cdot\nabla, e^{af}] = -i\boldsymbol{\alpha}\cdot(\nabla e^{af}) = -i\boldsymbol{\alpha}\cdot a(\nabla f)e^{af}$. Now (4.3.24) follows from (4.3.15) since $\|\nabla f\|_{L_\infty} = 1$. •

Lemma 4.3.8 *There exist $C_4 > 0$ and $C_0(a) > 0$ such that*

$$A_4 \leqslant C_4 a\|e^{af}\phi\|^2 + C_0(a)\|\phi\|^2_{H^{1/2}}. \quad (4.3.25)$$

We give a proof of Lemma 4.3.8 in Section 4.6.

Substituting the estimates (4.3.19), (4.3.21), (4.3.24), and (4.3.25) into (4.3.18), we conclude that

$$\Big(\varkappa(D,E) - \lambda - a\sum_{l=1}^{4} C_l\Big)\|e^{af}\phi\|^2 \leqslant C_0(a)\|\phi\|^2_{H^{1/2}}. \quad (4.3.26)$$

Now if

$$a < \min\left\{\frac{1}{2}, \Big(\sum_{l=1}^{4} C_l\Big)^{-1}\big(\varkappa(D,E) - \lambda\big)\right\},$$

then the expression in brackets on the l. h. s. of (4.3.26) is positive, and (4.3.26) implies (4.3.5) with a finite C independent of ϵ. Theorem 4.2.1 is proved.

4.4 Proof of Lemma 4.3.2

To prove (4.3.6) it is enough to show that $[\Lambda_1, e^{af}]e^{-af}$ is a bounded operator from $L_2(\mathbb{R}^3, \mathbb{C}^4)$ to $H^1(\mathbb{R}^3, \mathbb{C}^4)$ satisfying

$$\big\|[\Lambda_1, e^{af}]e^{-af}\big\|_{L_2(\mathbb{R}^3,\mathbb{C}^4)\to H^1(\mathbb{R}^3,\mathbb{C}^4)} \leqslant C(a_0)a, \quad a \in [0, 1). \quad (4.4.1)$$

The integral kernel of $[\Lambda_1, e^{af}]e^{-af} = \big[(\Lambda_1 - 1/2), e^{af}\big]e^{-af}$ is given by (see (3.3.9))

$$\big([\Lambda_1, e^{af}]e^{-af}\big)(\mathbf{x}, \mathbf{y}) = \mathcal{K}(\mathbf{x}, \mathbf{y})(1 - e^{a(f(\mathbf{x})-f(\mathbf{y}))}), \quad (4.4.2)$$

and its gradient in $\mathbf{x}$ is

$$\begin{aligned}\big(\nabla[\Lambda_1, e^{af}]e^{-af}\big)(\mathbf{x},\mathbf{y}) = (\nabla_{\mathbf{x}}\mathcal{K})(\mathbf{x},\mathbf{y})(1-e^{a(f(\mathbf{x})-f(\mathbf{y}))})\\ + a\mathcal{K}(\mathbf{x},\mathbf{y})(1-e^{a(f(\mathbf{x})-f(\mathbf{y}))})(\nabla f)(\mathbf{x}) - a\mathcal{K}(\mathbf{x},\mathbf{y})(\nabla f)(\mathbf{x}).\end{aligned} \tag{4.4.3}$$

We rewrite

$$1-e^{a(f(\mathbf{x})-f(\mathbf{y}))} = -a(\nabla f)(\mathbf{y})\cdot(\mathbf{x}-\mathbf{y}) + R_1(\mathbf{x},\mathbf{y}) + R_2(\mathbf{x},\mathbf{y}), \tag{4.4.4}$$

where

$$R_1(\mathbf{x},\mathbf{y}) := 1 + a\big(f(\mathbf{x})-f(\mathbf{y})\big) - e^{a(f(\mathbf{x})-f(\mathbf{y}))}, \tag{4.4.5}$$

and

$$R_2(\mathbf{x},\mathbf{y}) := a\big((\nabla f)(\mathbf{y})\cdot(\mathbf{x}-\mathbf{y}) + f(\mathbf{y}) - f(\mathbf{x})\big). \tag{4.4.6}$$

