The Classical Limit of Bohmian Mechanics

Semiclassical Wave Packets and an Application to
Many Particle Scattering Theory

Dissertation

vorgelegt von

Sarah Römer

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Zusammenfassung

Bohmsche Mechanik [4, 8, 19, 20, 22, 26] ist eine Quantentheorie über Teilchen in Bewegung (d.h. über Teilchen*bahnen*), die empirisch äquivalent zur orthodoxen Quantenmechanik ist, wenn immer letztere eindeutige Vorhersagen macht [20]. Da auch die Newtonsche Mechanik eine Theorie über Teilchenbahnen ist, lässt sich die Frage nach dem klassischen Limes in der Bohmschen Mechanik somit besonders einfach und klar formulieren: Wann sehen Bohmsche Bahnen wie Newtonsche Bahnen aus? Als ersten Schritt hin zu einer umfassenderen Antwort auf diese Frage zeigen wir im ersten Teil dieser Arbeit, dass die Bohmschen Bahnen, die zu semiklassischen Wellenpaketen (wie sie in [25] von Hagedorn definiert wurden) gehören, in einem angemessenen Skalenlimes zu der klassischen Bahn konvergieren, auf der sich der Ortserwartungswert des Wellenpakets bewegt (Kapitel 2).

Es gibt eine weitere Situation wo wir bereits wissen, dass sich Bohmsche Bahnen klassisch verhalten: Ein Teilchen, das an einem kurzreichweitigen Potential gestreut wird, bewegt sich asymptotisch frei, d.h. seine Geschwindigkeit wird für $t \to \infty$ konstant [34]. Im zweiten Teil dieser Arbeit (Kapitel 3) erweitern wir dieses Resultat auf den Fall von N nicht wechselwirkenden, möglicherweise verschränkten Teilchen (wie z.B. in einem EPR-Experiment). Vor allen Dingen aber benutzten wir diese Erweiterung, um eine der grundlegenden Fragen der Streutheorie zu beantworten: Wie kann man die Wahrscheinlichkeit bestimmen, dass Teilchen in einem gegebenen Raumwinkel detektiert werden?

In orthodoxer Quantenmechanik werden diese Wahrscheinlichkeiten mit Hilfe der S-Matrix-Theorie berechnet, wobei die tiefere Begründung der S-Matrix-Theorie allerdings ein in der Literatur viel diskutiertes Problem ist. Wir besprechen frühere Versuche, die Detektionswahrscheinlichkeiten aus grundlegenden Prinzipien abzuleiten, und begründen, inwiefern sich der Mehrteilchenfall vom Einteilchenfall so stark unterscheidet, dass er neuer Methoden bedarf. Mit Hilfe des asymptotisch klassischen Verhaltens der Bohmschen Bahnen zeigen wir schließlich, dass die Bohmschen Detektionswahrscheinlichkeiten zum üblichen S-Matrix-Ausdruck konvergieren wenn der Abstand zwischen den Detektoren und dem Streuzentrum unendlich groß wird.

Danksagung

Ich danke Herrn Prof. Dr. D. Dürr für inzwischen fast 10 Jahre an exemplarischer Klarheit in seinen Antworten und vor allen Dingen in seinen Fragen. Die Überzeugung, nicht nur an irgendeinem abstrakten „Problem“ sondern an einer klaren physikalischen Fragestellung zu arbeiten, hat mir über manche Durststrecke hinweggeholfen. Und wo das allein nicht genügte, hatte Herr Dürr immer Zeit für ein Gespräch. Ob direkt oder indirekt, ich habe unglaublich viel von ihm gelernt und kann mir keine bessere Betreuung vorstellen.
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Contents

Chapter 1

Introduction

1.1 A very brief overview

This work consists of two parts. In the first we are concerned with the classical limit of Bohmian mechanics per se: We prove a result about the Bohmian trajectories of semiclassical wave packets. In the second we apply a special instance of the classical limit to many particle scattering theory: We derive the detection statistics of N non-interacting, possibly entangled particles from first principles.

The key question of the classical limit is: How does the classical world of everyday's experience as it is described by Newtonian mechanics emerge out of quantum mechanics? Since orthodox quantum mechanics contains no particle trajectories while Newtonian mechanics is solely about particle trajectories, to answer this question one usually needs to either introduce in classical mechanics an observer and a commutative algebra of observables or to restrict the emergence of classical behavior to the time development of phase space densities.

Bohmian mechanics [4, 8, 19, 20, 22, 26], however, is a theory of particles in motion (i.e. a theory of particle *trajectories*) that is experimentally equivalent to quantum mechanics whenever the latter makes unambiguous predictions [20]. Thus, using Bohmian mechanics the question of the classical limit becomes as simple as it could possibly be: Under which circumstances are the trajectories of the particles of a system (close to) Newtonian trajectories? As a first step towards an answer to this question we show that in an appropriate scaling limit the trajectories associated with semiclassical wave packets (as defined by Hagedorn in [25]) tend to the classical trajectory tracked by the mean position of the wave packet (Chapter 2).

There is a second situation where we already know that Bohmian trajectories look like classical ones: Whenever a particle is scattered by a short range potential it becomes free asymptotically in the sense that its Bohmian velocity becomes constant as $t \to \infty$ [34]. In Chapter 3 we extend this result to the case of N non-interacting, possibly entangled particles (like, for example, in an EPR experiment). More importantly, we use this extension to answer one of the fundamental questions of scattering theory: How can one determine the probability that particles are detected in a given solid angle?

In orthodox quantum mechanics this is computed from S-matrix theory. The justification of S-matrix theory from first principles, however, is a recurrent problem in the literature. We discuss earlier attempts to derive the scattering probability from first principles and explain how many particle potential scattering is so different from one particle potential scattering that it calls for new methods. With the help of the asymptotic classicality of the Bohmian trajectories we prove that the Bohmian detection probability converges to the usual S-matrix expression whenever the distance between detectors and scattering potential tends to infinity.

We give a more detailed overview at the beginning of Chapter 2 and Chapter 3 each.

1.2 Bohmian mechanics

In Bohmian mechanics [4, 8, 19, 20, 22, 26] the state of N spinless, non-relativistic particles is described by their (normalized) quantum mechanical wave function $\psi(\boldsymbol{x},t) \in L^2(\mathbb{R}^{3N})$, where $\boldsymbol{x} = (\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N) \in \mathbb{R}^{3N}$, $t \in \mathbb{R}$, and by their actual configuration (positions) $\boldsymbol{X} = (\boldsymbol{X}_1, \ldots, \boldsymbol{X}_N) \in \mathbb{R}^{3N}$. The wave function evolves according to the Schrödinger equation

$$i\hbar \frac{\partial}{\partial t}\psi(\boldsymbol{x},t) = H\psi(\boldsymbol{x},t) \tag{1.1}$$

and governs the motion of the particle by ($l = 1, \ldots, N$)

$$\frac{d}{dt}\boldsymbol{X}_l^{\psi}(\boldsymbol{x}_0,t) = \boldsymbol{v}_l^{\psi}\left(\boldsymbol{X}^{\psi}(\boldsymbol{x}_0,t),t\right) =: \frac{\hbar}{m_l}\mathrm{Im}\left(\frac{\nabla_l\psi(\boldsymbol{X}^{\psi}(\boldsymbol{x}_0,t),t)}{\psi(\boldsymbol{X}^{\psi}(\boldsymbol{x}_0,t),t)}\right). \tag{1.2}$$

Here $\boldsymbol{x}_0$ is the particles' configuration at time $t = 0$, m_l is the mass of the lth particle and ∇_l is the gradient with respect to $\boldsymbol{x}_l$. In (1.1) H is the usual non-relativistic Schrödinger Hamiltonian

$$H = -\sum_{l=1}^{N}\frac{\hbar^2}{2m_l}\Delta_l + V(\boldsymbol{x}) =: H_0 + V(\boldsymbol{x}) \tag{1.3}$$

with the non-relativistic real valued potential[1] V.

The dynamical system defined by Bohmian mechanics is naturally associated with a family of finite measures $\mathbb{P}^{\psi(\cdot,t)}$ given by the densities $\rho^{\psi(\cdot,t)}(\boldsymbol{x}) := |\psi(\boldsymbol{x},t)|^2$ on configuration space $\mathbb{R}^{3N}$. If at time $t = 0$ we start with a random distribution on the configurations $\boldsymbol{x}$ of the system with density $\rho_0 = \rho^{\psi(\cdot,0)}$, for any other time t (1.2) transports this to a distribution with density $\rho_t = \rho^{\psi(\cdot,t)}$. This property is called equivariance. More precisely, let $\Phi^{\psi}_{t_2,t_1} : \mathbb{R}^{3N} \to \mathbb{R}^{3N}$ be the flow map of (1.2), i.e. $\boldsymbol{X}^{\psi}(\boldsymbol{x}_0,t_2) = \Phi^{\psi}_{t_2,t_1}\big(\boldsymbol{X}^{\psi}(\boldsymbol{x}_0,t_1)\big)$. Then the measure $\mathbb{P}^{\psi(\cdot,0)}$ is transported to $\mathbb{P}_t^{\psi(\cdot,0)} := \mathbb{P}^{\psi(\cdot,0)} \cdot \left(\Phi^{\psi}_{t,0}\right)^{-1} = \mathbb{P}^{\psi(\cdot,0)} \cdot \Phi^{\psi}_{0,t}$. We say that the functional $\psi(\cdot,t) \mapsto \mathbb{P}^{\psi(\cdot,t)}$ from wave functions to the finite measures $\mathbb{P}^{\psi(\cdot,t)}$ is equivariant if for all $t \in \mathbb{R}$

$$\mathbb{P}_t^{\psi(\cdot,0)} = \mathbb{P}^{\psi(\cdot,0)} \cdot \Phi^{\psi}_{0,t} = \mathbb{P}^{\psi(\cdot,t)}. \tag{1.4}$$

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[1] More rigorously: H is a self-adjoint extension of $H|_{C_0^\infty(\Omega)} = -\sum\limits_{l=1}^{N}\frac{\hbar^2}{2m_l}\Delta_l + V$ (with $V : \Omega \subset \mathbb{R}^{3N} \to \mathbb{R}$) on the Hilbert space $L^2(\Omega)$ with domain $\mathcal{D}(H)$.

On the family of measures $\mathbb{P}^{\psi(\cdot,t)}$ we bestow the role usually played by the stationary[2] "equilibrium measure": We call $\mathbb{P}^{\psi(\cdot,t)}$ the *quantum equilibrium* measure and say that a property is *typical*, resp. holds for *typical initial configurations* $\boldsymbol{x}_0$, if it holds for $\mathbb{P}^{\psi(\cdot,0)}$-almost all $\boldsymbol{x}_0 \in \mathbb{R}^{3N}$. By equivariance this notion of typicality is time independent. For an extensive treatment of quantum equilibrium and how it entails the usual quantum measurement formalism (including the collapse of the wave function) see [19, 20].

Since the Bohmian velocity field $\boldsymbol{v}_l^{\psi} = \frac{\hbar}{m_l}\mathrm{Im}\left(\frac{\nabla_l \psi}{\psi}\right)$ becomes obviously ill defined at the nodes of the wave function ψ, one might wonder whether the dynamic system of Bohmian mechanics is well defined. However, for a wide class of (sufficiently regular) potentials V and initial wave functions ψ $\mathbb{P}^{\psi}$-almost sure global existence of Bohmian mechanics was proved in [5] and [39]. In particular, typical Bohmian trajectories do not run into the nodes of the wave function. Both our settings below (Chapters 2 and 3) fall into the scope of Corollary 3.2 in [5] resp. Corollary 4 in [39].

Proposition 1. *Let $V \in C^{\infty}(\Omega, \mathbb{R})$ with $\Omega \subset \mathbb{R}^{3N}$ such that $\mathbb{R}^3 \setminus \Omega$ consists of at most finitely many points (i.e. the real valued potential V has got at most finitely many singularities). Further let $V = V_1 + V_2$ where V_1 is bounded below and V_2 is H_0-bounded with relative bound $a < 1$. Finally, assume that the initial wave function ψ is a C^{∞}-vector of H, $\psi \in C^{\infty}(H) := \bigcap_{n=1}^{\infty} \mathcal{D}(H^n)$, and is normalized. Then there exists a unique global solution of* (1.2) *for $\mathbb{P}^{\psi}$-almost all initial configurations $\boldsymbol{x}_0 \in \mathbb{R}^{3N}$.*

For a proof see Corollary 3.2 in [5] resp. Corollary 4 in [39]. In fact they are more general than Proposition 1 (they allow for more general singularities of the potential and are formulated in terms of quadratic forms instead of operators). The set of admissible initial wave functions $C^{\infty}(H)$ is dense in $L^2(\Omega)$ and invariant under the time evolution e^{-iHt}. Therefore it is a core, i.e. a domain of essential self adjointness of H. Examples for C^{∞}-vectors are eigenfunctions and wave functions $\psi \in \mathrm{Ran}(P_{[E_1,E_2]})$ of "finite energy", where $P_{[E_1,E_2]}$ denotes the spectral projection of H to the finite energy interval $[E_1, E_2]$. Since Ω and $\mathbb{R}^{3N}$ differ at most by a set of Lesbegue- and thus $\mathbb{P}^{\psi}$-measure zero we shall in the following no longer distinguish between them.

[2] Since in most cases the velocity field defined in (1.2) will be explicitly time dependent one cannot expect to find a stationary measure.

Chapter 2

Trajectories of Semiclassical Wave Packets

Under which circumstances are the Bohmian trajectories of the particles of a system (close to) Newtonian trajectories? In this chapter we study this question in the case of a system with three degrees of freedom only, so Schrödinger's equation (1.1) and the Bohmian equation of motion (1.2) read

$$i\hbar\frac{\partial}{\partial t}\psi(\boldsymbol{x},t) = H\psi(\boldsymbol{x},t) = -\frac{\hbar^2}{2m}\triangle\psi(\boldsymbol{x},t) + V(\boldsymbol{x})\psi(\boldsymbol{x},t),$$
$$\frac{d}{dt}\boldsymbol{X}^{\psi}(\boldsymbol{x}_0,t) = \boldsymbol{v}^{\psi}\left(\boldsymbol{X}^{\psi}(\boldsymbol{x}_0,t),t\right) = \frac{\hbar}{m}\mathrm{Im}\left(\frac{\nabla\psi(\boldsymbol{X}^{\psi}(\boldsymbol{x}_0,t),t)}{\psi(\boldsymbol{X}^{\psi}(\boldsymbol{x}_0,t),t)}\right), \quad \boldsymbol{X}^{\psi}(\boldsymbol{x}_0,0) = \boldsymbol{x}_0$$

with $\boldsymbol{x}$ and $\boldsymbol{X}^{\psi}$ in $\mathbb{R}^3$. Here one should not so much think of a single particle but rather of a macroscopic body in an external potential V whose center of mass coordinates $\boldsymbol{x}$ can be dynamically decoupled from its inner degrees of freedom[1]. Only for simplicity we henceforth call $\boldsymbol{X}^{\psi}$ and ψ the position respectively the wavefunction of a "particle".

Usually, physicists consider classical behavior of a quantum mechanical system as ensured by the limit $\hbar \to 0$, meaning by this

$$\hbar \ll A_0\,,$$

where A_0 is *some* characteristic action of the corresponding classical motion (see, e.g., [7, 30, 36]). We prefer, however, to use another, equivalent standard condition of classicality which involves the length scales of the motion (see, e.g., [29]): Suppose the de Broglie wave length λ is small with respect to the characteristic dimension L determined by the scale of variation of the potential V. Then on the *macroscopic* scale given by L the behavior of the system should be close to the behavior of a classical system in the same potential V. This is very reminiscent of how geometrical optics can be deduced from wave optics. We regard this condition, i.e.,

$$\lambda \ll L\,,$$

[1]See e.g. [3], Section 3, for conditions under which this is possible.

as the most natural condition of classicality since it relates in a completely transparent way a property of the state, namely its de Broglie wave length λ, and a property of the dynamics, namely the scale of variation of the potential L (cf. [3]).

It is a priori not clear how the scale of variation L of a given potential V should be defined. One way to circumvent this problem is to consider an arbitrary potential V and to rescale it as $V^\varepsilon(\boldsymbol{x}) := V(\varepsilon\boldsymbol{x})$. Then the limit $\varepsilon \to 0$ corresponds to the limit of slow variation of V^ε, no matter exactly how the scale of variation is defined.

Since we want to compare quantum and classical dynamics on the scale the potential lives on, we change from *microscopic* coordinates $(\boldsymbol{x}, t)$ to *macroscopic* coordinates $(\boldsymbol{x}', t') = (\varepsilon\boldsymbol{x}, \varepsilon t)$. Then the time-dependent Schrödinger equation becomes ($\psi^\varepsilon(\boldsymbol{x}', t') := \varepsilon^{-\frac{3}{2}}\psi(\frac{\boldsymbol{x}'}{\varepsilon}, \frac{t'}{\varepsilon})$ where $\varepsilon^{-\frac{3}{2}}$ is just a normalization factor)

$$i\varepsilon\hbar\frac{\partial}{\partial t'}\psi^\varepsilon(\boldsymbol{x}', t') = H^\varepsilon\psi^\varepsilon(\boldsymbol{x}', t') = -\frac{\varepsilon^2\hbar^2}{2m}\triangle'\,\psi^\varepsilon(\boldsymbol{x}', t') + V(\boldsymbol{x}')\,\psi^\varepsilon(\boldsymbol{x}', t') \tag{2.1}$$

while the Bohmian equation of motion reads

$$\begin{aligned} \frac{d}{dt'}\boldsymbol{X}'^{\psi^\varepsilon}(\boldsymbol{x}_0', t') &= \boldsymbol{v}^{\psi^\varepsilon}\left(\boldsymbol{X}'^{\psi^\varepsilon}(\boldsymbol{x}_0', t'), t'\right) = \frac{\varepsilon\hbar}{m}\mathrm{Im}\left(\frac{\nabla'\psi^\varepsilon(\boldsymbol{X}'^{\psi^\varepsilon}(\boldsymbol{x}_0', t'), t')}{\psi^\varepsilon(\boldsymbol{X}'^{\psi^\varepsilon}(\boldsymbol{x}_0', t'), t')}\right), \\ \boldsymbol{X}'^{\psi^\varepsilon}(\boldsymbol{x}_0', 0) &= \boldsymbol{x}_0'\,. \end{aligned} \tag{2.2}$$

Hence, in macroscopic coordinates, the limit $\varepsilon \to 0$ is mathematically equivalent to the limit $\hbar \to 0$. From now on we use natural units $\hbar = m = 1$. Moreover, since we shall stick to the macroscopic scale, we change the notation: For the remainder of this chapter $(\boldsymbol{x}, t)$ denotes the *macroscopic* (and no longer the microscopic) coordinates. For ease of notation we also write $\boldsymbol{X}$ instead of $\boldsymbol{X}^{\psi^\varepsilon}$.

We shall study the scaling limit $\varepsilon \to 0$ of the Bohmian trajectories associated with a special class of initial wave functions $\Phi^\varepsilon_{\boldsymbol{k}}(\boldsymbol{a}(0), \boldsymbol{\eta}(0), \cdot)$ in a sufficiently smooth potential V. The $\Phi^\varepsilon_{\boldsymbol{k}}$s are the semiclassical wave packets defined by Hagedorn in [24, 25]. Roughly speaking they are "narrow" non-isotropic three dimensional generalized Hermite functions (generalized Hermite polynomials of order $k := k_1 + k_2 + k_3,\ \boldsymbol{k} \in \mathbb{N}^3$ multiplied by a Gaussian wave packet) centered around some classical phase space point $(\boldsymbol{a}(0), \boldsymbol{\eta}(0))$. "Narrow" means that their standard deviation is of order $\sqrt{\varepsilon}$ both in position and momentum. Moreover, Hagedorn [24, 25] showed that they give a good approximation to the Schrödinger time evolution in the sense that, up to an error of order $\sqrt{\varepsilon}$ in L^2-norm, the solution $\psi^\varepsilon_{\boldsymbol{k}}(\boldsymbol{x}, t)$ of (2.1) with initial data $\psi^\varepsilon_{\boldsymbol{k}}(\boldsymbol{x}, 0) = \Phi^\varepsilon_{\boldsymbol{k}}(\boldsymbol{a}(0), \boldsymbol{\eta}(0), \boldsymbol{x})$ is given by $\Phi^\varepsilon_{\boldsymbol{k}}(\boldsymbol{a}(t), \boldsymbol{\eta}(t), \boldsymbol{x})$. Here $(\boldsymbol{a}(t), \boldsymbol{\eta}(t))$ is the corresponding classical phase space trajectory, that is the solution of the Newtonian law of motion with initial data $(\boldsymbol{a}(0), \boldsymbol{\eta}(0))$ (see subsection 2.1.2).

For this class of initial wave functions we show that for $\varepsilon \to 0$ $\mathbb{P}^{\psi^\varepsilon_{\boldsymbol{k}}(\cdot,0)}$-almost all Bohmian trajectories stay arbitrarily close to the corresponding classical trajectory $\boldsymbol{a}(t)$ and that the rate of convergence is of order $\sqrt{\varepsilon}$: For all $T > 0$ and $\gamma > 0$ there exists some $R < \infty$ such that

$$\mathbb{P}^{\psi^\varepsilon_{\boldsymbol{k}}(\cdot,0)}(\{\boldsymbol{x}_0 \in \mathbb{R}^3 \mid \max_{t\in[0,T]} |\boldsymbol{X}(\boldsymbol{x}_0, t) - \boldsymbol{a}(t)| \leq R\sqrt{\varepsilon}\}) > 1 - \gamma$$

for all ε small enough (cf. Theorem 1).

At first glance this looks like an easy corollary to Hagedorn's L^2-results. After all, they imply that for every time $t \in [0,T]$ not just the main support of $\Phi^\varepsilon_{\boldsymbol{k}}(\boldsymbol{a}(t), \boldsymbol{\eta}(t), \boldsymbol{x})$ but also that of $\psi^\varepsilon_{\boldsymbol{k}}(\boldsymbol{x},t)$ lies in a ball with radius $\sim \sqrt{\varepsilon}$ centered around the classical position $\boldsymbol{a}(t)$ at that time. But beware: This only implies that for ε small enough the set of initial positions $\boldsymbol{x}_0$ of Bohmian trajectories $\boldsymbol{X}(\boldsymbol{x}_0,t)$ that do not deviate more than order $\sqrt{\varepsilon}$ from the classical trajectory $\boldsymbol{a}(t)$ at some arbitrary but *fixed* time $t \in [0,T]$ has (nearly) full $\mathbb{P}^{\psi^\varepsilon_{\boldsymbol{k}}(\cdot,0)}$-measure. It does not imply that the set of initial positions $\boldsymbol{x}_0$ of Bohmian trajectories $\boldsymbol{X}(\boldsymbol{x}_0,t)$ that stay $\sqrt{\varepsilon}$-close to $\boldsymbol{a}(t)$ for *all* times $t \in [0,T]$ has (nearly) full $\mathbb{P}^{\psi^\varepsilon_{\boldsymbol{k}}(\cdot,0)}$-measure. There is still the possibility that the Bohmian trajectories "take turns" to escape the proximity of the classical trajectory $\boldsymbol{a}(t)$: While for every time $t \in [0,T]$ most of the Bohmian trajectories are close to the classical trajectory $\boldsymbol{a}(t)$, nevertheless (nearly) every Bohmian trajectory may leave the vicinity of $\boldsymbol{a}(t)$ at some time $t \in [0,T]$ (see Figure 2.1).

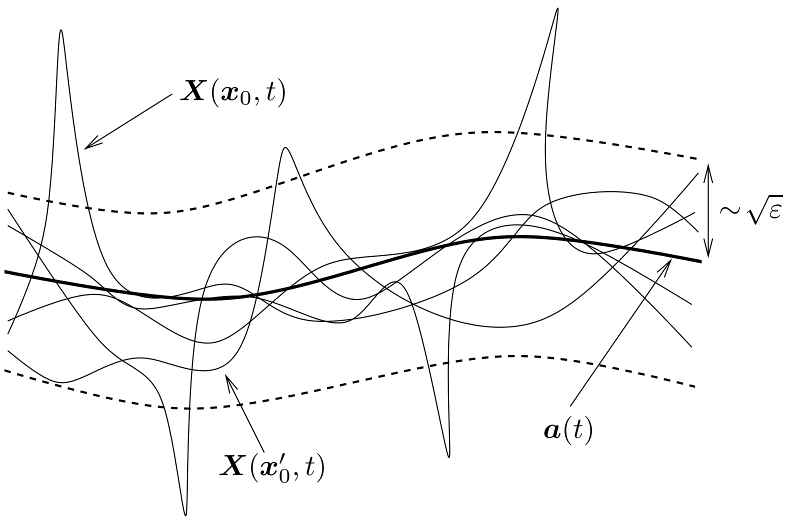

Figure 2.1: What might go wrong.

So we need more controll over the Bohmian trajectories $\boldsymbol{X}(\boldsymbol{x}_0,t)$ than available from L^2-results. In view of (2.2) this can be achieved by evaluating the wave function $\psi^\varepsilon_{\boldsymbol{k}}$ and its gradient *pointwise*. Thus the main *technical* result of this work is Lemma 1: $\psi^\varepsilon_{\boldsymbol{k}}(\boldsymbol{x},t)$ and $\Phi^\varepsilon_{\boldsymbol{k}}(\boldsymbol{a}(t), \boldsymbol{\eta}(t), \cdot)$ are close not only in L^2-norm but also pointwise and the same is true for their gradients.

For its proof we use a Gagliardo-Nirenberg inequality (i.e. a Sobolev-type inequality) that allows us to estimate the supremum norm of $(\nabla_x)\psi^\varepsilon_{\boldsymbol{k}} - (\nabla_x)\Phi^\varepsilon_{\boldsymbol{k}}$ by its L^2-norm and the L^2-norm of its second derivatives. The main difficulty then is to compute the latter. In particular, we have to commute differentiation (respectively $\boldsymbol{p} = -i\varepsilon\nabla$) with the Schrödinger time evolution $e^{-\frac{i}{\varepsilon}H^\varepsilon t}$ without loosing too many orders of ε. This is further complicated by the fact that $\psi^\varepsilon_{\boldsymbol{k}} - \Phi^\varepsilon_{\boldsymbol{k}}$ carries a rapidly varying phase factor of the form $e^{\frac{i}{\varepsilon}\langle \boldsymbol{\eta}, \boldsymbol{x}-\boldsymbol{a}\rangle}$ which blows up the estimates for the derivatives. To remedy this we use Gagliardo-Nirenberg not directly on $\psi^\varepsilon_{\boldsymbol{k}} - \Phi^\varepsilon_{\boldsymbol{k}}$ (resp. $\nabla_x\psi^\varepsilon_{\boldsymbol{k}} - \nabla_x\Phi^\varepsilon_{\boldsymbol{k}}$) but rather on

$e^{-\frac{i}{\varepsilon}\langle\boldsymbol{\eta},\boldsymbol{x}-\boldsymbol{a}\rangle}\left(\psi^\varepsilon_{\boldsymbol{k}}-\Phi^\varepsilon_{\boldsymbol{k}}\right)$. This, however, means that in the end we even have to compute[2] the higher order terms $\|D^\alpha e^{-\frac{i}{\varepsilon}\langle\boldsymbol{\eta},\boldsymbol{x}-\boldsymbol{a}\rangle}\left(\psi^\varepsilon_{\boldsymbol{k}}-\Phi^\varepsilon_{\boldsymbol{k}}\right)\|_2=\varepsilon^{-|\alpha|}\|(\boldsymbol{p}-\boldsymbol{\eta})^\alpha\left(\psi^\varepsilon_{\boldsymbol{k}}-\Phi^\varepsilon_{\boldsymbol{k}}\right)\|_2$ instead of $\|D^\alpha\left(\psi^\varepsilon_{\boldsymbol{k}}-\Phi^\varepsilon_{\boldsymbol{k}}\right)\|_2=\varepsilon^{-|\alpha|}\|\boldsymbol{p}^\alpha\left(\psi^\varepsilon_{\boldsymbol{k}}-\Phi^\varepsilon_{\boldsymbol{k}}\right)\|_2$ (see subsection 2.4.3).

The remainder of this chapter is organized as follows. In section 2.1 we give the mathematical setup: We briefly recount the different dynamics (classical and quantum) we want to compare (subsection 2.1.1) and introduce Hagedorn's wave packets (subsection 2.1.2). Section 2.2 contains our results about the classical behavior of the Bohmian trajectories and Lemma 1 about the pointwise closeness of $\psi^\varepsilon_{\boldsymbol{k}}(\boldsymbol{x},t)$ and $\Phi^\varepsilon_{\boldsymbol{k}}(\boldsymbol{a}(t),\boldsymbol{\eta}(t),\cdot)$. In section 2.3 we have collected some remarks and a short outlook on possible generalizations of our results. Last but not least we give the proofs (section 2.4).

2.1 Mathematical framework

2.1.1 Dynamics

In this subsection we collect the different kinds of particle dynamics we wish to compare. We look at particle motion in a macroscopic potential $V:\mathbb{R}^3\to\mathbb{R}$, which we always assume to be in $C^\infty(\mathbb{R}^3)$. Since we will habitually need to restrict the growth of the potential and its derivatives, we give the following

Definition 1. *We say that $V\in C^\infty(\mathbb{R}^3,\mathbb{R})$ is in G_V if for all multi-indices $\alpha\in\mathbb{N}^3$*

$$\max_{|\alpha|\le 4}\|D^\alpha V\|_\infty\le C_V \tag{2.3}$$

for some $C_V<\infty$ and if multiplication by V maps the Schwartz space $\mathcal{S}(\mathbb{R}^3)$ into itself, i.e. if $Vf\in\mathcal{S}(\mathbb{R}^3)$ for all $f\in\mathcal{S}(\mathbb{R}^3)$. Here D^α denotes the (weak) derivative $\partial^{\alpha_1}_{x_1}\partial^{\alpha_2}_{x_2}\partial^{\alpha_3}_{x_3}$.

Remark 1. The (quite mild) requirement that V maps $\mathcal{S}$ into itself is needed to get $\mathbb{P}^\psi$-almost sure global existence of Bohmian mechanics [5, 39] for initial wave functions $\psi\in\mathcal{S}$ (c.f. the beginning of the proof of Theorem 1). The boundedness of V and its derivatives will be needed in the proof of the pointwise closeness of $(\nabla)\psi^\varepsilon_{\boldsymbol{k}}$ and $(\nabla)\Phi^\varepsilon_{\boldsymbol{k}}$ when we commute $\boldsymbol{p}$ with $e^{-\frac{i}{\varepsilon}H^\varepsilon t}$.

The classical dynamics is given by Newtonian mechanics, so the classical state of a particle at the macroscopic time t is given by its classical position and velocity at that time, which we denote by $(\boldsymbol{a}(t),\boldsymbol{\eta}(t))$. For any given initial value $(\boldsymbol{a}(0),\ \boldsymbol{\eta}(0))$ it is the (unique global) solution[3] of the usual classical equations of motion:

$$\begin{aligned}\dot{\boldsymbol{a}}(t)&=\boldsymbol{\eta}(t)\,,\\ \dot{\boldsymbol{\eta}}(t)&=-\nabla V\left(\boldsymbol{a}(t)\right)\,.\end{aligned} \tag{2.4}$$

[2]We use the usual multi-index notation, $D^\alpha=\partial_1^{\alpha_1}\partial_2^{\alpha_2}\partial_3^{\alpha_3}$.

[3]Since $\max\limits_{|\alpha|=2}\|D^\alpha V\|_\infty\le C_V$, global existence and uniqueness of solutions to (2.4) is a standard result.

The quantum dynamics is given by Bohmian mechanics, so the particle's quantum mechanical state is given by its quantum mechanical position and wave function, $(\boldsymbol{X}(\boldsymbol{x}_0,t),\psi(\cdot,t))$ (cf. section 1.2). In macroscopic coordinates and natural units Schrödinger's equation and the Bohmian equation of motion read respectively (cf. the beginning of this chapter)

$$i\varepsilon\frac{\partial}{\partial t}\psi(\boldsymbol{x},t)=H^{\varepsilon}\,\psi(\boldsymbol{x},t)=\left(-\frac{\varepsilon^2}{2}\triangle+V(\boldsymbol{x})\right)\psi(\boldsymbol{x},t) \tag{2.1}$$

and

$$\frac{d}{dt}\boldsymbol{X}(\boldsymbol{x}_0,t)=\boldsymbol{v}^{\psi}(\boldsymbol{X}(\boldsymbol{x}_0,t),t)=\varepsilon\mathrm{Im}\left(\frac{\nabla\psi(\boldsymbol{X}(\boldsymbol{x}_0,t),t)}{\psi(\boldsymbol{X}(\boldsymbol{x}_0,t),t)}\right)\,,\quad \boldsymbol{X}(\boldsymbol{x}_0,0)=\boldsymbol{x}_0\,. \tag{2.2}$$

By $U^{\varepsilon}(t)$ we denote the unitary propagator generated by H^{ε}:

$$\frac{d}{dt}U^{\varepsilon}(t)|_{t=0}=-\frac{i}{\varepsilon}H^{\varepsilon} \tag{2.5}$$

To mediate between classical and quantum dynamics we follow Hagedorn [25] and use a second, "semiclassical" time evolution for the wave function, namely a Schrödinger evolution with truncated potential. To this end we Taylor-expand the potential V and introduce the following abbreviations.

Definition 2. *For any $l\leq m\in\mathbb{N}$, $V\in C^m(\mathbb{R}^3)$ define*

$$V_m\left(\boldsymbol{x},\boldsymbol{a}\right):=V(\boldsymbol{x})-\sum_{|\alpha|=0}^{m-1}\frac{1}{\alpha!}\left(D^{\alpha}V\right)(\boldsymbol{a})(\boldsymbol{x}-\boldsymbol{a})^{\alpha} \tag{2.6}$$

and

$$V_{l,m}\left(\boldsymbol{x},\boldsymbol{a}\right):=V_l\left(\boldsymbol{x},\boldsymbol{a}\right)-V_{m+1}\left(\boldsymbol{x},\boldsymbol{a}\right)=\sum_{|\alpha|=l}^{m}\frac{1}{\alpha!}\left(D^{\alpha}V\right)(\boldsymbol{a})(\boldsymbol{x}-\boldsymbol{a})^{\alpha}. \tag{2.7}$$

Then the truncated, time dependent (quadratic) Hamiltonian

$$\widetilde{H}^{\varepsilon}(t):=\widetilde{H}^{\varepsilon}(\boldsymbol{a}(t)):=-\frac{\varepsilon^2}{2}\triangle+V_{0,2}\left(\boldsymbol{x},\boldsymbol{a}(t)\right) \tag{2.8}$$

is the generator of a second unique unitary propagator, which we denote by $\widetilde{U}^{\varepsilon}(t,s)$:

$$\frac{d}{dt}\widetilde{U}^{\varepsilon}(t,s)|_{t=s}=-\frac{i}{\varepsilon}\widetilde{H}^{\varepsilon}(s)\;. \tag{2.9}$$

For a proof see [25].

2.1.2 Hagedorn's wave packets

In this subsection we recount the definition and the basic properties of Hagedorn's (n-dimensional) wave packets [24, 25]. They are semiclassical wave packets that form an orthonormal basis (ONB) of $L^2(\mathbb{R}^n)$ and come endowed with their very own time evolution, which is such that their mean position and momentum track a classical trajectory in phase space while their standard deviation is of order $\sqrt{\varepsilon}$ both in position and momentum. In fact we shall see that this time evolution is just that given by the truncated Hamiltonian $\widetilde{H}^\varepsilon$.

Like the eigenfunctions of the n-dimensional harmonic oscillator Hagedorn's wave packets can be constructed with the help of raising and lowering operators [25].

For this let $A_0, B_0 \in \mathbb{C}^{n\times n}$ such that[4]

$$\begin{aligned} A_0^t B_0 - B_0^t A_0 &= 0\,, \\ A_0^* B_0 + B_0^* A_0 &= 2\mathbb{1} \end{aligned} \tag{2.10}$$

and let $(A(t)\,, B(t)) \in \mathbb{C}^{n\times n} \times \mathbb{C}^{n\times n}$ be the solution[5] of ($V^{(2)}$ denotes the Hessian of V)

$$\begin{aligned} \dot{A}(t) &= iB(t)\,, \\ \dot{B}(t) &= iV^{(2)}(\boldsymbol{a}(t))A(t)\,, \end{aligned} \tag{2.11}$$

with initial data $(A(0), B(0)) = (A_0, B_0)$. Then also $A(t)$ and $B(t)$ fulfill (2.10). Moreover, (2.10) implies that

$$\begin{aligned} &A \text{ and } B \text{ are invertible}\,, \\ &BA^{-1} \text{ and } AB^{-1} \text{ are symmetric}\,, \\ &\mathrm{Re}(BA^{-1}) = (AA^*)^{-1} \text{ and } \mathrm{Re}(AB^{-1}) = (BB^*)^{-1}\,. \end{aligned} \tag{2.12}$$

For a proof see [25].

Next define (formal) vectors of lowering resp. raising operators acting on Schwartz space $\mathcal{S}(\mathbb{R}^n)$:

$$\begin{aligned} \mathcal{A}(A, B, \varepsilon, \boldsymbol{a}, \boldsymbol{\eta}) &:= \frac{1}{\sqrt{2\varepsilon}}\left[B^t(\boldsymbol{x}-\boldsymbol{a}) + iA^t(\boldsymbol{p}-\boldsymbol{\eta})\right] \\ \mathcal{A}^*(A, B, \varepsilon, \boldsymbol{a}, \boldsymbol{\eta}) &:= \frac{1}{\sqrt{2\varepsilon}}\left[B^*(\boldsymbol{x}-\boldsymbol{a}) - iA^*(\boldsymbol{p}-\boldsymbol{\eta})\right] \end{aligned} \tag{2.13}$$

They fulfill the commutator relations ($j, l \in \{1\,, \dots\,, n\}$)

$$\begin{aligned} \left[\mathcal{A}_j,\, A_l\right] &= \left[\mathcal{A}_j^*,\, A_l^*\right] = 0\,, \\ \left[\mathcal{A}_j,\, A_l^*\right] &= \delta_{jl}\,. \end{aligned}$$

Here $\boldsymbol{p} = -i\varepsilon\nabla$ is the momentum and $\boldsymbol{x}$ is the (macroscopical) position operator.

[4] A^t is the transposed of A, A^* its adjoint and $\bar{A}$ its complex conjugate.

[5] Since $\max\limits_{|\alpha|=3} \|D^\alpha V\|_\infty \le C_V$, such a solution exists and is unique.

Remark 2. Note that $\mathcal{A}$ and $\mathcal{A}^*$ are only formal vectors. In particular, $\mathcal{A}^*$ is the vector consisting of the adjoint components of $\mathcal{A}$; that is why in the definition of $\mathcal{A}^*$ we find A^* and B^* instead of the probably expected $\bar{B}$ resp. $\bar{A}$.

Then Hagedorn's wave packets are given by

Definition 3 (Hagedorn's wave packets)**.** *Let $\varepsilon > 0$, $\boldsymbol{k} \in \mathbb{N}^n$ and let $\boldsymbol{a}(t)$, $\boldsymbol{\eta}(t)$ be solutions of* (2.4) *and $A(t)$, $B(t)$ solutions of* (2.11) *with initial data A_0, B_0 fulfilling* (2.10)*. Define*

$$\Phi^\varepsilon_{\boldsymbol{k}}(\boldsymbol{x},t) := \Phi_{\boldsymbol{k}}(A(t),B(t),\varepsilon,\boldsymbol{a}(t),\boldsymbol{\eta}(t),\boldsymbol{x}) := \frac{1}{\sqrt{\boldsymbol{k}!}}\mathcal{A}^*(A,B,\varepsilon,\boldsymbol{a},\boldsymbol{\eta})^{\boldsymbol{k}}\Phi^\varepsilon_0(\boldsymbol{x},t) \tag{2.14}$$

where the ground state Φ^ε_0 is given by

$$\begin{aligned}\Phi^\varepsilon_0(\boldsymbol{x},t) &:= \Phi_0\left(A(t),B(t),\varepsilon,\boldsymbol{a}(t),\boldsymbol{\eta}(t),\boldsymbol{x}\right)\\ &:= e^{\frac{i}{\varepsilon}S(t)}\frac{(\pi\varepsilon)^{-\frac{n}{4}}}{\sqrt{\det(A)}}\exp\left[-\frac{1}{2\varepsilon}\left\langle(\boldsymbol{x}-\boldsymbol{a}),\, BA^{-1}(\boldsymbol{x}-\boldsymbol{a})\right\rangle + \frac{i}{\varepsilon}\left\langle\boldsymbol{\eta},\,(\boldsymbol{x}-\boldsymbol{a})\right\rangle\right],\end{aligned} \tag{2.15}$$

$S(t) = \int_0^t \left[\frac{1}{2}\eta^2(s) - V(\boldsymbol{a}(s))\right]ds$ *denotes the usual classical action and $\langle\cdot,\,\cdot\rangle$ is the canonical scalar product on $\mathbb{C}^n$.*

Since it appears only as a global (if time dependent) phase factor we choose not to denote dependence on $S(t)$.

The basic properties of Hagedorn's wave packets we shall need in the course of our analysis are collected in the following two propositions.

Proposition 2. *Let $\varepsilon > 0$, $\boldsymbol{a}$, $\boldsymbol{\eta} \in \mathbb{R}^n$ and A, $B \in \mathbb{C}^{n\times n}$ such that* (2.10) *holds. Then*

(i) Hagedorn's wave packets $\{\Phi_{\boldsymbol{k}} \mid \boldsymbol{k} \in \mathbb{N}^n\}$ form an orthonormal basis (ONB) of $L^2(\mathbb{R}^n)$. The lowering resp. raising operators act on them as follows:

$$\begin{aligned}\mathcal{A}_j(A,B,\varepsilon,\boldsymbol{a},\boldsymbol{\eta})\Phi_{\boldsymbol{k}}\left(A,B,\varepsilon,\boldsymbol{a},\boldsymbol{\eta},\boldsymbol{x}\right) &= \sqrt{k_j}\Phi_{\boldsymbol{k}'}\left(A,B,\varepsilon,\boldsymbol{a},\boldsymbol{\eta},\boldsymbol{x}\right),\\ \mathcal{A}^*_j(A,B,\varepsilon,\boldsymbol{a},\boldsymbol{\eta})\Phi_{\boldsymbol{k}}\left(A,B,\varepsilon,\boldsymbol{a},\boldsymbol{\eta},\boldsymbol{x}\right) &= \sqrt{k_j+1}\Phi_{\widetilde{\boldsymbol{k}}}\left(A,B,\varepsilon,\boldsymbol{a},\boldsymbol{\eta},\boldsymbol{x}\right).\end{aligned} \tag{2.16}$$

where $\boldsymbol{k}' = (k_1,\dots,k_{j-1},k_j-1,k_{j+1},\dots,k_n)$, $\widetilde{\boldsymbol{k}} = (k_1,\dots,k_{j-1},k_j+1,k_{j+1},\dots,k_n)$.

(ii) The Φ_ks can be written as generalized Hermite functions, i.e. as products of generalized Hermite polynomials and the ground state Φ_0: Let $\{\widehat{e}_1,\widehat{e}_2,\dots,\widehat{e}_n\}$ be the standard ONB of $\mathbb{R}^n$ and $A = R_A U_A$ the polar decomposition of A (i.e. $R_A = \sqrt{AA^*}$ and U_A is unitary). Then[6]

$$\begin{aligned}\Phi_{\boldsymbol{k}}\left(A,B,\varepsilon,\boldsymbol{a},\boldsymbol{\eta},\boldsymbol{x}\right) &= \frac{2^{-\frac{k}{2}}}{\sqrt{\boldsymbol{k}!}}\mathcal{H}_{\boldsymbol{k}}\left(U_A;\, R_A^{-1}\frac{\boldsymbol{x}-\boldsymbol{a}}{\sqrt{\varepsilon}}\right)\Phi_0\left(A,B,\varepsilon,\boldsymbol{a},\boldsymbol{\eta},\boldsymbol{x}\right)\\ \textit{with}\qquad \mathcal{H}_{\boldsymbol{k}}\left(U_A;\,\boldsymbol{x}\right) &:= \widetilde{\mathcal{H}}_k(\underbrace{U_A\widehat{e}_1,\dots,U_A\widehat{e}_1}_{k_1\ \textit{times}},\dots,\underbrace{U_A\widehat{e}_n,\dots,U_A\widehat{e}_n}_{k_n\ \textit{times}};\,\boldsymbol{x}).\end{aligned} \tag{2.17}$$

[6]Note that R_A^{-1} is well defined by (2.12).

Here the $\widetilde{\mathcal{H}}_m(\boldsymbol{v}_1,\ldots,\boldsymbol{v}_m;\,\cdot)$ *(*$m\in\mathbb{N}$, $\boldsymbol{v}_1,\ldots,\boldsymbol{v}_m\in\mathbb{C}^n$*) are the generalized* n*-dimensional Hermite polynomials defined by Hagedorn in [24]:*

$$\begin{aligned}
&\widetilde{\mathcal{H}}_0(\boldsymbol{x}) := 1\,, \quad \widetilde{\mathcal{H}}_1(\boldsymbol{v}_1;\,\boldsymbol{x}) := 2\,\langle \boldsymbol{v}_1,\,\boldsymbol{x}\rangle\,,\\
&\widetilde{\mathcal{H}}_m(\boldsymbol{v}_1,\ldots,\boldsymbol{v}_m;\,\boldsymbol{x}) := 2\,\langle \boldsymbol{v}_m,\,\boldsymbol{x}\rangle\,\widetilde{\mathcal{H}}_{m-1}(\boldsymbol{v}_1,\ldots,\boldsymbol{v}_{m-1};\,\boldsymbol{x})\\
&\qquad\qquad -2\sum_{i=1}^{m-1}\langle \boldsymbol{v}_m,\,\bar{\boldsymbol{v}}_i\rangle \widetilde{\mathcal{H}}_{m-2}(\boldsymbol{v}_1,\ldots,\widehat{\boldsymbol{v}}_i,\ldots,\boldsymbol{v}_{m-1};\,\boldsymbol{x})\,.
\end{aligned} \tag{2.18}$$

(iii) For any multi-index $\alpha\in\mathbb{N}^n$ *(we abuse notation and write* $\langle\cdot,\,\cdot\rangle$ *also for the scalar product on* $L^2(\mathbb{R}^n)$*)*

$$\begin{aligned}
&\left(\frac{\boldsymbol{x}-\boldsymbol{a}}{\sqrt{\varepsilon}}\right)^{\alpha}\Phi_{\boldsymbol{k}}\left(A,B,\varepsilon,\boldsymbol{a},\boldsymbol{\eta},\boldsymbol{x}\right)\\
&=\sum_{\substack{|\boldsymbol{k}-\boldsymbol{k}'|\le|\alpha|\\ |\boldsymbol{k}-\boldsymbol{k}'|+|\alpha|\ \text{even}}}\langle\Phi_{\boldsymbol{k}'}(U_A,\mathbb{1},1,0,0,\boldsymbol{x}),\,(R_A\boldsymbol{x})^{\alpha}\Phi_{\boldsymbol{k}}(U_A,\mathbb{1},1,0,0,\boldsymbol{x})\rangle\,\Phi_{\boldsymbol{k}'}\big(A,B,\varepsilon,\boldsymbol{a},\boldsymbol{\eta},\boldsymbol{x}\big)
\end{aligned} \tag{2.19}$$

and

$$\begin{aligned}
&\left(\frac{\boldsymbol{p}-\boldsymbol{\eta}}{\sqrt{\varepsilon}}\right)^{\alpha}\Phi_{\boldsymbol{k}}\left(A,B,\varepsilon,\boldsymbol{a},\boldsymbol{\eta},\boldsymbol{x}\right)\\
&=\sum_{\substack{|\boldsymbol{k}-\boldsymbol{k}'|\le|\alpha|\\ |\boldsymbol{k}-\boldsymbol{k}'|+|\alpha|\ \text{even}}}\langle\Phi_{\boldsymbol{k}'}(\mathbb{1},U_B,1,0,0,\boldsymbol{x}),\,(R_B\boldsymbol{p})^{\alpha}\Phi_{\boldsymbol{k}}(\mathbb{1},U_B,1,0,0,\boldsymbol{x})\rangle\,\Phi_{\boldsymbol{k}'}\big(A,B,\varepsilon,\boldsymbol{a},\boldsymbol{\eta},\boldsymbol{x}\big)\,.
\end{aligned} \tag{2.20}$$

For a proof of (i) see [25] (Theorem 3.3). For a proof of (ii) see [24] (cf. also Remark 3.2 in [25]). Parts of (iii) can be found in [24] (Remark 2) and [25] (equation (2.41)). For the sake of completeness we give a short synopsis of the proof of *(iii)* in subsection 2.4.4.

Proposition 3. *Let* $\varepsilon>0$*, let* $\boldsymbol{a}(t)$*,* $\boldsymbol{\eta}(t)$ *be solutions of* (2.4) *and* $A(t)$*,* $B(t)$ *solutions of* (2.11) *with initial data* A_0*,* B_0 *fulfilling* (2.10)*. Then*

(i) Hagedorn's wave packets $\Phi^{\varepsilon}_{\boldsymbol{k}}$ *evolve according to the Schrödinger evolution with the truncated (quadratic) Hamiltonian* $\widetilde{H}^{\varepsilon}$ *defined in subsection 2.1.1. That is for any* $t\,,s\in\mathbb{R}$

$$\Phi^{\varepsilon}_{\boldsymbol{k}}(\boldsymbol{x},t)=\widetilde{U}^{\varepsilon}(t,s)\Phi^{\varepsilon}_{\boldsymbol{k}}(\boldsymbol{x},s)\,. \tag{2.21}$$

Moreover, they track the classical phase space trajectory $(\boldsymbol{a}(t),\,\boldsymbol{\eta}(t))$ *in the sense that (for all* $t\in\mathbb{R}$*),*

$$\begin{aligned}
\langle\Phi^{\varepsilon}_{\boldsymbol{k}}(\boldsymbol{x},t),\,\boldsymbol{x}\,\Phi^{\varepsilon}_{\boldsymbol{k}}(\boldsymbol{x},t)\rangle&=\boldsymbol{a}(t)\,,\\
\langle\Phi^{\varepsilon}_{\boldsymbol{k}}(\boldsymbol{x},t),\,\boldsymbol{p}\,\Phi^{\varepsilon}_{\boldsymbol{k}}(\boldsymbol{x},t)\rangle&=\boldsymbol{\eta}(t)
\end{aligned} \tag{2.22}$$

and for any multi-index $\alpha \in \mathbb{N}^n$ there are $C_1 < \infty$ and $C_2 < \infty$ (depending on $\boldsymbol{k}, \alpha$ and the matrix norm $\|A(t)\|$ resp. on $\boldsymbol{k}, \alpha$ and $\|B(t)\|$) such that

$$\begin{aligned} \|(\boldsymbol{x} - \boldsymbol{a}(t))^\alpha \Phi^\varepsilon_{\boldsymbol{k}}(\boldsymbol{x}, t)\|_2 &\leq C_1 \varepsilon^{\frac{|\alpha|}{2}} , \\ \|(\boldsymbol{p} - \boldsymbol{\eta}(t))^\alpha \Phi^\varepsilon_{\boldsymbol{k}}(\boldsymbol{x}, t)\|_2 &\leq C_2 \varepsilon^{\frac{|\alpha|}{2}} . \end{aligned} \tag{2.23}$$

Here $\| \cdot \|_2$ denotes the L^2-norm.

(ii) The $\Phi^\varepsilon_{\boldsymbol{k}}$s and their gradients scale in ε as follows: For all $T > 0$ there are constants $C < \infty$, $C' < \infty$ (depending on $\boldsymbol{k}$, $A(t)$ and $B(t)$) such that

$$\begin{aligned} |\Phi^\varepsilon_{\boldsymbol{k}}(\boldsymbol{x}, t)| &= \varepsilon^{-\frac{n}{4}} \Big| \Phi_{\boldsymbol{k}}\Big(A(t), B(t), 1, 0, 0, \frac{\boldsymbol{x} - \boldsymbol{a}(t)}{\sqrt{\varepsilon}}\Big)\Big| \\ &\leq \varepsilon^{-\frac{n}{4}} C \Big(1 + \frac{|\boldsymbol{x} - \boldsymbol{a}(t)|}{\sqrt{\varepsilon}}\Big)^k e^{-\frac{1}{2} C \left(\frac{|\boldsymbol{x} - \boldsymbol{a}(t)|}{\sqrt{\varepsilon}}\right)^2} \leq C' \varepsilon^{-\frac{n}{4}} \end{aligned} \tag{2.24}$$

and

$$\begin{aligned} \Big|\nabla \Phi^\varepsilon_{\boldsymbol{k}}(\boldsymbol{x}, t) - \frac{i}{\varepsilon} \boldsymbol{\eta}(t) \Phi^\varepsilon_{\boldsymbol{k}}(\boldsymbol{x}, t)\Big| &= \varepsilon^{-\frac{1}{2}} \Big| \frac{\boldsymbol{p} - \boldsymbol{\eta}(t)}{\sqrt{\varepsilon}} \Phi^\varepsilon_{\boldsymbol{k}}(\boldsymbol{x}, t)\Big| \\ &\leq \varepsilon^{-\left(\frac{n}{4} + \frac{1}{2}\right)} C \Big(1 + \frac{|\boldsymbol{x} - \boldsymbol{a}(t)|}{\sqrt{\varepsilon}}\Big)^{k+1} e^{-\frac{1}{2} C \left(\frac{|\boldsymbol{x} - \boldsymbol{a}(t)|}{\sqrt{\varepsilon}}\right)^2} \leq C' \varepsilon^{-\left(\frac{n}{4} + \frac{1}{2}\right)} \end{aligned} \tag{2.25}$$

for all $t \in [0, T]$ and $\boldsymbol{x} \in \mathbb{R}^n$. Remember that with the usual multi-index notation $k = |\boldsymbol{k}| = k_1 + \ldots + k_n$.

For a proof of (i) see [25]. Note that (2.22) and (2.23) are direct consequences of Proposition 2 (iii) and the fact that the $\Phi^\varepsilon_{\boldsymbol{k}}$s are orthonormal. (ii) follows from Proposition 2 (ii) by a straightforward calculation (cf. subsection 2.4.4). The idea is that, as generalized n-dimensional Hermite function, every $\Phi^\varepsilon_{\boldsymbol{k}}$ is a product of a (generalized n-dimensional Hermite) polynomial of order k in the components of $\frac{\boldsymbol{x} - \boldsymbol{a}(t)}{\sqrt{\varepsilon}}$ and a *normalized* Gaussian wave packet centered at $\boldsymbol{a}(t)$ and with width $\sim \sqrt{\varepsilon}$. Thus the $\varepsilon^{-\frac{n}{4}}$ is in fact just a normalization constant. Regarding (2.25) one should think of $\frac{\boldsymbol{p} - \boldsymbol{\eta}(t)}{\sqrt{\varepsilon}}$ as a liner combination of a lowering and a *raising* operator, so we end up with having to estimate a polynomial of order $k + 1$ times a Gaussian.

2.2 Bohmian trajectories of semiclassical wave packets

We return to $n = 3$ and consider Hamiltonians $H^\varepsilon = -\frac{\varepsilon^2}{2} \triangle + V(\boldsymbol{x})\,,\ \mathcal{D}(H^\varepsilon) \subset L^2(\mathbb{R}^3)$, with $V \in G_V$ and wave functions $\psi^\varepsilon_{\boldsymbol{k}}(\boldsymbol{x}, t)$ that are solutions of the Schrödinger equation (2.1) with initial wave function $\psi^\varepsilon_{\boldsymbol{k}}(\boldsymbol{x}, 0) = \Phi^\varepsilon_{\boldsymbol{k}}(\boldsymbol{x}, 0)$:

$$\psi^\varepsilon_{\boldsymbol{k}}(\boldsymbol{x}, t) = U^\varepsilon(t) \Phi^\varepsilon_{\boldsymbol{k}}(\boldsymbol{x}, 0) \qquad \text{for all } t \in \mathbb{R}.$$

For these wave functions we get that in the limit $\varepsilon \to 0$ $\mathbb{P}^{\psi^\varepsilon_{\boldsymbol{k}}(\cdot,0)}$-almost every Bohmian trajectory becomes classical in the sense that it stays close to the corresponding classical trajectory for arbitrary long time.

Theorem 1. *Let $V \in G_V$. Then*

(i) the Bohmian trajectories $\boldsymbol{X}(\boldsymbol{x}_0, t)$ exist uniquely and globally in time for $\mathbb{P}^{\psi^\varepsilon_{\boldsymbol{k}}(\cdot,0)}$-almost all initial positions $\boldsymbol{x}_0 \in \mathbb{R}^3$,

(ii) for all $T > 0$, $\gamma > 0$ and all multi-indices $\boldsymbol{k} \in \mathbb{N}^3$ there exists some $R < \infty$ and some $\varepsilon_0 > 0$ such that

$$\mathbb{P}^{\psi^\varepsilon_{\boldsymbol{k}}(\cdot,0)}(\{\boldsymbol{x}_0 \in \mathbb{R}^3 \mid \max_{t\in[0,T]} |\boldsymbol{X}(\boldsymbol{x}_0,t) - \boldsymbol{a}(t)| \le R\sqrt{\varepsilon}\}) > 1 - \gamma \tag{2.26}$$

for all $0 < \varepsilon \le \varepsilon_0$.

For the proof we shall use that the probability that a Bohmian trajectory crosses a certain surface (here the moving sphere $S_{R\sqrt{\varepsilon}}(\boldsymbol{a}(t))$) is bounded by the quantum probability flux across this surface (see subsection 2.4.1). So we will need pointwise estimates on the quantum probability current density $\boldsymbol{j}^{\psi^\varepsilon_{\boldsymbol{k}}} = \boldsymbol{v}^{\psi^\varepsilon_{\boldsymbol{k}}} |\psi^\varepsilon_{\boldsymbol{k}}|^2 = \varepsilon \mathrm{Im}[(\psi^\varepsilon_{\boldsymbol{k}})^* \nabla \psi^\varepsilon_{\boldsymbol{k}}]$, that is on $\psi^\varepsilon_{\boldsymbol{k}}$ and $\nabla\psi^\varepsilon_{\boldsymbol{k}}$. In [24, 25] Hagedorn showed that the semiclassical time evolution of the wave packets $\Phi^\varepsilon_{\boldsymbol{k}}(\boldsymbol{x},t) = \widetilde{U}^\varepsilon(t,0)\Phi^\varepsilon_{\boldsymbol{k}}(\boldsymbol{x},0)$ is a good approximation for the Schrödinger time evolution $\psi^\varepsilon_{\boldsymbol{k}}(\boldsymbol{x},t) = U^\varepsilon(t)\Phi^\varepsilon_{\boldsymbol{k}}(\boldsymbol{x},0)$; in L^2-norm the error is of order $\sqrt{\varepsilon}$ better than the leading order term $\Phi^\varepsilon_{\boldsymbol{k}}$. That the same holds true also pointwise is the main *technical* result of this work.

Lemma 1. *Let $V \in G_V$. Then for all multi-indices $\boldsymbol{k} \in \mathbb{N}^3$ and all $T > 0$ there exists some constant $C < \infty$ such that*

$$\max_{t\in[0\,,T]} \|\psi^\varepsilon_{\boldsymbol{k}}(\cdot\,,t) - \Phi^\varepsilon_{\boldsymbol{k}}(\cdot\,,t)\|_\infty \le C\varepsilon^{-\frac{1}{4}} \tag{2.27}$$

and

$$\max_{t\in[0\,,T]} \|\,|\nabla\psi^\varepsilon_{\boldsymbol{k}}(\cdot\,,t) - \nabla\Phi^\varepsilon_{\boldsymbol{k}}(\cdot\,,t)|\,\|_\infty \le C\varepsilon^{-\frac{5}{4}}\,. \tag{2.28}$$

Here $\|\cdot\|_\infty = \sup_{\boldsymbol{x}\in\mathbb{R}^3} |\cdot|$ denotes the sup-norm (not just the L^∞-norm).

For the proof see subsection 2.4.3.

Remark 3. Note that on the macroscopic scale the wave packets' supremum norm $\|\Phi^\varepsilon_{\boldsymbol{k}}\|_\infty$ tend to infinity for $\varepsilon \to 0$. More precisely, by (2.24) and (2.25) $\|\Phi^\varepsilon_{\boldsymbol{k}}\|_\infty \sim \varepsilon^{-\frac{3}{4}}$ resp. $\|\,|\nabla\Phi^\varepsilon_{\boldsymbol{k}}|\,\|_\infty \sim \varepsilon^{-\frac{7}{4}}$. Thus the pointwise errors (2.27) and (2.28) are indeed of order $\sqrt{\varepsilon}$ better than the leading order terms.

Theorem 1 is a result about a particle's typical Bohmian trajectory, i.e. about its position. But what about its velocity?

While we believe that a statement analogous to (2.26) is true also for a particle's velocity, i.e.

$$\mathbb{P}^{\psi^\varepsilon_{\boldsymbol{k}}(\cdot,0)}(\{\boldsymbol{x}_0 \in \mathbb{R}^3 \mid \max_{t\in[0,T]} |\boldsymbol{v}^{\psi^\varepsilon_{\boldsymbol{k}}}(\boldsymbol{X}(\boldsymbol{x}_0,t),t) - \boldsymbol{\eta}(t)| \leq C\sqrt{\varepsilon}\}) > 1-\gamma \tag{2.29}$$

for some $C < \infty$ and all ε small enough, there is a major technical difficulty in proving it for general $\boldsymbol{k} \in \mathbb{N}^3$. The problem is that we cannot sufficiently controll the Bohmian velocity field $\boldsymbol{v}^{\psi^\varepsilon_{\boldsymbol{k}}} = \varepsilon \mathrm{Im}\left(\frac{\nabla\psi^\varepsilon_{\boldsymbol{k}}}{\psi^\varepsilon_{\boldsymbol{k}}}\right)$ in the vicinity of the wave function's nodes. For (2.29) we need that

$$\left|\boldsymbol{v}^{\psi^\varepsilon_{\boldsymbol{k}}} - \boldsymbol{\eta}\right| = \left|\mathrm{Im}\frac{\varepsilon\nabla\psi^\varepsilon_{\boldsymbol{k}} - i\boldsymbol{\eta}\psi^\varepsilon_{\boldsymbol{k}}}{\psi^\varepsilon_{\boldsymbol{k}}}\right| \leq \frac{|\varepsilon\nabla\psi^\varepsilon_{\boldsymbol{k}} - i\boldsymbol{\eta}\psi^\varepsilon_{\boldsymbol{k}}|}{|\psi^\varepsilon_{\boldsymbol{k}}|}$$

– evaluated on a typical Bohmian trajectory $\boldsymbol{X}(\boldsymbol{x}_0,t)$ – is well behaved (i.e. of order $\sqrt{\varepsilon}$). For the numerator we can find an upper bound that scales like $\varepsilon^{-\frac{1}{4}}$ and holds even for all $\boldsymbol{x} \in \mathbb{R}^3$. Regarding the denominator we know that for ε small enough $|\psi^\varepsilon_{\boldsymbol{k}}| \approx |\Phi^\varepsilon_{\boldsymbol{k}}|$ pointwise (Lemma 1) and that by (2.25) $|\Phi^\varepsilon_{\boldsymbol{k}}(\boldsymbol{x},t)| = \varepsilon^{-\frac{3}{4}}|\Phi_{\boldsymbol{k}}(A(t),B(t),1,0,0,\frac{\boldsymbol{x}-\boldsymbol{a}(t)}{\sqrt{\varepsilon}})|$ scales like $\varepsilon^{-\frac{3}{4}}$. So we indeed get what we desire *as long as the trajectory* $\boldsymbol{X}(\boldsymbol{x}_0,t)$ *does not come too close to a node of* $\psi^\varepsilon_{\boldsymbol{k}}$ *resp.* $\Phi^\varepsilon_{\boldsymbol{k}}$ (as long as $\left|\Phi_{\boldsymbol{k}}\big(A(t),B(t),1,0,0,\frac{\boldsymbol{X}(\boldsymbol{x}_0,t)-\boldsymbol{a}(t)}{\sqrt{\varepsilon}}\big)\right| > \delta > 0$):

Lemma 2. *Let* $V \in G_V$*. Then for all* $T > 0\,,\delta > 0$ *and all multi-indices* $\boldsymbol{k} \in \mathbb{R}^3$ *there exists some* $C < \infty$ *and some* $\varepsilon_0 > 0$ *such that for all* $0 < \varepsilon \leq \varepsilon_0$

$$|\boldsymbol{v}^{\psi^\varepsilon_{\boldsymbol{k}}}(\boldsymbol{x},t) - \boldsymbol{\eta}(t)| \leq C\sqrt{\varepsilon} \tag{2.30}$$

for all $t \in [0,T]$ *and all*

$$\boldsymbol{x} \in G^\varepsilon_{\boldsymbol{k},\delta}(t) := \left\{\boldsymbol{x} \in \mathbb{R}^3 \mid |\Phi^\varepsilon_{\boldsymbol{k}}(\boldsymbol{x},t)| > \varepsilon^{-\frac{3}{4}}\delta\right\}. \tag{2.31}$$

For the proof see subsection 2.4.2. So the real difficulty consists in showing that a typical Bohmian trajectory stays away far enough from the nodes of $\psi^\varepsilon_{\boldsymbol{k}}$: For all $T > 0$, $\gamma > 0$, $\boldsymbol{k} \in \mathbb{N}^3$ there exists some $\delta_{T,\boldsymbol{k}}(\gamma) > 0$ such that

$$\mathbb{P}^{\psi^\varepsilon_{\boldsymbol{k}}(\cdot,0)}\left(\left\{\boldsymbol{x}_0 \in \mathbb{R}^3 \mid \left|\Phi^\varepsilon_{\boldsymbol{k}}\big(\boldsymbol{X}(\boldsymbol{x}_0,t),t\big)\right| > \varepsilon^{-\frac{3}{4}}\delta_{T,\boldsymbol{k}}(\gamma) \text{ for all } t \in [0,T]\right\}\right) > 1-\gamma \tag{2.32}$$

for all ε small enough. Now, we already know the following. Since the Bohmian trajectories $\boldsymbol{X}(\boldsymbol{x}_0,t)$ exist uniquely and globally in time for $\mathbb{P}^{\psi^\varepsilon_{\boldsymbol{k}}(\cdot,0)}$-almost all initial positions $\boldsymbol{x}_0 \in \mathbb{R}^3$ (Theorem 1 (i)), a typical Bohmian trajectory cannot run into a node of $\psi^\varepsilon_{\boldsymbol{k}}$ (where the velocity field is ill defined, see also the end of section 1.2): For all $\gamma > 0$, $\varepsilon > 0$, $\boldsymbol{k} \in \mathbb{N}^3$ there is some $\delta^\varepsilon_{\boldsymbol{k}}(\gamma) > 0$ such that

$$\mathbb{P}^{\psi^\varepsilon_{\boldsymbol{k}}(\cdot,0)}\left(\left\{\boldsymbol{x}_0 \in \mathbb{R}^3 \mid |\psi^\varepsilon_{\boldsymbol{k}}(\boldsymbol{X}(\boldsymbol{x}_0,t),t)| > \delta^\varepsilon_{\boldsymbol{k}}(\gamma) \text{ for all } t \in \mathbb{R}\right\}\right) > 1-\gamma\,. \tag{2.33}$$

While this is a weaker statement than (2.32), by taking apart its proof in [6] one should be able to extract the ε-dependence of $\delta^\varepsilon_{\boldsymbol{k}}(\gamma)$ and thus to sharpen (2.33) to (2.32) (the proof in [39] is too abstract for that purpose). This, however, is beyond the scope of this work[7]. While we do not prove (2.29) for general $\boldsymbol{k} \in \mathbb{N}^3$, for the ground state $\boldsymbol{k} = 0$ it is an easy corollary to Theorem 1 and Lemma 2. Since Φ_0^ε is just a Gaussian, it does not possess any nodes. Neither does ψ_0^ε (for ε small enough). Thus:

Corollary 1. *Let $V \in G_V$. Then for all $T > 0$ and all $\gamma > 0$ there exists some $R < \infty$ and some $\varepsilon_0 > 0$ such that*

$$\mathbb{P}^{\psi_0^\varepsilon(\cdot,0)}\Big(\big\{\boldsymbol{x}_0 \in \mathbb{R}^3 \mid \max_{t\in[0,T]}|\boldsymbol{X}(\boldsymbol{x}_0,t) - \boldsymbol{a}(t)| \le R\sqrt{\varepsilon} \\ \wedge \max_{t\in[0,T]} |\boldsymbol{v}^{\psi_0^\varepsilon}(\boldsymbol{X}(\boldsymbol{x}_0,t),t) - \boldsymbol{\eta}(t)| \le R\sqrt{\varepsilon}\big\}\Big) > 1-\gamma \tag{2.34}$$

for all $0 < \varepsilon \le \varepsilon_0$.

For the proof see subsection 2.4.2.

The above notwithstanding, we remark that Theorem 1 indeed does give rise to a (somewhat weaker but *empirically* satisfying) statement on Bohmian velocities for any $\boldsymbol{k} \in \mathbb{N}^3$. Since a typical Bohmian trajectory may not deviate too much from its corresponding classical one, at least the time-averaged Bohmian velocity has to stay close to its classical counterpart. More precisely, for any macroscopic time interval $0 < \delta t \le \frac{T}{2}$ define the *time-averaged Bohmian and classical velocities* ($t \in [\delta t, T-\delta t]$)

$$\boldsymbol{v}_{\delta t}^{\psi_{\boldsymbol{k}}^\varepsilon}(\boldsymbol{x}_0,t) := \frac{1}{2\delta t}\int_{t-\delta t}^{t+\delta t} \boldsymbol{v}^{\psi_{\boldsymbol{k}}^\varepsilon}(\boldsymbol{X}(\boldsymbol{x}_0,s),s)\,ds\,,$$

$$\boldsymbol{\eta}_{\delta t}(t) := \frac{1}{2\delta t}\int_{t-\delta t}^{t+\delta t} \boldsymbol{\eta}(s)ds\,.$$

Now suppose $\boldsymbol{x}_0 \in \mathbb{R}^3$ is such that $\max_{t\in[0,T]} |\boldsymbol{X}(\boldsymbol{x}_0,t) - \boldsymbol{a}(t)| \le R\sqrt{\varepsilon}$. Then

$$\begin{aligned}|\boldsymbol{v}_{\delta t}^{\psi_{\boldsymbol{k}}^\varepsilon}(\boldsymbol{x}_0,t) - \boldsymbol{\eta}_{\delta t}(t)| &= \frac{1}{2\delta t}\Big|\int_{t-\delta t}^{t+\delta t}\big(\boldsymbol{v}^{\psi_{\boldsymbol{k}}^\varepsilon}(\boldsymbol{X}(\boldsymbol{x}_0,s),s) - \boldsymbol{\eta}(s)\big)ds\Big| \\ &\le \frac{1}{2\delta t}\big[\,|\boldsymbol{X}(\boldsymbol{x}_0,t+\delta t) - \boldsymbol{a}(t+\delta t)| + |\boldsymbol{X}(\boldsymbol{x}_0,t-\delta t) - \boldsymbol{a}(t-\delta t)|\,\big] \\ &\le \frac{R}{\delta t}\sqrt{\varepsilon}\,.\end{aligned}$$

So by Theorem 1 (*ii*) we immediately get

[7]Note that because of $|\psi_{\boldsymbol{k}}^\varepsilon| \approx |\Phi_{\boldsymbol{k}}^\varepsilon|$, the nodes of $\psi_{\boldsymbol{k}}^\varepsilon$ are essentially those of (the generalized Hermite functions) $\Phi_{\boldsymbol{k}}^\varepsilon$ and thus those of the generalized Hermite polynomials $\mathcal{H}_{\boldsymbol{k}}\Big(U_{A(t)}; R_{A(t)}\frac{\boldsymbol{x}-\boldsymbol{a}(t)}{\sqrt{\varepsilon}}\Big)$ (cf. (2.17)). Therefore |node of $\psi_{\boldsymbol{k}}^\varepsilon(\boldsymbol{x},t) - \boldsymbol{a}(t)| \sim \sqrt{\varepsilon}$, i.e. the nodes of $\psi_{\boldsymbol{k}}^\varepsilon$ live on the *same scale* as a typical Bohmian trajectoy and there is no "simple" scaling-like proof of (2.32).

Corollary 2. *Let $V \in G_V$. Then for all $T > 0$, $\gamma > 0$ and all multi-indices $\boldsymbol{k} \in \mathbb{N}^3$ there exists some $R < \infty$ and some $\varepsilon_0 > 0$ such that for any $0 < \delta t \leq \frac{T}{2}$*

$$\mathbb{P}^{\psi^{\varepsilon}_{\boldsymbol{k}}(\cdot,0)}\left(\left\{\boldsymbol{x}_0 \in \mathbb{R}^3 \mid \max_{t\in[\delta t, T-\delta t]} |\boldsymbol{v}^{\psi^{\varepsilon}_{\boldsymbol{k}}}_{\delta t}(\boldsymbol{x}_0, t) - \boldsymbol{\eta}_{\delta t}(t)| \leq \frac{R}{\delta t}\sqrt{\varepsilon}\right\}\right) > 1 - \gamma \tag{2.35}$$

for all $0 < \varepsilon \leq \varepsilon_0$.

Note that measuring macroscopic velocities generically involves some kind of macroscopic time averaging (as, for example, when calculating an object's velocity by measuring its time of flight across a given distance). So Corollary 2 in fact implies that *empirically* the Bohmian velocity along a typical trajectory cannot be distinguished from its classical counterpart in the limit $\varepsilon \to 0$.

2.3 Some remarks and a short outlook

We have presented results on a single "particle", that is on the center of mass of a single macroscopic body in an external potential. We remark that our method works also for more than one such "particle", i.e. in higher dimensions $n = 3N,\ N > 1$. Since we use an instance of Gagliardo-Nirenberg (a Sobolev-type) inequality to prove the pointwise estimates of Lemma 1, one would, however, need L^2-estimates for higher order derivatives of $\psi^{\varepsilon}_{\boldsymbol{k}} - \Phi^{\varepsilon}_{\boldsymbol{k}}$. As explained at the end of the overview at the very beginning of this chapter this necessitates commuting correspondingly higher powers of $\boldsymbol{p}$ with the Schrödinger time evolution $e^{-\frac{i}{\varepsilon}H^{\varepsilon}t}$, which then leads to more severe restrictions on the potential V, namely that also higher (than fourth) order derivatives of V must be uniformly bounded.

In this context note also that Lemma 1 is most probable a stronger result than necessary to get Theorem 1. Remember that we prove that a typical Bohmian trajectory stays in a neighborhood of the classical trajectory $\boldsymbol{a}(t)$ by showing that the probability flux out of this neighborhood is negligible. So we in fact need pointwise estimates analogous to (2.27) and (2.28) and thus control over the Bohmian velocity field resp. the flux only in a sufficiently big neighborhood of the classical trajectory $\boldsymbol{a}(t),\ t \in [0, T]$. In other words: Since we expect typical Bohmian trajectories to stay close to $\boldsymbol{a}(t)$, we should have no need of knowledge on the velocity field far away from $\boldsymbol{a}(t)$. But then also the potential far away from $\boldsymbol{a}(t)$ should not play too big a role, i.e. it should be possible to replace the requirement of uniform boundedness of the potential and its derivatives by boundedness on an appropriate compactum. The latter, however, is already a consequence of the potential's regularity.

So far we have talked only about Bohmian trajectories made by wave functions that are initially a Hagedorn wave packet $\Phi^{\varepsilon}_{\boldsymbol{k}}$. But what about more general wave functions? What are the next steps towards a more general classical limit of Bohmian mechanics? In [3] Allori et al. outlined a general program for the classical limit of Bohmian mechanics where they also argued that one should be able to reduce the case of general initial wave functions to that of semiclassical wave packets (like, for example, Hagedorn's). Summarized the idea is that due to the (for $\varepsilon \to 0$ dominating) dispersive character of the free Schrödinger evolution a general initial wave function should evolve into a so called local plane wave on a *microscopic* time scale. Here a local plane wave is essentially a sum of semiclassical wave packets that evolve "side by side" without appreciably interfering with each other. Since a particle's actual Bohmian position is always in the support of one wave packet only, this implies that one should be able to neglect the "empty" wave packets' effects on the particle's evolution, that is that one should be able to effectively collapse the local plane wave to just one semiclassical wave packet. Allori et al. also took care of the caveat that this simple scheme generally breaks down at the "first caustic time" of the classical dynamics: Remember that this is the first time at which the classical action becomes multivalued which corresponds to a crossing of classical trajectories in configuration space[8]. Since the semiclassical wave packets (that make up the local plane wave) follow the classical trajectories, they will interfere and one can thus no longer neglect the "empty" wave packets[9]. It is at this point where one has to abandon the idealization of the isolated particle and invoke the effects of the environment (i.e. decoherence) to get a *stable* collapse of the local plane wave to the wave packet containing the particle's actual position.

A prominent example for the formation of local plane waves is given by the free Schrödinger evolution respectively by the asymptotically free Schrödinger evolution in scattering situations. In chapter 3 we show that this indeed yields classical behavior of the Bohmian trajectories (Theorems 2 and 4).

2.4 Proof

2.4.1 Proof of Theorem 1

(i) is a direct consequence of Proposition 1 if we can show that the initial wave function $\psi^\varepsilon_{\boldsymbol{k}}(\cdot,0) = \Phi^\varepsilon_{\boldsymbol{k}}(\cdot,0)$ is a C^∞-vector of H^ε, $\Phi^\varepsilon_{\boldsymbol{k}}(\cdot,0) \in C^\infty(H^\varepsilon) = \bigcap_{n=1}^{\infty} \mathcal{D}\left((H^\varepsilon)^n\right)$. Note that $V \in G_V$ guarantees that H^ε maps the Schwartz space $\mathcal{S}(\mathbb{R}^3)$ into itself. Consequently $\mathcal{S}(\mathbb{R}^3) \subset C^\infty(H^\varepsilon)$. Since obviously $\Phi^\varepsilon_{\boldsymbol{k}}(\cdot,0) \in \mathcal{S}(\mathbb{R}^3)$, we are done.