Since

$$|e^z - 1 - z| \leqslant (e-2)z^2 \quad \text{for} \quad |z| \leqslant 1$$

and

$$\|\nabla f\|_{L_\infty} \leqslant 1 \tag{4.4.7}$$

(uniformly in ϵ) we have

$$\big|R_1(\mathbf{x},\mathbf{y})\big| \leqslant (e-2)a^2\big(f(\mathbf{x})-f(\mathbf{y})\big)^2 \leqslant (e-2)a^2|\mathbf{x}-\mathbf{y}|^2, \text{ for } |\mathbf{x}-\mathbf{y}| \leqslant a^{-\frac{1}{2}}. \tag{4.4.8}$$

On the other hand, since $a < a_0 < 1$, for $|\mathbf{x}-\mathbf{y}| > a^{-\frac{1}{2}}$ the functions

$$\big|\mathcal{K}(\mathbf{x},\mathbf{y})R_1(\mathbf{x},\mathbf{y})\big| \quad \text{and} \quad \big|\nabla_{\mathbf{x}}\mathcal{K}(\mathbf{x},\mathbf{y})R_1(\mathbf{x},\mathbf{y})\big|$$

are integrable in $\mathbf{x}$ or $\mathbf{y}$ with the integrals bounded by $C(a_0)a$, as follows from (3.3.10), (3.3.11), and (4.4.7). Since $f \in C^2(\mathbb{R}^3)$, by the Taylor formula we have

$$f(\mathbf{x}) - f(\mathbf{y}) = (\nabla f)(\mathbf{y})\cdot(\mathbf{x}-\mathbf{y}) + \langle(\mathcal{D}f)\big(\xi\mathbf{x}+(1-\xi)\mathbf{y}\big)(\mathbf{x}-\mathbf{y}), (\mathbf{x}-\mathbf{y})\rangle_{\mathbb{R}^3},$$

where $\mathcal{D}f$ is the Hess matrix (i. e. the matrix of the second partial derivatives of f) and $\xi \in [0,1]$. Hence

$$\big|R_2(\mathbf{x},\mathbf{y})\big| = a\Big|\langle(\mathcal{D}f)\big(\xi\mathbf{x}+(1-\xi)\mathbf{y}\big)(\mathbf{x}-\mathbf{y}), (\mathbf{x}-\mathbf{y})\rangle_{\mathbb{R}^3}\Big| \leqslant a\|\mathcal{D}f\|_{L_\infty}|\mathbf{x}-\mathbf{y}|^2, \tag{4.4.9}$$

where $\|\mathcal{D}f\|_{L_\infty}$ is bounded uniformly in ϵ by (4.3.4) and (4.3.3). Substituting (4.4.4) into (4.4.2) and (4.4.3), and using the estimates (4.4.8) — (4.4.9) we obtain (4.4.1) by Theorems 3.3.1 and 3.3.3.

The proof of (4.3.7) is completely analogous since the integral kernel of

$$e^{-af}[\Lambda_1, e^{af}] = e^{-af}\big[(\Lambda_1 - 1/2), e^{af}\big]$$

is

$$\mathcal{K}(\mathbf{x},\mathbf{y})(e^{a(f(\mathbf{y})-f(\mathbf{x}))} - 1)$$

(compare with (4.4.2)).

4.5 Proof of Lemma 4.3.4

Let $\eta \in C^\infty\big(\mathbb{R}^3, [0,1]\big)$ with

$$\eta(\mathbf{x}) \equiv \begin{cases} 0, & \mathbf{x} \in B_{2R}, \\ 1, & \mathbf{x} \in \mathbb{R}^3 \setminus B_{3R}. \end{cases}$$

Since Λ_1 is a bounded operator in $H^{1/2}(\mathbb{R}^3, \mathbb{C}^4)$, by Lemma 3.4.3 we have

$$\begin{aligned} \|\Lambda_1\psi\|_{H^{1/2}(B_R,\mathbb{C}^4)} &\leqslant \big\|\Lambda_1(1-\eta)\psi\big\|_{H^{1/2}(B_R,\mathbb{C}^4)} + \|\Lambda_1\eta\psi\|_{H^{1/2}(B_R,\mathbb{C}^4)} \\ &\leqslant C(R)\|\psi\|_{H^{1/2}(B_{3R},\mathbb{C}^4)} + \|\Lambda_1\eta\psi\|_{H^1(B_R,\mathbb{C}^4)}. \end{aligned} \tag{4.5.1}$$