We proceed with the proof of (ii). Let $\gamma > 0$. For $\varepsilon > 0$ and $R > 0$ define

$$G^\varepsilon_R := \left\{ \boldsymbol{x}_0 \in \mathbb{R}^3 \mid \max_{t\in[0,T]} |\boldsymbol{X}(\boldsymbol{x}_0,t) - \boldsymbol{a}(t)| < R\sqrt{\varepsilon} \right\}.$$

Our task is to show that, for suitable R and ε, the measure of $(G^\varepsilon_R)^c$ is smaller than γ. The idea is to show that $\mathbb{P}^{\psi^\varepsilon_{\boldsymbol{k}}(\cdot,0)}$-almost no trajectory starts outside a ball with radius $\sim \sqrt{\varepsilon}$ and center $\boldsymbol{a}(0)$ (easy L^2-result) and to use the quantum probability flux to see that a trajectory with starting point in this ball nearly never leaves a $\sqrt{\varepsilon}$-neighborhood

[8] In confining potentials this *typically* happens.

[9] Put differently: At the "edges" of a confining potential the dispersive character of the free Schrödinger evolution is no longer dominating, so the local plane wave structure breaks down.

of the classical trajectory $\boldsymbol{a}(t)$. Thus we write

$$\begin{aligned}
&\mathbb{P}^{\psi^\varepsilon_{\boldsymbol{k}}(\cdot,0)}\big((G^\varepsilon_R)^c\big)\\
&\leq \mathbb{P}^{\psi^\varepsilon_{\boldsymbol{k}}(\cdot,0)}\left(\left\{\boldsymbol{x}_0 \in \mathbb{R}^3 \mid |\boldsymbol{x}_0 - \boldsymbol{a}(0)| \geq R\sqrt{\varepsilon}\right\}\right)\\
&\quad + \mathbb{P}^{\psi^\varepsilon_{\boldsymbol{k}}(\cdot,0)}\left(\left\{\boldsymbol{x}_0 \mid |\boldsymbol{x}_0 - \boldsymbol{a}(0)| < R\sqrt{\varepsilon} \wedge \exists\, t \in (0,T] : |\boldsymbol{X}(\boldsymbol{x}_0,t) - \boldsymbol{a}(t)| \geq R\sqrt{\varepsilon}\right\}\right)\\
&=: \mathbb{P}^{\psi^\varepsilon_{\boldsymbol{k}}(\cdot,0)}\left(B_{R\sqrt{\varepsilon}}(\boldsymbol{a}(0))^c\right) + \mathbb{P}^{\psi^\varepsilon_{\boldsymbol{k}}(\cdot,0)}\left(\mathcal{M}^T_{R\sqrt{\varepsilon}}(\boldsymbol{a}(0))\right) .
\end{aligned} \tag{2.36}$$

Regarding the first summand note that $\psi^\varepsilon_{\boldsymbol{k}}(\cdot,0) = \Phi^\varepsilon_{\boldsymbol{k}}(\cdot,0)$ and that by (2.24)

$$|\Phi^\varepsilon_{\boldsymbol{k}}(\boldsymbol{x},t)| = \varepsilon^{-\frac{3}{4}}\left|\Phi_{\boldsymbol{k}}\Big(A(t), B(t), 1, 0, 0, \frac{\boldsymbol{x}-\boldsymbol{a}(t)}{\sqrt{\varepsilon}}\Big)\right|$$

for any $t \in \mathbb{R}$. Substituting $\boldsymbol{y} = \frac{\boldsymbol{x}-\boldsymbol{a}(0)}{\sqrt{\varepsilon}}$ this in particular yields ($y := |\boldsymbol{y}|$)

$$\mathbb{P}^{\psi^\varepsilon_{\boldsymbol{k}}(\cdot,0)}\left(B_{R\sqrt{\varepsilon}}(\boldsymbol{a}(0))^c\right) = \int\limits_{|\boldsymbol{x}-\boldsymbol{a}(0)|\geq R\sqrt{\varepsilon}} |\Phi^\varepsilon_{\boldsymbol{k}}(\boldsymbol{x},0)|^2\, d^3x = \int\limits_{y\geq R} |\Phi_{\boldsymbol{k}}(A(0), B(0), 1, 0, 0, \boldsymbol{y})|^2\, d^3y\,.$$

Since $\Phi_{\boldsymbol{k}}(A(0), B(0), 1, 0, 0, \cdot)$ is square summable (in fact it is normalized) we see that there is some $R' < \infty$ *independent* of ε such that

$$\mathbb{P}^{\psi^\varepsilon_{\boldsymbol{k}}(\cdot,0)}\left(B_{R\sqrt{\varepsilon}}(\boldsymbol{a}(0))^c\right) \leq \frac{\gamma}{2} \tag{2.37}$$

for all $R > R'$. Thus we are left with the task to find a suitable estimate for $\mathbb{P}^{\psi^\varepsilon_{\boldsymbol{k}}(\cdot,0)}\big(\mathcal{M}^T_{R\sqrt{\varepsilon}}(\boldsymbol{a}(0))\big)$.

Since $\boldsymbol{X}(\boldsymbol{x}_0,t)$ (as a solution of (2.2)) is continuous in t, $x_0 \in \mathcal{M}^T_{R\sqrt{\varepsilon}}(\boldsymbol{a}(0))$ implies that $\boldsymbol{X}(\boldsymbol{x}_0,t)$ crosses the moving sphere $S_{R\sqrt{\varepsilon}}(\boldsymbol{a}(t))$ at least once and outwards in $(0,T]$. Therefore $\mathbb{P}^{\psi^\varepsilon_{\boldsymbol{k}}(\cdot,0)}\big(\mathcal{M}^T_{R\sqrt{\varepsilon}}(\boldsymbol{a}(0))\big)$ is bounded from above by the probability that some trajectory crosses $S_{R\sqrt{\varepsilon}}(\boldsymbol{a}(t))$ in any direction in $(0,T]$. In Subsection 2.3.2 of [6] Berndl invoked the probabilistic meaning of the quantum probability current density

$$\begin{aligned}
J^\psi(\boldsymbol{x},t) &= \big(\boldsymbol{j}^\psi(\boldsymbol{x},t),\, |\psi(\boldsymbol{x},t)|^2\big)\\
&:= \big(\boldsymbol{v}^\psi(\boldsymbol{x},t)|\psi(\boldsymbol{x},t)|^2,\, |\psi(\boldsymbol{x},t)|^2\big) = \big(\varepsilon \mathrm{Im}\big(\psi^*(\boldsymbol{x},t)\nabla\psi(\boldsymbol{x},t)\big),\, |\psi(\boldsymbol{x},t)|^2\big)
\end{aligned}$$

to prove that the expected number of crossings[10] of a smooth surface Σ in configuration-space-time by the random configuration-space-time trajectory $(\boldsymbol{X}(\cdot,t)\,,\, t)$ is given by the modulus of the flux across this surface,

$$\int\limits_\Sigma \left|J^\psi(\boldsymbol{x},t)\cdot \boldsymbol{U}\right|\, d\sigma\,,$$

where $\boldsymbol{U}$ denotes the local unit normal vector at $(\boldsymbol{x},t)$ (see also the argument given in [5], p. 11.). Since any trajectory $(\boldsymbol{X}(\boldsymbol{x}_0,t)\,,\, t)$ crosses Σ an integral number of times

[10]This also includes tangential "crossings" in which the trajectory remains on the same side of Σ.

(including 0 and ∞) this expected value gives an upper bound for the probability that $(\boldsymbol{X}(\boldsymbol{x}_0, t)\,,\, t)$ crosses Σ. So in our case we obtain

$$\mathbb{P}^{\psi^\varepsilon_{\boldsymbol{k}}(\cdot,0)}\Big(\mathcal{M}^T_{R\sqrt{\varepsilon}}(\boldsymbol{a}(0))\Big) \le \int_{\Sigma^\varepsilon_T} \Big|J^{\psi^\varepsilon_{\boldsymbol{k}}}(\boldsymbol{x},t)\cdot \boldsymbol{U}\Big|\, d\sigma \tag{2.38}$$

where

$$\Sigma^\varepsilon_T = \{(\boldsymbol{x},\, t) \mid\; t\in[0,T],\, \boldsymbol{x}\in S_{R\sqrt{\varepsilon}}(\boldsymbol{a}(t))\}$$

and $\boldsymbol{U} = \frac{1}{\sqrt{1+\langle \boldsymbol{\eta}(t),\, \widehat{e}_r\rangle^2}}\Big(\widehat{e}_r, -\langle \boldsymbol{\eta}(t),\, \widehat{e}_r\rangle\Big)$, $d\sigma = \sqrt{1+\langle \boldsymbol{\eta}(t),\, \widehat{e}_r\rangle^2}\,\varepsilon R^2 d\Omega\, dt$. Here we have used spatial polar coordinates centered at $\boldsymbol{a}(t)$ so that $\widehat{e}_r = (\cos\varphi\sin\theta, \sin\varphi\sin\theta, \cos\theta)$ and $d\Omega = \sin\theta\, d\varphi\, d\theta$. Thus

$$\begin{aligned} |J^{\psi^\varepsilon_{\boldsymbol{k}}}(\boldsymbol{x},t)\cdot\boldsymbol{U}|\, d\sigma &= \big|\big\langle \boldsymbol{j}^{\psi^\varepsilon_{\boldsymbol{k}}}(\boldsymbol{x},t) - |\psi^\varepsilon_{\boldsymbol{k}}(\boldsymbol{x},t)|^2\boldsymbol{\eta}(t),\, \widehat{e}_r\big\rangle\big|\,\varepsilon R^2 d\Omega \\ &\le |\boldsymbol{j}^{\psi^\varepsilon_{\boldsymbol{k}}}(\boldsymbol{x},t) - |\psi^\varepsilon_{\boldsymbol{k}}(\boldsymbol{x},t)|^2\boldsymbol{\eta}(t)|\varepsilon R^2 d\Omega \end{aligned} \tag{2.39}$$

where $\boldsymbol{j}^{\psi^\varepsilon_{\boldsymbol{k}}}(\boldsymbol{x},t) - |\psi^\varepsilon_{\boldsymbol{k}}(\boldsymbol{x},t)|^2\boldsymbol{\eta}(t)$ is evaluated at points $(\boldsymbol{x},t)\in\Sigma^\varepsilon_T$. By the definition of $\boldsymbol{j}^\psi$ and since $\boldsymbol{\eta}(t)$ is always real

$$\begin{aligned} \big|\boldsymbol{j}^{\psi^\varepsilon_{\boldsymbol{k}}}(\boldsymbol{x},t) - |\psi^\varepsilon_{\boldsymbol{k}}(\boldsymbol{x},t)|^2\boldsymbol{\eta}(t)\big| &= \big|\mathrm{Im}\big[(\psi^\varepsilon_{\boldsymbol{k}})^*(\boldsymbol{x},t)\big(\varepsilon\nabla\psi^\varepsilon_{\boldsymbol{k}}(\boldsymbol{x},t) - i\boldsymbol{\eta}(t)\psi^\varepsilon_{\boldsymbol{k}}(\boldsymbol{x},t)\big)\big]\big| \\ &\le |\psi^\varepsilon_{\boldsymbol{k}}(\boldsymbol{x},t)|\,|\varepsilon\nabla\psi^\varepsilon_{\boldsymbol{k}}(\boldsymbol{x},t) - i\boldsymbol{\eta}(t)\psi^\varepsilon_{\boldsymbol{k}}(\boldsymbol{x},t)| \\ &\le \Big(|\Phi^\varepsilon_{\boldsymbol{k}}(\boldsymbol{x},t)| + |\psi^\varepsilon_{\boldsymbol{k}}(\boldsymbol{x},t) - \Phi^\varepsilon_{\boldsymbol{k}}(\boldsymbol{x},t)|\Big)\Big(\varepsilon|\nabla\psi^\varepsilon_{\boldsymbol{k}}(\boldsymbol{x},t) - \nabla\Phi^\varepsilon_{\boldsymbol{k}}(\boldsymbol{x},t)| \\ &\qquad + \eta(t)\,|\psi^\varepsilon_{\boldsymbol{k}}(\boldsymbol{x},t) - \Phi^\varepsilon_{\boldsymbol{k}}(\boldsymbol{x},t)| + |\varepsilon\nabla\Phi^\varepsilon_{\boldsymbol{k}}(\boldsymbol{x},t) - i\boldsymbol{\eta}(t)\Phi^\varepsilon_{\boldsymbol{k}}(\boldsymbol{x},t)|\Big)\,. \end{aligned}$$

Then by (2.24), (2.25) and Lemma 1

$$\begin{aligned} &\big|\boldsymbol{j}^{\psi^\varepsilon_{\boldsymbol{k}}}(\boldsymbol{x},t) - |\psi^\varepsilon_{\boldsymbol{k}}(\boldsymbol{x},t)|^2\boldsymbol{\eta}(t)\big| \\ &\quad\le \left[C\varepsilon^{-\frac34}\left(1+\frac{|\boldsymbol{x}-\boldsymbol{a}(t)|}{\sqrt{\varepsilon}}\right)^k e^{-\frac12 C\left(\frac{|\boldsymbol{x}-\boldsymbol{a}(t)|}{\sqrt{\varepsilon}}\right)^2} + C\varepsilon^{-\frac14}\right] \\ &\qquad\qquad \left[C\varepsilon^{-\frac14} + C\varepsilon^{-\frac14}\left(1+\frac{|\boldsymbol{x}-\boldsymbol{a}(t)|}{\sqrt{\varepsilon}}\right)^{k+1} e^{-\frac12 C\left(\frac{|\boldsymbol{x}-\boldsymbol{a}(t)|}{\sqrt{\varepsilon}}\right)^2}\right] \\ &\quad\le C\left[\varepsilon^{-1}(1+R)^{2k+1}e^{-\frac12 CR^2} + \varepsilon^{-\frac12}\right] \end{aligned}$$

where we have used that $\eta(t)$ is continuous and thus bounded on $[0,T]$ and that $(\boldsymbol{x},t)\in\Sigma^\varepsilon_T$ entails $\frac{|\boldsymbol{x}-\boldsymbol{a}(t)|}{\sqrt{\varepsilon}} = R$. Plugging this into (2.39), we see that

$$\big|J^{\psi^\varepsilon_{\boldsymbol{k}}}(\boldsymbol{x},t)\cdot\boldsymbol{U}\big|\; d\sigma \le C\left[(1+R)^{2k+1}e^{-\frac12 CR^2} + \sqrt{\varepsilon}\right] R^2 d\Omega\,.$$

Thus by (2.38)

$$\begin{aligned} \mathbb{P}^{\psi^\varepsilon_{\boldsymbol{k}}(\cdot,0)}\Big(\mathcal{M}^T_{R\sqrt{\varepsilon}}(\boldsymbol{a}(0))\Big) &\le \int_0^T dt\int_0^{2\pi} d\varphi\int_0^\pi d\theta\sin(\theta)CR^2\left[(1+R)^{2k+1}e^{-\frac12 CR^2} + \sqrt{\varepsilon}\right] \\ &\le 2\pi TC\left[R^2(1+R)^{2k+1}e^{-\frac12 CR^2} + R^2\sqrt{\varepsilon}\right] < \frac{\gamma}{2} \end{aligned} \tag{2.40}$$

for R big and ε small enough.

Together (2.37) and (2.40) give the desired result:

$$\mathbb{P}^{\psi^\varepsilon_{\boldsymbol{k}}(\cdot,0)}\left(G^\varepsilon_R\right) = 1 - \mathbb{P}^{\psi^\varepsilon_{\boldsymbol{k}}(\cdot,0)}\left((G^\varepsilon_R)^c\right) > 1-\gamma$$

for all R big and all ε small enough.

2.4.2 Proof of Corollary 1 and Lemma 2

With Lemma 2 we can use the fact that the ground state Φ^ε_0 possesses no nodes to prove Corollary 1.

Proof of Corollary 1. Let $\gamma > 0$ and $T > 0$. By Theorem 1 there exists some $R < \infty$ and some $\varepsilon_0 > 0$ such that

$$\mathbb{P}^{\psi^\varepsilon_0}(\{\boldsymbol{x}_0 \in \mathbb{R}^3 \mid \max_{t\in[0,T]} |\boldsymbol{X}(\boldsymbol{x}_0,t) - \boldsymbol{a}(t)| \leq R\sqrt{\varepsilon}\}) > 1-\gamma$$

for all $0 < \varepsilon \leq \varepsilon_0$. Now let $\boldsymbol{x}_0 \in \mathbb{R}^3$ such that $\max\limits_{t\in[0,T]} |\boldsymbol{X}(\boldsymbol{x}_0,t) - \boldsymbol{a}(t)| \leq R\sqrt{\varepsilon}$. Then with the help of (2.12) (2.15) gives

$$\begin{aligned}
|\Phi^\varepsilon_0(\boldsymbol{X}(\boldsymbol{x}_0,t),t)| &= (\pi\varepsilon)^{-\frac{3}{4}} |\det(A(t))|^{-\frac{1}{2}}\, e^{-\frac{1}{2\varepsilon}\left\langle \boldsymbol{X}(\boldsymbol{x}_0,t)-\boldsymbol{a}(t),\, \mathrm{Re}(B(t)A(t)^{-1})(\boldsymbol{X}(\boldsymbol{x}_0,t)-\boldsymbol{a}(t))\right\rangle} \\
&\overset{(2.12)}{=} (\pi\varepsilon)^{-\frac{3}{4}} |\det(A(t))|^{-\frac{1}{2}}\, e^{-\frac{1}{2}\left|A(t)^{-1}\frac{\boldsymbol{X}(\boldsymbol{x}_0,t)-\boldsymbol{a}(t)}{\sqrt{\varepsilon}}\right|^2} \\
&\geq (\pi\varepsilon)^{-\frac{3}{4}} |\det(A(t))|^{-\frac{1}{2}}\, e^{-\frac{1}{2}\|A(t)\|^{-2}R^2}\,.
\end{aligned}$$

Since $A(t)$ is continuous (it solves (2.11)) and always invertible (cf. (2.12)), $\min\limits_{t\in[0,T]} |\det(A(t))|^{-\frac{1}{2}} > 0$ and $\min\limits_{t\in[0,T]} \|A(t)\|^{-2} > 0$. So there exists some $\delta > 0$ such that

$$\min_{t\in[0,T]} |\Phi^\varepsilon_0(\boldsymbol{X}(\boldsymbol{x}_0,t),t)| > \varepsilon^{-\frac{3}{4}}\delta\,,$$

i.e. such that $\boldsymbol{X}(\boldsymbol{x}_0,t) \in G^\varepsilon_{\boldsymbol{k},\delta}(t)$ for all $t \in [0,T]$. Then by Lemma 2

$$|\boldsymbol{v}^{\psi^\varepsilon_0}(\boldsymbol{X}(\boldsymbol{x}_0,t),t) - \boldsymbol{\eta}(t)| \leq C\sqrt{\varepsilon}$$

for some $C < \infty$ and all $t \in [0,T]$. □

So we are left to prove Lemma 2.

Proof of Lemma 2. Since $V \in G_V$ implies not only $V \in C^\infty(\mathbb{R}^3)$ but also $\psi^\varepsilon_{\boldsymbol{k}}(\boldsymbol{x},0) = \Phi^\varepsilon_{\boldsymbol{k}}(\boldsymbol{x},0) \in C^\infty(H^\varepsilon)$ (see beginning of proof of Theorem 1), one can use methods of elliptic regularity to show that $\psi^\varepsilon_{\boldsymbol{k}}(\boldsymbol{x},t) \in C^\infty(\mathbb{R}^3\times\mathbb{R})$ (Lemma 6.1 in [5]). Thus $\boldsymbol{v}^{\psi^\varepsilon_{\boldsymbol{k}}}(\boldsymbol{x},t)$ is well defined and C^∞ on $(\mathbb{R}^3\times\mathbb{R})\setminus\mathcal{N}$ where $\mathcal{N} = \{(\boldsymbol{x},t) \in \mathbb{R}^3\times\mathbb{R} \mid \psi^\varepsilon_{\boldsymbol{k}}(\boldsymbol{x},t) = 0\}$ is the set of nodes of $\psi^\varepsilon_{\boldsymbol{k}}$. Now let $t \in [0,T]\,, \boldsymbol{x} \in G^\varepsilon_{\boldsymbol{k},\delta}(t)$. Then by the definition (2.31) of $G^\varepsilon_{\boldsymbol{k},\delta}(t)$ and Lemma 1

$$|\psi^\varepsilon_{\boldsymbol{k}}(\boldsymbol{x},t)| \geq |\Phi^\varepsilon_{\boldsymbol{k}}(\boldsymbol{x},t)| - |\psi^\varepsilon_{\boldsymbol{k}}(\boldsymbol{x},t) - \Phi^\varepsilon_{\boldsymbol{k}}(\boldsymbol{x},t)| > \varepsilon^{-\frac{3}{4}}(\delta - C\sqrt{\varepsilon}) \geq \varepsilon^{-\frac{3}{4}}\frac{\delta}{2} > 0 \qquad (2.41)$$

for all $\varepsilon > 0$ small enough, i.e. $\boldsymbol{x} \in G^\varepsilon_{\boldsymbol{k},\delta}(t)$ guarantees not only $\Phi^\varepsilon_{\boldsymbol{k}}(\boldsymbol{x},t) \neq 0$ but also $\psi^\varepsilon_{\boldsymbol{k}}(\boldsymbol{x},t) \neq 0$ and thus that $\boldsymbol{v}^{\psi^\varepsilon_{\boldsymbol{k}}}(\boldsymbol{x},t) = \varepsilon \mathrm{Im}(\frac{\nabla\psi^\varepsilon_{\boldsymbol{k}}(\boldsymbol{x},t)}{\psi^\varepsilon_{\boldsymbol{k}}(\boldsymbol{x},t)})$ is well defined. So we may write

$$
\begin{aligned}
|\boldsymbol{v}^{\psi^\varepsilon_{\boldsymbol{k}}}(\boldsymbol{x},t) - \boldsymbol{\eta}(t)| &= \Big|\mathrm{Im}\Big(\frac{\varepsilon\nabla\psi^\varepsilon_{\boldsymbol{k}}(\boldsymbol{x},t) - i\boldsymbol{\eta}(t)\psi^\varepsilon_{\boldsymbol{k}}(\boldsymbol{x},t)}{\psi^\varepsilon_{\boldsymbol{k}}(\boldsymbol{x},t)}\Big)\Big| \\
&\leq \frac{\varepsilon|\nabla\psi^\varepsilon_{\boldsymbol{k}}(\boldsymbol{x},t) - \nabla\Phi^\varepsilon_{\boldsymbol{k}}(\boldsymbol{x},t)| + \eta(t)\,|\psi^\varepsilon_{\boldsymbol{k}}(\boldsymbol{x},t) - \Phi^\varepsilon_{\boldsymbol{k}}(\boldsymbol{x},t)| + |\varepsilon\nabla\Phi^\varepsilon_{\boldsymbol{k}}(\boldsymbol{x},t) - i\boldsymbol{\eta}(t)\Phi^\varepsilon_{\boldsymbol{k}}(\boldsymbol{x},t)|}{|\psi^\varepsilon_{\boldsymbol{k}}(\boldsymbol{x},t)|}\,.
\end{aligned}
$$

Using (2.25), that is

$$
|\varepsilon\nabla\Phi^\varepsilon_{\boldsymbol{k}}(\boldsymbol{x},t) - i\boldsymbol{\eta}(t)\Phi^\varepsilon_{\boldsymbol{k}}(\boldsymbol{x},t)| \leq C\varepsilon^{-\frac{1}{4}}\,,
$$

(2.41) and Lemma 1 we get ($\eta^T := \max_{t\in[0,T]}\eta(t) < \infty$ since $\boldsymbol{\eta}(t)$ is continuous)

$$
|\boldsymbol{v}^{\psi^\varepsilon_{\boldsymbol{k}}}(x,t) - \boldsymbol{\eta}(t)| \leq \frac{2}{\delta}\varepsilon^{\frac{3}{4}}[C\varepsilon^{-\frac{5}{4}+1} + C\eta^T\varepsilon^{-\frac{1}{4}} + C\varepsilon^{-\frac{1}{4}}] < C\sqrt{\varepsilon}
$$

for all $t \in [0,T]$ and $\boldsymbol{x} \in G^\varepsilon_{\boldsymbol{k},\delta}(t)$, i.e. we are done. □

2.4.3 Proof of Lemma 1

We give a rough outline of the proof of (2.27) (that of (2.28) is completely analogous). Using Cook's method (aka Duhamel's formula) our starting point is (remember $H^\varepsilon - \widetilde{H}^\varepsilon = V_3$)

$$
\psi^\varepsilon_{\boldsymbol{k}}(\boldsymbol{x},t) - \Phi^\varepsilon_{\boldsymbol{k}}(\boldsymbol{x},t) = \Big[U^\varepsilon(t) - \widetilde{U}^\varepsilon(t,0)\Big]\,\Phi^\varepsilon_{\boldsymbol{k}}(\boldsymbol{x},0) = -\frac{i}{\varepsilon}\int_0^t U^\varepsilon(t-s)V_3(\boldsymbol{x},\boldsymbol{a}(s))\Phi^\varepsilon_{\boldsymbol{k}}(\boldsymbol{x},s)d\,s\,.
$$

This gives the desired result (2.27) if $\|U^\varepsilon V_3\Phi^\varepsilon_{\boldsymbol{k}}\|_\infty \sim \varepsilon^{\frac{3}{4}}$. Indeed, we shall show (Lemma 3) that for every $m \in \mathbb{N}$

$$
\max_{s,t\in[0,T]}\|U^\varepsilon(t-s)V_m(\cdot,\boldsymbol{a}(s))\Phi^\varepsilon_{\boldsymbol{k}}(\cdot,s)\|_\infty \leq C\varepsilon^{\frac{m}{2}-\frac{3}{4}}\,.
$$

That $\|V_m\Phi^\varepsilon_{\boldsymbol{k}}\|_\infty \sim \varepsilon^{\frac{m}{2}-\frac{3}{4}}$ is comparatively easy to see. To get rid of the *unitary* (on $L^2(\mathbb{R}^3)$) time evolution $U^\varepsilon(t-s) = e^{-\frac{i}{\varepsilon}H^\varepsilon(t-s)}$ we use an instance of the Gagliardo-Nirenberg inequality ([23, 31], see (2.48) below) and $\boldsymbol{p} = -i\varepsilon\nabla$,

$$
\begin{aligned}
\|U^\varepsilon V_m\Phi^\varepsilon_{\boldsymbol{k}}\|_\infty &\leq C\|U^\varepsilon V_m\Phi^\varepsilon_{\boldsymbol{k}}\|_2^{\frac{1}{4}}\max_{|\alpha|=2}\|D^\alpha U^\varepsilon V_m\Phi^\varepsilon_{\boldsymbol{k}}\|_2^{\frac{3}{4}} \\
&= C\varepsilon^{-\frac{3}{2}}\|V_m\Phi^\varepsilon_{\boldsymbol{k}}\|_2^{\frac{1}{4}}\max_{|\alpha|=2}\|\boldsymbol{p}^\alpha U^\varepsilon V_m\Phi^\varepsilon_{\boldsymbol{k}}\|_2^{\frac{3}{4}}\,.
\end{aligned}
\tag{2.42}
$$

Then $\|U^\varepsilon V_m\Phi^\varepsilon_{\boldsymbol{k}}\|_\infty \sim \varepsilon^{\frac{m}{2}-\frac{3}{4}}$ if $\|\boldsymbol{p}^\alpha U^\varepsilon V_m\Phi^\varepsilon_{\boldsymbol{k}}\|_2 \sim \varepsilon^{\frac{m+|\alpha|}{2}}$.

The latter, however, is *false* in general. Remember that $V_m(\boldsymbol{x},\boldsymbol{a})$ is the mth remainder term of the Taylor expansion of V about $\boldsymbol{a}$, that is roughly $V_m(\boldsymbol{x},\boldsymbol{a}) \sim (\boldsymbol{x}-\boldsymbol{a})^m$. Since

$\frac{\boldsymbol{x}-\boldsymbol{a}}{\sqrt{\varepsilon}}$ acts on $\Phi^\varepsilon_{\boldsymbol{k}}$ as a combination of lowering and raising operators (cf. Proposition 2 (iii)), this means that

$$V_m \Phi^\varepsilon_{\boldsymbol{k}} \sim \varepsilon^{\frac{m}{2}} \sum_{|\boldsymbol{k}'-\boldsymbol{k}|\le m} \Phi^\varepsilon_{\boldsymbol{k}'} \,.$$

Moreover, since by Proposition 3 $\boldsymbol{p}^\alpha \Phi^\varepsilon_{\boldsymbol{k}'} \sim \boldsymbol{\eta}^\alpha \Phi^\varepsilon_{\boldsymbol{k}'}$, this implies that even

$$\|\boldsymbol{p}^\alpha V_m \Phi^\varepsilon_{\boldsymbol{k}}\|_2 \sim \varepsilon^{\frac{m}{2}} \|\boldsymbol{p}^\alpha \Phi^\varepsilon_{\boldsymbol{k}'}\|_2 \sim \varepsilon^{\frac{m}{2}} \|\boldsymbol{\eta}^\alpha \Phi^\varepsilon_{\boldsymbol{k}'}\|_2 \sim \varepsilon^{\frac{m}{2}}$$

is of order $\varepsilon^{-\frac{|\alpha|}{2}}$ worse than what we need.

To circumvent this impasse we use a trick: We substract the leading order, that is instead of $\boldsymbol{p}^\alpha \Phi^\varepsilon_{\boldsymbol{k}'}$ we contrive to use $(\boldsymbol{p}-\boldsymbol{\eta})^\alpha \Phi^\varepsilon_{\boldsymbol{k}'}$, which by Proposition 3 is exactly of order $\varepsilon^{\frac{|\alpha|}{2}}$ better than $\boldsymbol{p}^\alpha \Phi^\varepsilon_{\boldsymbol{k}'}$. Indeed, since $|e^{-\frac{i}{\varepsilon}\langle \eta,\, \boldsymbol{x}-\boldsymbol{a}\rangle} U^\varepsilon V_m \Phi^\varepsilon_{\boldsymbol{k}}| = |U^\varepsilon V_m \Phi^\varepsilon_{\boldsymbol{k}}|$ and $|\boldsymbol{p}^\alpha e^{-\frac{i}{\varepsilon}\langle \eta,\, \boldsymbol{x}-\boldsymbol{a}\rangle} U^\varepsilon V_m \Phi^\varepsilon_{\boldsymbol{k}}| = |(\boldsymbol{p}-\boldsymbol{\eta})^\alpha U^\varepsilon V_m \Phi^\varepsilon_{\boldsymbol{k}}|$, instead of (2.42) we may also write

$$\|U^\varepsilon V_m \Phi^\varepsilon_{\boldsymbol{k}}\|_\infty \le C\varepsilon^{-\frac{3}{2}} \|V_m \Phi^\varepsilon_{\boldsymbol{k}}\|_2^{\frac{1}{4}} \max_{|\alpha|=2} \|(\boldsymbol{p}-\boldsymbol{\eta})^\alpha U^\varepsilon V_m \Phi^\varepsilon_{\boldsymbol{k}}\|_2^{\frac{3}{4}} \,.$$

Thus $\|U^\varepsilon V_m \Phi^\varepsilon_{\boldsymbol{k}}\|_\infty \sim \varepsilon^{\frac{m}{2}-\frac{3}{4}}$ if $\|(\boldsymbol{p}-\boldsymbol{\eta})^\alpha U^\varepsilon V_m \Phi^\varepsilon_{\boldsymbol{k}}\|_2 \sim \varepsilon^{\frac{m+|\alpha|}{2}}$.

The latter is the content of Lemma 4 and is proven in two steps. First we use $\frac{p^2}{2} = H^\varepsilon - V$, the fact that $[H^\varepsilon, U^\varepsilon] = 0$ and brute force to commute $\boldsymbol{p}^\alpha$ and U^ε and consequently show that indeed $\|\boldsymbol{p}^\alpha U^\varepsilon V_m \Phi^\varepsilon_{\boldsymbol{k}}\|_2 \sim \|\boldsymbol{p}^\alpha V_m \Phi^\varepsilon_{\boldsymbol{k}}\|_2 \sim \varepsilon^{\frac{m}{2}}$. Since $\boldsymbol{\eta}(t)$ is bounded on $[0,T]$ this implies that also $\|(\boldsymbol{p}-\boldsymbol{\eta})^\alpha U^\varepsilon V_m \Phi^\varepsilon_{\boldsymbol{k}}\|_2$ is at least of order $\varepsilon^{\frac{m}{2}}$. In a second step we apply Cook's trick once more to construct a bootstrapping argument that allows us to sharpen this non-optimal estimate to the desired $\|(\boldsymbol{p}-\boldsymbol{\eta})^\alpha U^\varepsilon V_m \Phi^\varepsilon_{\boldsymbol{k}}\|_2 \sim \varepsilon^{\frac{m+|\alpha|}{2}}$.

We now give the details of the proof. As mentioned above our starting point is $(t \in [0,T])$

$$\psi^\varepsilon_{\boldsymbol{k}}(\boldsymbol{x},t) - \Phi^\varepsilon_{\boldsymbol{k}}(\boldsymbol{x},t) = -\frac{i}{\varepsilon}\int_0^t U^\varepsilon(t-s) V_3(\boldsymbol{x},\boldsymbol{a}(s))\Phi^\varepsilon_{\boldsymbol{k}}(\boldsymbol{x},s)d\,s \,. \tag{2.43}$$

A priori equality in (2.43) holds in the sense of L^2-functions, i.e. for almost every $\boldsymbol{x} \in \mathbb{R}^3$, only. In the course of our proof (Lemma 3 below) we shall however see that $U^\varepsilon V_3 \Phi^\varepsilon_{\boldsymbol{k}}$ is continuously differentiable[11] with respect to $\boldsymbol{x}$ and that $U^\varepsilon V_3 \Phi^\varepsilon_{\boldsymbol{k}}$ and $\nabla U^\varepsilon V_3 \Phi^\varepsilon_{\boldsymbol{k}}$ are bounded for all $s,t \in [0,T]$ and $\boldsymbol{x} \in \mathbb{R}^3$. So by dominated convergence also $\psi^\varepsilon_{\boldsymbol{k}} - \Phi^\varepsilon_{\boldsymbol{k}}$ (and thus $\psi^\varepsilon_{\boldsymbol{k}}$) is continuously differentiable[12] with

$$\begin{aligned}\nabla\psi^\varepsilon_{\boldsymbol{k}}(\boldsymbol{x},t) - \nabla\Phi^\varepsilon_{\boldsymbol{k}}(\boldsymbol{x},t) &= -\frac{i}{\varepsilon}\nabla\int_0^t U^\varepsilon(t-s) V_3(\boldsymbol{x},\boldsymbol{a}(s))\Phi^\varepsilon_{\boldsymbol{k}}(\boldsymbol{x},s)d\,s \\ &= -\frac{i}{\varepsilon}\int_0^t \nabla U^\varepsilon(t-s) V_3(\boldsymbol{x},\boldsymbol{a}(s))\Phi^\varepsilon_{\boldsymbol{k}}(\boldsymbol{x},s)d\,s \,.\end{aligned} \tag{2.44}$$

---

[11] When we say that some $f \in L^2$ is r times continuously differentiable we of course mean that there is some $\widetilde{f} \in C^r$ such that $\widetilde{f}(\boldsymbol{x}) = f(\boldsymbol{x})$ for almost every $\boldsymbol{x}$. Since, however, such a $\widetilde{f}$ is always unique, we can safely identify (the equivalence class) f with (its smooth representative) $\widetilde{f}$.

[12] In fact even $\psi^\varepsilon_{\boldsymbol{k}} \in C^\infty(\mathbb{R}^3 \times \mathbb{R})$. See the beginning of the proof of Lemma 2.

Moreover, by continuity (2.43) and(2.44) hold in fact pointwise for *all* $\boldsymbol{x} \in \mathbb{R}^3$.

Let us state our results on $(\nabla)U^\varepsilon V_3 \Phi^\varepsilon_{\boldsymbol{k}}$.

Lemma 3. *Let $V \in G_V$ and $T > 0$, $m \in \mathbb{N}$, $\boldsymbol{k} \in \mathbb{N}^3$. Then $U^\varepsilon(t-s)V_m(\cdot, \boldsymbol{a}(s))\Phi^\varepsilon_{\boldsymbol{k}}(\cdot, s)$ is continuously differentiable for all s, $t \in [0,T]$ and there exists some $C < \infty$ such that*

$$\max_{s,t\in[0,T]} \|U^\varepsilon(t-s)V_m(\cdot\,, \boldsymbol{a}(s))\Phi^\varepsilon_{\boldsymbol{k}}(\cdot\,, s)\|_\infty \leq C\varepsilon^{\frac{m}{2}-\frac{3}{4}} \tag{2.45}$$

and

$$\max_{s,t\in[0,T]} \|\,|\nabla U^\varepsilon(t-s)V_m(\cdot\,, \boldsymbol{a}(s))\Phi^\varepsilon_{\boldsymbol{k}}(\cdot\,, s)|\,\|_\infty \leq C\varepsilon^{\frac{m}{2}-\frac{7}{4}}\,. \tag{2.46}$$

Then, plugging (2.45) and (2.46) into (2.43) and (2.44) immediately yields Lemma 1, i.e.

$$\max_{t\in[0\,,T]} \|\psi^\varepsilon_{\boldsymbol{k}}(\cdot\,,t) - \Phi^\varepsilon_{\boldsymbol{k}}(\cdot\,,t)\|_\infty \leq \frac{T}{\varepsilon} \max_{s,t\in[0,T]} \|U^\varepsilon(t-s)V_3(\cdot\,, \boldsymbol{a}(s))\Phi^\varepsilon_{\boldsymbol{k}}(\cdot\,, s)\|_\infty \leq CT\varepsilon^{-\frac{1}{4}}$$

and

$$\begin{aligned}\max_{t\in[0\,,T]} \|\,|\nabla\psi^\varepsilon_{\boldsymbol{k}}(\cdot\,,t) - \nabla\Phi^\varepsilon_{\boldsymbol{k}}(\cdot\,,t)|\,\|_\infty &\leq \frac{T}{\varepsilon} \max_{s,t\in[0,T]} \|\,|\nabla U^\varepsilon(t-s)V_3(\cdot\,, \boldsymbol{a}(s))\Phi^\varepsilon_{\boldsymbol{k}}(\cdot\,, s)|\,\|_\infty \\ &\leq CT\varepsilon^{-\frac{5}{4}}\,.\end{aligned}$$

As explained in the outline above to prove Lemma 3 we need L^2-estimates of $(\boldsymbol{p}-\boldsymbol{\eta})^\alpha U^\varepsilon V_m \Phi^\varepsilon_{\boldsymbol{k}}$. They are collected in

Lemma 4. *Let $V \in G_V$. For every $T > 0$, $m \in \mathbb{N}$ and $\boldsymbol{k} \in \mathbb{N}^3$ there exists some $C < \infty$ such that*

$$\max_{s,t\in[0,T]} \|(\boldsymbol{p}-\boldsymbol{\eta}(t))^\alpha\, U^\varepsilon(t-s)V_m(\cdot\,, \boldsymbol{a}(s))\Phi^\varepsilon_{\boldsymbol{k}}(\cdot\,, s)\|_2 \leq C\varepsilon^{\frac{m+|\alpha|}{2}} \tag{2.47}$$

for all multi-indices $0 \leq |\alpha| \leq 3$.

Remark 4. For $m = 0$ and $s = 0$ Lemma 4 in particular implies

$$\max_{t\in[0,T]} \|(\boldsymbol{p}-\boldsymbol{\eta}(t))^\alpha\, \psi^\varepsilon_{\boldsymbol{k}}(\cdot\,, t)\|_2 \leq C\varepsilon^{\frac{|\alpha|}{2}}$$

for some $C < \infty$ and all $0 \leq |\alpha| \leq 3$. So we have, for example, that regarding momentum not only the $\Phi^\varepsilon_{\boldsymbol{k}}(\boldsymbol{x},t)$'s but also the $\psi^\varepsilon_{\boldsymbol{k}}(\boldsymbol{x},t)$'s standard deviation is of order $\sqrt{\varepsilon}$. Since the momentum operator $\boldsymbol{p}$ is unbounded this is not a consequence of Hagedorn's results $\|\psi^\varepsilon_{\boldsymbol{k}} - \Phi^\varepsilon_{\boldsymbol{k}}\|_2 \sim \sqrt{\varepsilon}$ and $\|(\boldsymbol{p}-\boldsymbol{\eta}(t))^\alpha\, \Phi^\varepsilon_{\boldsymbol{k}}\|_2 \sim \varepsilon^{\frac{|\alpha|}{2}}$ ([24, 25]; see also Proposition 3).

With Lemma 4 we may go on to the

Proof of Lemma 3.
Let

$$g^\varepsilon_{m,\boldsymbol{k}}(\boldsymbol{x},t,s) := U^\varepsilon(t-s)V_m(\boldsymbol{x}, \boldsymbol{a}(s)\Phi^\varepsilon_{\boldsymbol{k}}(\boldsymbol{x}, s),$$

and

$$\widetilde{g}^{\varepsilon}_{m,\boldsymbol{k}}(\boldsymbol{x},t,s) := e^{-\frac{i}{\varepsilon}\langle \boldsymbol{\eta}(t),\, \boldsymbol{x}-\boldsymbol{a}(t)\rangle} g^{\varepsilon}_{m,\boldsymbol{k}}(\boldsymbol{x},t,s).$$

We use an instance of Gagliardo-Nirenberg's inequality [23, 31]: For every $n \in \mathbb{N}$ and $l > \frac{n}{2}$ there is some $C < \infty$ such that for every $f \in W^{l,2}(\mathbb{R}^n) = \{f \in L^2(\mathbb{R}^n) \mid \max_{|\alpha|\le l} \|D^\alpha f\|_2 < \infty\}$

$$\|f\|_\infty \le C\Big(\max_{|\alpha|=l} \|D^\alpha f\|_2\Big)^{\frac{n}{2l}} \|f\|_2^{1-\frac{n}{2l}}\,. \tag{2.48}$$

Moreover, $f \in C^r(\mathbb{R}^n)$ for all $0 \le r < l - \frac{n}{2}$.

First, to prove (2.45) we apply (2.48) to $\widetilde{g}^{\varepsilon}_{m,k}$. Since $|g^{\varepsilon}_{m,\boldsymbol{k}}(\boldsymbol{x},t,s)| = |\widetilde{g}^{\varepsilon}_{m,\boldsymbol{k}}(\boldsymbol{x},t,s)|$ (2.48) with $n = 3$ and $l = 2$ gives

$$\begin{aligned}\max_{s,t\in[0,T]} \|g^{\varepsilon}_{m,\boldsymbol{k}}(\cdot,t,s)\|_\infty &= \max_{s,t\in[0,T]} \|\widetilde{g}^{\varepsilon}_{m,\boldsymbol{k}}(\cdot,t,s)\|_\infty \\ &\le C \max_{|\alpha|=2} \|D^\alpha \widetilde{g}^{\varepsilon}_{m,\boldsymbol{k}}(\cdot,t,s)\|_2^{\frac{3}{4}} \|\widetilde{g}^{\varepsilon}_{m,\boldsymbol{k}}(\cdot,t,s)\|_2^{\frac{1}{4}}\,.\end{aligned} \tag{2.49}$$

So we need to calculate $\|D^\alpha \widetilde{g}^{\varepsilon}_{m,\boldsymbol{k}}\|_2$ for multi-indices $\alpha \in \mathbb{N}^3$ with $|\alpha| = 0$ and$|\alpha| = 2$. Note however, that

$$\begin{aligned}D^\alpha \widetilde{g}^{\varepsilon}_{m,\boldsymbol{k}}(x,t,s) &= \sum_{|\beta|=0}^{|\alpha|} \binom{\alpha}{\beta} \Big(D^\beta e^{-\frac{i}{\varepsilon}\langle \boldsymbol{\eta}(t),\, \boldsymbol{x}-\boldsymbol{a}(t)\rangle}\Big) D^{\alpha-\beta} g^{\varepsilon}_{m,\boldsymbol{k}}(x,t,s) \\ &= e^{-\frac{i}{\varepsilon}\langle \boldsymbol{\eta}(t),\, \boldsymbol{x}-\boldsymbol{a}(t)\rangle} \sum_{|\beta|=0}^{|\alpha|} \binom{\alpha}{\beta} \Big(-\frac{i}{\varepsilon}\boldsymbol{\eta}(t)\Big)^\beta \Big(\frac{i}{\varepsilon}\boldsymbol{p}\Big)^{\alpha-\beta} g^{\varepsilon}_{m,\boldsymbol{k}}(x,t,s) \\ &= \Big(\frac{i}{\varepsilon}\Big)^{|\alpha|} e^{-\frac{i}{\varepsilon}\langle \boldsymbol{\eta}(t),\, \boldsymbol{x}-\boldsymbol{a}(t)\rangle} (\boldsymbol{p}-\boldsymbol{\eta}(t))^\alpha g^{\varepsilon}_{m,\boldsymbol{k}}(x,t,s)\end{aligned}$$

and thus by Lemma 4

$$\max_{s,t\in[0,T]} \|D^\alpha \widetilde{g}^{\varepsilon}_{m,\boldsymbol{k}}(\cdot,t,s)\|_2 = \varepsilon^{-|\alpha|} \max_{s,t\in[0,T]} \|\,(\boldsymbol{p}-\boldsymbol{\eta}(t))^\alpha g^{\varepsilon}_{m,\boldsymbol{k}}(\cdot,t,s)\|_2 \le C\varepsilon^{\frac{m-|\alpha|}{2}}\,. \tag{2.50}$$

With (2.49) this yields (2.45):

$$\max_{s,t\in[0,T]} \|g^{\varepsilon}_{m,\boldsymbol{k}}(\cdot,t,s)\|_\infty \le C\varepsilon^{\frac{m-2}{2}\frac{3}{4}+\frac{m}{2}\frac{1}{4}} = C\varepsilon^{\frac{m}{2}-\frac{3}{4}}\,.$$

The proof of (2.46) is analogous. By (2.48) (with $n = 3$ and $l = 2$)

$$\begin{aligned}\max_{s,t\in[0,T]} \|\,|\nabla g^{\varepsilon}_{m,\boldsymbol{k}}(\cdot,t,s)|\,\|_\infty &\le 3\max_{\substack{s,t\in[0,T]\\|\beta|=1}} \Big\|e^{-\frac{i}{\varepsilon}\langle \boldsymbol{\eta}(t),\, \boldsymbol{x}-\boldsymbol{a}(t)\rangle} D^\beta g^{\varepsilon}_{m,\boldsymbol{k}}(\cdot,t,s)\Big\|_\infty \\ &\le C \max_{\substack{|\alpha|=2\\|\beta|=1}} \|D^\alpha e^{-\frac{i}{\varepsilon}\langle \boldsymbol{\eta}(t),\, \boldsymbol{x}-\boldsymbol{a}(t)\rangle} D^\beta g^{\varepsilon}_{m,\boldsymbol{k}}(\cdot,t,s)\|_2^{\frac{3}{4}} \max_{|\beta|=1} \|D^\beta g^{\varepsilon}_{m,\boldsymbol{k}}(\cdot,t,s)\|_2^{\frac{1}{4}}\,.\end{aligned}$$

However by Lemma 4 we get

$$\begin{aligned}\left\|D^\alpha e^{-\frac{i}{\varepsilon}\langle\boldsymbol{\eta}(t),\,\boldsymbol{x}-\boldsymbol{a}(t)\rangle} D^\beta g^\varepsilon_{m,\boldsymbol{k}}(\cdot,t,s)\right\|_2 &= \varepsilon^{-(|\alpha|+|\beta|)}\left\|\,(\boldsymbol{p}-\boldsymbol{\eta}(t))^\alpha\,\boldsymbol{p}^\beta g^\varepsilon_{m,\boldsymbol{k}}(\cdot,t,s)\right\|_2\\ &\le \varepsilon^{-(|\alpha|+1)}\Big(\left\|\,(\boldsymbol{p}-\boldsymbol{\eta}(t))^{\alpha+\beta}\,g^\varepsilon_{m,\boldsymbol{k}}(\cdot,t,s)\right\|_2+\max_{t\in[0,T]}|\boldsymbol{\eta}(t)|\left\|\,(\boldsymbol{p}-\boldsymbol{\eta}(t))^{\alpha}\,g^\varepsilon_{m,\boldsymbol{k}}(\cdot,t,s)\right\|_2\Big)\\ &\le C\varepsilon^{\frac{m-|\alpha|-1}{2}}\end{aligned}$$

and thus (2.46). □

Remark 5. Instead of the Gagliardo-Nirenberg inequality (2.48) we could also use canonical Sobolev inequalities. However, then we get results that are not of optimal order in ε,

$$\|U^\varepsilon V_m\Phi^\varepsilon_{\boldsymbol{k}}\|_\infty \le C\Big[\sum_{|\alpha|=0}^{2}\varepsilon^{-|\alpha|}\,\|(\boldsymbol{p}-\boldsymbol{\eta}(t))^\alpha U^\varepsilon V_m\Phi^\varepsilon_{\boldsymbol{k}}\|_2^2\Big]^{\frac12}\le \widetilde{C}\varepsilon^{\frac{m}{2}-1}$$

and

$$\|\,|\nabla U^\varepsilon V_m\Phi^\varepsilon_{\boldsymbol{k}}|\,\|_\infty \le C\Big[\sum_{|\alpha|=0}^{3}\varepsilon^{-|\alpha|}\,\|(\boldsymbol{p}-\boldsymbol{\eta}(t))^\alpha U^\varepsilon V_m\Phi^\varepsilon_{\boldsymbol{k}}\|_2^2\Big]^{\frac12}\le \widetilde{C}\varepsilon^{\frac{m}{2}-2}\,.$$

Note that also this weaker results suffice to get convergence to classical behavior in the sense of Theorem 1 – but with a lower rate of convergence. More precisely, instead of (2.26) one gets

$$\mathbb{P}^{\psi^\varepsilon_{\boldsymbol{k}}(\cdot,0)}(\{\boldsymbol{x}\in\mathbb{R}^3\mid \max_{t\in[0,T]}|\boldsymbol{X}(\boldsymbol{x}_0,t)-\boldsymbol{a}(t)|\le R\varepsilon^{\frac14}\})>1-\gamma\,.$$

We conclude the proof of Lemma 1 with the

Proof of Lemma 4. We expand the notation of Lemma 3 to:

$$\begin{aligned} f^\varepsilon_{m,\boldsymbol{k}}(\boldsymbol{x},s) &:= V_m\left(\boldsymbol{x},\boldsymbol{a}(s)\right)\Phi^\varepsilon_{\boldsymbol{k}}(\boldsymbol{x},s) \quad\text{resp.}\quad f^\varepsilon_{(m,l),\boldsymbol{k}}(\boldsymbol{x},s):=V_{m,l}\left(\boldsymbol{x},\boldsymbol{a}(s)\right)\Phi^\varepsilon_{\boldsymbol{k}}(\boldsymbol{x},s)\,,\\ g^\varepsilon_{m,\boldsymbol{k}}(\boldsymbol{x},t,s) &= U^\varepsilon(t-s)f^\varepsilon_{m,\boldsymbol{k}}(\boldsymbol{x},s) \quad\text{resp.}\quad g^\varepsilon_{(m,l),\boldsymbol{k}}(\boldsymbol{x},t,s):=U^\varepsilon(t-s)f^\varepsilon_{(m,l),k}(\boldsymbol{x},s)\,.\end{aligned}$$

In the following we set $\|\cdot\|=\|\cdot\|_2$. We first prove the weaker result ($|\alpha|\le 3$)

$$\max_{s,t\in[0,T]}\left\|(\boldsymbol{p}-\boldsymbol{\eta}(t))^\alpha\,g^\varepsilon_{m,\boldsymbol{k}}(\cdot,t,s)\right\|\le C\varepsilon^{\frac{m}{2}} \tag{2.51}$$

and then use a bootstrapping argument to arrive at (2.47).

Since $\boldsymbol{\eta}(t)$ is bounded on $[0,T]$, instead of (2.51) it suffices to prove that

$$\max_{s,t\in[0,T]}\left\|\boldsymbol{p}^\alpha g^\varepsilon_{m,\boldsymbol{k}}(\cdot,t,s)\right\|\le C\varepsilon^{\frac{m}{2}} \tag{2.52}$$

for some $C<\infty$ and all $|\alpha|\le 3$. For that we first get rid of the (unitary) time evolution U^ε, i.e. we express $\|\boldsymbol{p}^\alpha g^\varepsilon_{m,\boldsymbol{k}}\|$ in terms of $\|f^\varepsilon_{m,\boldsymbol{k}}\|$, $\|H^\varepsilon f^\varepsilon_{m,\boldsymbol{k}}\|$ and $\|(H^\varepsilon)^2 f^\varepsilon_{m,\boldsymbol{k}}\|$. We then mimic the proof of (2.38) in [25] to find estimates for the latter.

Since U^ε is unitary

$$\|g^\varepsilon_{m,\boldsymbol{k}}(\cdot,t,s)\| = \|f^\varepsilon_{m,\boldsymbol{k}}(\cdot,s)\|\,. \tag{2.53}$$

Since $\boldsymbol{p} = -i\varepsilon\nabla$ is self-adjoint, by Schwarz's inequality and (2.53)

$$\begin{aligned}\max_{|\alpha|=1}\|\boldsymbol{p}^\alpha g^\varepsilon_{m,\boldsymbol{k}}(\cdot,t,s)\| &= \max_j \left\langle g^\varepsilon_{m,\boldsymbol{k}}(\cdot,t,s),\, p_j^2 g^\varepsilon_{m,\boldsymbol{k}}(\cdot,t,s)\right\rangle^{\frac12}\\ &\le \left(\|f^\varepsilon_{m,\boldsymbol{k}}(\cdot,s)\|\,\|p^2 g^\varepsilon_{m,\boldsymbol{k}}(\cdot,t,s)\|\right)^{\frac12}\ ,\\ \max_{|\alpha|=2}\|\boldsymbol{p}^\alpha g^\varepsilon_{m,\boldsymbol{k}}(\cdot,t,s)\| &\le \|p^2 g^\varepsilon_{m,\boldsymbol{k}}(\cdot,t,s)\|\end{aligned} \tag{2.54}$$

and

$$\max_{|\alpha|=3}\|\boldsymbol{p}^\alpha g^\varepsilon_{m,\boldsymbol{k}}(\cdot,t,s)\| \le \left(\|p^2 g^\varepsilon_{m,\boldsymbol{k}}(\cdot,t,s)\|\|p^4 g^\varepsilon_{m,\boldsymbol{k}}(\cdot,t,s)\|\right)^{\frac12}\ .$$

Thus we get (2.52) if we can show that $\|f^\varepsilon_{m,\boldsymbol{k}}\|$, $\|p^2 g^\varepsilon_{m,\boldsymbol{k}}\|$ and $\|p^4 g^\varepsilon_{m,\boldsymbol{k}}\|$ are of order $\varepsilon^{\frac{m}{2}}$. Write $p^2 = 2(H^\varepsilon - V)$. Since $[H^\varepsilon, U^\varepsilon] = 0$ and V is bounded by C_V (cf. Definition 1),

$$\begin{aligned}\|p^2 g^\varepsilon_{m,\boldsymbol{k}}(\cdot,t,s)\| &= 2\|(H^\varepsilon - V)g^\varepsilon_{m,\boldsymbol{k}}(\cdot,t,s)\|\\ &\le 2\left[\|H^\varepsilon U^\varepsilon(t-s) f^\varepsilon_{m,\boldsymbol{k}}(\cdot,s)\| + \|V\|_\infty\|g^\varepsilon_{m,\boldsymbol{k}}(\cdot,t,s)\|\right]\\ &\le 2\left[\|H^\varepsilon f^\varepsilon_{m,\boldsymbol{k}}(\cdot,s)\| + C_V\|f^\varepsilon_{m,\boldsymbol{k}}(\cdot,s)\|\right]\ .\end{aligned} \tag{2.55}$$

In the same way

$$\begin{aligned}\|p^4 g^\varepsilon_{m,\boldsymbol{k}}(\cdot,t,s)\| &= 4\|(H^\varepsilon - V)^2 g^\varepsilon_{m,\boldsymbol{k}}(\cdot,t,s)\|\\ &\le 4\Big[\|(H^\varepsilon)^2 f^\varepsilon_{m,\boldsymbol{k}}(\cdot,s)\| + 2\|V\|_\infty\|H^\varepsilon f^\varepsilon_{m,\boldsymbol{k}}(\cdot,s)\| + \|V\|^2_\infty\|f^\varepsilon_{m,\boldsymbol{k}}(\cdot,s)\|\\ &\qquad + \|[H^\varepsilon, V]g^\varepsilon_{m,\boldsymbol{k}}(\cdot,t,s)\|\Big]\\ &\le 4\Big[\|(H^\varepsilon)^2 f^\varepsilon_{m,\boldsymbol{k}}(\cdot,s)\| + 2C_V\|H^\varepsilon f^\varepsilon_{m,\boldsymbol{k}}(\cdot,s)\| + C_V^2\|f^\varepsilon_{m,\boldsymbol{k}}(\cdot,s)\|\\ &\qquad + \varepsilon\|\left\langle \nabla V,\, p\right\rangle g^\varepsilon_{m,\boldsymbol{k}}(\cdot,t,s)\| + \frac{\varepsilon^2}{2}\|\triangle V\|_\infty\|f^\varepsilon_{m,\boldsymbol{k}}(\cdot,s)\|\Big]\end{aligned}$$

Since $V \in G_V$ implies that also ∇V and $\triangle V$ are bounded by C_V, this yields

$$\begin{aligned}\|p^4 g^\varepsilon_{m,\boldsymbol{k}}(\cdot,t,s)\| &= 4\|(H^\varepsilon - V)^2 g^\varepsilon_{m,\boldsymbol{k}}(\cdot,t,s)\|\\ &\overset{(2.54)}{\le} 4\Big[\|(H^\varepsilon)^2 f^\varepsilon_{m,\boldsymbol{k}}(\cdot,s)\| + 2C_V\|H^\varepsilon f^\varepsilon_{m,\boldsymbol{k}}(\cdot,s)\| + C_V(C_V + \frac{\varepsilon^2}{2})\|f^\varepsilon_{m,\boldsymbol{k}}(\cdot,s)\|\\ &\qquad + \varepsilon C_V\left(\|f^\varepsilon_{m,\boldsymbol{k}}(\cdot,s)\|\,\|p^2 g^\varepsilon_{m,\boldsymbol{k}}(\cdot,t,s)\|\right)^{\frac12}\Big]\\ &\overset{(2.55)}{\le} 4\Big[\|(H^\varepsilon)^2 f^\varepsilon_{m,\boldsymbol{k}}(\cdot,s)\| + 2C_V\|H^\varepsilon f^\varepsilon_{m,\boldsymbol{k}}(\cdot,s)\| + C_V(C_V + \frac{\varepsilon^2}{2})\|f^\varepsilon_{m,\boldsymbol{k}}(\cdot,s)\|\\ &\qquad + \sqrt{2}\varepsilon C_V\|f^\varepsilon_{m,\boldsymbol{k}}(\cdot,s)\|^{\frac12}\left(\|H^\varepsilon f^\varepsilon_{m,\boldsymbol{k}}(\cdot,s)\| + C_V\|f^\varepsilon_{m,\boldsymbol{k}}(\cdot,s)\|\right)^{\frac12}\Big]\,.\end{aligned}$$

Thus we get (2.52) if we can show that $\|f^\varepsilon_{m,\boldsymbol{k}}\|$, $\|H^\varepsilon f^\varepsilon_{m,\boldsymbol{k}}\|$ and $\|(H^\varepsilon)^2 f^\varepsilon_{m,\boldsymbol{k}}\|$ are of order $\varepsilon^{\frac{m}{2}}$. We mimic the proof of (2.38) in [25] and introduce the following splitting ($R > 0$):

$$\|f^\varepsilon_{m,\boldsymbol{k}}(\cdot,s)\|^2 = \int\limits_{|\boldsymbol{x}-\boldsymbol{a}(s)|\le R} \left|V_m(\boldsymbol{x},\boldsymbol{a}(s))\Phi^\varepsilon_{\boldsymbol{k}}(\boldsymbol{x},s)\right|^2 d^3x \; + \int\limits_{|\boldsymbol{x}-\boldsymbol{a}(s)|> R} \left|V_m(\boldsymbol{x},\boldsymbol{a}(s))\Phi^\varepsilon_{\boldsymbol{k}}(\boldsymbol{x},s)\right|^2 d^3x =: \mathrm{I} + \mathrm{II}\,.$$

Recall Definition 2, i.e. that V_m is the remainder

$$V_m(\boldsymbol{x},\boldsymbol{a}) = V(\boldsymbol{x}) - \sum_{|\alpha|=0}^{m-1} \frac{1}{\alpha!}(D^\alpha V)(\boldsymbol{a})(\boldsymbol{x}-\boldsymbol{a})^\alpha = \sum_{|\alpha|=m} \frac{1}{\alpha!}(D^\alpha V)\left(\xi(\boldsymbol{x},\boldsymbol{a})\right)(\boldsymbol{x}-\boldsymbol{a})^\alpha$$

where $\xi(\boldsymbol{x},\boldsymbol{a}) = \boldsymbol{a} + \lambda(\boldsymbol{x}-\boldsymbol{a})$ for some $\lambda \in (0,1)$. Remember also that $\boldsymbol{a}(s)$ is continuous in s. Since V is C^∞ this implies

$$\max_{\substack{s\in[0,T]\\ |\alpha|\le m-1}} |(D^\alpha V)(\boldsymbol{a}(s))| < \infty$$

and

$$\max_{\substack{s\in[0,T]\\ |\alpha|= m}} \max_{|\boldsymbol{x}-\boldsymbol{a}(s)|\le R} |(D^\alpha V)\left(\xi(\boldsymbol{x},\boldsymbol{a}(s))\right)| < \infty\,.$$

Since $\|V\|_\infty \le C_V$, there thus is some $C < \infty$ such that for all $s \in [0,T]$

$$\begin{aligned}|V_m(\boldsymbol{x},\boldsymbol{a}(s))| &\le \|V\|_\infty + \left[\max_{\substack{s\in[0,T]\\ |\alpha|\le m-1}} |(D^\alpha V)(\boldsymbol{a}(s))|\right] \sum_{l=0}^{m-1}\sum_{|\alpha|=l} \frac{l!}{\alpha!}\,\frac{|\boldsymbol{x}-\boldsymbol{a}(s)|^l}{l!} \\ &\le C_V + \left[\max_{\substack{s\in[0,T]\\ |\alpha|\le m-1}} |(D^\alpha V)(\boldsymbol{a}(s))|\right] \sum_{l=0}^{\infty} \frac{\left(3\,|\boldsymbol{x}-\boldsymbol{a}(s)|\right)^l}{l!} \le Ce^{3|\boldsymbol{x}-\boldsymbol{a}(s)|}\end{aligned}$$

and

$$\max_{|\boldsymbol{x}-\boldsymbol{a}(s)|\le R} |V_m(\boldsymbol{x},\boldsymbol{a}(s))| \le C|\boldsymbol{x}-\boldsymbol{a}(s)|^m\,,$$

where we have used that $\sum\limits_{|\alpha|=l} \frac{l!}{\alpha!} = n^l$ for all n-dimensional multi-indices $\alpha \in \mathbb{N}^n$. Substituting $\boldsymbol{y} := \frac{\boldsymbol{x}-\boldsymbol{a}(s)}{\sqrt{\varepsilon}}$, with the above and (2.24) we get

$$\mathrm{II} \le C \int_{\frac{R}{\sqrt{\varepsilon}}}^{\infty} (1+y)^{2k}\, e^{-y(Cy-6\sqrt{\varepsilon})} dy \;\le Ce^{-\frac{C}{\sqrt{\varepsilon}}}$$

and

$$\mathrm{I} \le C \int_0^{\frac{R}{\sqrt{\varepsilon}}} \varepsilon^m y^{2m}(1+y)^{2k}\, e^{-Cy^2} dy \;\le C\varepsilon^m$$

for some $C < \infty$. So
$$\max_{s\in[0,T]} \|f^\varepsilon_{m,\boldsymbol{k}}(\cdot,s)\| = \mathcal{O}(\varepsilon^{\frac{m}{2}})\,. \tag{2.56}$$

To estimate $\|H^\varepsilon f^\varepsilon_{m,\boldsymbol{k}}\|$ write
$$H^\varepsilon f^\varepsilon_{m,\boldsymbol{k}}(\boldsymbol{x},s) = V_m(\boldsymbol{x},\boldsymbol{a}(s))H^\varepsilon\Phi^\varepsilon_{\boldsymbol{k}}(\boldsymbol{x},s) + [H^\varepsilon, V_m(\boldsymbol{x},\boldsymbol{a}(s))]\Phi^\varepsilon_{\boldsymbol{k}}(\boldsymbol{x},s)\,.$$

With $E_{cl} = \frac{1}{2}\eta(s)^2 + V\left(\boldsymbol{a}(s)\right)$ and $[H^\varepsilon, V_m] = -i\varepsilon\left\langle \nabla V_m,\, \boldsymbol{p}\right\rangle - \frac{\varepsilon^2}{2}(\triangle V_m)$ this gives (where there is no risk of confusion we suppress dependence on $\boldsymbol{x}$ and s respectively $\boldsymbol{a}(s)$)

$$\begin{aligned}
H^\varepsilon f^\varepsilon_{m,\boldsymbol{k}} &= E_{cl}f^\varepsilon_{m,\boldsymbol{k}} + V_m(H^\varepsilon - E_{cl})\Phi^\varepsilon_{\boldsymbol{k}} - i\varepsilon\left\langle \nabla V_m,\, \boldsymbol{p}\right\rangle\,\Phi^\varepsilon_{\boldsymbol{k}} - \frac{\varepsilon^2}{2}(\triangle V_m)\Phi^\varepsilon_{\boldsymbol{k}}\\
&= E_{cl}f^\varepsilon_{m,\boldsymbol{k}} + \frac{1}{2}V_m(p^2-\eta^2)\Phi^\varepsilon_{\boldsymbol{k}} + V_m(V(\boldsymbol{x}) - V(\boldsymbol{a}))\Phi^\varepsilon_{\boldsymbol{k}}\\
&\qquad\qquad - i\varepsilon\left\langle \nabla V_m,\, \boldsymbol{\eta}\right\rangle\,\Phi^\varepsilon_{\boldsymbol{k}} - i\varepsilon\left\langle \nabla V_m,\, \boldsymbol{p}-\boldsymbol{\eta}\right\rangle\,\Phi^\varepsilon_{\boldsymbol{k}} - \frac{\varepsilon^2}{2}(\triangle V_m)\Phi^\varepsilon_{\boldsymbol{k}}\\
&= E_{cl}f^\varepsilon_{m,\boldsymbol{k}} + \frac{1}{2}V_m(\boldsymbol{p}-\boldsymbol{\eta})^2\Phi^\varepsilon_{\boldsymbol{k}} + V_m\left\langle \boldsymbol{\eta},\, \boldsymbol{p}-\boldsymbol{\eta}\right\rangle\Phi^\varepsilon_{\boldsymbol{k}} + V_mV_1\Phi^\varepsilon_{\boldsymbol{k}}\\
&\qquad\qquad - i\varepsilon\left\langle \nabla V_m,\, \boldsymbol{\eta}\right\rangle\,\Phi^\varepsilon_{\boldsymbol{k}} - i\varepsilon\left\langle \nabla V_m,\, \boldsymbol{p}-\boldsymbol{\eta}\right\rangle\,\Phi^\varepsilon_{\boldsymbol{k}} - \frac{\varepsilon^2}{2}(\triangle V_m)\Phi^\varepsilon_{\boldsymbol{k}}\,.
\end{aligned}$$

Now, by (2.20) we see that $(\boldsymbol{p}-\boldsymbol{\eta})\Phi^\varepsilon_{\boldsymbol{k}}$ is $\sqrt{\varepsilon}$ times a (vector of) linear combination(s) of $\Phi^\varepsilon_{\boldsymbol{k}'}$'s with $|\boldsymbol{k}-\boldsymbol{k}'| = 1$ and $(\boldsymbol{p}-\boldsymbol{\eta})^2\Phi^\varepsilon_{\boldsymbol{k}}$ is ε times a linear combination of $\Phi^\varepsilon_{\boldsymbol{k}'}$'s with $|\boldsymbol{k}-\boldsymbol{k}'| \in \{0,2\}$. Thus $H^\varepsilon f^\varepsilon_{m,\boldsymbol{k}}$ is a sum of terms of the form
$$C(\boldsymbol{\eta})\widetilde{f}^\varepsilon_{m,\boldsymbol{k}'} = C(\boldsymbol{\eta})\widetilde{V}^\varepsilon_m\Phi^\varepsilon_{\boldsymbol{k}'}$$
where $C(\boldsymbol{\eta})$ is either a constant or some function of $\boldsymbol{\eta}$, $|\boldsymbol{k}-\boldsymbol{k}'| \le 2$ and $\widetilde{V}^\varepsilon_m$ is a wild card for V_m, εV_m, $\sqrt{\varepsilon}V_m$, V_mV_1, $\varepsilon(\partial_j V_m)$, $\varepsilon^{\frac{3}{2}}(\partial_j V_m)$ or $\varepsilon^2(\partial_j^2 V_m)$ $(j=1,2,3)$. Note that

$$\begin{aligned}
(D^\alpha V_m)(\boldsymbol{x},\boldsymbol{a}) &= (D^\alpha V)(\boldsymbol{x}) - \sum_{|\beta|=0}^{m-1}\frac{1}{\beta!}\left(D^\beta V\right)(\boldsymbol{a})D^\alpha(\boldsymbol{x}-\boldsymbol{a})^\beta\\
&= (D^\alpha V)(\boldsymbol{x}) - \sum_{|\beta'|=0}^{m-|\alpha|-1}\frac{1}{\beta'!}\left(D^{\beta'}D^\alpha V\right)(\boldsymbol{a})(\boldsymbol{x}-\boldsymbol{a})^{\beta'} = (D^\alpha V)_{m-|\alpha|}(\boldsymbol{x},\boldsymbol{a})\,,
\end{aligned}$$

so $\widetilde{V}^\varepsilon_m$ is either V_mV_1 or of the form $\varepsilon^{\frac{l}{2}}\widetilde{V}_{m-r}$ where the "new" potential $\widetilde{V}$ is a placeholder for V, $\partial_j V$ or $\partial_j^2 V$ and $l, r \in \mathbb{N}$ are such that $l-r \ge 0$. Now, since $V \in G_V$ implies $\widetilde{V} \in C^\infty$ and $\|\widetilde{V}\|_\infty \le \max_{|\alpha|\le 2}\|D^\alpha V\|_\infty \le C_V$, not only the proof of $\|V_mV_1\Phi^\varepsilon_{\boldsymbol{k}'}\| = \mathcal{O}(\varepsilon^{\frac{m+1}{2}})$ but also that of $\|\widetilde{V}_{m-r}\Phi^\varepsilon_{\boldsymbol{k}'}\| = \mathcal{O}(\varepsilon^{\frac{m-r}{2}})$ is completely analogous to that of (2.56). Therefore, $\|\widetilde{f}^\varepsilon_{m,\boldsymbol{k}'}\|$ is either of order $\varepsilon^{\frac{m+1}{2}}$ $(\widetilde{V}^\varepsilon_m = V_mV_1)$ or of order $\varepsilon^{\frac{m+l-r}{2}} \le \varepsilon^{\frac{m}{2}}$ $(\widetilde{V}^\varepsilon_m = \varepsilon^{\frac{l}{2}}\widetilde{V}_{m-r})$, that is we get
$$\max_{s\in[0,T]}\|H^\varepsilon f^\varepsilon_{m,\boldsymbol{k}}(\cdot,s)\| \le \sum\max_{s\in[0,T]}|C(\boldsymbol{\eta})|\,\|\widetilde{f}^\varepsilon_{m,\boldsymbol{k}'}(\cdot,s)\| = \mathcal{O}(\varepsilon^{\frac{m}{2}})\,. \tag{2.57}$$

Finally, $\|(H^\varepsilon)^2 f^\varepsilon_{m,\boldsymbol{k}}\| = \mathcal{O}(\varepsilon^{\frac{m}{2}})$ clearly follows if we can show that, for each of the above $\widetilde{f}^\varepsilon_{m,\boldsymbol{k}'}$, $\|H^\varepsilon\widetilde{f}^\varepsilon_{m\boldsymbol{k}'}\|$ is (at least) of order $\varepsilon^{\frac{m}{2}}$. The proof of the latter, however, is completely analogous to that of (2.57). Just note that this time we get up to fourth order derivatives of V as "new" potentials $\widetilde{V}$, which is why in the definition of G_V we required that $\|D^\alpha V\|_\infty \le C_V$ for $|\alpha| \le 4$.

So we have shown that (2.52) and thus also (2.51) holds. To get (2.47) we split V_m into $V_m = V_{m,m} + V_{m+1}$ (cf. Definition 2). Then by (2.51)

$$\begin{aligned}
&\| (\boldsymbol{p} - \boldsymbol{\eta}(t))^\alpha g^\varepsilon_{m,\boldsymbol{k}}(\cdot, t, s)\| \\
&\qquad \le \| (\boldsymbol{p} - \boldsymbol{\eta}(t))^\alpha \, g^\varepsilon_{(m,m),k}(\cdot, t, s)\| + \| (\boldsymbol{p} - \boldsymbol{\eta}(t))^\alpha \, g^\varepsilon_{m+1,\boldsymbol{k}}(\cdot, t, s)\| \\
&\qquad \le \| (\boldsymbol{p} - \boldsymbol{\eta}(t))^\alpha \, g^\varepsilon_{(m,m),\boldsymbol{k}}(\cdot, t, s)\| + C\varepsilon^{\frac{m+1}{2}} \, .
\end{aligned} \tag{2.58}$$

To estimate $(\boldsymbol{p} - \boldsymbol{\eta})^\alpha \, g^\varepsilon_{(m,m),\boldsymbol{k}}$ note that by definition

$$\begin{aligned}
g^\varepsilon_{(m,m),\boldsymbol{k}}(\boldsymbol{x}, t, s) &= U^\varepsilon(t-s) V_{m,m}(\boldsymbol{x}, \boldsymbol{a}(s) \Phi^\varepsilon_{\boldsymbol{k}}(\boldsymbol{x}, s) \\
&= \varepsilon^{\frac{m}{2}} U^\varepsilon(t-s) \sum_{|\beta|=m} \frac{1}{\beta!} \left(D^\beta V\right)(a(s)) \left(\frac{\boldsymbol{x} - \boldsymbol{a}(s)}{\sqrt{\varepsilon}}\right)^\beta \Phi^\varepsilon_{\boldsymbol{k}}(x, s)
\end{aligned}$$

and that $\left(\frac{\boldsymbol{x}-\boldsymbol{a}}{\sqrt{\varepsilon}}\right)^\beta \Phi^\varepsilon_{\boldsymbol{k}}$ is a finite sum of $\Phi^\varepsilon_{\boldsymbol{k}'}$s with $|\boldsymbol{k} - \boldsymbol{k}'| \le m$ and coefficients that are independent of ε and uniformly bounded on $[0,T]$ (cf. (2.19)). Since also $\left(D^\beta V\right)(\boldsymbol{a}(s))$ is uniformly bounded on $[0,T]$ ($V \in C^\infty(\mathbb{R}^3)$ and $\boldsymbol{a}(s)$ continuous in s) it thus suffices to estimate

$$\varepsilon^{\frac{m}{2}} \, (\boldsymbol{p} - \boldsymbol{\eta}(t))^\alpha \, U^\varepsilon(t-s) \Phi^\varepsilon_{\boldsymbol{k}'}(\boldsymbol{x}, s)$$

for $|\boldsymbol{k} - \boldsymbol{k}'| \le m$. For this we use once more Cook's method, i.e.

$$\begin{aligned}
U^\varepsilon(t-s)\Phi^\varepsilon_{\boldsymbol{k}'}(\boldsymbol{x}, s) &= \Phi^\varepsilon_{\boldsymbol{k}'}(\boldsymbol{x}, t) - \frac{i}{\varepsilon} \int_s^t U^\varepsilon(t-\tau) V_3\left(\boldsymbol{x}, \boldsymbol{a}(\tau)\right) \Phi^\varepsilon_{\boldsymbol{k}'}(\boldsymbol{x}, \tau) \, d\tau \\
&= \Phi^\varepsilon_{\boldsymbol{k}'}(\boldsymbol{x}, t) - \frac{i}{\varepsilon} \int_s^t g^\varepsilon_{3,\boldsymbol{k}'}(\boldsymbol{x}, t, \tau) \, d\tau \, .
\end{aligned}$$

Since by (2.51) $\| (\boldsymbol{p} - \boldsymbol{\eta}(t))^\alpha \, g^\varepsilon_{3,\boldsymbol{k}'}(\cdot, t, \tau)\| < C\varepsilon^{\frac{3}{2}}$, changing the order of differentiation ($\boldsymbol{p} = -i\varepsilon\nabla$) and integration in

$$\| (\boldsymbol{p} - \boldsymbol{\eta}(t))^\alpha \int_s^t g^\varepsilon_{3,\boldsymbol{k}'}(\cdot, t, \tau) \, d\tau\| = \| \int_s^t (\boldsymbol{p} - \boldsymbol{\eta}(t))^\alpha \, g^\varepsilon_{3,\boldsymbol{k}'}(\cdot, t, \tau) \, d\tau\|$$

is justified by dominated convergence and we thus get (for any $s, t \in [0,T]$)

$$\begin{aligned}
&\varepsilon^{\frac{m}{2}} \| (\boldsymbol{p} - \boldsymbol{\eta}(t))^\alpha U^\varepsilon(t-s) \Phi^\varepsilon_{\boldsymbol{k}'}(\cdot, s)\| \\
&\qquad \le \varepsilon^{\frac{m}{2}} \| (\boldsymbol{p} - \boldsymbol{\eta}(t))^\alpha \, \Phi^\varepsilon_{\boldsymbol{k}'}(\cdot, t)\| + \varepsilon^{\frac{m}{2}-1} \int_s^t \| (\boldsymbol{p} - \boldsymbol{\eta}(t))^\alpha \, g^\varepsilon_{3,\boldsymbol{k}'}(\cdot, t, \tau)\| \, d\tau \\
&\qquad \le \varepsilon^{\frac{m+|\alpha|}{2}} \left\| \left(\frac{\boldsymbol{p} - \boldsymbol{\eta}(t)}{\sqrt{\varepsilon}}\right)^\alpha \Phi^\varepsilon_{\boldsymbol{k}'}(\cdot, t)\right\| + \varepsilon^{\frac{m+1}{2}} CT \, .
\end{aligned}$$

By (2.23) this yields

$$\varepsilon^{\frac{m}{2}} \| (\boldsymbol{p}-\boldsymbol{\eta}(t))^{\alpha} U^{\varepsilon}(t-s)\Phi^{\varepsilon}_{\boldsymbol{k}'}(\cdot,s)\| \leq C\left(\varepsilon^{\frac{m+|\alpha|}{2}}+\varepsilon^{\frac{m+1}{2}}\right)$$

and thus also

$$\| (\boldsymbol{p}-\boldsymbol{\eta}(t))^{\alpha} g^{\varepsilon}_{(m,m),\boldsymbol{k}}(\cdot,t,s)\| \leq C\left(\varepsilon^{\frac{m+|\alpha|}{2}}+\varepsilon^{\frac{m+1}{2}}\right).$$

Putting this into (2.58) we see that we can sharpen (2.51) to

$$\max_{s,t\in[0,T]} \left\|(\boldsymbol{p}-\boldsymbol{\eta}(t))^{\alpha} g^{\varepsilon}_{m,\boldsymbol{k}}(\cdot,t,s)\right\| \leq C\left(\varepsilon^{\frac{m+|\alpha|}{2}}+\varepsilon^{\frac{m+1}{2}}\right) \leq C\varepsilon^{\frac{m+1}{2}}.$$

Repeating this bootstrapping argument several times we finally arrive at

$$\max_{s,t\in[0,T]} \left\|(\boldsymbol{p}-\boldsymbol{\eta}(t))^{\alpha} g^{\varepsilon}_{m,\boldsymbol{k}}(\cdot,t,s)\right\| \leq C\left(\varepsilon^{\frac{m+|\alpha|}{2}}+\varepsilon^{\frac{m+|\alpha|}{2}}\right),$$

i.e. at (2.47).