By (3.3.10) we can estimate the second term on the r. h. s. of (4.5.1) as

$$\begin{aligned} &\|\Lambda_1\eta\psi\|^2_{H^1(B_R,\mathbb{C}^4)} \\ &= \int\limits_{B_R} \bigg(\Big| \int\limits_{|\mathbf{y}|>2R} K(\mathbf{x},\mathbf{y})\eta(\mathbf{y})\psi(\mathbf{y})d\mathbf{y}\Big|^2 + \Big| \int\limits_{|\mathbf{y}|>2R} \nabla_{\mathbf{x}} K(\mathbf{x},\mathbf{y})\eta(\mathbf{y})\psi(\mathbf{y})d\mathbf{y}\Big|^2 \bigg) d\mathbf{x} \\ &\leqslant \frac{4}{3}\pi R^3 \sup_{\mathbf{x}\in B_R} \bigg(\Big| \int_{|\mathbf{y}|>2R} K(\mathbf{x},\mathbf{y})\eta(\mathbf{y})\psi(\mathbf{y})d\mathbf{y}\Big|^2 \\ &+ \Big| \int_{|\mathbf{y}|>2R} \nabla_{\mathbf{x}} K(\mathbf{x},\mathbf{y})\eta(\mathbf{y})\psi(\mathbf{y})d\mathbf{y}\Big|^2 \bigg) \\ &\leqslant \frac{4}{3}\pi R^3 \bigg(\int_{|\mathbf{y}|>2R} \Big(\sup_{\mathbf{x}\in B_R} \big|K(\mathbf{x},\mathbf{y})\big| + \sup_{\mathbf{x}\in B_R} \big|\nabla_{\mathbf{x}} K(\mathbf{x},\mathbf{y})\big| \Big) \big|\psi(\mathbf{y})\big| d\mathbf{y} \bigg)^2 \\ &\leqslant \frac{4}{3}\pi R^3 \bigg(\int_{|\mathbf{y}|>2R} G\big(|\mathbf{y}|-R\big)\big|\psi(\mathbf{y})\big| d\mathbf{y} \bigg)^2 \\ &\leqslant \frac{4}{3}\pi R^3 \bigg(\int_{|\mathbf{y}|>2R} G^{1-2a}\big(|\mathbf{y}|-R\big) d\mathbf{y} \bigg) \bigg(\int_{|\mathbf{y}|>2R} G^{1+2a}\big(|\mathbf{y}|-R\big)\big|\psi(\mathbf{y})\big|^2 d\mathbf{y} \bigg). \end{aligned}$$

Since $a < 1/2$ and $f(\mathbf{x}) \leqslant |\mathbf{x}|$, we conclude from (3.3.11) that there exists $C(a,R)$ such that

$$\|\Lambda_1\eta\psi\|_{H^1(B_R,\mathbb{C}^4)} \leqslant C(a,R)\|e^{-2af}\psi\|_{L_2(\mathbb{R}^3,\mathbb{C}^4)},$$

and (4.3.9) follows by (4.5.1).

4.6 Proof of Lemma 4.3.8

For $j = 2, \dots, N$ we have

$$\begin{aligned} &\langle \Lambda_1 e^{af}\Lambda_1 e^{af}\phi, U_{1j}\phi\rangle = \langle U_{1j}e^{af}\phi, e^{af}\phi\rangle \\ &+ \langle U_{1j}e^{-af}[\Lambda_1, e^{af}]\Lambda_1 e^{af}\phi, e^{af}\phi\rangle + \langle U_{1j}[\Lambda_1, e^{af}]\phi, e^{af}\phi\rangle. \end{aligned} \tag{4.6.1}$$

The first term on the r. h. s. of (4.6.1) is nonnegative by (4.1.4). Applying (4.1.5), Lemma 4.3.2, and Schwarz inequality we can estimate the last two terms by $Ca\|e^{af}\phi\|^2$. Hence by (4.3.16)

$$A_4 \leqslant Ca\|e^{af}\phi\|^2 + \big|\langle \Lambda_1 e^{af}\Lambda_1 e^{af}\phi, V_1\phi\rangle\big| \tag{4.6.2}$$

and it remains to estimate the last term on the r. h. s. of (4.6.2).