□

2.4.4 Completing the proofs of Propositions 2 and 3

Proof of Proposition 2 (iii). We start with the proof of (2.19). Since the $\Phi_{\boldsymbol{k}}$s form an ONB this is equivalent to showing that

$$\begin{aligned}\left\langle \Phi_{\boldsymbol{k}'}(A,B,\varepsilon,\boldsymbol{a},\boldsymbol{\eta},\boldsymbol{x}),\ \left(\frac{\boldsymbol{x}-\boldsymbol{a}}{\sqrt{\varepsilon}}\right)^{\alpha}\Phi_{\boldsymbol{k}}(A,B,\varepsilon,\boldsymbol{a},\boldsymbol{\eta},\boldsymbol{x})\right\rangle \\ = \langle \Phi_{\boldsymbol{k}'}(U_A,\mathbb{1},1,0,0,\boldsymbol{x}),\ (R_A\boldsymbol{x})^{\alpha}\Phi_{\boldsymbol{k}}(U_A,\mathbb{1},1,0,0,\boldsymbol{x})\rangle\end{aligned} \tag{2.59}$$

for all $\boldsymbol{k}$, $\boldsymbol{k}'$, $\alpha\in\mathbb{N}^n$ and

$$\langle \Phi_{\boldsymbol{k}'}(U_A,\mathbb{1},1,0,0,\boldsymbol{x}),\ (R_A\boldsymbol{x})^{\alpha}\Phi_{\boldsymbol{k}}(U_A,\mathbb{1},1,0,0,\boldsymbol{x})\rangle = 0$$

for all $\boldsymbol{k}$, $\boldsymbol{k}'$, $\alpha\in\mathbb{N}^n$ with $|\boldsymbol{k}-\boldsymbol{k}'|>|\alpha|$ or $|\boldsymbol{k}-\boldsymbol{k}'|+|\alpha|$ odd. Since the scalar product is sesquilinear the latter is equivalent to proving that

$$\langle \Phi_{\boldsymbol{k}'}(U_A,\mathbb{1},1,0,0,\boldsymbol{x}),\ \boldsymbol{x}^{\alpha}\Phi_{\boldsymbol{k}}(U_A,\mathbb{1},1,0,0,\boldsymbol{x})\rangle = 0 \tag{2.60}$$

for all $\boldsymbol{k}$, $\boldsymbol{k}'$, $\alpha\in\mathbb{N}^n$ with $|\boldsymbol{k}-\boldsymbol{k}'|>|\alpha|$ or $|\boldsymbol{k}-\boldsymbol{k}'|+|\alpha|$ odd.

Writing $\Phi_{\boldsymbol{k}}$ as generalized Hermite function (cf. (2.15) and (2.17)) we get

$$\begin{aligned}&\left\langle \Phi_{\boldsymbol{k}'}(A,B,\varepsilon,\boldsymbol{a},\boldsymbol{\eta},\boldsymbol{x}),\ \left(\frac{\boldsymbol{x}-\boldsymbol{a}}{\sqrt{\varepsilon}}\right)^{\alpha}\Phi_{\boldsymbol{k}}(A,B,\varepsilon,\boldsymbol{a},\boldsymbol{\eta},\boldsymbol{x})\right\rangle \\ &= \frac{(\pi\varepsilon)^{-\frac{n}{2}}}{|\det(A)|}\frac{2^{-\frac{k+k'}{2}}}{\sqrt{\boldsymbol{k}'!\boldsymbol{k}!}} \\ &\quad\times \int_{\mathbb{R}^n} \mathcal{H}^{*}_{\boldsymbol{k}'}(U_A;\ R_A^{-1}\frac{\boldsymbol{x}-\boldsymbol{a}}{\sqrt{\varepsilon}})\mathcal{H}_{\boldsymbol{k}}(U_A;\ R_A^{-1}\frac{\boldsymbol{x}-\boldsymbol{a}}{\sqrt{\varepsilon}})\left(\frac{\boldsymbol{x}-\boldsymbol{a}}{\sqrt{\varepsilon}}\right)^{\alpha} e^{-\left\langle\frac{\boldsymbol{x}-\boldsymbol{a}}{\sqrt{\varepsilon}},\,\mathrm{Re}(BA^{-1})\frac{\boldsymbol{x}-\boldsymbol{a}}{\sqrt{\varepsilon}}\right\rangle} d^n x \\ &\overset{R_A\boldsymbol{y}=\frac{\boldsymbol{x}-\boldsymbol{a}}{\sqrt{\varepsilon}}}{=} \pi^{-\frac{n}{2}}\frac{2^{-\frac{k+k'}{2}}}{\sqrt{\boldsymbol{k}'!\boldsymbol{k}!}}\int_{\mathbb{R}^n}\mathcal{H}^{*}_{\boldsymbol{k}'}(U_A;\ \boldsymbol{y})\mathcal{H}_{\boldsymbol{k}}(U_A;\ \boldsymbol{y})\,(R_A\boldsymbol{y})^{\alpha}\,e^{-y^2}d^n y\,.\end{aligned}$$

In the last step we have used (2.12), i.e. $\mathrm{Re}(BA^{-1}) = (AA^*)^{-1} = R_A^{-2}$, and $\frac{|\det(R_A)|}{|\det(A)|} = \frac{1}{|\det(U_A)|} = 1$. Note that $\mathrm{Re}(U_A^{-1}) = \mathbb{1}$ and thus $\pi^{-\frac{n}{2}} e^{-y^2} = \frac{\pi^{-\frac{n}{2}}}{|\det(U_A)|} e^{-\langle \boldsymbol{y}, \mathrm{Re}(U_A)\boldsymbol{y}\rangle} = |\Phi_0(U_A, \mathbb{1}, 1, 0, 0, R_A^{-1}\boldsymbol{y})|^2$. So, using (2.17) once more, we see that

$$\left\langle \Phi_{\boldsymbol{k}'}(A, B, \varepsilon, \boldsymbol{a}, \boldsymbol{\eta}, \boldsymbol{x}), \left(\frac{\boldsymbol{x}-\boldsymbol{a}}{\sqrt{\varepsilon}}\right)^{\alpha} \Phi_{\boldsymbol{k}}(A, B, \varepsilon, \boldsymbol{a}, \boldsymbol{\eta}, \boldsymbol{x}) \right\rangle = \\ = \langle \Phi_{\boldsymbol{k}'}(U_A, \mathbb{1}, 1, 0, 0, \boldsymbol{x}), (R_A \boldsymbol{x})^{\alpha} \Phi_{\boldsymbol{k}}(U_A, \mathbb{1}, 1, 0, 0, \boldsymbol{x}) \rangle ,$$

i.e. that (2.59) holds.

To prove (2.60), note that with the help of (2.13) we may write $\boldsymbol{x}$ as a sum of lowering and raising operators (cf. [25] (3.28)):

$$\boldsymbol{x} = \frac{1}{\sqrt{2}} \left(U_A \mathcal{A}^*(U_A, \mathbb{1}, 1, 0, 0) + \overline{U}_A \mathcal{A}(U_A, \mathbb{1}, 1, 0, 0) \right) .$$

Then (2.60) follows by a straightforward induction on $|\alpha|$.

Finally (2.20) is an easy consequence of (2.19) (resp. of (2.59) and (2.60)) and the fact that (see [24] Lemma 2.2 resp. [25] (3.19))

$$(\mathcal{F}_\varepsilon \Phi_{\boldsymbol{k}}(A, B, \varepsilon, \boldsymbol{a}, \boldsymbol{\eta}, \cdot))(\boldsymbol{\xi}) = (-i)^k e^{-\frac{i}{\varepsilon}\langle \boldsymbol{a}, \boldsymbol{\eta}\rangle} \Phi_{\boldsymbol{k}}(B, A, \varepsilon, \boldsymbol{\eta}, -\boldsymbol{a}, \boldsymbol{\xi})$$

where the scaled Fourier transform $\mathcal{F}_\varepsilon$ is defined as

$$(\mathcal{F}_\varepsilon \psi)(\boldsymbol{\xi}) = (2\pi\varepsilon)^{-\frac{n}{2}} \int e^{-\frac{i}{\varepsilon}\langle \boldsymbol{x}, \boldsymbol{\xi}\rangle} \psi(\boldsymbol{x}) d^n x .$$

Then, using Plancherel's theorem, $\mathcal{F}_\varepsilon(p\psi)(\boldsymbol{\xi}) = \boldsymbol{\xi}(\mathcal{F}_\varepsilon\psi)(\boldsymbol{\xi})$ and (2.59),

$$\begin{aligned} &\left\langle \Phi_{\boldsymbol{k}'}(A, B, \varepsilon, \boldsymbol{a}, \boldsymbol{\eta}, \boldsymbol{x}), \left(\frac{\boldsymbol{p}-\boldsymbol{\eta}}{\sqrt{\varepsilon}}\right)^{\alpha} \Phi_{\boldsymbol{k}}(A, B, \varepsilon, \boldsymbol{a}, \boldsymbol{\eta}, \boldsymbol{x}) \right\rangle \\ &\quad = i^{k'-k} \left\langle \Phi_{\boldsymbol{k}'}(B, A, \varepsilon, \boldsymbol{\eta}, -\boldsymbol{a}, \boldsymbol{\xi}), \left(\frac{\boldsymbol{\xi}-\boldsymbol{\eta}}{\sqrt{\varepsilon}}\right)^{\alpha} \Phi_{\boldsymbol{k}}(B, A, \varepsilon, \boldsymbol{\eta}, -\boldsymbol{a}, \boldsymbol{\xi}) \right\rangle \\ &\quad = i^{k'-k} \langle \Phi_{\boldsymbol{k}'}(U_B, \mathbb{1}, 1, 0, 0, \boldsymbol{\xi}), (R_B \boldsymbol{\xi})^{\alpha} \Phi_{\boldsymbol{k}}(U_B, \mathbb{1}, 1, 0, 0, \boldsymbol{\xi}) \rangle \\ &\quad = \langle \Phi_{\boldsymbol{k}'}(\mathbb{1}, U_B, 1, 0, 0, \boldsymbol{x}), (R_B \boldsymbol{p})^{\alpha} \Phi_{\boldsymbol{k}}(\mathbb{1}, U_B, 1, 0, 0, \boldsymbol{x}) \rangle . \end{aligned}$$

Similarly, we can use (2.60) to get

$$\langle \Phi_{\boldsymbol{k}'}(\mathbb{1}, U_B, 1, 0, 0, \boldsymbol{x}), \boldsymbol{p}^{\alpha} \Phi_{\boldsymbol{k}}(\mathbb{1}, U_B, 1, 0, 0, \boldsymbol{x}) \rangle = 0$$

for all $\boldsymbol{k}$, $\boldsymbol{k}'$, $\alpha \in \mathbb{N}^n$ with $|\boldsymbol{k} - \boldsymbol{k}'| > |\alpha|$ or $|\boldsymbol{k} - \boldsymbol{k}'| + |\alpha|$ odd. Thus (2.20) holds. □

Proof of Proposition 3 (ii). According to part (ii) of Proposition 2

$$|\Phi_{\boldsymbol{k}}^{\varepsilon}(\boldsymbol{x}, t)| = \frac{2^{-\frac{k}{2}}}{\sqrt{\boldsymbol{k}!}} \left| \mathcal{H}_{\boldsymbol{k}}\left(U_{A(t)};\, R_{A(t)}^{-1} \frac{\boldsymbol{x} - \boldsymbol{a}(t)}{\sqrt{\varepsilon}} \right) \right| |\Phi_0^{\varepsilon}(\boldsymbol{x}, t)|$$

and

$$\left|\Big(\nabla - \frac{i}{\varepsilon}\boldsymbol{\eta}(t)\Big)\Phi^{\varepsilon}_{\boldsymbol{k}}(\boldsymbol{x},t)\right| \leq \frac{2^{-\frac{k}{2}}}{\sqrt{\boldsymbol{k}!}}\Bigg[\left|\nabla\mathcal{H}_{\boldsymbol{k}}\Big(U_{A(t)};\, R^{-1}_{A(t)}\frac{\boldsymbol{x}-\boldsymbol{a}(t)}{\sqrt{\varepsilon}}\Big)\right|\,|\Phi^{\varepsilon}_0(\boldsymbol{x},t)|$$
$$+\left|\mathcal{H}_{\boldsymbol{k}}\Big(U_{A(t)};\, R^{-1}_{A(t)}\frac{\boldsymbol{x}-\boldsymbol{a}(t)}{\sqrt{\varepsilon}}\Big)\right|\left|\Big(\nabla - \frac{i}{\varepsilon}\boldsymbol{\eta}(t)\Big)\Phi^{\varepsilon}_0(\boldsymbol{x},t)\right|\Bigg].$$

By the definition of $\mathcal{H}_{\boldsymbol{k}}$ (equations (2.17) and (2.18)) we see that $\mathcal{H}_{\boldsymbol{k}}(U_{A(t)};\, R^{-1}_{A(t)}\frac{\boldsymbol{x}-\boldsymbol{a}(t)}{\sqrt{\varepsilon}})$ is a polynomial of kth order in the components of $\frac{\boldsymbol{x}-\boldsymbol{a}(t)}{\sqrt{\varepsilon}}$ with coefficients depending on $A(t)$ resp. $A(t)^{-1}$. Since $A(t)$ is continuous and invertible for all $t\in\mathbb{R}$ (cf. (2.11) and (2.12)), i.e. since $0 < \min\limits_{t\in[0,T]}\|A(t)\|$ and $\max\limits_{t\in[0,T]}\|A(t)\| < \infty$, this implies that there is some $C<\infty$ such that

$$\left|\mathcal{H}_{\boldsymbol{k}}\Big(U_{A(t)};\, R^{-1}_{A(t)}\frac{\boldsymbol{x}-\boldsymbol{a}(t)}{\sqrt{\varepsilon}}\Big)\right| \leq C\Big(1+\frac{|\boldsymbol{x}-\boldsymbol{a}(t)|}{\sqrt{\varepsilon}}\Big)^k$$

and

$$\left|\nabla\mathcal{H}_{\boldsymbol{k}}\Big(U_{A(t)};\, R^{-1}_{A(t)}\frac{\boldsymbol{x}-\boldsymbol{a}(t)}{\sqrt{\varepsilon}}\Big)\right| \leq \frac{1}{\sqrt{\varepsilon}}C\Big(1+\frac{|\boldsymbol{x}-\boldsymbol{a}(t)|}{\sqrt{\varepsilon}}\Big)^{k-1}$$

for all $t\in[0,T]$. Similar, by (2.15) there is some $C<\infty$ (depending also on $B(t)$) such that (remember $\mathrm{Re}(BA^{-1}) = (AA^*)^{-1}$)

$$|\Phi^{\varepsilon}_0(\boldsymbol{x},t)| = \frac{(\pi\varepsilon)^{-\frac{n}{4}}}{\sqrt{|\det(A(t))|}}\, e^{-\frac{1}{2}\left\langle\frac{\boldsymbol{x}-\boldsymbol{a}(t)}{\sqrt{\varepsilon}},\,\mathrm{Re}\left(B(t)A(t)^{-1}\right)\frac{\boldsymbol{x}-\boldsymbol{a}(t)}{\sqrt{\varepsilon}}\right\rangle}$$
$$=\varepsilon^{-\frac{n}{4}}\left|\Phi_0\Big(A(t),B(t),1,0,0,\frac{\boldsymbol{x}-\boldsymbol{a}(t)}{\sqrt{\varepsilon}}\Big)\right| \leq \varepsilon^{-\frac{n}{4}}Ce^{-\frac{1}{2}C\left(\frac{|\boldsymbol{x}-\boldsymbol{a}(t)|}{\sqrt{\varepsilon}}\right)^2}$$

and

$$\left|\Big(\nabla - \frac{i}{\varepsilon}\boldsymbol{\eta}(t)\Big)\Phi^{\varepsilon}_0(\boldsymbol{x},t)\right| = \frac{(\pi\varepsilon)^{-\frac{n}{4}}}{\sqrt{|\det(A)|}}\left|B(t)A(t)^{-1}\frac{\boldsymbol{x}-\boldsymbol{a}(t)}{\varepsilon}\right|\, e^{-\frac{1}{2}\left\langle\frac{\boldsymbol{x}-\boldsymbol{a}(t)}{\sqrt{\varepsilon}},\,\mathrm{Re}\left(B(t)A(t)^{-1}\right)\frac{\boldsymbol{x}-\boldsymbol{a}(t)}{\sqrt{\varepsilon}}\right\rangle}$$
$$\leq \varepsilon^{-(\frac{n}{4}+\frac{1}{2})}C\Big(1+\frac{|\boldsymbol{x}-\boldsymbol{a}(t)|}{\sqrt{\varepsilon}}\Big)\, e^{-\frac{1}{2}C\left(\frac{|\boldsymbol{x}-\boldsymbol{a}(t)|}{\sqrt{\varepsilon}}\right)^2}$$

for all $t\in[0,T]$. Thus

$$|\Phi^{\varepsilon}_{\boldsymbol{k}}(\boldsymbol{x},t)| = \varepsilon^{-\frac{n}{4}}\left|\Phi_{\boldsymbol{k}}\Big(A(t),B(t),1,0,0,\frac{\boldsymbol{x}-\boldsymbol{a}(t)}{\sqrt{\varepsilon}}\Big)\right|$$
$$\leq \varepsilon^{-\frac{n}{4}}C\left(1+\frac{|\boldsymbol{x}-\boldsymbol{a}(t)|}{\sqrt{\varepsilon}}\right)^k e^{-\frac{1}{2}C\left(\frac{|\boldsymbol{x}-\boldsymbol{a}(t)|}{\sqrt{\varepsilon}}\right)^2}$$

and

$$\left|\nabla\Phi^{\varepsilon}_{\boldsymbol{k}}(\boldsymbol{x},t) - \frac{i}{\varepsilon}\boldsymbol{\eta}(t)\Phi^{\varepsilon}_{\boldsymbol{k}}(\boldsymbol{x},t)\right| \leq \varepsilon^{-\left(\frac{n}{4}+\frac{1}{2}\right)}C\left(1+\frac{|\boldsymbol{x}-\boldsymbol{a}(t)|}{\sqrt{\varepsilon}}\right)^{k+1} e^{-\frac{1}{2}C\left(\frac{|\boldsymbol{x}-\boldsymbol{a}(t)|}{\sqrt{\varepsilon}}\right)^2},$$

i.e. we get the first parts of (2.24) and (2.25). Noting that $\sup\limits_{r\geq 0}(1+r)^k e^{-\frac{1}{2}Cr^2} < \infty$ (for every $k\in\mathbb{N}$) gives the rest. □

Chapter 3

On the Detection Statistics of Many Particle Quantum Scattering

In this chapter we use the asymptotically classical behavior of Bohmian trajectories in scattering situations to derive from first principles the detection probability of particles in a given solid angle.

The central quantity in a scattering experiment is the cross section, whose derivation is based on the probability that particles are detected in a given solid angle. To calculate this probability one usually relies on two things: First, one uses the asymptotic S-matrix formalism. The working physicist's justification for this is that *"an experimentalist generally prepares a state ... at $t \to -\infty$, and then measures what this state looks like at $t \to +\infty$"* (cf. [41], p. 113), pretending that the asymptotic expressions are "all there is" – as if they weren't the asymptotics of some other expression, however complicated, describing the scattering process as it really is, namely happening at finite distances and at finite times. Second, one ignores the presence of detectors, i.e. one neglects possible influences of the detection process on the statistics of the detection. In short, one calculates the unmeasured statistics.

Clearly a justification of the S-matrix formalism must be based on a physically realistic, i.e. *finite*, setup that contains the S-matrix formalism as an appropriate limit case and it must consider the possible influence of the detection process on the measured results. Concerning the former, there have been various attempts to base the S-matrix formalism on realistic expressions. In section 3.1 we briefly discuss two such approaches, namely Dollard's scattering into cones, and the flux across surfaces theorems, which have received much attention in recent years. However, both these approaches do not come to grips with the physically realistic situation which succinctly can be summarized by the observation that the scattered particles arrive at the detectors at random times. Within Bohmian mechanics this is easily described (although not easily computed!). In a first step we calculate the exit statistics of Bohmian particles through surfaces which we may think of as detector surfaces, but we ignore the detectors as parts of the physical system. In a second step we address the exit statistics when the detectors are physically present.

Our first object is therefore the joint first exit statistics, i.e. the probability

$$\mathbb{P}^{\psi}\left(\text{the first exit of the } l\text{th particle is in } R\Sigma_l,\ l=1,\ldots,N\right), \tag{3.1}$$

where $\Sigma_l \subset S^2$ are subsets of the three-dimensional unit sphere and the $R\Sigma_l := \{\boldsymbol{x} \in \mathbb{R}^3 \mid \boldsymbol{x} = R\boldsymbol{\omega},\ \boldsymbol{\omega} \in \Sigma_l\}$ denote the corresponding pieces of the spherical surface with radius R covering the solid angles Σ_l. The relevant parameter is the distance R of the detectors from the scattering center. More precisely let $\boldsymbol{X}_l^{\psi}(\boldsymbol{x}_0, t_{\text{ex}}^{B_{l,R}}) \in \mathbb{R}^3$ denote[1] the position of the lth particle at the first exit time $t_{\text{ex}}^{B_{l,R}}$ when it leaves the ball $x_l < R$ for the first time (cf. (3.17)). We shall prove that

$$\lim_{R\to\infty} \mathbb{P}^{\psi}\left(\boldsymbol{X}_l^{\psi}(\boldsymbol{x}_0, t_{\text{ex}}^{B_{l,R}}) \in R\Sigma_l\ \forall\, l \in \{1,\ldots,N\}\right) = \int\limits_{C_{\Sigma_1}} \cdots \int\limits_{C_{\Sigma_N}} \left|\widehat{\psi}_{\text{out}}(\boldsymbol{k})\right|^2 d^3k_1 \cdots d^3k_N \tag{3.2}$$

where $\boldsymbol{k} = (\boldsymbol{k}_1, \ldots, \boldsymbol{k}_N) \in \mathbb{R}^{3N}$ and $C_{\Sigma_l} := \{\boldsymbol{k}_l \in \mathbb{R}^3 \mid \frac{\boldsymbol{k}_l}{k_l} \in \Sigma_l\}$ is the cone given by Σ_l (see Figure 3.1). Furthermore $\widehat{\ }$ denotes the Fourier transform and ψ_{out} is the outgoing asymptote corresponding to the scattering wave function ψ. Note that the right hand side of (3.2) is the formula resulting from the S-matrix formalism.

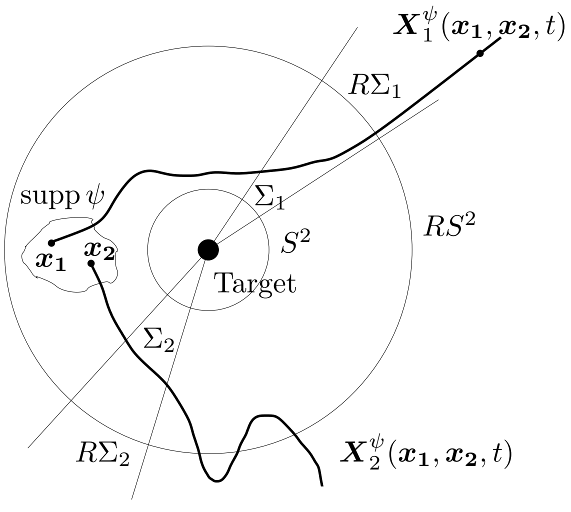

Figure 3.1: Sketch of the scattering situation for $N = 2$.

We remark that our theorem is formulated in terms of the realistic spatial limit rather than a temporal one, as it is often done in scattering theory (see also [33] for a note on this).

The idea for proving (3.2) is rather simple and, from a Bohmian point of view, the most immediate one: One expects that for large times, i.e. far away from the scattering center, the particles' trajectories become classical straight lines. In fact we shall show that for large times the velocity $\dot{\boldsymbol{X}}^{\psi}(\boldsymbol{x}_0, t) = (\dot{\boldsymbol{X}}_1^{\psi}(\boldsymbol{x}_0, t), \ldots, \dot{\boldsymbol{X}}_N^{\psi}(\boldsymbol{x}_0, t))$ converges to the asymptotic velocity

$$\boldsymbol{v}_{\infty}^{\psi} := \lim_{t\to\infty} \frac{\dot{\boldsymbol{X}}^{\psi}(\boldsymbol{x}_0, t)}{t},$$

[1]In this chapter we switch back to the default notation of section 1.2.

which is $|\widehat{\psi}_{\text{out}}|^2$-distributed,[2] i.e. for $A \in \mathbb{R}^{3N}$

$$\mathbb{P}^{\psi}\left(\boldsymbol{v}_{\infty}^{\psi} \in A\right) = \int\limits_{A} |\widehat{\psi}_{\text{out}}(\boldsymbol{k})|^2 \, d^{3N}k. \tag{3.3}$$

Moreover, we shall show that the difference between actual and asymptotic velocity is so well behaved, that the exit statistics for large R is given by the asymptotic velocity. With the distribution (3.3) this then leads to (3.2).

The asymptotic form of the velocity field is no surprise since (as is well known)

$$\lim_{t\to\infty}\left\| e^{-iHt}\psi - (it)^{-\frac{3N}{2}} e^{i\frac{x^2}{2t}} \widehat{\psi}_{\text{out}}\left(\frac{\boldsymbol{x}}{t}\right)\right\| = 0$$

and thus at least in the L^2-sense $\psi(\cdot, t)$ is close to the local plane wave $(it)^{-\frac{3N}{2}} e^{i\frac{x^2}{2t}} \widehat{\psi}_{\text{out}}\left(\frac{\boldsymbol{x}}{t}\right)$. For large times the latter yields a velocity field of straight paths. Now one can expect that under certain conditions this closeness in L^2 results also in a closeness of the corresponding velocity fields.

In a second step we analyze the exit statistics (the detection statistics),

$$\mathbb{P}^{\psi}\left(\text{the } l\text{th particle hits a detector surface } R\Sigma_l,\ l = 1, \ldots, N\right), \tag{3.4}$$

when the detectors are physically present. The effect of detection is of course backscattering through the interaction with the detector and the collapse of the wave function. We do not elaborate on the backscattering, which is already present in one particle scattering, and which will be argued to be small. On the other hand the effect of collapse cannot be argued away, collapse will happen, and when the particles' wave function is entangled, as it is generically the case, one must show that the collapse does not affect the exit statistics we discussed above. The problem is the following: As was stressed before, particles arrive at the detectors at random times. When the first particle is detected the other particles are still on their way. But the detection of the first particle collapses the wave function. Why doesn't that affect the motion of the as yet undetected particles? In view of Bell's nonlocality this question possesses no trivial answer. The answer lies within the "quasi"-product structure of the local plane waves $(it)^{-\frac{3N}{2}} e^{i\frac{x^2}{2t}} \widehat{\psi}_{\text{out}}\left(\frac{\boldsymbol{x}}{t}\right)$ that the scattered wave functions tend to in the scattering regime. In these local plane waves all particles move on straight lines and remain to do so even after the collapse. Indeed we shall prove[3] that, analogous to (3.2),

$$\lim_{R\to\infty} \mathbb{P}^{\psi}\left(\boldsymbol{X}_l^R(\boldsymbol{x}_0, t_l^R(\boldsymbol{x}_0)) \in R\Sigma_l \ \forall\, l \in \{1, 2, \ldots, N\}\right) = \int\limits_{C_{\Sigma_1}} \ldots \int\limits_{C_{\Sigma_N}} \left|\widehat{\psi}_{\text{out}}(\boldsymbol{k})\right|^2 d^3k_1 \cdots d^3k_N\,, \tag{3.5}$$

where the position $\boldsymbol{X}_l^R(\boldsymbol{x}_0, t_l^R(\boldsymbol{x}_0))$ of the lth particle at the first exit time $t_l^R(\boldsymbol{x}_0)$ when it leaves the ball $x_l < R$ (i.e. hits one of the detector surfaces that among them cover

[2] We again use natural units $\hbar = m_l = 1$ where $\boldsymbol{p} = \boldsymbol{k} = \boldsymbol{v}$.

[3] For ease of notation we in fact prove (3.5) only for $N = 2$. The generalization to $N \geq 3$ is, however straightforward, cf. footnote 9.

RS^2) for the first time is now calculated using the collapsed wave function (see subsection 3.4.2).

This remainder of this chapter is organized as follows. We briefly discuss Dollard's scattering into cones and the flux-across-surfaces theorems as attempts to justify the S-matrix formalism (section 3.1). We describe the mathematical framework, that is the setup of many particle potential scattering (section 3.2). In section 3.3 we state our result on the asymptotically classical behavior of the unmeasured Bohmian trajectories of N scattered particles (Theorem 2). Section 3.4 contains our main results: We state and prove the unmeasured instance of the first exit statistics theorem (Theorem 3), give the asymptotically classical behavior of the measured Bohmian trajectories of N scattered particles (Theorem 4) and state and prove the measured instance of the first exit statistics theorem (Theorem 5). We give a short outlook (section 3.5) on the extension to the case of interacting particles. Finally, we prove our results on the asymptotically classical behavior of Bohmian trajectories, i.e. Theorems 2 and 4 (section 3.6).

3.1 Previous works on the foundations of scattering formalism

First works on a deeper justification of the asymptotic S-matrix formalism go back to Dollard [15, 16]. With his scattering-into-cones theorem he gave a first connection between position and momentum space:

$$\lim_{t\to\infty}\int_{C_{\Sigma_1}} d^3x_1 \ldots \int_{C_{\Sigma_N}} d^3x_N\, |\psi(\boldsymbol{x},t)|^2 = \int_{C_{\Sigma_1}} d^3k_1 \ldots \int_{C_{\Sigma_N}} d^3k_N \left|\widehat{\psi}_{\text{out}}(\boldsymbol{k})\right|^2 ,$$

i.e. the probability of finding the scattered particles at large times in the cones $C_{\Sigma_1}, \ldots,$ C_{Σ_N} is given by the probability that the momenta of the outgoing asymptotes lay in the cones $C_{\Sigma_1}, \ldots, C_{\Sigma_N}$, respectively. However, the connection to (3.1) resp. the left hand side of (3.2) is still missing. Crucial in this context is that the time of detection is random and not given by the experimenter. Only R is given. Thus one has to consider a spatial rather than a temporal limit. While the latter may be technical convenient, it is not mirroring the actual physical situation.

For the case of one particle, the next step was taken by Combes, Newton, Shtokhamer [10] who proposed the so called flux-across-surfaces theorem (FAST). It states that

$$\lim_{R\to\infty}\int_0^\infty \int_{R\Sigma} \boldsymbol{j}^\psi(\boldsymbol{x},t)\cdot d\boldsymbol{\sigma} dt = \lim_{R\to\infty}\int_0^\infty \int_{R\Sigma} |\boldsymbol{j}^\psi(\boldsymbol{x},t)\cdot d\boldsymbol{\sigma}| dt = \int_{C_\Sigma} \left|\widehat{\psi}_{\text{out}}(\boldsymbol{k})\right|^2 d^3k,$$

where the quantum mechanical probability current density (short the flux) $\boldsymbol{j}^\psi$ is given by

$$\boldsymbol{j}^\psi(\boldsymbol{x},t) = \text{Im}\left(\psi^*(\boldsymbol{x},t)\nabla\psi(\boldsymbol{x},t)\right) .$$

Hence, asymptotically the flux points outwards and the integrated flux gives rise to the asymptotic S-matrix formalism. It is hard to resist to identify the first exit probability, i.e. the left hand side of (3.2) (with $N = 1$), with the integrated flux, i.e. with

$$\int_0^\infty \int_{R\Sigma} \boldsymbol{j}^\psi(\boldsymbol{x},t) \cdot d\boldsymbol{\sigma} dt\,.$$

For general R, however, this is not true. In general the integrated flux is not positive and therefore not a probability (in fact not even the integrated absolute value of the flux is a probability). Only asymptotically (for large R) does the integrated flux turn into a probability. But the probability of what? If the meaning of the integrated flux is, at least in the usual quantum formalism, not clear for finite R, how can one possibly divine its meaning for $R \to \infty$?

This loophole is closed in Bohmian mechanics, where the integrated flux has got also a non-asymptotic meaning. For that one introduces the number of crossings of a trajectory through an oriented surface. If one denotes by $N^\psi_{\text{sig}}(R\Sigma, \Delta T)$ the signed crossings through $R\Sigma$ during the time interval ΔT, i.e. the difference between outward crossings and inward crossings, one can show that (cf. also subsection 2.4.1)

$$\mathbb{E}^\psi(N^\psi_{\text{sig}}(R\Sigma, \Delta T)) = \int_{\Delta T} \int_{R\Sigma} \boldsymbol{j}^\psi(\boldsymbol{x},t) \cdot d\boldsymbol{\sigma} dt, \tag{3.6}$$

where $d\boldsymbol{\sigma} = \frac{\boldsymbol{x}}{x} d\sigma$ is the infinitesimal surface element. Similarly one has that[4]

$$\mathbb{E}^\psi(N^\psi_{\text{tot}}(R\Sigma, \Delta T)) = \int_{\Delta T} \int_{R\Sigma} |\boldsymbol{j}^\psi(\boldsymbol{x},t) \cdot d\boldsymbol{\sigma}| dt, \tag{3.7}$$

where N^ψ_{tot} denotes the total crossings through $R\Sigma$, i.e. the sum of outward crossings and inward crossings. Hence, with the FAST

$$\lim_{R\to\infty} \mathbb{E}^\psi(N^\psi_{\text{tot}}(R\Sigma, [0,\infty))) = \lim_{R\to\infty} \mathbb{E}^\psi(N^\psi_{\text{sig}}(R\Sigma, [0,\infty)))\,.$$

This means that the scattered particle crosses distant surfaces only outwards and thus at most once. Then one can easily show that (3.2) holds (see [17], Section 3, and [13, 11, 12, 22] for more details). It is this non-asymptotic meaning of the flux in Bohmian mechanics together with the FAST, which in the one-particle case leads to a satisfying exit statistics theorem. First proofs of the FAST can be found in [13, 11, 12]. More results are in [38, 37]. The most recent result on the FAST including a review of the existing results can be found in [18].

The corresponding problem for the N-particle case, however, is different: It was shown in [21] that there the quantum flux looses its significance. That is so because each particle has got its own exit time and thus a multi-time setup is needed. In such a setup, however, it is no longer possible to establish an N-particle statement corresponding to (3.6) or (3.7), which is basic for the exit statistics theorem if one wants to use the flux. This is why one has to take an alternative approach like the direct use of the asymptotically classical behavior of the Bohmian trajectories presented above.

[4] The proof can be found in [5], pp. 34-37, see also [17], Section 3, for a heuristic approach.

3.2 N-particle potential scattering

We consider a system of N non-interacting particles with configuration space $\mathbb{R}^{3N}$ and Hamiltonian

$$H = H_0 + V(\boldsymbol{x}) \,, \quad V(\boldsymbol{x}) = \sum_{l=1}^{N} V_l(\boldsymbol{x}_l) \tag{3.8}$$

where each V_l is a short-range scattering potential $V_l \in (V)_n$ ($n \in \mathbb{N}$):

Definition 4. *For $n \in \mathbb{N}$ $V \in (V)_n$ if*

(i) $V \in L^2(\mathbb{R}^3, \mathbb{R})$,

(ii) V *is* C^∞ *except, perhaps, at finitely many singularities,*

(iii) there exist $\delta > 0,\ C > 0,\ R_0 > 0$ *such that*

$$|V(\boldsymbol{x})| \leq C\langle x\rangle^{-n-\delta} \text{ for } x \geq R_0,$$

where $\langle\cdot\rangle := (1 + (\cdot)^2)^{\frac{1}{2}}$.

Then the potential $V(\boldsymbol{x})$ is H_0-bounded with arbitrarily small bound and H is self-adjoint on $D(H) = D(H_0) = W^2(\mathbb{R}^{3N})$ with $W^2(\mathbb{R}^{3N}) = \{f \in L^2(\mathbb{R}^{3N}) : \int |k^2 \widehat{f}(\boldsymbol{k})|^2 d^{3N}k < \infty\}$ the second Sobolev-space (Kato's theorem, see, e.g., [32] Theorem X.16). Since there is no interaction we may also write

$$H = \sum_{l=1}^{N} H_l = \sum_{l=1}^{N} \big(-\frac{1}{2}\Delta_l + V_l(\boldsymbol{x}_l)\big) = \sum_{l=1}^{N} (H_{0,l} + V_l(\boldsymbol{x}_l)) \ .$$

In the following, we abuse notation and do not distinguish between, say H_l as a multi-particle operator (defined on $L^2(\mathbb{R}^{3N})$) and H_l as a one-particle operator (defined on $L^2(\mathbb{R}^3)$). Now, for every $l \in \{1, \dots, N\}$, the wave operators $\Omega_{\pm,l} : L^2(\mathbb{R}^3) \to \mathrm{Ran}(\Omega_{\pm,l})$

$$\Omega_{\pm,l} := \operatorname*{s-lim}_{t\to\pm\infty} e^{iH_l t} e^{-iH_{0,l}t}$$

exist[5] and are asymptotically complete (see, e.g., [33]), i.e.

$$\mathrm{Ran}(\Omega_{\pm,l}) = \mathcal{H}_{\mathrm{cont}}(H_l) = \mathcal{H}_{\mathrm{a.c.}}(H_l) \,,$$

where $\mathcal{H}_{\mathrm{cont}}(H_l)$ resp. $\mathcal{H}_{\mathrm{a.c.}}(H_l)$ denotes the spectral subspace of $L^2(\mathbb{R}^3)$ that belongs to the continuous resp. the absolutely continuous spectrum of the Hamiltonian H_l. Thus $L^2(\mathbb{R}^3)$ is the orthogonal sum of $\mathcal{H}_{\mathrm{a.c.}}(H_l)$ and $\mathcal{H}_{\mathrm{p.p.}}(H_l)$ (the subspace that belongs to the pure point spectrum of H_l), $\mathcal{H}_{\mathrm{a.c.}}(H_l)$ and $\mathcal{H}_{\mathrm{p.p.}}(H_l)$ are invariant under the time evolution $U_l(t) = e^{-iH_l t}$ and for every scattering wave function $\psi \in \mathcal{H}_{\mathrm{a.c.}}(H_l)$ there exists a unique outgoing/incoming asymptote

$$\psi_{\mathrm{out/in},l} := \Omega_{\pm,l}^{-1}\psi \tag{3.9}$$

[5] s - lim denotes the limit in L^2-sense.

that evolves according to the free time evolution $e^{-iH_{0,l}t}$, i.e. for which

$$\lim_{t\to\pm\infty} \|e^{-iH_{0,l}t}\psi_{\text{out/in},l} - e^{-iH_l t}\psi\| = 0\,.$$

Since H contains no interaction potentials the time evolution $U(t) = e^{-iHt}$ on $L^2(\mathbb{R}^{3N})$ trivially factorizes,

$$U(t) = \prod_{l=1}^{N} U_l(t) = \prod_{l=1}^{N} e^{-iH_l t}\,,$$

and there is a natural splitting of $L^2(\mathbb{R}^{3N})$,

$$L^2(\mathbb{R}^{3N}) \cong \bigotimes_{l=1}^{N} L^2(\mathbb{R}^3) = \bigotimes_{l=1}^{N} \Big(\mathcal{H}_{\text{a.c.}}(H_l) \oplus \mathcal{H}_{\text{p.p.}}(H_l)\Big) \cong \mathcal{H}_{\text{s}}(H) \oplus \mathcal{H}_{\text{rest}}(H),$$

where

$$\mathcal{H}_{\text{s}}(H) :\cong \bigotimes_{l=1}^{N} \mathcal{H}_{\text{a.c.}}(H_l)$$

and $\cong$ is defined by the canonical isomorphism between $L^2(\mathbb{R}^{3N})$ and $\bigotimes_{l=1}^{N} L^2(\mathbb{R}^3)$. Then $\mathcal{H}_{\text{s}}(H)$ and $\mathcal{H}_{\text{rest}}(H)$ are invariant under the time evolution $U(t) = e^{-iHt}$ and $\mathcal{H}_{\text{s}}(H)$ contains the "pure" scattering wave functions, i.e. those wave functions for which all N particles are free asymptotically (for $t \to \pm\infty$) while $\mathcal{H}_{\text{rest}}(H)$ contains those wave functions where either all or at least some particles stay bound. For simplicity we restrict ourselves to the case where the initial wave function is a pure scattering wave function, $\psi \in \mathcal{H}_{\text{s}}(H)$. Then the relevant wave operators are $\Omega_\pm^{(N)} := \text{s-}\lim_{t\to\pm\infty} e^{iHt}e^{-iH_0 t}$. Indeed, observe that

$$\Omega_\pm^{(N)} = \prod_{l=1}^{N} \Omega_{\pm,l}\,,$$

which implies that $\text{Ran}(\Omega_\pm^{(N)}) = \mathcal{H}_{\text{s}}(H)$ and that for every pure scattering wave function $\psi \in \mathcal{H}_{\text{s}}(H)$ there exists a unique outgoing/incoming asymptote

$$\psi_{\text{out/in}} := \left(\Omega_\pm^{(N)}\right)^{-1} \psi \tag{3.10}$$

that evolves according to the free time evolution $e^{-iH_0 t}$.

3.3 Asymptotic behavior of Bohmian trajectories in scattering situations

We first present the result on the asymptotically classical behavior of the Bohmian trajectories we wish to employ in the proof of the exits statistics theorem (3.2). It is an extension of that for one particle in [34]. In Definition 5 we define the set $\mathcal{G}^{(N)}$ of "good" initial wave functions, for which we can proof our results. This set is optimized for generality and occurred in a similar form already in [18, 34] (for $N = 1$).

Definition 5. *A function* $f : \mathbb{R}^{3N} \to \mathbb{C}$ *is in* $\mathcal{G}_0^{(N)}$, *if*

$$\begin{aligned} & f \in \mathcal{H}_s(H) \cap C^\infty(H), \\ & \langle x \rangle^{\frac{3N+1}{2}+\beta} H^n f \in L^2(\mathbb{R}^{3N}), \qquad \beta \in \{N+1, N+2, \ldots, 2N\},\ n \in \{0,1,2,\ldots,4N-\beta\}, \\ & \langle x \rangle^{\frac{3N+1}{2}+N} H^n f \in L^2(\mathbb{R}^{3N}), \qquad n \in \{2N, 2N+1, \ldots, 3N\}. \end{aligned}$$

Then $\mathcal{G}^{(N)} := \bigcup_{t\in\mathbb{R}} e^{-iHt}\mathcal{G}_0^{(N)}$. *Here* $C^\infty(H) = \bigcap_{n=1}^{\infty} D(H^n)$.

For $\psi \in \mathcal{G}^{(N)}$ we get the desired asymptotically classical behavior of the Bohmian trajectories.

Theorem 2. *Let* $V_l \in (V)_4$ *and let zero be neither a resonance nor an eigenvalue of* H_l $(l = 1, \ldots, N)$. *Let* $\psi \in \mathcal{G}^{(N)}$ *with* $\|\psi\| = 1$. *Then:*

(i) The Bohmian trajectories $\boldsymbol{X}^\psi(\boldsymbol{x}_0, t)$ *exist uniquely and globally in time for* $\mathbb{P}^\psi$*-almost all initial configurations* $\boldsymbol{x}_0 \in \mathbb{R}^{3N}$.

(ii) For $\mathbb{P}^\psi$*-almost all Bohmian trajectories the asymptotic velocity* $\lim_{t\to\infty} \boldsymbol{v}^\psi\left(\boldsymbol{X}^\psi(\boldsymbol{x}_0,t),t\right)$ *is given by* $\boldsymbol{v}_\infty^\psi(\boldsymbol{x}_0) := \lim_{t\to\infty} \frac{\boldsymbol{X}^\psi(\boldsymbol{x}_0,t)}{t}$. *More precisely,* $\boldsymbol{v}_\infty^\psi$ *exists for* $\mathbb{P}^\psi$*-almost all* $\boldsymbol{x}_0 \in \mathbb{R}^{3N}$ *and for all* $\epsilon > 0$ *there exist some* $T < \infty$ *and some* $C < \infty$ *such that*

$$\mathbb{P}^\psi\left(\left\{\boldsymbol{x} \in \mathbb{R}^{3N} \mid \left|\boldsymbol{v}^\psi\left(\boldsymbol{X}^\psi(\boldsymbol{x}_0,t),t\right) - \boldsymbol{v}_\infty^\psi(\boldsymbol{x}_0)\right| < Ct^{-\frac{1}{2}} \quad \forall\, t \geq T\right\}\right) > 1-\epsilon\,. \tag{3.11}$$

(iii) $\boldsymbol{v}_\infty^\psi$ *is randomly distributed with density* $|\widehat{\psi}_{out}(\cdot)|^2$, *i.e. for every measurable set* $A \subset \mathbb{R}^{3N}$

$$\mathbb{P}^\psi\left(\left\{\boldsymbol{x}_0 \in \mathbb{R}^{3N} \mid \boldsymbol{v}_\infty^\psi(\boldsymbol{x}_0) \in A\right\}\right) = \int_A |\widehat{\psi}_{out}(\boldsymbol{k})|^2\, d^{3N}k\,. \tag{3.12}$$

The proof of Theorem 2 can be found in subsection 3.6.1.

Remark 6. Zero is a resonance of H if there exists a solution f of $Hf = 0$ such that $\langle\cdot\rangle^{-\gamma} f \in L^2(\mathbb{R}^3)$ for any $\gamma > \frac{1}{2}$ but not for $\gamma = 0$.[6] The occurrence of a zero eigenvalue or resonance is an exceptional event: For Hamiltonians $H(c) = H_0 + cV$ the set of parameters $c \in \mathbb{R}$, for which zero is an eigenvalue or a resonance, is discrete (see e.g. [2], p. 20 and [28], p. 589).

It is well known that, in L^2-sense, the large time asymptote of a scattering wave function $\psi(\boldsymbol{x},t)$ is given by $\Phi(\boldsymbol{x},t) := (it)^{-\frac{3N}{2}} e^{i\frac{\boldsymbol{x}^2}{2t}} \widehat{\psi}_{\text{out}}\left(\frac{\boldsymbol{x}}{t}\right)$. Moreover, one easily sees that the Bohmian velocity field of $\Phi(\boldsymbol{x},t)$ is essentially that of straight paths (cf. [34]):

$$\boldsymbol{v}^\Phi(\boldsymbol{x},t) = \mathrm{Im}\frac{\nabla\Phi(\boldsymbol{x},t)}{\Phi(\boldsymbol{x},t)} = \frac{\boldsymbol{x}}{t} + \frac{1}{t}\mathrm{Im}\frac{\nabla\widehat{\psi}_{\text{out}}(\boldsymbol{y})}{\widehat{\psi}_{\text{out}}(\boldsymbol{y})}\bigg|_{\boldsymbol{y}=\frac{\boldsymbol{x}}{t}} \overset{t\text{ big}}{\approx} \frac{\boldsymbol{x}}{t}\,.$$

[6] There are various definitions, see e.g. [42], p. 552, [2], p.20 and [28], p. 584.

Thus the main technical difficulty in proving Theorem 2 is to show that the velocity field (1.2) of $\psi(\boldsymbol{x},t)$ is approximated sufficiently well by that of its asymptote $\Phi(\boldsymbol{x},t)$, i.e. that $\psi(\boldsymbol{x},t)$ and $\Phi(\boldsymbol{x},t)$ are close not only in the L^2-sense but also in the stronger sense of velocity fields. For that one needs detailed *pointwise* estimates on $\psi(\boldsymbol{x},t)$ and its gradient. They are collected in the following

Lemma 5. *Let $V_l \in (V)_4$ and zero be neither a resonance nor an eigenvalue of H_l $(l=1,\dots,N)$. Let $\psi \in \mathcal{G}^{(N)}$. Then for all $0<a<b<\infty$ there exist constants $T<\infty$ and $C<\infty$ such that for all $t>T$ and $a<\frac{x_l}{t}<b$, $l=1,\dots,N$*

$$|\psi(\boldsymbol{x},t)-\Phi(\boldsymbol{x},t)| \le Ct^{-\frac{3N+1}{2}} \tag{3.13}$$

and

$$\left|\nabla\psi(\boldsymbol{x},t)-i\frac{\boldsymbol{x}}{t}\Phi(\boldsymbol{x},t)\right| \le Ct^{-\frac{3N+1}{2}}\,. \tag{3.14}$$

The proof of Lemma 5 can be found in subsection 3.6.3. The idea is to use the method of expansion in generalized eigenfunctions, i.e. in functions $\varphi_+^{(N)}$ that are solutions of the stationary Schrödinger equation

$$H\varphi_+^{(N)}(\boldsymbol{x},\boldsymbol{k}) = \frac{k^2}{2}\varphi_+^{(N)}(\boldsymbol{x},\boldsymbol{k})$$

with the boundary condition $\lim\limits_{x\to\infty}\left|\varphi_+^{(N)}(\boldsymbol{x},\boldsymbol{k})-e^{i\boldsymbol{k}\cdot\boldsymbol{x}}\right|=0$. The generalized eigenfunctions $\varphi_+^{(N)}$ diagonalize H on $\mathcal{H}_{\mathrm{s}}(H)$ as the plane waves $e^{i\boldsymbol{k}\cdot\boldsymbol{x}}$ diagonalize H_0. Thus one can define a generalized Fourier transform connecting the outgoing asymptote ψ_{out} and the pure scattering wave function $\psi\in\mathcal{H}_{\mathrm{s}}(H)$ via[7]

$$\psi(\boldsymbol{x}) = (2\pi)^{-\frac{3N}{2}}\,\mathrm{l.\,i.\,m.}\int \varphi_+^{(N)}(\boldsymbol{x},\boldsymbol{k})\widehat{\psi}_{\mathrm{out}}(\boldsymbol{k})d^{3N}k$$

and

$$\widehat{\psi}_{\mathrm{out}}(\boldsymbol{k}) = (2\pi)^{-\frac{3N}{2}}\,\mathrm{l.\,i.\,m.}\int \left(\varphi_+^{(N)}\right)^*(\boldsymbol{x},\boldsymbol{k})\psi(\boldsymbol{x})d^{3N}x\,. \tag{3.15}$$

Moreover,

$$\psi(\boldsymbol{x},t) = (2\pi)^{-\frac{3N}{2}}\,\mathrm{l.\,i.\,m.}\int e^{-i\frac{k^2t}{2}}\varphi_+^{(N)}(\boldsymbol{x},\boldsymbol{k})\widehat{\psi}_{\mathrm{out}}(\boldsymbol{k})d^{3N}k\,. \tag{3.16}$$

We elaborate on that and the properties of the generalized eigenfunctions $\varphi_\pm^{(N)}$ in subsection 3.6.2. With the help of stationary phase methods (3.16) will give us the desired pointwise estimates on $(\nabla)\psi(\boldsymbol{x},t)$ whenever $\widehat{\psi}_{\mathrm{out}}$ and the generalized eigenfunctions $\varphi_+^{(N)}$ are sufficiently regular (subsection 3.6.3).

[7] $\mathrm{l.\,i.\,m.}\int$ is a shorthand notation for $\operatorname*{s\text{-}lim}\limits_{R\to\infty}\int_{B_R}$, where s - lim denotes the limit in the L^2-norm and B_R is a ball with radius R around the origin.

Note, however, that it is important to impose any emerging technical conditions on the scattering wave function ψ rather than its asymptote ψ_{out}, since it is the former not the latter that is prepared in an experiment. Thus, we shall use (3.15) to infer how smoothness properties of ψ map to the desired smoothness properties of $\widehat{\psi}_{\text{out}}$ (subsection 3.6.3, Lemma 10). Of course, also this mapping crucially depends on the regularity properties of the generalized eigenfunctions. This regularity, however, is very poor in general. Thus one can use only weak requirements on $\widehat{\psi}_{\text{out}}$, which in turn makes the application of stationary phase methods to (3.16) quite a tricky business. Nevertheless, for $N = 1$ the above program was successfully carried out in [18]. For general N and *interacting* particles, however, not enough is known about the generalized eigenfunctions (cf. section 3.5). This is why we restrict ourselves to non-interacting particles and pure scattering wave functions $\psi \in \mathcal{H}_{\text{s}}(H)$. In this case we can show that ψ can be expanded in N-particle eigenfunctions $\varphi_+^{(N)}$ which are products of the one-particle generalized eigenfunctions $\varphi_{+,l}$ (cf. equation (3.52)) which gives us all the leverage on the $\varphi_+^{(N)}$s we need.[8]

3.4 Exit statistics

3.4.1 The first exit statistics theorem

The first task is to find a formalized expression for the (unmeasured) joint first exit probability (3.1). To explain what is meant by "the first exit of the lth particle is in $R\Sigma_l$" we define the first exit time $t_{\text{ex}}^A(\boldsymbol{x}_0)$ at which the trajectory $\{\boldsymbol{X}^\psi(\boldsymbol{x}_0, t),\, t \geq 0\}$ leaves an open subset $A \subset \mathbb{R}^{3N}$ for the first time:

$$t_{\text{ex}}^A(\boldsymbol{x}_0) := \inf\big\{t \geq 0 \mid \boldsymbol{X}^\psi(\boldsymbol{x}_0, s) \in A \;\forall s \in [0,t) \text{ and } \boldsymbol{X}^\psi(\boldsymbol{x}_0, t) \notin A\big\}\,, \tag{3.17}$$

where we set $t_{\text{ex}}^A(\boldsymbol{x}_0) = 0$ if the above set is empty. t_{ex}^A is a random variable on the space $\mathbb{R}^{3N}$ of initial configurations (cf. [6], Lemma 4.2). Clearly, $B_{l,R} := \{\boldsymbol{x} \in \mathbb{R}^{3N} \mid x_l < R\}$ is open and $\{\boldsymbol{X}^\psi(\boldsymbol{x}_0, t),\, t \geq 0\}$ leaves $B_{l,R}$ exactly when the lth particle's trajectory leaves the open ball $B_R = \{\boldsymbol{x} \in \mathbb{R}^3 \mid x < R\}$. Moreover, continuity of $\boldsymbol{X}^\psi(\boldsymbol{x}_0, t)$ in t (as a solution of (1.2)) implies $\boldsymbol{X}_l^\psi(\boldsymbol{x}_0, t_{\text{ex}}^{B_{l,R}}(\boldsymbol{x}_0)) \in \delta B_R = RS^2$, so "the first exit of the lth particle is in $R\Sigma_l$" if and only if $\boldsymbol{X}_l^\psi(\boldsymbol{x}_0, t_{\text{ex}}^{B_{l,R}}(\boldsymbol{x}_0)) \in R\Sigma_l$. Hence

$$\begin{aligned}\mathbb{P}^\psi&(\text{the first exit of the } l\text{th particle is in } R\Sigma_l,\; l = 1, \ldots, N) \\ &= \mathbb{P}^\psi\left(\boldsymbol{X}_l^\psi(\boldsymbol{x}_0, t_{\text{ex}}^{B_{l,R}}(\boldsymbol{x}_0)) \in R\Sigma_l \quad \forall l \in \{1, \ldots, N\}\right).\end{aligned}$$

We remark that "problematical crossings" (tangential crossings where the velocity $\dot{\boldsymbol{X}}_l^\psi(\boldsymbol{x}_0, t)$ is orthogonal to the orientation of $R\Sigma_l$) have measure zero and need not concern us, see [6], pp. 28-34.

With the above we can formulate the first exit statistics theorem.

[8] In fact we don't even need to explicitly apply stationary phase methods to (3.16) but can directly fall back on results for the one particle case, see subsection 3.6.3.

Theorem 3. *Let $V_l \in (V)_4$ and let zero be neither a resonance nor an eigenvalue of H_l $(l = 1, \dots, N)$. Let $\psi \in \mathcal{G}^{(N)}$ with $\|\psi\| = 1$. Then:*

$$\lim_{R\to\infty} \mathbb{P}^\psi\Big(\Big\{\boldsymbol{x}_0 \in \mathbb{R}^{3N} \mid \boldsymbol{X}_l^\psi(\boldsymbol{x}_0, t_{ex}^{B_{l,R}}(\boldsymbol{x})) \in R\Sigma_l\,,\, l = 1, 2, \dots, N\Big\}\Big) = \int_{C_{\Sigma_1}} d^3k_1 \,\dots \int_{C_{\Sigma_N}} d^3k_N \,\left|\widehat{\psi}_{out}(\boldsymbol{k})\right|^2 . \tag{3.2}$$

Proof of Theorem 3. Because of Theorem 2 (iii) we are done if we can show that

$$\lim_{R\to\infty} \mathbb{P}^\psi \left(\boldsymbol{X}_l^\psi(\cdot, t_{\rm ex}^{B_{l,R}}) \in R\Sigma_l\,,\ l = 1, 2, \dots, N\right) = \mathbb{P}^\psi\left(\boldsymbol{v}_\infty^\psi \in C_{\Sigma_1} \times \dots \times C_{\Sigma_N}\right) , \tag{3.18}$$

i.e. that each particle's trajectory $\boldsymbol{X}_l^\psi$ leaves the ball B_R for the first time through $R\Sigma_l$ if and only if the asymptotic velocity $\boldsymbol{v}_{\infty,l}^\psi$ is in C_{Σ_l}. For that it suffices that the actual trajectory $\boldsymbol{X}^\psi$ differs not too much from the "ideal" trajectory $\boldsymbol{v}_\infty^\psi t$. But this is a simple consequence of Theorem 2. Let $\varepsilon > 0$. Integrating (3.11) we get that there is some $C_\varepsilon < \infty$ and some $T_\varepsilon < \infty$ such that

$$\mathbb{P}^\psi\left(\left\{\boldsymbol{x}_0 \in \mathbb{R}^{3N} \mid |\boldsymbol{X}^\psi(\boldsymbol{x}_0, t) - \boldsymbol{X}^\psi(\boldsymbol{x}_0, T) - \boldsymbol{v}_\infty^\psi(\boldsymbol{x})(t - T)| < C_\varepsilon\sqrt{t},\ \forall t \geq T\right\}\right) > 1 - \frac{\epsilon}{3}$$

for all $T > T_\varepsilon$. Since Theorem 2 (i), i.e. global existence of Bohmian mechanics, guarantees that $\mathbb{P}^\psi$-almost no trajectory reaches spatial infinity in finite time we also know that

$$\mathbb{P}^\psi\Big(\big\{\boldsymbol{x}_0 \in \mathbb{R}^{3N} \mid \sup_{0\leq t\leq T_\varepsilon} |\boldsymbol{X}^\psi(\boldsymbol{x}_0, t)| < C_{T_\varepsilon}\big\}\Big) > 1 - \frac{\epsilon}{3}$$

for some $C_{T_\varepsilon} < \infty$. Moreover, by Theorem 2 (iii) and since $\widehat{\psi}_{\rm out} \in L^2(\mathbb{R}^{3N})$

$$\mathbb{P}^\psi\left(v_\infty^\psi < b_\varepsilon\right) = \int_{k<b_\varepsilon} |\widehat{\psi}_{\rm out}(\boldsymbol{k})|^2\, d^{3N}k > 1 - \frac{\epsilon}{3}$$

for $b_\varepsilon > 0$ big enough. So, noting that

$$\left|\boldsymbol{X}^\psi(\boldsymbol{x}_0, t) - \boldsymbol{v}_\infty^\psi(\boldsymbol{x}_0)t\right| \leq \sup_{0\leq t\leq T_\varepsilon} |\boldsymbol{X}^\psi(\boldsymbol{x}_0, t)| + v_\infty^\psi(\boldsymbol{x}_0)T_\varepsilon < C_{T_\varepsilon} + b_\varepsilon T_\varepsilon$$

for $0 \leq t \leq T_\varepsilon$,

$$\begin{aligned}\left|\boldsymbol{X}^\psi(\boldsymbol{x}_0, t) - \boldsymbol{v}_\infty^\psi(\boldsymbol{x}_0)t\right| &\\ &\leq \left|\boldsymbol{X}^\psi(\boldsymbol{x}_0, t) - \boldsymbol{X}^\psi(\boldsymbol{x}_0, T_\varepsilon) - \boldsymbol{v}_\infty^\psi(\boldsymbol{x}_0)(t - T_\varepsilon)\right| + |\boldsymbol{X}^\psi(\boldsymbol{x}_0, T_\varepsilon)| + v_\infty^\psi(\boldsymbol{x}_0)T_\varepsilon \\ &< C_\varepsilon\sqrt{t} + C_{T_\varepsilon} + b_\varepsilon T_\varepsilon\end{aligned}$$

for $t > T_\varepsilon$ and $\mathbb{P}^\psi(A \cap B \cap C) \geq \mathbb{P}^\psi(A) + \mathbb{P}^\psi(B) + \mathbb{P}^\psi(B) - 2$ for all measurable sets $A, B, C \subset \mathbb{R}^{3N}$, we finally see that

$$\mathbb{P}^\psi\left(\left\{\boldsymbol{x}_0 \in \mathbb{R}^{3N} \Big| \left|\boldsymbol{X}^\psi(\boldsymbol{x}_0,t) - \boldsymbol{v}^\psi_\infty(\boldsymbol{x}_0)t\right| < C_\varepsilon(1+\sqrt{t}), \quad \forall t \geq 0\right\}\right) > 1-\epsilon \tag{3.19}$$

for some $C_\varepsilon < \infty$.

Now the idea of the proof is straightforward: If $0 \neq \boldsymbol{v}^\psi_\infty$ lies in $C_{\Sigma_1} \times \ldots \times C_{\Sigma_N}$, the "ideal" trajectory $\boldsymbol{v}^\psi_{\infty,l}t$ of the lth particle crosses the surface $R\Sigma_l$ at time $\frac{R}{v^\psi_{\infty,l}}$. Thus the "ideal" time of crossing grows linear with the distance R. As does the distance between the point where $\boldsymbol{v}^\psi_{\infty,l}t$ crosses $R\Sigma_l$ and the boundary of $R\Sigma_l$. However, since the difference between the actual and the "ideal" trajectory grows only sublinear in time, it also grows sublinear with R, if evaluated at the "ideal" time of crossing. So if R is big enough, the distance between the point of crossing of the "ideal" trajectory and the boundary of $R\Sigma_l$ is larger than the distance between $\boldsymbol{X}^\psi_l$ and $\boldsymbol{v}^\psi_{\infty,l}t$ at the "ideal" time of crossing. Since the trajectory is continuous in t this implies that $\boldsymbol{X}^\psi_l$ crosses RS^2 first in $R\Sigma_l$, if and only if $\boldsymbol{v}^\psi_{\infty,l}$ lies in C_{Σ_l} (see Figure 3.2). To render this idea more precise, we introduce two sets M_C and M'_C:

$$M_C := \left\{\boldsymbol{x}_0 \in \mathbb{R}^{3N} \mid 0 \neq \boldsymbol{v}^\psi_\infty(\boldsymbol{x}_0) \in C_{\Sigma_1} \times C_{\Sigma_2} \times \ldots \times C_{\Sigma_N}\right\} \cap G_C$$
$$M'_C := \left\{\boldsymbol{x}_0 \in \mathbb{R}^{3N} \mid 0 \neq \boldsymbol{v}^\psi_\infty(\boldsymbol{x}_0) \in \left(\overline{C_{\Sigma_1} \times C_{\Sigma_2} \times \ldots \times C_{\Sigma_N}}\right)^c\right\} \cap G_C$$

where

$$G_C := \left\{\boldsymbol{x}_0 \in \mathbb{R}^{3N} \Big| \left|\boldsymbol{X}^\psi(\boldsymbol{x}_0,t) - \boldsymbol{v}^\psi_\infty(\boldsymbol{x}_0)t\right| < C(1+\sqrt{t})\,,\ \forall t \geq 0\right\}$$

and $\overline{C_{\Sigma_1} \times \ldots \times C_{\Sigma_N}} = \overline{C}_{\Sigma_1} \times \ldots \times \overline{C}_{\Sigma_N}$ denotes the closure of $C_{\Sigma_1} \times \ldots \times C_{\Sigma_N}$. We shall show that

(i) for all $C > 0$

$$\boldsymbol{x}_0 \in M_C \quad \Rightarrow \quad \exists R' > 0 : \boldsymbol{X}^\psi_l(\boldsymbol{x}_0, t^{B_{l,R}}_{\text{ex}}(\boldsymbol{x}_0)) \in R\Sigma_l \quad \forall R \geq R',\, l \in \{1,\ldots,N\}\,,$$
$$\boldsymbol{x}_0 \in M'_C \quad \Rightarrow \quad \exists R'' > 0,\, l \in \{1,\ldots,N\} : \boldsymbol{X}^\psi_l(\boldsymbol{x}_0, t^{B_{l,R}}_{\text{ex}}(\boldsymbol{x}_0)) \notin R\Sigma_l \quad \forall R \geq R''\,,$$

(ii) for all $\epsilon > 0$ there exists a $C_\varepsilon < \infty$ such that

$$\mathbb{P}^\psi\left(M_{C_\varepsilon}\right) > \mathbb{P}^\psi\left(\boldsymbol{v}^\psi_\infty \in C_{\Sigma_1} \times \ldots \times C_{\Sigma_N}\right) - \epsilon\,,$$
$$\mathbb{P}^\psi(M'_{C_\varepsilon}) > 1 - \mathbb{P}^\psi\left(\boldsymbol{v}^\psi_\infty \in C_{\Sigma_1} \times \ldots \times C_{\Sigma_N}\right) - \epsilon\,.$$

Then, for all $\varepsilon > 0$,

$$\begin{aligned}\lim_{R\to\infty} \mathbb{P}^\psi\left(\boldsymbol{X}^\psi_l(\boldsymbol{x}_0, t^{B_{l,R}}_{\text{ex}}(\boldsymbol{x}_0)) \in R\Sigma_l\,,\ l = 1,2,\ldots,N\right) &\overset{(i)}{\geq} \mathbb{P}^\psi(M_{C_\varepsilon}) \\ &\overset{(ii)}{>} \mathbb{P}^\psi\left(\boldsymbol{v}^\psi_\infty \in C_{\Sigma_1} \times \ldots \times C_{\Sigma_N}\right) - \varepsilon\end{aligned}$$

and

$$\begin{aligned}&\lim_{R\to\infty} \mathbb{P}^\psi\left(\boldsymbol{X}^\psi_l(\boldsymbol{x}_0, t^{B_{l,R}}_{\text{ex}}(\boldsymbol{x}_0)) \in R\Sigma_l\ \forall l \in \{1,\ldots,N\}\right) \\ &\qquad = 1 - \lim_{R\to\infty} \mathbb{P}^\psi\left(\exists l \in \{1,\ldots,N\}:\ \boldsymbol{X}^\psi_l(\boldsymbol{x}_0, t^{B_{l,R}}_{\text{ex}}(\boldsymbol{x}_0)) \notin R\Sigma_l\right) \\ &\qquad \overset{(i)}{\leq} 1 - \mathbb{P}^\psi(M'_{C_\varepsilon}) \overset{(ii)}{<} \mathbb{P}^\psi\left(\boldsymbol{v}^\psi_\infty \in C_{\Sigma_1} \times \ldots \times C_{\Sigma_N}\right) + \varepsilon\,,\end{aligned}$$

which together gives (3.18).

Now to the proof of (i) and (ii). (ii) is a direct consequence of (3.19) and the fact that by Theorem 2 (iii) the image measure $\mathbb{P}^{\psi}_{\boldsymbol{v}^{\psi}_{\infty}}(A) := \mathbb{P}^{\psi}(\boldsymbol{v}^{\psi}_{\infty} \in A)$ is absolutely continuous with respect to Lebesgue measure:

$$\mathbb{P}^{\psi}\left(M_{C_\varepsilon}\right) > \mathbb{P}^{\psi}\big(0 \neq \boldsymbol{v}^{\psi}_{\infty} \in C_{\Sigma_1} \times \ldots \times C_{\Sigma_N}\big) - \varepsilon = \mathbb{P}^{\psi}\big(\boldsymbol{v}^{\psi}_{\infty} \in C_{\Sigma_1} \times \ldots \times C_{\Sigma_N}\big) - \varepsilon$$

and

$$\begin{aligned}\mathbb{P}^{\psi}(M'_{C_\varepsilon}) &> \mathbb{P}^{\psi}\big(0 \neq \boldsymbol{v}^{\psi}_{\infty} \in \big(\overline{C_{\Sigma_1} \times \ldots \times C_{\Sigma_N}}\big)^c\big) - \varepsilon = \mathbb{P}^{\psi}\big(\boldsymbol{v}^{\psi}_{\infty} \in \big(\overline{C_{\Sigma_1} \times \ldots \times C_{\Sigma_N}}\big)^c\big) - \varepsilon \\ &= 1 - \mathbb{P}^{\psi}\big(\boldsymbol{v}^{\psi}_{\infty} \in C_{\Sigma_1} \times \ldots \times C_{\Sigma_N}\big) - \varepsilon\end{aligned}$$

for some $C_\varepsilon < \infty$.

Thus we are left with (i). We just prove the first implication. Since $\big(\overline{C_{\Sigma_1} \times C_{\Sigma_2} \times \ldots \times C_{\Sigma_N}}\big)^c = \big(C_{S^2\setminus\overline{\Sigma}_1} \times C_{S^2} \times \ldots \times C_{S^2}\big) \cup \ldots \cup \big(C_{S^2} \times \ldots \times C_{S^2} \times C_{S^2\setminus\overline{\Sigma}_N}\big)$ and $R(S^2 \setminus \overline{\Sigma}_l) \subset R(S^2 \setminus \Sigma_l) = (R\Sigma_l)^c$ the second implication is in fact a consequence of the first.

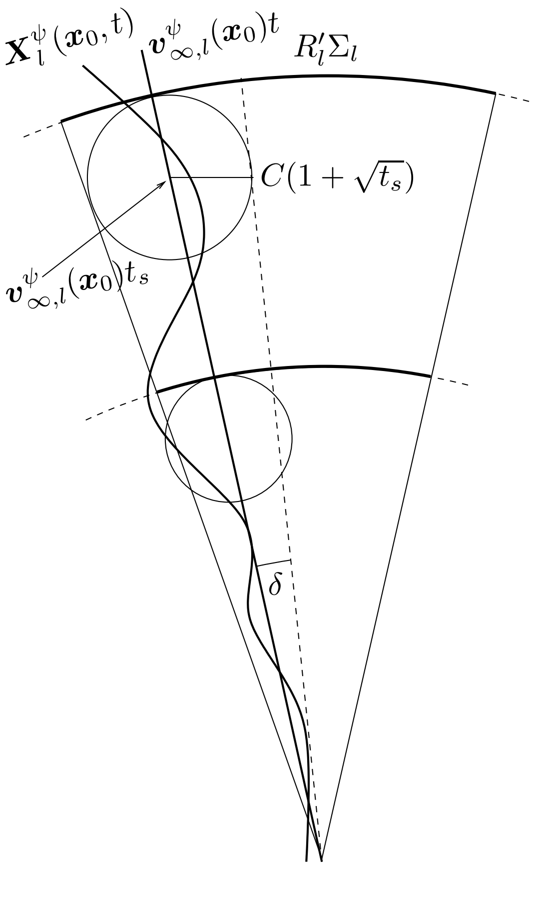

Figure 3.2: Real and "ideal" trajectory.

Let $\boldsymbol{x}_0 \in M_C$ and $C > 0$. We show that for every $l \in \{1, \ldots, N\}$ there is an $R'_l < \infty$ such that $\boldsymbol{X}^{\psi}_{l}(\boldsymbol{x}_0, t^{B_{l,R}}_{\text{ex}}(\boldsymbol{x}_0)) \in R\Sigma_l$ for all $R \geq R'_l$. Then (iii) holds with $R' = \max\{R'_1, \ldots, R'_N\}$. Since $0 \neq \boldsymbol{v}^{\psi}_{\infty,l} \in C_{\Sigma_l}$ and C_{Σ_l} is open, there exists a cone $C_{l,\delta}$ around the axis $\boldsymbol{v}^{\psi}_{\infty,l}$ with apex in the origin and apex angle $0 < \delta < \pi$ such that $C_{l,\delta} \subset C_{\Sigma_l}$. By the definition of M_C the trajectory $\boldsymbol{X}^{\psi}_{l}(\boldsymbol{x}_0, t)$ stays in the ball around $\boldsymbol{v}^{\psi}_{\infty,l}t$ with radius $C(1 + \sqrt{t})$. This ball fits entirely into the cone $C_{l,\delta}$ whenever $v^{\psi}_{\infty,l}(\boldsymbol{x})t \sin\delta > C(1 + \sqrt{t})$. Obviously the latter holds for all t big enough, $t > t_s$ for appropriate $0 < t_s < \infty$. So if $R'_l = v^{\psi}_{\infty,l}(\boldsymbol{x}_0)t_s + C(1 + \sqrt{t_s})$, the (continuous!) trajectory $\boldsymbol{X}^{\psi}_{l}(\boldsymbol{x}_0, t)$ — just like the "ideal" trajectory $\boldsymbol{v}^{\psi}_{\infty,l}t$ — leaves the ball B_R for the first time through the surface $R\Sigma_l$ for all $R \geq R'_l$. Moreover, this clearly happens at a finite time. Hence, $\boldsymbol{X}^{\psi}_{l}(\boldsymbol{x}_0, t^{B_{l,R}}_{\text{ex}}(\boldsymbol{x}_0)) \in R\Sigma_l$ for all $R \geq R'_l$ and we are done.

□

3.4.2 Extension to measured statistics

All of the above concerns *unmeasured* statistics: We did not take into account the effects a detector in a real life experiment might have on the scattered particles (resp. their wave function). In N-particle scattering the presence of detectors could affect the exit statistics in two ways, the first pertaining also to one-particle scattering ($N = 1$), the second unique to "real" multi-particle scattering ($N \geq 2$).

First, in order to detect anything at all every detector must interact with the scattered particles, i.e. due to their interaction potential the presence of detectors might change the time evolution of the scattered particles' wave function and thus the particles' trajectories even before any particle hits a detector ("backscattering"). Second, once one of the scattered particles hits a detector the particles' wave function will collapse, which (since the wave function typically is entangled) might result in a change in the remaining particles' motion.

Regarding the first point one has to argue why the interaction between the detector and the particle is sufficiently small. In a scattering experiment one is interested in a good angle resolution, which is proportional to $\frac{\Delta x}{R}$, where Δx is the spatial resolution of the detector and R its distance from the scattering center. Hence, in the scattering regime, where R tends to infinity, one can achieve microscopic angle resolution with macroscopic spatial resolution. Macroscopic spatial resolution, however, corresponds to weak interaction between detector and particle. Here we do not elaborate on this point but just assume that the detectors are such that we can safely neglect any effects of backscattering.

Regarding the second point the idea is to prove that the collapse of the scattered particles' wave function due to the detection of one particle *far away from the scattering center* does not noticeably alter the velocity field of the remaining particles. But then also the remaining particles' trajectories stay unchanged, i.e. if one of the remaining particles hits a detector it does so *at the same place and time* as it would have if the first particle hadn't been detected. And – as before – this second detection does not alter the trajectories of the still remaining $N - 2$ particles. So in the end we may conclude that the measured exit statistics is the same as the unmeasured one.