Let $\chi_1 \in C^\infty\big(\mathbb{R}^3, [0,1]\big)$ be a function supported in $\mathbb{R}^3 \setminus B_1$ such that it is equal to 1 on $\mathbb{R}^3 \setminus B_2$. For $R > 1$ and $n = 1, \dots, N$ let

$$\chi_{n,R}(\mathbf{X}) := \chi_{n,R}(\mathbf{x}_n) := \chi_1(\mathbf{x}_n/R). \tag{4.6.3}$$

We have

$$\begin{aligned} \big|\langle \Lambda_1 e^{af}\Lambda_1 e^{af}\phi, V_1\phi\rangle\big| &\leqslant \big|\langle e^{-af}\Lambda_1 e^{af}\Lambda_1 e^{af}\phi, \chi_{1,R}V_1 e^{af}\phi\rangle\big| \\ &+ \big|\langle (1-\chi_{1,R})\Lambda_1 e^{af}\Lambda_1 e^{af}\phi, V_1\phi\rangle\big|. \end{aligned} \tag{4.6.4}$$

By Lemma 4.3.3,

$$\|e^{-af}\Lambda_1 e^{af}\Lambda_1 e^{af}\phi\| \leqslant C\|e^{af}\phi\|. \tag{4.6.5}$$

Since $\chi_{1,R}$ is supported outside B_R, by (4.1.8) we have

$$\|\chi_{1,R}V_1 e^{af}\phi\| \leqslant \varepsilon(R)\|e^{af}\phi\|, \quad \varepsilon(R) \underset{R\to\infty}{\longrightarrow} 0. \tag{4.6.6}$$

According to (4.1.2) there exists $C > 0$ such that

$$\big|\langle (1-\chi_{1,R})\Lambda_1 e^{af}\Lambda_1 e^{af}\phi, V_1\phi\rangle\big| \leqslant C\big\|(1-\chi_{1,R})\Lambda_1 e^{af}\Lambda_1 e^{af}\phi\big\|_{H_1^{1/2}}\|\phi\|_{H_1^{1/2}}. \tag{4.6.7}$$

Since $(1-\chi_{1,R})$ is a smooth function supported in $\big\{|\mathbf{x}_1| \leqslant 2R\big\}$, by Lemmata 3.4.3 and 4.3.4 we have

$$\begin{aligned} &\big\|(1-\chi_{1,R})\Lambda_1 e^{af}\Lambda_1 e^{af}\phi\big\|_{H_1^{1/2}} \leqslant C(R)\|\Lambda_1 e^{af}\Lambda_1 e^{af}\phi\|_{H_1^{1/2}(B_{2R}\times\mathbb{R}^{3N-3},\mathbb{C}^{4^N})} \\ &\leqslant C(R)\|e^{af}\Lambda_1 e^{af}\phi\|_{H_1^{1/2}(B_{6R}\times\mathbb{R}^{3N-3},\mathbb{C}^{4^N})} + C(a,R)\|e^{-af}\Lambda_1 e^{af}\phi\|_{L_2(\mathbb{R}^{3N},\mathbb{C}^{4^N})}. \end{aligned} \tag{4.6.8}$$

By Lemma 4.3.3 the second term on the r. h. s. of (4.6.8) can be estimated by $C(a,R)\|\phi\|$. Applying Lemma 4.3.4 to the first term we obtain

$$\begin{aligned} &C(R)\|e^{af}\Lambda_1 e^{af}\phi\|_{H_1^{1/2}(B_{6R}\times\mathbb{R}^{3N-3},\mathbb{C}^{4^N})} \\ &\leqslant C(a,R)\|\Lambda_1 e^{af}\phi\|_{H_1^{1/2}(B_{6R}\times\mathbb{R}^{3N-3},\mathbb{C}^{4^N})} \\ &\leqslant C(a,R)\|e^{af}\phi\|_{H_1^{1/2}(B_{18R}\times\mathbb{R}^{3N-3},\mathbb{C}^{4^N})} + C(a,R)\|e^{-af}\phi\|_{L_2(\mathbb{R}^{3N},\mathbb{C}^{4^N})} \\ &\leqslant C(a,R)\|\phi\|_{H^{1/2}(\mathbb{R}^{3N},\mathbb{C}^{4^N})}. \end{aligned} \tag{4.6.9}$$