Elaborating on this idea we proceed as follows. For ease of notation we restrict ourselves to the case of two particles[9]. We model the collapse of the particles's wave function due to the detection of one particle, which leads to the definition of the particles' measured Bohmian trajectories (Definition 6). We prove that, whenever the detectors are far away from the scattering center, for large times the velocity along a typical measured (configuration-space) trajectory is close to the asymptotic velocity v_∞^ψ of the corresponding unmeasured trajectory (Theorem 4). Here corresponding means that the measured and the unmeasured trajectory start with the same configuration $\boldsymbol{x}_0$. Finally, we show that the closeness expressed in Theorem 4 suffices to guarantee agreement of the measured with the unmeasured exit statistics (Theorem 5).

[9]If the collapse due to one particle's detection does not alter the exit statistics there is no reason why the collapse due to a second particle's detection should. Indeed, the extension of our proof to $N \geq 3$ is mostly evident. Where not we have commented on it.

In the following let $N = 2$. Since we neglect backscattering, before any of the two particles hits a detector surface the particles measured dynamics is the same as the unmeasured one, i.e. at first $\psi^{\text{measured}}(\boldsymbol{x}, t) = \psi(\boldsymbol{x}, t)$ and $\boldsymbol{X}^{\text{measured}}(\boldsymbol{x}_0, t) = \boldsymbol{X}^{\psi}(\boldsymbol{x}_0, t)$. By $T^R(\boldsymbol{x}_0)$ denote the time at which the first particle arrives at one of the detector surfaces (which together cover all of RS^2). Say it is the $\boldsymbol{x}_1$-particle that reaches RS^2 first. Let us assume that at $T^R(\boldsymbol{x}_0)$ the detectors perform an ideal sharp position measurement on the $\boldsymbol{x}_1$-particle. Since its position at that time is $\boldsymbol{X}_1^{\psi}(\boldsymbol{x}_0, T^R(\boldsymbol{x}_0))$, the outcome of this measurement will be, of course, $\boldsymbol{X}_1^{\psi}(\boldsymbol{x}_0, T^R(\boldsymbol{x}_0))$. Then the standard calculus of quantum mechanics gives us the following expression for the collapsed wave function of the $\boldsymbol{x}_2$-particle[10]:

$$\psi^{\text{measured}}(\boldsymbol{x}_2, T^R(\boldsymbol{x}_0)) = \frac{\psi\left(\boldsymbol{X}_1^{\psi}(\boldsymbol{x}_0, T^R(\boldsymbol{x}_0)), \boldsymbol{x}_2, T^R(\boldsymbol{x}_0)\right)}{\left\|\psi\left(\boldsymbol{X}_1^{\psi}(\boldsymbol{x}_0, T^R(\boldsymbol{x}_0)), \cdot, T^R(\boldsymbol{x}_0)\right)\right\|_{L^2(\mathbb{R}^3_{x_2})}}$$

resp. $(t \geq T^R(\boldsymbol{x}_0))$

$$\psi^{\text{measured}}(\boldsymbol{x}_2, t) = \frac{e^{-iH_2(t-T^R(\boldsymbol{x}_0))}\psi\left(\boldsymbol{X}_1^{\psi}(\boldsymbol{x}_0, T^R(\boldsymbol{x}_0)), \boldsymbol{x}_2, T^R(\boldsymbol{x}_0)\right)}{\left\|\psi\left(\boldsymbol{X}_1^{\psi}(\boldsymbol{x}_0, T^R(\boldsymbol{x}_0)), \cdot, T^R(\boldsymbol{x}_0)\right)\right\|_{L^2(\mathbb{R}^3_{x_2})}}.$$

Here $L^2(\mathbb{R}^3_{x_2})$ is a shorthand notation for $L^2(\mathbb{R}^3, d^3x_2)$. Thus the $\boldsymbol{x}_2$-particle's Bohmian trajectory after the collapse due to the $\boldsymbol{x}_1$-particle's detection is given by the velocity field

$$\boldsymbol{v}^{\psi^{\text{measured}}}(\boldsymbol{x}_2, t) = \operatorname{Im}\frac{\nabla_2 e^{-iH_2(t-T^R(\boldsymbol{x}_0))}\psi\left(\boldsymbol{X}_1^{\psi}(\boldsymbol{x}_0, T^R(\boldsymbol{x}_0)), \boldsymbol{x}_2, T^R(\boldsymbol{x}_0)\right)}{e^{-iH_2(t-T^R(\boldsymbol{x}_0))}\psi\left(\boldsymbol{X}_1^{\psi}(\boldsymbol{x}_0, T^R(\boldsymbol{x}_0)), \boldsymbol{x}_2, T^R(\boldsymbol{x}_0)\right)}.$$

Regarding the $\boldsymbol{x}_1$-particle's Bohmian trajectory, since we do not want one and the same particle to be detected more than once, we assume that the detectors are such that no detected particle may leave them (think e.g. of a photographic plate or a photomultiplier). Then we can safely neglect the $\boldsymbol{x}_1$-particle's evolution after $T^R(\boldsymbol{x}_0)$. Indeed, we shall simply truncate it at $T^R(\boldsymbol{x}_0)$, $\boldsymbol{X}_1^{\text{measured}}(\boldsymbol{x}_0, t) := \boldsymbol{X}_1^{\psi}(\boldsymbol{x}_0, T^R(\boldsymbol{x}_0))$ for all $t \geq T^R(\boldsymbol{x}_0)$.

Keeping in mind that it might as well have been the $\boldsymbol{x}_2$-particle that was detected first, with the above considerations we arrive at the following definition for the measured Bohmian trajectories:

[10] As mentioned in section 1.2 in Bohmian mechanics the collapse of the wave function in measurement-like situations is an emerging feature of the theory that holds in an effective sense. See [20] for an extensive treatment of the emergence out of Bohmian mechanics of the measurement formalism (including operators as observables) of orthodox quantum mechanics.

Definition 6. *Let V_1, $V_2 \in (V)_4$ and let zero be neither a resonance nor an eigenvalue of H_1, H_2. Let $\psi \in \mathcal{G}^{(2)}$ with $\|\psi\| = 1$.*
For every $R > 0$ and every initial configuration $\boldsymbol{x}_0$ define the time of first measurement

$$T^R(\boldsymbol{x}_0) := \min\{t_{ex}^{B_{1,R}}(\boldsymbol{x}_0),\, t_{ex}^{B_{2,R}}(\boldsymbol{x}_0)\} \tag{3.20}$$

where $t_{ex}^{B_{l,R}}(\boldsymbol{x}_0)$ is the exit time defined at the beginning of subsection 3.4.1. Further define the measured (time evolution of the) wave function[11] ψ

$$\psi^R_{\boldsymbol{x}_0}(\boldsymbol{x},t) := \begin{cases} \psi(\boldsymbol{x},t) = (e^{-iHt}\psi)(\boldsymbol{x}) & \text{if } t < T^R(\boldsymbol{x}_0) \\ \psi\left(\boldsymbol{X}_1^\psi(\boldsymbol{x}_0, T^R(\boldsymbol{x}_0)), \boldsymbol{x}_2; T^R(\boldsymbol{x}_0), t\right) & \text{if } t \geq T^R(\boldsymbol{x}_0),\, t_{ex}^{B_{1,R}}(\boldsymbol{x}_0) < t_{ex}^{B_{2,R}}(\boldsymbol{x}_0) \\ \psi\left(\boldsymbol{x}_1, \boldsymbol{X}_2^\psi(\boldsymbol{x}_0, T^R(\boldsymbol{x}_0)); t, T^R(\boldsymbol{x}_0)\right) & \text{if } t \geq T^R(\boldsymbol{x}_0),\, t_{ex}^{B_{2,R}}(\boldsymbol{x}_0) < t_{ex}^{B_{1,R}}(\boldsymbol{x}_0) \\ \psi\left(\boldsymbol{X}^\psi(\boldsymbol{x}_0, T^R(\boldsymbol{x}_0)), T^R(\boldsymbol{x}_0)\right) & \text{if } t \geq T^R(\boldsymbol{x}_0),\, t_{ex}^{B_{1,R}}(\boldsymbol{x}_0) = t_{ex}^{B_{2,R}}(\boldsymbol{x}_0) \end{cases}$$

where $\boldsymbol{X}^\psi$ is the standard Bohmian (configuration-space-)trajectory of the preceding sections and

$$\psi(\boldsymbol{x}_1, \boldsymbol{x}_2; t_1, t_2) := \left(e^{-iH_1t_1}e^{-iH_2t_2}\psi\right)(\boldsymbol{x}_1, \boldsymbol{x}_2)\,.$$

Finally, the measured Bohmian (configuration-space-)trajectory *is defined as the solution of*

$$\frac{d}{dt}\boldsymbol{X}^R(\boldsymbol{x}_0,t) = \boldsymbol{v}^{\psi^R_{\boldsymbol{x}_0}}(\boldsymbol{X}^R(\boldsymbol{x}_0,t),t), \qquad \boldsymbol{X}^R(\boldsymbol{x}_0,0) = \boldsymbol{x}_0 \tag{3.21}$$

where the measured Bohmian velocity field *is given by*

$$\boldsymbol{v}^{\psi^R_{\boldsymbol{x}_0}}(\boldsymbol{x},t) = \operatorname{Im}\left(\frac{\nabla\psi^R_{\boldsymbol{x}_0}(\boldsymbol{x},t)}{\psi^R_{\boldsymbol{x}_0}(\boldsymbol{x},t)}\right).$$

In particular, for $l \in \{1,2\}$ such that $t_{ex}^{B_{l,R}}(\boldsymbol{x}_0) = T^R(\boldsymbol{x}_0)$ we have

$$\boldsymbol{v}_l^{\psi^R_{\boldsymbol{x}_0}}(\boldsymbol{X}^R(\boldsymbol{x}_0,t),t) = 0$$

for all $t > T^R(\boldsymbol{x}_0)$, i. e.

$$\boldsymbol{X}_l^R(\boldsymbol{x}_0,t) = \boldsymbol{X}_l^R(\boldsymbol{x}_0, T^R(\boldsymbol{x}_0))$$

for all $t \geq T^R(\boldsymbol{x}_0)$.

We now formulate our results on the asymptotically classical behavior of the measured Bohmian trajectories.

[11]Since the Bohmian velocity field is projective, we neglect any normalization constants. Further, for ease of notation we write $\psi^R_{\boldsymbol{x}_0}(\boldsymbol{x},t)$ even when $\psi^R_{\boldsymbol{x}_0}$ depends only on $\boldsymbol{x}_1$ or $\boldsymbol{x}_2$.

Theorem 4. *Let V_1, $V_2 \in (V)_4$ and let zero be neither a resonance nor an eigenvalue of H_1, H_2. Let $\psi \in \mathcal{G}^{(2)}$ with $\|\psi\| = 1$. Then:*

(i) For all $R > 0$ the measured trajectories $\boldsymbol{X}^R(\boldsymbol{x}_0, t)$ exist uniquely and globally in time for $\mathbb{P}^\psi$-almost all initial configurations $\boldsymbol{x}_0 \in \mathbb{R}^6$.

(ii) Let $v^\psi_\infty(\boldsymbol{x}_0)$ the asymptotic velocity defined in Theorem 2. For $R > 0, T > 0$ and $C > 0$ define $\boldsymbol{x}_0$ to be in $\mathcal{V}_{RTC}$ whenever

$$\begin{aligned} T^R(\boldsymbol{x}_0) > T\,, \\ \left|\boldsymbol{v}^{\psi^R_{\boldsymbol{x}_0}}(\boldsymbol{X}^R(\boldsymbol{x}_0, t), t) - v^\psi_\infty(\boldsymbol{x}_0)\right| \leq \frac{C}{\sqrt{t}} \end{aligned} \tag{3.22}$$

for all $T \leq t < T^R(\boldsymbol{x}_0)$ and

$$\left|\boldsymbol{v}_l^{\psi^R_{\boldsymbol{x}_0}}(\boldsymbol{X}^R(\boldsymbol{x}_0, t), t) - \boldsymbol{v}^\psi_{\infty,l}(\boldsymbol{x}_0)\right| \leq \frac{C}{\sqrt{T^R(\boldsymbol{x}_0)}} \tag{3.23}$$

for all $t \geq T^R(\boldsymbol{x}_0)$ and $l \in \{1, 2\}$ such that $T^R(\boldsymbol{x}_0) < t^{B_l,R}_{ex}(\boldsymbol{x}_0)$. Then for all $\varepsilon > 0$ there exist $T < \infty$, $C < \infty$ and some $R_T < \infty$ such that

$$\mathbb{P}^\psi(\mathcal{V}_{RTC}) > 1 - \varepsilon$$

for all $R > R_T$.

The proof of Theorem 4 can be found in subsection 3.6.1. Note that we choose to compare the measured velocity $\boldsymbol{v}^{\psi^R_{\boldsymbol{x}_0}}$ directly to the *unmeasured* asymptotic velocity $\boldsymbol{v}^\psi_\infty$. Theorem 4 (ii) should be understood as follows: If R is big enough most velocities are already close to the unmeasured asymptotic ones even before the first particle hits a detector. Moreover, the rate of convergence is (of course) the same as in the unmeasured case (equation (3.22)). After the first particle's detection the remaining particle's velocity still converges to an asymptotic one, but to one that might be slightly different, namely $\boldsymbol{v}^R_{l,\infty} := \lim\limits_{t\to\infty} \frac{\boldsymbol{X}^R_l}{t}$. While the convergence rate of the remaining particle's velocity to this *measured* asymptotic velocity $\boldsymbol{v}^R_{l,\infty}$ is still of order $\frac{1}{\sqrt{t}}$, the difference between $\boldsymbol{v}^R_{l,\infty}$ and the unmeasured asymptotic velocity $\boldsymbol{v}^\psi_\infty$ is of order $\frac{1}{\sqrt{T^R(\boldsymbol{x}_0)}}$, which gives equation (3.23).

As in the unmeasured case, if we wish to control the Bohmian velocity field, we need pointwise estimates on the (gradient of the) relevant wave function $\psi^R_{\boldsymbol{x}_0}$, that is on $(\nabla)\psi(\boldsymbol{x}; t_1, t_2)$ (cf. Definition 6). They are collected in

Lemma 6. *Let V_1, $V_2 \in (V)_4$ and let zero be neither a resonance nor an eigenvalue of H_1, H_2. Let $\psi \in \mathcal{G}^{(2)}$. Then for all $0 < a < b < \infty$ there exist constants $T < \infty$ and $C < \infty$ such that for all $t_1, t_2 \geq T$ and $a < \frac{x_1}{t_1}, \frac{x_2}{t_2} < b$*

$$\begin{aligned} &|\psi(\boldsymbol{x}; t_1, t_2) - \Phi(\boldsymbol{x}; t_1, t_2)| \leq C\,(t_1 t_2)^{-\frac{3}{2}}\,(\min\{t_1, t_2\})^{-\frac{1}{2}}\,, \\ &|\psi(\boldsymbol{x}; t_1, t_2) - \Phi_{1/2}(\boldsymbol{x}; t_1, t_2)| \leq C\,(t_{1/2})^{-2}(t_{2/1})^{-\frac{3}{2}} \end{aligned} \tag{3.24}$$

and

$$|\nabla_{1/2}\psi(\boldsymbol{x}; t_1, t_2) - i\frac{\boldsymbol{x}_{1/2}}{t_{1/2}}\Phi_{1/2}(\boldsymbol{x}; t_1, t_2)| \leq C\,(t_{1/2})^{-2}(t_{2/1})^{-\frac{3}{2}}\,. \tag{3.25}$$

Here

$$\Phi(\boldsymbol{x}; t_1, t_2) := (it_1)^{-\frac{3}{2}}(it_2)^{-\frac{3}{2}}\, e^{\frac{i}{2}\left(\frac{x_1^2}{t_1} + \frac{x_2^2}{t_2}\right)}\, \widehat{\psi}_{out}\left(\frac{\boldsymbol{x}_1}{t_1}, \frac{\boldsymbol{x}_2}{t_2}\right)$$

and

$$\begin{aligned} \Phi_1(\boldsymbol{x}; t_1, t_2) &:= (it_1)^{-\frac{3}{2}}\, e^{\frac{ix_1^2}{2t_1}}\,(\mathcal{F}_{+,1}\psi)\left(\frac{\boldsymbol{x}_1}{t_1}, \boldsymbol{x}_2; 0, t_2\right)\,, \\ \Phi_2(\boldsymbol{x}; t_1, t_2) &:= (it_2)^{-\frac{3}{2}}\, e^{\frac{ix_2^2}{2t_2}}\,(\mathcal{F}_{+,2}\psi)\left(\boldsymbol{x}_1, \frac{\boldsymbol{x}_2}{t_2}; t_1, 0\right)\,. \end{aligned}$$

The proof of Lemma 6 can be found in subsection 3.6.3. Note that the collapse preserves the wave function's asymptotic local plane wave structure in the degrees of freedom belonging to the not yet detected particle: Suppose the $\boldsymbol{x}_1$-particle is detected first. Then for large t the collapsed wave function

$$\psi^R_{\boldsymbol{x}_0}(\boldsymbol{x}, t) = \psi\big(\boldsymbol{X}^\psi_1(\boldsymbol{x}_0, T^R(\boldsymbol{x}_0)), \boldsymbol{x}_2; T^R(\boldsymbol{x}_0), t\big)$$

is approximately given by the local plane wave

$$\begin{aligned} \Phi_2\big(&\boldsymbol{X}^\psi_1(\boldsymbol{x}_0, T^R(\boldsymbol{x}_0)), \boldsymbol{x}_2; T^R(\boldsymbol{x}_0), t\big) \\ &= (it)^{-\frac{3}{2}}\, e^{\frac{ix_2^2}{2t}}\,\big(\mathcal{F}_{+,2}\psi\big)\big(\boldsymbol{X}^\psi_1(\boldsymbol{x}_0, T^R(\boldsymbol{x}_0)), \frac{\boldsymbol{x}_2}{t}; T^R(\boldsymbol{x}_0), 0\big) \end{aligned}$$

with an error of order $T^R(\boldsymbol{x}_0)^{-\frac{3}{2}}t^{-2}$ (second line of (3.24) and (3.25)). Since at first glance the appearance of $T^R(\boldsymbol{x}_0)^{-\frac{3}{2}}t^{-2}$ in the latter might seem a little bit surprising, we remark that the leading order term of

$$\big(\mathcal{F}_{+,2}\psi\big)\big(\boldsymbol{X}^\psi_1(\boldsymbol{x}_0, T^R(\boldsymbol{x}_0)), \frac{\boldsymbol{x}_2}{t}; T^R(\boldsymbol{x}_0), 0\big)$$

will be given by

$$(iT^R(\boldsymbol{x}_0))^{-\frac{3}{2}}\, e^{\frac{i\boldsymbol{X}^\psi_1(\boldsymbol{x}_0, T^R(\boldsymbol{x}_0))^2}{2T^R(\boldsymbol{x}_0)}}\, \widehat{\psi}_{\text{out}}\big(\frac{\boldsymbol{X}^\psi_1(\boldsymbol{x}_0, T^R(\boldsymbol{x}_0))}{T^R(\boldsymbol{x}_0)}, \frac{\boldsymbol{x}_2}{t}\big),$$

so the former is of order $T^R(\boldsymbol{x}_0)^{-\frac{3}{2}}$ and thus $\Phi_2\big(\boldsymbol{X}^\psi_1(\boldsymbol{x}_0, T^R(\boldsymbol{x}_0)), \boldsymbol{x}_2; T^R(\boldsymbol{x}_0), t\big)$ is of order $T^R(\boldsymbol{x}_0)^{-\frac{3}{2}}t^{-\frac{3}{2}}$.

Having established the asymptotically classical behavior of the measured Bohmian trajectories we may now turn to the measured exit statistics (i.e. the exit statistics in the presence of collapse). As in the unmeasured case we first give a formalized expression for the (joint) detection probability (3.4): We say that "the lth particle hits a detector surface $R\Sigma_l$" if and only if $\boldsymbol{X}_l^R(\boldsymbol{x}_0, t_l^R(\boldsymbol{x}_0)) \in R\Sigma_l$, where $t_l^R(\boldsymbol{x}_0)$ denotes the time at which the lth particle first leaves the open ball $B_R \subset \mathbb{R}^3$ (i.e. at which $\{\boldsymbol{X}^R(\boldsymbol{x}_0, t),\, t \geq 0\}$ first leaves $B_{l,R}$, cf. subsection 3.4.1):

$$t_l^R(\boldsymbol{x}_0) := \inf\left\{t \geq 0 \mid \boldsymbol{X}^R(\boldsymbol{x}_0, s) \in B_{l,R}\, \forall s \in [0,t) \text{ and } \boldsymbol{X}^R(\boldsymbol{x}_0, t) \notin B_{l,R}\right\}\,,$$

where we set $t_l^R(\boldsymbol{x}_0) = 0$ if the above set is empty. Note that for the particle that is detected first this should and indeed does coincide with the unmeasured first exit time defined at the beginning of subsection 3.4.1 and thus with the time of first measurement, $t_l^R(\boldsymbol{x}_0) = t_{\text{ex}}^{B_{l,R}}(\boldsymbol{x}_0) = T^R(\boldsymbol{x}_0)$.

Now we can formulate the measured first exit statistics theorem.

Theorem 5. *Let V_1, $V_2 \in (V)_4$ and let zero be neither a resonance nor an eigenvalue of H_1, H_2. Let $\psi \in \mathcal{G}^{(2)}$ with $\|\psi\| = 1$. Then:*

$$\begin{aligned}\lim_{R\to\infty} \mathbb{P}^\psi\Big(\Big\{\boldsymbol{x}_0 \in \mathbb{R}^6 \mid \boldsymbol{X}_l^R(\boldsymbol{x}_0, t_l^R(\boldsymbol{x}_0)) \in R\Sigma_l \quad \forall l \in \{1,2,\}\Big\}\Big) \\ = \int_{C_{\Sigma_1}} d^3k_1 \int_{C_{\Sigma_2}} d^3k_2\, \left|\widehat{\psi}_{out}(\boldsymbol{k})\right|^2 .\end{aligned} \tag{3.26}$$

Proof of Theorem 5. The proof is analogous to that of Theorem 3: Because of Theorem 2 (iii) we are done if we can show that

$$\begin{aligned}\lim_{R\to\infty} \mathbb{P}^\psi\Big(\Big\{\boldsymbol{x}_0 \in \mathbb{R}^6 \mid \boldsymbol{X}_l^R(\boldsymbol{x}_0, t_l^R(\boldsymbol{x}_0)) \in R\Sigma_l \quad \forall l \in \{1,2,\}\Big\}\Big) \\ = \mathbb{P}^\psi\left(\boldsymbol{v}_{\infty,l}^\psi \in C_{\Sigma_l}\, \forall l \in \{1,2\}\right) .\end{aligned} \tag{3.27}$$

Using Theorem 4 we see that, analogous to (3.19), for every $\varepsilon > 0$ there is some $C < \infty$ such that

$$\begin{aligned}\mathbb{P}^\psi\left(|\boldsymbol{X}_l^R(\boldsymbol{x}_0, t) - \boldsymbol{v}_{\infty,l}^\psi(\boldsymbol{x}_0)t| < \begin{cases} C(1+\sqrt{t}) & \text{if } 0 \leq t < T^R(\boldsymbol{x}_0)\,, \\ C\big(1+\frac{t}{\sqrt{T^R(\boldsymbol{x}_0)}}\big) & \text{if } T^R(\boldsymbol{x}_0) \leq t \leq t_l^R(\boldsymbol{x}_0) \end{cases} \quad l = 1,2\right) \\ > 1-\epsilon\,.\end{aligned} \tag{3.28}$$

Then (3.27) follows from (3.28) just as (3.18) followed from (3.19):

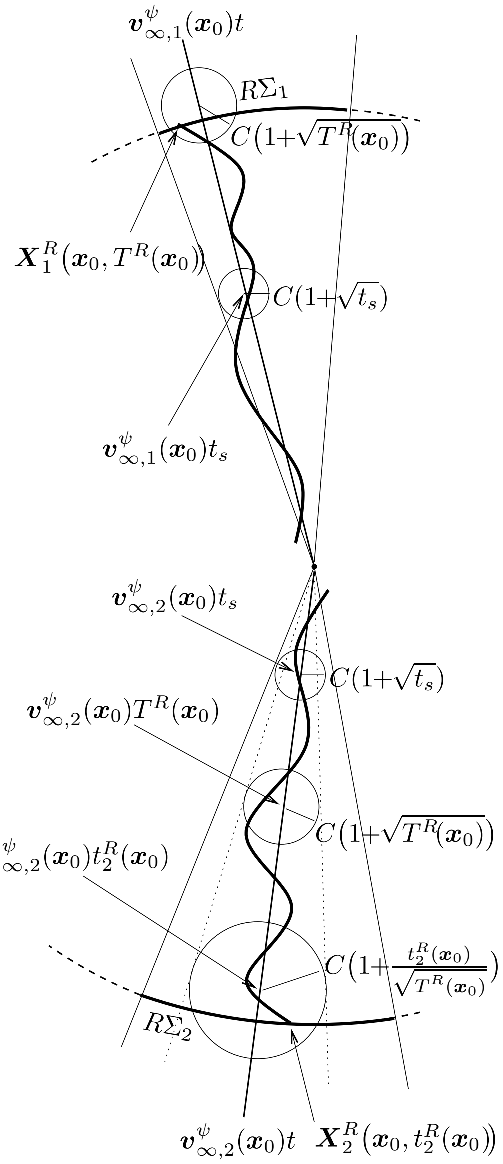

Figure 3.3: Real and “ideal” trajectories of two measured particles.

Suppose that the $\boldsymbol{x}_1$-particle is detected first ($T^R(\boldsymbol{x}_0) = t_{\text{ex}}^{B_{1,R}}(\boldsymbol{x}_0) = t_1^R(\boldsymbol{x}_0)$). Before this first detection both particles' real trajectories $\boldsymbol{X}^R_l$ are contained in moving balls $B_{C(1+\sqrt{t})}(\boldsymbol{v}^{\psi}_{\infty,l}t)$ around the "ideal" trajectories $\boldsymbol{v}^{\psi}_{\infty,l}t$ with radius growing sub-linear in time. Since the distance between the "ideal" trajectories $\boldsymbol{v}^{\psi}_{\infty,l}t$ and the boundary of C_{Σ_l} grows linear in time, this means that for times t big enough, $t > t_s$ for some appropriate $0 < t_s < \infty$, both balls $B_{C(1+\sqrt{t})}(\boldsymbol{v}^{\psi}_{\infty,1}t)$ and $B_{C(1+\sqrt{t})}(\boldsymbol{v}^{\psi}_{\infty,2}t)$ will be contained entirely in the cones C_{Σ_1} and C_{Σ_2}, respectively. For R and thus $T^R(\boldsymbol{x}_0)$ big enough we may choose $t_s < T^R(\boldsymbol{x}_0)$ and thus guarantee that the $\boldsymbol{x}_1$-particle (i.e. the first particle to be detected) reaches RS^2 while contained in the cone C_{Σ_1}, i.e. somewhere in $R\Sigma_1$. Now, after the detection of the $\boldsymbol{x}_1$-particle (i.e. for $t \geq T^R(\boldsymbol{x}_0)$) the moving ball's radius that contains the $\boldsymbol{x}_2$-particle's real trajectory $\boldsymbol{X}^R_2$ may grow linear in time. However, since this ball already was contained in C_{Σ_2} at time $T^R(\boldsymbol{x}_0)$ (and the distance between the "ideal" trajectory $\boldsymbol{v}^{\psi}_{\infty,2}t$ and the boundary of C_{Σ_2} of course still grows linear in time) it will nevertheless stay contained in C_{Σ_2}. Thus also the $\boldsymbol{x}_2$-particle will reach RS^2 somewhere in $R\Sigma_2$ (cf. Figure 3.3). □

3.5 Outlook

With Theorems 3 and 5 we have presented results on the exit statistics of N non-interacting particles. For an extension to interacting particles one needs detailed estimates on generalized eigenfunctions also for potentials with interaction terms. Remember that the fundamental Theorems 2 and 4 about the asymptotic classicality of the Bohmian trajectories rely heavily on the detailed estimates of Lemmas 5 and 6, respectively, which in turn are based on the method of expansion in generalized eigenfunctions. However, while there are results about generalized eigenfunctions in higher dimensions (see e.g. [1, 35, 40]) they hold only for potentials with sufficiently rapid decay at infinity. And potentials with interacting terms do not fall off at infinity in certain directions: A typical potential for a pair of interacting particles is of the form $V(\boldsymbol{x}) = V(\boldsymbol{x}_1 - \boldsymbol{x}_2)$ which does not fall off at all on the "diagonal" $\boldsymbol{x}_1 \approx \boldsymbol{x}_2$. However, at least for repulsive potentials one should be able to show that the absent fall off on the diagonal is negligible in some appropriate sense. After all, when the particles repulse each other, their wave function will typically be concentrated away from the diagonal. Thus one could probably approximate the actual potential by truncated potentials that decay also on the diagonal, i.e. for which the existing results about generalized eigenfunctions become applicable. But beware: The exit statistics is a statement about trajectories, not a L^2 statement for which one could apply "dense-in-L^2" arguments. So one would have to be very careful about the appropriate sense of convergence in which the truncated potentials approximate the actual one.

3.6 Asymptotic behavior of Bohmian trajectories: Proofs

The goal of this section is the proof of Theorems 2 and 4. In subsection 3.6.1 we present the main body of the proof using the pointwise estimates on $(\nabla)\psi$ given in Lemmas 5 and 6, respectively. In subsection 3.6.2 we list the properties of the generalized eigenfunctions we use in subsection 3.6.3 to finally prove Lemmas 5 and 6.

3.6.1 Proof of Theorems 2 and 4

Since the standard Bohmian trajectories $\boldsymbol{X}^{\psi}$ and the measured ones $\boldsymbol{X}^{R}$ are closely related, we merge the proofs of Theorems 2 and 4 to avoid repetitions. Rather we split the proof into that of Theorem 2 (i) and 4 (i) ($\mathbb{P}^{\psi}$-almost sure global existence and uniqueness of $\boldsymbol{X}^{\psi}$ resp. $\boldsymbol{X}^{R}$) and that of Theorem 2 (ii), (iii) and Theorem 4 (ii) (asymptotically classical behavior of $\boldsymbol{X}^{\psi}$ resp. $\boldsymbol{X}^{R}$).

Proof of Theorem 2 (i) and 4 (i). Theorem 2 (i), i.e. $\mathbb{P}^{\psi}$-almost sure global existence and uniqueness of $\boldsymbol{X}^{\psi}(\boldsymbol{x}_0, t)$, is a direct consequence Proposition 1. Regarding Theorem 4 (i) note that $\psi^{R}_{\boldsymbol{x}_0}(\boldsymbol{x}, t) = \psi(\boldsymbol{x}, t)$ for $t < T^R(\boldsymbol{x}_0)$ implies $\boldsymbol{X}^R(\boldsymbol{x}_0, t) = \boldsymbol{X}^{\psi}(\boldsymbol{x}_0, t)$ for $t \leq T^R(\boldsymbol{x}_0)$. Moreover, since $t_{\text{ex}}^{B_{l,R}}$ $(l = 1, 2)$ are well defined random variables on the space of initial configurations $\boldsymbol{x}_0$ (cf. subsection 3.4.1), so is $T^R(\boldsymbol{x}_0) = \min\{t_{\text{ex}}^{B_{1,R}}(\boldsymbol{x}_0), t_{\text{ex}}^{B_{2,R}}(\boldsymbol{x}_0)\}$. Thus we already have that for $\mathbb{P}^{\psi}$-almost all $\boldsymbol{x}_0$ $\boldsymbol{X}^R(\boldsymbol{x}_0, t)$ is well defined up to (the also well defined) time $T^R(\boldsymbol{x}_0)$ and our task really is to extend this to times $t > T^R(\boldsymbol{x}_0)$.

Split the set of "good" initial configurations for the standard Bohmian dynamics,

$$\begin{aligned}\mathcal{G}^{\psi} :&= \{\boldsymbol{x}_0 \in \mathbb{R}^6 \mid \boldsymbol{X}^{\psi}(\boldsymbol{x}_0, t) \text{ exists and is unique for all } t \in \mathbb{R}\} \\ &\subset \{\boldsymbol{x}_0 \in \mathbb{R}^6 \mid \boldsymbol{X}^{R}(\boldsymbol{x}_0, t) \text{ exists and is unique for all } t \leq T^R(\boldsymbol{x}_0)\},\end{aligned}$$

into the three disjoint subsets

$$\begin{aligned}D_1^R &:= \{\boldsymbol{x}_0 \in \mathcal{G}^\psi \mid T^R(\boldsymbol{x}_0) = t_{\text{ex}}^{B_{1,R}}(\boldsymbol{x}_0) < t_{\text{ex}}^{B_{2,R}}(\boldsymbol{x}_0)\}\,,\\ D_2^R &:= \{\boldsymbol{x}_0 \in \mathcal{G}^\psi \mid T^R(\boldsymbol{x}_0) = t_{\text{ex}}^{B_{2,R}}(\boldsymbol{x}_0) < t_{\text{ex}}^{B_{1,R}}(\boldsymbol{x}_0)\}\,,\\ D_{12}^R &:= \{\boldsymbol{x}_0 \in \mathcal{G}^\psi \mid T^R(\boldsymbol{x}_0) = t_{\text{ex}}^{B_{1,R}}(\boldsymbol{x}_0) = t_{\text{ex}}^{B_{2,R}}(\boldsymbol{x}_0)\}\end{aligned}$$

and denote by $\mathcal{G}^R$ the set of "good" initial configurations for the measured dynamics, i.e.

$$\mathcal{G}^R := \{\boldsymbol{x}_0 \in \mathbb{R}^6 \mid \boldsymbol{X}^R(\boldsymbol{x}_0, t) \text{ exists and is unique for all } t \in \mathbb{R}\}\,.$$

We shall show

$$\mathbb{P}^\psi(D_{12}^R) = 0 \tag{3.29}$$

and

$$\mathbb{P}^\psi(D_1^R \cap \mathcal{G}^R) = \mathbb{P}^\psi(D_1^R)\,, \qquad \mathbb{P}^\psi(D_2^R \cap \mathcal{G}^R) = \mathbb{P}^\psi(D_2^R)\,. \tag{3.30}$$

Then

$$\mathbb{P}^\psi(\mathcal{G}^R) \geq \mathbb{P}^\psi(D_1^R \cap \mathcal{G}^R) + \mathbb{P}^\psi(D_2^R \cap \mathcal{G}^R) = \mathbb{P}^\psi(D_1^R) + \mathbb{P}^\psi(D_2^R) + \mathbb{P}^\psi(D_{12}^R) = \mathbb{P}^\psi(\mathcal{G}^\psi) = 1\,,$$

i.e. we have $\mathbb{P}^\psi$-almost sure global existence and uniqueness of the measured dynamics, $\mathbb{P}^\psi(\mathcal{G}^R) = 1$.

First, suppose both particles arrive at the detectors at the same time, i.e. $\boldsymbol{x}_0 \in D_{12}^R$. Since $X_l^R(\boldsymbol{x}_0, t_{\text{ex}}^{B_{l,R}}(\boldsymbol{x}_0)) = X_l^\psi(\boldsymbol{x}_0, t_{\text{ex}}^{B_{l,R}}(\boldsymbol{x}_0)) = R$ we have

$$D_{12}^R \subset \widetilde{D}_{12}^R := \{\boldsymbol{x}_0 \in \mathcal{G}^\psi \mid X_1^\psi(\boldsymbol{x}_0, t) = R = X_2^\psi(\boldsymbol{x}_0, t) \text{ for some } t \in \mathbb{R}\}\,.$$

$\widetilde{D}_{12}^R$, however, clearly (is contained in a submanifold of $\mathbb{R}^6$ that) has at least codimension one, i.e. $\widetilde{D}_{12}^R$ and thus D_{12}^R has Lebesgue measure zero. Since $\mathbb{P}^\psi$ is absolutely continuous with respect to Lebesgue measure this gives (3.29): $\mathbb{P}^\psi(D_{12}^R) = 0$.

We remark that by Definition 6 $\boldsymbol{x}_0 \in D_{12}^R$ entails $\boldsymbol{X}^R(\boldsymbol{x}_0, t) = \boldsymbol{X}^R(\boldsymbol{x}_0, T^R(\boldsymbol{x}_0))$ for all $t > T^R(\boldsymbol{x}_0)$, that is we trivially have $D_{12}^R \subset \mathcal{G}^R$ and thus

$$\mathbb{P}^\psi(D_{12}^R \cap \mathcal{G}^R) = \mathbb{P}^\psi(D_{12}^R)\,. \tag{3.29'}$$

This, together with (3.30), of course also gives $\mathbb{P}^\psi(\mathcal{G}^R) = 1$ and one might wonder why we use (3.29) instead of the trivial (3.29'). The reason is that in the case of more than two scattered particles ($N > 2$) (3.29) easily generalizes to

$$\mathbb{P}^\psi(\{\boldsymbol{x}_0 \in \mathcal{G}^\psi \subset \mathbb{R}^{3N} \mid T^R(\boldsymbol{x}_0) = t_{\text{ex}}^{B_{l,R}}(\boldsymbol{x}_0) \text{ for at least two different } l = 1, 2, \ldots, N\}) = 0\,.$$

While this, together with the higher dimensional analogue of (3.30), does still suffice to get $\mathbb{P}^\psi(\mathcal{G}^R) = 1$, the analogue of (3.29'),

$$\begin{aligned}&\mathbb{P}^\psi(\{\boldsymbol{x}_0 \in \mathcal{G}^\psi \mid T^R(\boldsymbol{x}_0) = t_{\text{ex}}^{B_{l,R}}(\boldsymbol{x}_0) \text{ for all } l = 1, 2, \ldots, N\} \cap \mathcal{G}^R)\\ &\qquad\qquad = \mathbb{P}^\psi(\{\boldsymbol{x}_0 \in \mathcal{G}^\psi \mid T^R(\boldsymbol{x}_0) = t_{\text{ex}}^{B_{l,R}}(\boldsymbol{x}_0) \text{ for all } l = 1, 2, \ldots, N\})\,,\end{aligned}$$

does not.