Thus by (4.6.7) — (4.6.9)

$$\left|\langle(1-\chi_{1,R})\Lambda_1 e^{af}\Lambda_1 e^{af}\phi, V_1\phi\rangle\right| \leqslant C(a,R)\|\phi\|^2_{H^{1/2}}. \tag{4.6.10}$$

Estimating the r. h. s. of (4.6.4) according to (4.6.5), (4.6.6), and (4.6.10) and substituting the result into (4.6.2) we obtain

$$A_4 \leqslant Ca\|e^{af}\phi\|^2 + C\varepsilon(R)\|e^{af}\phi\|^2 + C(a,R)\|\phi\|^2_{H^{1/2}}. \tag{4.6.11}$$

Choosing R so that $\varepsilon(R) \leqslant a$ we arrive at (4.3.25). Lemma 4.3.8 is proved.

Part 5
Appendices

A Some Properties of Modified Bessel Functions

The modified Bessel (McDonald) functions are related to the Hankel functions by the formula

$$K_\nu(z) = \frac{\pi}{2} e^{i\pi(\nu+1)/2} H_\nu^{(1)}(iz).$$

These functions are positive and decaying for $z \in (0, \infty)$. Their asymptotics are (see [10] 8.446, 8.447.3, 8.451.6)

$$\begin{aligned} &K_\nu(z) = \sqrt{\frac{\pi}{2z}} e^{-z} \left(1 + O\Big(\frac{1}{z}\Big)\right), \quad z \to +\infty; \\ &K_0(z) = -\log z\big(1 + o(1)\big), \quad K_1(z) = \frac{1}{z}\big(1 + o(1)\big), \quad z \to +0. \end{aligned} \tag{5.1.1}$$

The derivatives of these functions are (see [10] 8.486.12, 8.486.18)

$$K_0'(z) = -K_1(z), \quad K_1'(z) = -K_0(z) - \frac{1}{z} K_1(z), \quad z \in (0, \infty). \tag{5.1.2}$$

B Proof of Lemma 3.5.2

Let $f \in L_2(\mathbb{R}^{3N})$, $\operatorname{supp} f \subset [-R, R]^{3N}$. Then

$$f(\mathbf{x}) = \sum_{\mathbf{k} \in \mathbb{Z}_+^{3N}} c_{\mathbf{k}} \prod_{i=1}^{3N} \varphi_{k_i}(x_i),$$

where

$$\varphi_k(x) = \begin{cases} \dfrac{1}{\sqrt{R}} \sin\left(\pi k \Big(\dfrac{1}{2} + \dfrac{x}{2R}\Big)\right), & x \in [-R, R], \\ 0, & x \notin [-R, R], \end{cases}$$

and $c_{\mathbf{k}}$ are the Fourier coefficients of $f|_{[-R,R]^{3N}}$.

For the Fourier transform of f we have

$$\hat{f}(\mathbf{p}) = \sum_{\mathbf{k} \in \mathbb{Z}_+^{3N}} c_{\mathbf{k}} \prod_{i=1}^{3N} \hat{\varphi}_{k_i}(p_i), \tag{5.2.1}$$

where

$$\hat{\varphi}_k(p) = \frac{2\sqrt{2\pi R} k e^{i\frac{\pi}{2}(k-1)} \sin\left(\frac{\pi k}{2} - pR\right)}{\pi^2 k^2 - 4p^2 R^2}. \tag{5.2.2}$$

Let

$$L := \frac{768RNM}{\pi^3} + 1. \tag{5.2.3}$$

Assume that f is orthogonal to the linear span of L^{3N} functions

$$\left\{ \prod_{i=1}^{3N} \varphi_{k_i}(x_i), \quad k_i \in [0, L-1] \cap \mathbb{Z}, \quad i = 1, \dots 3N \right\}.$$

Then the summation in (5.2.1) can be restricted to

$$\mathbf{k} \in \bigcup_{j=1}^{3N} \gamma_j, \quad \gamma_j := \bigcap_{l=1}^{j-1} \{\mathbf{k} \in \mathbb{Z}_+^{3N} | k_l < L\} \cap \{\mathbf{k} \in \mathbb{Z}_+^{3N} | k_j \geqslant L\}.$$

Obviously $\|\hat{f}\|^2_{L_2(\mathbb{R}^{3N})} = \sum\limits_{\mathbf{k} \in \bigcup\limits_{j=1}^{3N} \gamma_j} |c_{\mathbf{k}}|^2$. On the other hand,

$$\begin{aligned}
\|\hat{f}\|_{L_2(W_M)} &\leqslant \sum_{j=1}^{3N} \Big\| \sum_{\mathbf{k} \in \gamma_j} c_{\mathbf{k}} \prod_{i=1}^{3N} \varphi_{k_i}(p_i) \Big\|_{L_2(\{|p_j| \leqslant M\})} \\
&= \sum_{j=1}^{3N} \left(\sum_{\mathbf{k}, \mathbf{k}' \in \gamma_j} \langle c_{\mathbf{k}}, c_{\mathbf{k}'} \rangle \int_{-M}^{M} \varphi_{k_j}(p_j) \overline{\varphi_{k'_j}(p_j)} dp_j \prod_{\substack{i=1 \\ i \neq j}}^{3N} \int_{\mathbb{R}} \varphi_{k_i}(p_i) \overline{\varphi_{k'_i}(p_i)} dp_i \right)^{1/2} \\
&= \sum_{j=1}^{3N} \left(\sum_{\substack{k_i=1 \\ i<j}}^{L} \sum_{\substack{k_i=1 \\ i>j}}^{\infty} \sum_{k_j, k'_j = L}^{\infty} \langle c_{(k_1, \dots, k_j, \dots, k_{3N})}, c_{(k_1, \dots, k'_j, \dots, k_{3N})} \rangle \int\limits_{-M}^{M} \varphi_{k_j}(p) \overline{\varphi_{k'_j}(p)} dp \right)^{\frac{1}{2}}.
\end{aligned}$$

Since

$$k_j,\, k'_j \geqslant L > \frac{2\sqrt{2} MR}{\pi}, \tag{5.2.4}$$

we can estimate

$$\begin{aligned}
&\Big| \int_{-M}^{M} \varphi_{k_j}(p) \overline{\varphi_{k'_j}(p)} dp \Big| \\
&\leqslant 8\pi R k_j k'_j \int_{-M}^{M} \frac{1}{|\pi^2 k_j^2 - 4p^2 R^2| |\pi^2 k'^2_j - 4p^2 R^2|} dp \\
&\leqslant 8\pi R k_j k'_j \cdot 2M \cdot \frac{2}{\pi^2 k_j^2} \cdot \frac{2}{\pi^2 k'^2_j} = \frac{64RM}{\pi^3 k_j k'_j}.
\end{aligned}$$

Applying Schwarz inequality, we arrive at

$$\begin{aligned}
&\Big| \sum_{k_j, k_j' = L}^{\infty} \langle c_{(k_1,\dots,k_j,\dots,k_{3N})}, c_{(k_1,\dots,k_j',\dots,k_{3N})} \rangle \int_{-M}^{M} \varphi_{k_j}(p) \overline{\varphi_{k_j'}(p)} dp \Big| \\
&\leqslant \frac{64RM}{\pi^3} \sum_{k_j'=L}^{\infty} |c_{(k_1,\dots,k_j',\dots,k_{3N})}|^2 \cdot \sum_{k_j=L}^{\infty} k_j^{-2} \\
&\leqslant \frac{64RM}{\pi^3(L-1)} \sum_{k_j'=L}^{\infty} |c_{(k_1,\dots,k_j',\dots,k_{3N})}|^2 .
\end{aligned}$$

Therefore

$$\begin{aligned}
\|\hat{f}\|_{L_2(W_M)} &\leqslant \sum_{j=1}^{3N} \left(\frac{64RM}{\pi^3(L-1)} \sum_{\mathbf{k} \in \gamma_j} |c_{\mathbf{k}}|^2 \right)^{1/2} \\
&\leqslant \sqrt{\frac{192RNM}{\pi^3(L-1)}} \|\hat{f}\|_{L_2(\mathbb{R}^{3N})} = \frac{1}{2} \|\hat{f}\|_{L_2(\mathbb{R}^{3N})} .
\end{aligned}$$

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