Now, suppose that $\boldsymbol{x}_0 \in D_1^R$, i.e. the $\boldsymbol{x}_1$-particle arrives at the detectors before the $\boldsymbol{x}_2$-particle[12]. By Definition 6 this entails $\boldsymbol{X}_1^R(\boldsymbol{x}_0, t) = \boldsymbol{X}_1^R(\boldsymbol{x}_0, T^R(\boldsymbol{x}_0))$ for all $t > T^R(\boldsymbol{x}_0)$, i.e. we only need to ensure that $\boldsymbol{X}_2^R(\boldsymbol{x}_0, t)$ is well defined for $t > T^R(\boldsymbol{x}_0)$. Then the $\boldsymbol{x}_2$-particle's dynamics for $t \geq T^R(\boldsymbol{x}_0)$ (as defined in Definition 6) is actually a standard Bohmian one-particle dynamics: Write

$$\psi_{\boldsymbol{X}_1,T}(\boldsymbol{y},\tau) := \left(e^{-iH_2\tau}\psi_{\boldsymbol{X}_1,T}\right)(\boldsymbol{y}), \qquad \psi_{\boldsymbol{X}_1,T}(\boldsymbol{y}) := \frac{\psi(\boldsymbol{X}_1,\boldsymbol{y},T)}{\|\psi(\boldsymbol{X}_1,\cdot,T)\|_{L^2(\mathbb{R}^3_y)}}.$$

Setting $T = T^R(\boldsymbol{x}_0)$ and $\boldsymbol{X}_1 = \boldsymbol{X}_1^R(\boldsymbol{x}_0, T)$ this yields $(t \geq T)$

$$\boldsymbol{X}_2^R(\boldsymbol{x}_0,t) = \boldsymbol{Y}^{\psi_{\boldsymbol{X}_1,T}}(\boldsymbol{X}_2^R(\boldsymbol{x}_0,T), t-T) \tag{3.31}$$

where $\boldsymbol{Y}^{\psi_{\boldsymbol{X}_1,T}}$ is the solution of the one-particle Bohmian equation of motion

$$\begin{aligned} &\frac{d}{d\tau}\boldsymbol{Y}^{\psi_{\boldsymbol{X}_1,T}}(\boldsymbol{y}_0,\tau) = \boldsymbol{v}^{\psi_{\boldsymbol{X}_1,T}}(\boldsymbol{Y}^{\psi_{\boldsymbol{X}_1,T}}(\boldsymbol{y}_0,\tau),\tau), \\ &\boldsymbol{v}^{\psi_{\boldsymbol{X}_1,T}}(\boldsymbol{y},\tau) = \operatorname{Im}\left(\frac{\nabla_y\psi_{\boldsymbol{X}_1,T}(\boldsymbol{y},\tau)}{\psi_{\boldsymbol{X}_1,T}(\boldsymbol{y},\tau)}\right), \qquad \boldsymbol{Y}^{\psi_{\boldsymbol{X}_1,T}}(\boldsymbol{y}_0,0) = \boldsymbol{y}_0\,. \end{aligned} \tag{3.32}$$

Note however, that the guiding wave function $\psi_{\boldsymbol{X}_1,T} = \psi_{\boldsymbol{X}_1^R(\boldsymbol{x}_0,T^R(\boldsymbol{x}_0)),T^R(\boldsymbol{x}_0)}$ and thus also the Bohmian dynamics (3.32) is *random.* So first of all we need to show that $\psi \in \mathcal{G}^{(2)}$ is sufficiently regular such that $\boldsymbol{x}_0 \in D_1^R$ yields $\psi_{\boldsymbol{X}_1^R(\boldsymbol{x}_0,T^R(\boldsymbol{x}_0)),T^R(\boldsymbol{x}_0)}$ for which the dynamics (3.32) is reasonably well defined. In fact we shall show that

(a) $\psi \in \mathcal{G}^{(2)}$ implies $\psi_{\boldsymbol{X}_1,T} \in C^\infty(H_2) \subset L^2(\mathbb{R}^3_y)$ *for all* $\boldsymbol{X}_1 \in \mathbb{R}^3$, $T \in \mathbb{R}$

which again by Proposition 1 gives $\mathbb{P}^{\psi_{\boldsymbol{X}_1,T}}$-almost sure global existence and uniqueness of the Bohmian dynamics (3.32). But also the initial position $\boldsymbol{y}_0 = \boldsymbol{X}_2^R(\boldsymbol{x}_0, T^R(\boldsymbol{x}_0))$ is random, that is we need to show even more, namely that (at least $\mathbb{P}^\psi$-almost) all $\boldsymbol{x}_0 \in D_1^R$ lead to $\boldsymbol{y}_0 = \boldsymbol{X}_2^R(\boldsymbol{x}_0, T^R(\boldsymbol{x}_0))$ in the set of "good" initial positions ($T = T^R(\boldsymbol{x}_0)$, $\boldsymbol{X}_1 = \boldsymbol{X}_1^R(\boldsymbol{x}_0, T)$)

$$\mathcal{G}^{\psi_{\boldsymbol{X}_1,T}} := \{\boldsymbol{y}_0 \in \mathbb{R}^3 \mid \boldsymbol{Y}^{\psi_{\boldsymbol{X}_1,T}}(\boldsymbol{y}_0,\tau) \text{ exists and is unique for all } \tau \in \mathbb{R}\}$$

of the random dynamics (3.32). Indeed, with the help of (a) we shall show

(b) $\mathbb{P}^\psi\left(\left\{\boldsymbol{x}_0 \in D_1^R \mid \boldsymbol{X}_2^R(\boldsymbol{x}_0, T^R(\boldsymbol{x}_0)) \in \mathcal{G}^{\psi_{\boldsymbol{X}_1^R(\boldsymbol{x}_0,T^R(\boldsymbol{x}_0)),T^R(\boldsymbol{x}_0)}}\right\}\right) = \mathbb{P}^\psi(D_1^R)$.

By (3.31) this then immediately implies

$$\mathbb{P}^\psi\left(\left\{\boldsymbol{x}_0 \in D_1^R \mid \boldsymbol{X}_2^R(\boldsymbol{x}_0,t) \text{ exists and is unique for all } t > T^R(\boldsymbol{x}_0)\right\}\right) = \mathbb{P}^\psi(D_1^R)$$

and thus

$$\mathbb{P}^\psi(D_1^R \cap \mathcal{G}^R) = \mathbb{P}^\psi(D_1^R)\,.$$

Thus we are left with the proof of (a) and (b). We start with (a). Let $\psi \in \mathcal{G}^{(2)}$. Then, for any $T \in \mathbb{R}$, also $\psi(\cdot, T) \in \mathcal{G}^{(2)}$, i.e. it suffices to show that

[12] Since the reverse case, $\boldsymbol{x}_0 \in D_2^R$, is completely analogous we do not treat it separately.

$$\psi \in \mathcal{G}^{(2)} \text{ implies } \psi_{\boldsymbol{X}_1} := \psi_{\boldsymbol{X}_1,0} = \psi(\boldsymbol{X}_1,\cdot) \in C^\infty(H_2) \text{ for all } \boldsymbol{X}_1 \in \mathbb{R}^3.$$

This is most readily proved using the spectral theorem. More precisely, since $\mathcal{G}^{(2)} \subset \mathcal{H}_{\mathrm{s}}(H) \cong \mathcal{H}_{\mathrm{a.c.}}(H_1) \otimes \mathcal{H}_{\mathrm{a.c.}}(H_2)$, we may use the explicit diagonalization of $H_{1/2}$ on $\mathcal{H}_{\mathrm{a.c.}}(H_{1/2})$ resp. H on $\mathcal{H}_{\mathrm{s}}(H)$ given by the generalized Fourier transform $\mathcal{F}_{+,1/2}$ resp. $\mathcal{F}_+^{(2)}$ defined in subsection 3.6.2 (cf. Proposition 4 (iv) resp. equation (3.55)):

$$\begin{aligned} H_{1/2}\big|_{\mathcal{H}_{\mathrm{a.c.}}(H_{1/2})} &= \mathcal{F}_{+,1/2}^{-1}\frac{k_{1/2}^2}{2}\mathcal{F}_{+,1/2} \\ H\big|_{\mathcal{H}_{\mathrm{s}}(H)} &= \left(\mathcal{F}_+^{(2)}\right)^{-1}\frac{k^2}{2}\mathcal{F}_+^{(2)}\,. \end{aligned} \tag{3.33}$$

Then $\psi_{\boldsymbol{X}_1} \in C^\infty(H_2)$ if and only if $\left(\frac{k_2^2}{2}\right)^n \mathcal{F}_{+,2}\psi_{\boldsymbol{X}_1} \in L^2(\mathbb{R}^3_{k_2})$, i.e. if and only if $\varphi_n(\boldsymbol{X}_1,\cdot) := H_2^n\psi_{\boldsymbol{X}_1} = \mathcal{F}_{+,2}^{-1}\left(\frac{k_2^2}{2}\right)^n \mathcal{F}_{+,2}\psi_{\boldsymbol{X}_1} \in L^2(\mathbb{R}^3_{x_2})$ for all $n \in \mathbb{N}$.

Let $n \in \mathbb{N}$. Since $\mathcal{G}^{(2)} \subset C^\infty(H)$ and $\mathcal{F}_+^{(2)} = \mathcal{F}_{+,1}\mathcal{F}_{+,2}$ (3.33) gives[13]

$$\begin{aligned} \|H_1\varphi_n\|_{L^2(\mathbb{R}^6_x)} &= \left\|\frac{k_1^2}{2}\mathcal{F}_{+,1}\mathcal{F}_{+,2}^{-1}\left(\frac{k_2^2}{2}\right)^n\mathcal{F}_{+,2}\psi\right\|_{L^2(\mathbb{R}^3_{k_1}\times\mathbb{R}^3_{x_2})} = \left\|\frac{k_1^2}{2}\left(\frac{k_2^2}{2}\right)^n\mathcal{F}_+^{(2)}\psi\right\|_{L^2(\mathbb{R}^6_k)} \\ &\le \left\|\left(\frac{k^2}{2}\right)^{n+1}\mathcal{F}_+^{(2)}\psi\right\|_{L^2(\mathbb{R}^6_k)} = \left\|H^{n+1}\psi\right\|_{L^2(\mathbb{R}^6_x)} < \infty\,. \end{aligned} \tag{3.34}$$

Since $\|H_1\varphi_n\|^2_{L^2(\mathbb{R}^6_x)} = \int_{\mathbb{R}^3}\|(H_1\varphi_n)(\cdot,\boldsymbol{x}_2)\|^2_{L^2(\mathbb{R}^3_{x_1})}d^3x_2$ this implies $\|(H_1\varphi_n)(\cdot,\boldsymbol{x}_2)\|_{L^2(\mathbb{R}^3_{x_1})} < \infty$ for almost every (with respect to Lebesgue measure) $\boldsymbol{x}_2 \in \mathbb{R}^3$ and thus

$$\varphi_n(\cdot,\boldsymbol{x}_2) \in \mathcal{D}(H_1) = \mathcal{D}(H_{0,1}) = W^2(\mathbb{R}^3_{x_1}) \qquad \text{for a.e. } \boldsymbol{x}_2 \in \mathbb{R}^3\,.$$

Thus we can apply an instance of Gagliardo-Nirenberg inequality [23, 31] (seealso the proof of Lemma 3 in subsection 2.4.3), namely

$$\|u\|_{L^\infty(\mathbb{R}^3)} \le C\|D^2u\|^{\frac{3}{4}}_{L^2(\mathbb{R}^3)}\|u\|^{\frac{1}{4}}_{L^2(\mathbb{R}^3)}$$

with $\|D^mu\|_{L^2(\mathbb{R}^3)} := \max_{|\alpha|=m}\|D^\alpha u\|_{L^2(\mathbb{R}^3)}$ and $C < \infty$ independent of $u \in W^2(\mathbb{R}^3)$, to get

$$\|\varphi_n(\cdot,\boldsymbol{x}_2)\|_{L^\infty(\mathbb{R}^3_{x_1})} \le C\|D^2_{x_1}\varphi_n(\cdot,\boldsymbol{x}_2)\|^{\frac{3}{4}}_{L^2(\mathbb{R}^3_{x_1})}\|\varphi_n(\cdot,\boldsymbol{x}_2)\|^{\frac{1}{4}}_{L^2(\mathbb{R}^3_{x_1})} \qquad \text{for a.e. } \boldsymbol{x}_2 \in \mathbb{R}^3\,.$$

[13] We abuse notation and do not distinguish between, say, H_2 defined on $L^2(\mathbb{R}^3_{x_2})$ and H_2 ($\mathbb{1}\otimes H_2$) defined on $L^2(\mathbb{R}^6)$ ($L^2(\mathbb{R}^3_{x_1})\otimes L^2(\mathbb{R}^3_{x_2})$).

Then, using Hölder in the second to last step,

$$\begin{aligned}\|\varphi_n(\boldsymbol{X}_1,\cdot)\|^2_{L^2(\mathbb{R}^3_{\boldsymbol{x}_2})} &= \int_{\mathbb{R}^3} |\varphi_n(\boldsymbol{X}_1,\boldsymbol{x}_2)|^2 d^3x_2 \le \int_{\mathbb{R}^3} \|\varphi_n(\cdot,\boldsymbol{x}_2)\|^2_{L^\infty(\mathbb{R}^3_{x_1})} d^3x_2 \\ &\le C^2 \int_{\mathbb{R}^3} \|D^2_{x_1}\varphi_n(\cdot,\boldsymbol{x}_2)\|^{\frac{3}{2}}_{L^2(\mathbb{R}^3_{x_1})} \|\varphi_n(\cdot,\boldsymbol{x}_2)\|^{\frac{1}{2}}_{L^2(\mathbb{R}^3_{x_1})} d^3x_2 \\ &\le C^2 \left[\int_{\mathbb{R}^3} \|D^2_{x_1}\varphi_n(\cdot,\boldsymbol{x}_2)\|^{\frac{3}{2}\cdot\frac{4}{3}}_{L^2(\mathbb{R}^3_{x_1})} d^3x_2\right]^{\frac{3}{4}} \left[\int_{\mathbb{R}^3} \|\varphi_n(\cdot,\boldsymbol{x}_2)\|^{\frac{1}{2}\cdot 4}_{L^2(\mathbb{R}^3_{x_1})} d^3x_2\right]^{\frac{1}{4}} \\ &\le C^2 \|D^2\varphi_n\|^{\frac{3}{2}}_{L^2(\mathbb{R}^6_x)} \|\varphi_n\|^{\frac{1}{2}}_{L^2(\mathbb{R}^6_x)}\end{aligned}$$

for every $\boldsymbol{X}_1 \in \mathbb{R}^3$. Moreover, since analog to (3.34) $\|H\varphi_n\|_{L^2(\mathbb{R}^6_x)} < \infty$, i.e. $\varphi_n \in \mathcal{D}(H) = \mathcal{D}(H_0) = W^2(\mathbb{R}^6)$, the last term is finite, i.e. we have just shown that indeed $\varphi_n(\boldsymbol{X}_1,\cdot) \in L^2(\mathbb{R}^3_{\boldsymbol{x}_2})$ for arbitrary $\boldsymbol{X}_1 \in \mathbb{R}^3$ and $n \in \mathbb{N}$.

Note that, like Sobolev inequalities Gagliardo-Nirenberg inequalities depend on the dimension of the space the functions to be estimated are defined on, so one might worry wether this makes our argument void for $N > 2$. However, since we apply Gagliardo-Nirenberg to $\varphi_n(\cdot,\boldsymbol{x}_2) : \mathbb{R}^3 \to \mathbb{C}$ only, this is not the case: Also the higher dimensional analogue $\varphi_n(\cdot,\boldsymbol{x}_2,\ldots,\boldsymbol{x}_n)$ is a function on $\mathbb{R}^3$.

We turn to the proof of (b). Let

$$G_2^R := \left\{\boldsymbol{x}_0 \in \mathcal{G}^\psi \mid \boldsymbol{X}_2^\psi(\boldsymbol{x}_0, T^R(\boldsymbol{x}_0)) \in \mathcal{G}^{\psi_{\boldsymbol{X}_1^R(\boldsymbol{x}_0,T^R(\boldsymbol{x}_0)),T^R(\boldsymbol{x}_0)}}\right\}.$$

Since $\mathbb{P}(A) = 1$ implies[14] $\mathbb{P}(A \cap B) = \mathbb{P}(B)$ for any measurable sets A, B and $\boldsymbol{X}_2^R(\boldsymbol{x}_0, T^R(\boldsymbol{x}_0)) = \boldsymbol{X}_2^\psi(\boldsymbol{x}_0, T^R(\boldsymbol{x}_0))$ we get (b) if we can show that

$$\mathbb{P}^\psi(G_2^R) = 1\,. \tag{3.35}$$

By the definition of conditional probability[15]

$$\begin{aligned}\mathbb{P}^\psi(G_2^R) &= \int_{\mathbb{R}^3\times[0,\infty)} \mathbb{P}^\psi\left(G_2^R \mid \left(\boldsymbol{X}_1^\psi(\cdot,T^R),T^R\right) = (\boldsymbol{x}_1,T)\right) \mathbb{P}^\psi_{(\boldsymbol{X}_1^\psi(\cdot,T^R),T^R)}(d^3x_1 dT) \\ &= \int_{\mathbb{R}^3\times[0,\infty)} \mathbb{P}^\psi\left(\boldsymbol{X}_2^\psi(\cdot,T) \in \mathcal{G}^{\psi_{\boldsymbol{x}_1,T}} \mid \left(\boldsymbol{X}_1^\psi(\cdot,T),T^R\right) = (\boldsymbol{x}_1,T)\right) \mathbb{P}^\psi_{(\boldsymbol{X}_1^\psi(\cdot,T^R),T^R)}(d^3x_1 dT)\end{aligned} \tag{3.36}$$

where, for any random variable or vector Y and measurable set A,

$$\mathbb{P}_Y(A) := \mathbb{P}(Y \in A) := \mathbb{P}(\{\omega \mid Y(\omega) \in A\})\,.$$

[14] $\mathbb{P}(B) \ge \mathbb{P}(A \cap B)$ is trivial and thus $\mathbb{P}(B) = 1 - \mathbb{P}(B^c) \le \mathbb{P}(A) - \mathbb{P}(A \cap B^c) = \mathbb{P}(A \cap B)$ implies $\mathbb{P}(A \cap B) = \mathbb{P}(B)$.

[15] We follow [9], where, however, the image measure $\mathbb{P}_Y$ is denoted $\widehat{\mathbf{P}}$.

Let Φ^{ψ}_{t,t_0} denote the flow map of (1.2), i.e. $\Phi^{\psi}_{t,t_0}(\boldsymbol{X}^{\psi}(\boldsymbol{x}_0,t_0)) = \boldsymbol{X}^{\psi}(\boldsymbol{x}_0,t)$ and in particular $\Phi^{\psi}_{t,0}(\boldsymbol{x}_0) = \boldsymbol{X}^{\psi}(\boldsymbol{x}_0,t)$ (cf. section 1.2). We shall show that ($A \subset \mathbb{R}^6$ measurable)

$$\mathbb{P}^{\psi}(A \mid Y = y) = \mathbb{P}^{\psi(\cdot,T)}\left(\Phi^{\psi}_{T,0}(A) \mid Y \circ \Phi^{\psi}_{0,T} = y\right) \tag{3.37}$$

for all $T \in \mathbb{R}$ and ($A \subset \mathbb{R}^3$ measurable)

$$\mathbb{P}^{\psi}\left(\boldsymbol{X}_2 \in A \mid (\boldsymbol{X}_1, Y) = (\boldsymbol{x}_1, y)\right) = \mathbb{P}^{\psi_{\boldsymbol{x}_1}}\left(A \mid Y(\boldsymbol{x}_1,\cdot) = y\right) \tag{3.38}$$

where the random vectors $\boldsymbol{X}_l$ are given by $\boldsymbol{X}_l(\boldsymbol{x}) = \boldsymbol{X}_l(\boldsymbol{x}_1,\boldsymbol{x}_2) := \boldsymbol{x}_l$ and, as before, $\psi_{\boldsymbol{x}_1}(\boldsymbol{x}_2) = \frac{\psi(\boldsymbol{x}_1,\boldsymbol{x}_2)}{\|\psi(\boldsymbol{x}_1,\cdot)\|_{L^2(\mathbb{R}^3_{x_2})}}$. Then

$$\begin{aligned}
&\mathbb{P}^{\psi}\left(\boldsymbol{X}^{\psi}_2(\cdot,T) \in \mathcal{G}^{\psi_{\boldsymbol{x}_1,T}} \mid \left(\boldsymbol{X}^{\psi}_1(\cdot,T), T^R\right) = (\boldsymbol{x}_1,T)\right)\\
&\quad\overset{(3.37)}{=} \mathbb{P}^{\psi(\cdot,T)}\left(\boldsymbol{X}_2 \in \mathcal{G}^{\psi_{\boldsymbol{x}_1,T}} \mid \left(\boldsymbol{X}_1, T^R \circ \Phi^{\psi}_{0,T}\right) = (\boldsymbol{x}_1,T)\right)\\
&\quad\overset{(3.38)}{=} \mathbb{P}^{\psi_{\boldsymbol{x}_1,T}}\left(\mathcal{G}^{\psi_{\boldsymbol{x}_1,T}} \mid \left(T^R \circ \Phi^{\psi}_{0,T}\right)(\boldsymbol{x}_1,\cdot) = T\right).
\end{aligned}$$

Since, however, $\mathbb{P}(A) = 1$ implies[16] $\mathbb{P}(A \mid Y = y) = 1$ (for any random variable or vector Y), with (a) this gives

$$\mathbb{P}^{\psi}\left(\boldsymbol{X}^{\psi}_2(\cdot,T) \in \mathcal{G}^{\psi_{\boldsymbol{x}_1,T}} \mid \left(\boldsymbol{X}^{\psi}_1(\cdot,T), T^R\right) = (\boldsymbol{x}_1,T)\right) = 1\,.$$

Put into (3.36) this yields (3.35),

$$\mathbb{P}^{\psi}(G^R_2) = \int\limits_{\mathbb{R}^3\times[0,\infty)} \mathbb{P}^{\psi}_{(\boldsymbol{X}^{\psi}_1(\cdot,T^R),T^R)}(d^3x_1 dT) = 1\,,$$

and we are left to prove (3.37) and (3.38).

The proof of (3.37) is standard. Recall that by definition every measurable function $\varphi(y)$ with $\int_B \varphi(y)\mathbb{P}^{\psi}_Y(dy) = \mathbb{P}^{\psi}(A, Y \in B)$ for every measurable B is a version of $\mathbb{P}^{\psi}(A \mid Y = y)$. Using equivariance, i.e. $\mathbb{P}^{\psi} = \mathbb{P}^{\psi(\cdot,T)} \circ \Phi^{\psi}_{T,0}$ (cf. equation (1.4)), and $\left(\Phi^{\psi}_{T,0}\right)^{-1} = \Phi^{\psi}_{0,T}$ we get

$$\mathbb{P}^{\psi}_Y(B) = \mathbb{P}^{\psi}\left(\{\boldsymbol{x} \mid Y(\boldsymbol{x}) \in B\}\right) = \mathbb{P}^{\psi(\cdot,T)}\left(\left\{\boldsymbol{x} \mid Y\left(\Phi^{\psi}_{0,T}(\boldsymbol{x})\right) \in B\right\}\right) = \mathbb{P}^{\psi(\cdot,T)}_{Y\circ\Phi^{\psi}_{0,T}}(B)$$

and hence (using equivariance once more in the last step)

$$\begin{aligned}
&\int\limits_B \mathbb{P}^{\psi(\cdot,T)}\left(\Phi^{\psi}_{T,0}(A) \mid Y \circ \Phi^{\psi}_{0,T} = y\right)\mathbb{P}^{\psi}_Y(dy)\\
&\quad= \int\limits_B \mathbb{P}^{\psi(\cdot,T)}\left(\Phi^{\psi}_{T,0}(A) \mid Y \circ \Phi^{\psi}_{0,T} = y\right)\mathbb{P}^{\psi(\cdot,T)}_{Y\circ\Phi^{\psi}_{0,T}}(dy) = \mathbb{P}^{\psi(\cdot,T)}\left(\Phi^{\psi}_{T,0}(A), Y \circ \Phi^{\psi}_{0,T} \in B\right)\\
&\quad= \mathbb{P}^{\psi(\cdot,T)}\left(\Phi^{\psi}_{T,0}\left(A \cap \{\boldsymbol{x} \mid Y(\boldsymbol{x}) \in B\}\right)\right) = \mathbb{P}^{\psi}(A, Y \in B)\,.
\end{aligned}$$

[16] Since $\mathbb{P}(A) = 1$, we have $\mathbb{P}(A, Y \in B) = \mathbb{P}(Y \in B) = \int_B \mathbb{P}_Y(dy)$, i.e. $\mathbb{P}(A \mid Y = y) = 1$.

We turn to the proof of (3.38). Note that (relative to Lesbegue measure) $\mathbb{P}^{\psi}$ ($\mathbb{P}^{\psi_{\boldsymbol{x}_1}}$) has got the density $|\psi(\boldsymbol{x})|^2$ ($|\psi_{\boldsymbol{x}_1}(\boldsymbol{x}_2)|^2 = \frac{|\psi(\boldsymbol{x}_1,\boldsymbol{x}_2)|^2}{\|\psi(\boldsymbol{x}_1,\cdot)\|^2_{L^2(\mathbb{R}^3_{x_2})}}$). Then, by Fubini,

$$\mathbb{P}^{\psi}_{(\boldsymbol{X}_1,Y)}(B\times C) = \int\limits_{\{\boldsymbol{x}|\boldsymbol{x}_1\in B, Y(\boldsymbol{x})\in C\}} |\psi(\boldsymbol{x})|^2 d^6x = \int\limits_{B} d^3x_1\, \|\psi(\boldsymbol{x}_1,\cdot)\|^2_{L^2(\mathbb{R}^3_{x_2})} \int\limits_{\{\boldsymbol{x}_2|Y(\boldsymbol{x}_1,\boldsymbol{x}_2)\in C\}} d^3x_2\, |\psi_{\boldsymbol{x}_1}(\boldsymbol{x}_2)|^2$$
$$= \int\limits_{B} d^3x_1\, \|\psi(\boldsymbol{x}_1,\cdot)\|^2_{L^2(\mathbb{R}^3_{x_2})} \mathbb{P}^{\psi_{\boldsymbol{x}_1}}_{Y(\boldsymbol{x}_1,\cdot)}(C)\,,$$

i.e.

$$\mathbb{P}^{\psi}_{(\boldsymbol{X}_1,Y)}(d^3x_1 dy) = \|\psi(\boldsymbol{x}_1,\cdot)\|^2_{L^2(\mathbb{R}^3_{x_2})} \mathbb{P}^{\psi_{\boldsymbol{x}_1}}_{Y(\boldsymbol{x}_1,\cdot)}(dy) d^3x_1\,.$$

Thus (once more using Fubini)

$$\int\limits_{D} \mathbb{P}^{\psi_{\boldsymbol{x}_1}}(A \mid Y(\boldsymbol{x}_1,\cdot) = y) \mathbb{P}^{\psi}_{(\boldsymbol{X}_1,Y)}(d^3x_1 dy)$$
$$= \int\limits_{\mathbb{R}^3} d^3x_1\, \|\psi(\boldsymbol{x}_1,\cdot)\|^2_{L^2(\mathbb{R}^3_{x_2})} \int\limits_{\{\boldsymbol{x}_2|(\boldsymbol{x}_1,Y(\boldsymbol{x}_1,\boldsymbol{x}_2))\in D\}} \mathbb{P}^{\psi_{\boldsymbol{x}_1}}(A \mid Y(\boldsymbol{x}_1,\cdot) = y) \mathbb{P}^{\psi_{\boldsymbol{x}_1}}_{Y(\boldsymbol{x}_1,\cdot)}(dy)$$
$$= \int\limits_{\mathbb{R}^3} d^3x_1\, \|\psi(\boldsymbol{x}_1,\cdot)\|^2_{L^2(\mathbb{R}^3_{x_2})} \mathbb{P}^{\psi_{\boldsymbol{x}_1}}(A, Y(\boldsymbol{x}_1,\cdot) \in \{y \mid (\boldsymbol{x}_1, y) \in D\})$$
$$= \int\limits_{\mathbb{R}^3} d^3x_1\, \|\psi(\boldsymbol{x}_1,\cdot)\|^2_{L^2(\mathbb{R}^3_{x_2})} \int\limits_{\{\boldsymbol{x}_2\in A|(\boldsymbol{x}_1,Y(\boldsymbol{x}_1,\boldsymbol{x}_2))\in D\}} d^3x_2\, |\psi_{\boldsymbol{x}_1}(\boldsymbol{x}_2)|^2$$
$$= \int\limits_{\{\boldsymbol{x}|\boldsymbol{x}_2\in A,(\boldsymbol{x}_1,Y(\boldsymbol{x}))\in D\}} |\psi(\boldsymbol{x})|^2 d^6x = \mathbb{P}^{\psi}\left(\boldsymbol{X}_2 \in A, (\boldsymbol{X}_1, Y) \in D\right)\,,$$

i.e. we get (3.38). □

Proof of Theorem 2 (ii), (iii) and Theorem 4 (ii). The proof is analogous to that of Theorem 1 in [34] (the corresponding result for the unmeasured case with $N = 1$). By comparison we see that Theorem 2 (ii), (iii) and Theorem 4 (ii) hold if we can show that the following three conditions are satisfied:

(I) Pointwise estimates of ψ and $\nabla\psi$:

Lemmas 5 and 6 hold.

(II) L^2-estimates of ψ:

$$\lim_{t\to\infty} \|\psi(\cdot,t) - \Phi(\cdot,t)\| = 0\,. \tag{3.39}$$

(III) Regularity of $\widehat{\psi}_{\text{out}}$:

$$\widehat{\psi}_{\text{out}}(\boldsymbol{k}) \text{ is continuous and bounded for } \boldsymbol{k} \notin \mathcal{N}\,. \tag{3.40}$$

For a better understanding we sketch the main steps of the proof and explain how conditions (I) to (III) enter into it. Note that in the following $\boldsymbol{x}_0$, $\boldsymbol{X}^\psi$, $\boldsymbol{k}$ and $\boldsymbol{v}^\psi$ might be both in $\mathbb{R}^{3N}$ for general N (whenever we prove assertions of Theorem 2) and in $\mathbb{R}^6 = \mathbb{R}^{3N}$ for $N = 2$ (whenever we prove assertions of Theorem 4).

Condition (I) gives estimates for $\boldsymbol{v}^\psi(\boldsymbol{x}, t)$ and $\boldsymbol{v}^{\psi_{\boldsymbol{x}_1,t_1}}(\boldsymbol{x}_2, t_2)$ resp. $\boldsymbol{v}^{\psi_{\boldsymbol{x}_2,t_2}}(\boldsymbol{x}_1, t_1)$: For $\delta_1 > 0$ and $0 < a < b < \infty$ define

$$B_{\delta_1 ab} := \{\boldsymbol{k} | \, |\widehat{\psi}_{\text{out}}(\boldsymbol{k})| > \delta_1 \text{ and } a < k_l < b\,,\ l = 1, 2, \ldots, N\}\,.$$

Then there exist $T < \infty$, $C < \infty$ such that for all $t, t_1, t_2 \geq T$ and $\frac{\boldsymbol{x}}{t}$, $\left(\frac{\boldsymbol{x}_1}{t_1}, \frac{\boldsymbol{x}_2}{t_2}\right) \in B_{\delta_1 ab}$

$$\begin{aligned}
\left|\boldsymbol{v}^\psi(\boldsymbol{x}, t) - \frac{\boldsymbol{x}}{t}\right| &= \left|\text{Im}\left(\frac{\nabla\psi(\boldsymbol{x}, t) - i\frac{\boldsymbol{x}}{t}\psi(\boldsymbol{x}, t)}{\psi(\boldsymbol{x}, t)}\right)\right| \\
&\leq \frac{\left|\nabla\psi(\boldsymbol{x}, t) - i\frac{\boldsymbol{x}}{t}\Phi(\boldsymbol{x}, t)\right| + \frac{x}{t}|\psi(\boldsymbol{x}, t) - \Phi(\boldsymbol{x}, t)|}{|\Phi(\boldsymbol{x}, t)| - |\psi(\boldsymbol{x}, t) - \Phi(\boldsymbol{x}, t)|} \\
&\overset{\text{Lemma 5}}{\leq} \frac{C'\left(1 + \frac{x}{t}\right) t^{-\frac{3N+1}{2}}}{t^{-\frac{3N}{2}}|\widehat{\psi}_{\text{out}}(\frac{\boldsymbol{x}}{t})| - C' t^{-\frac{3N+1}{2}}} \leq C t^{-\frac{1}{2}}\,, \qquad (3.41)
\end{aligned}$$

$$\left|\boldsymbol{v}^{\psi_{\boldsymbol{x}_1,t_1}}(\boldsymbol{x}_2, t_2) - \frac{\boldsymbol{x}_2}{t_2}\right| = \left|\text{Im}\left(\frac{\nabla_2\psi(\boldsymbol{x}; t_1, t_2) - i\frac{\boldsymbol{x}_2}{t_2}\psi(\boldsymbol{x}; t_1, t_2)}{\psi(\boldsymbol{x}; t_1, t_2)}\right)\right| \overset{\text{Lemma 6}}{\leq} C t_1^{-\frac{1}{2}}\,,$$

$$\left|\boldsymbol{v}^{\psi_{\boldsymbol{x}_2,t_2}}(\boldsymbol{x}_1, t_1) - \frac{\boldsymbol{x}_1}{t_1}\right| \overset{\text{Lemma 6}}{\leq} C t_2^{-\frac{1}{2}}\,.$$

The latter two are of interest since for $t > T^R(\boldsymbol{x}_0)$ the measured velocity field $\boldsymbol{v}_{1/2}^{\psi^R_{\boldsymbol{x}_0}}(\boldsymbol{x}, t)$ is either identically zero (if $T^R(\boldsymbol{x}_0) = t_{\text{ex}}^{B_{1/2,R}}(\boldsymbol{x}_0)$) or equal to $\boldsymbol{v}^{\psi_{\boldsymbol{X}_{2/1},T}}(\boldsymbol{x}_{1/2}, t)$ (if $T^R(\boldsymbol{x}_0) < t_{\text{ex}}^{B_{1/2,R}}(\boldsymbol{x}_0)$ and with $T = T^R(\boldsymbol{x}_0)$, $\boldsymbol{X}_{2/1} = \boldsymbol{X}^\psi_{2/1}(\boldsymbol{x}_0, T)$). Now let $\delta_2 > 0$ and define (B_{δ_2} denotes the open ball with radius δ_2)

$$\begin{aligned}
B_{\delta_1\delta_2 ab} &: = \{\boldsymbol{k} \in B_{\delta_1 ab} \mid B_{\delta_2}(\boldsymbol{k}) \subset B_{\delta_1 ab}\}\,, \\
G^\psi_{\delta_1\delta_2 ab}(T) &: = \left\{\boldsymbol{x}_0 \mid \frac{\boldsymbol{X}^\psi(\boldsymbol{x}_0, T)}{T} \in B_{\delta_1\delta_2 ab}\right\}, \\
G^R_{\delta_1\delta_2 ab}(T) &: = G^\psi_{\delta_1\delta_2 ab}(T) \cap \{\boldsymbol{x}_0 \mid T^R(\boldsymbol{x}_0) \geq T\}\,.
\end{aligned}$$

Then, for T big enough, $G^\psi_{\delta_1\delta_2 ab}(T)$ resp. $G^R_{\delta_1\delta_2 ab}(T)$ is a set of "good" initial configurations in the sense that $\boldsymbol{x}_0 \in G^\psi_{\delta_1\delta_2 ab}(T)$ resp. $\boldsymbol{x}_0 \in G^R_{\delta_1\delta_2 ab}(T)$ implies that

> $v^\psi_\infty(\boldsymbol{x}_0)$ exists and $|\boldsymbol{v}^\psi\left(\boldsymbol{X}^\psi(\boldsymbol{x}_0, t), t\right) - v^\psi_\infty(\boldsymbol{x}_0)| \leq C t^{-\frac{1}{2}}$ for all $t \geq T$ and some $C < \infty$

resp.

> $v^\psi_\infty(\boldsymbol{x}_0)$ exists and $\boldsymbol{x}_0 \in \mathcal{V}_{RTC}$ for some $C < \infty$, i.e.
>
> $T^R(\boldsymbol{x}_0) > T$,
>
> $|\boldsymbol{v}^{\psi^R_{\boldsymbol{x}_0}}(\boldsymbol{X}^R(\boldsymbol{x}_0, t), t) - v^\psi_\infty(\boldsymbol{x}_0)| \leq \frac{C}{\sqrt{t}}$ for all $T \leq t \leq T^R(\boldsymbol{x}_0)$ and
>
> $|\boldsymbol{v}_l^{\psi^R_{\boldsymbol{x}_0}}(\boldsymbol{X}^R(\boldsymbol{x}_0, t), t) - \boldsymbol{v}^\psi_{\infty,l}(\boldsymbol{x}_0)| \leq \frac{C}{\sqrt{T^R(\boldsymbol{x}_0)}}$ for all $t > T^R(\boldsymbol{x}_0)$ and $l = 1, 2$ s.t. $T^R(\boldsymbol{x}_0) < t_{\text{ex}}^{B_{l,R}}(\boldsymbol{x}_0)$.

Since the above implications are the crucial parts of the respective proofs we elaborate on them. First, let $\boldsymbol{x}_0 \in G^{\psi}_{\delta_1\delta_2 ab}(T)$. Note that (3.41) (first equality) implies that $\left(\frac{\boldsymbol{X}^{\psi}(\boldsymbol{x}_0,t)}{t}\right)_{t\geq T}$ is Cauchy as long as it stays in $B_{\delta_1 ab}$: For $T \leq t_1 < t_2$ such that $\frac{\boldsymbol{X}^{\psi}(\boldsymbol{x}_0,s)}{s} \in B_{\delta_1 ab}$ for all $t_1 \leq s < t_2$

$$\begin{aligned}\Big|\frac{\boldsymbol{X}^{\psi}(\boldsymbol{x}_0,t_1)}{t_1} - \frac{\boldsymbol{X}^{\psi}(\boldsymbol{x}_0,t_2)}{t_2}\Big| &\leq \int_{t_1}^{t_2} \Big|\frac{d}{ds}\frac{\boldsymbol{X}^{\psi}(\boldsymbol{x}_0,s)}{s}\Big| ds \\ &\leq \int_{t_1}^{t_2} \frac{1}{s}\Big|\boldsymbol{v}^{\psi}\left(\boldsymbol{X}^{\psi}(\boldsymbol{x}_0,s),s\right) - \frac{\boldsymbol{X}^{\psi}(\boldsymbol{x}_0,s)}{s}\Big| ds \\ &\overset{(3.41)}{\leq} C\int_{t_1}^{t_2} s^{-\frac{3}{2}} ds \leq 2Ct_1^{-\frac{1}{2}} \leq 2CT^{-\frac{1}{2}}\,.\end{aligned} \tag{3.42}$$

Since $\frac{\boldsymbol{X}^{\psi}(\boldsymbol{x}_0,t)}{t}$ is continuous in t this in particular implies that, whenever T is big enough, $|\frac{\boldsymbol{X}^{\psi}(\boldsymbol{x}_0,T)}{T} - \frac{\boldsymbol{X}^{\psi}(\boldsymbol{x}_0,t)}{t}| < \delta_2$, i.e. $\frac{\boldsymbol{X}^{\psi}(\boldsymbol{x}_0,t)}{t}$ stays in $B_{\delta_2}(\frac{\boldsymbol{X}^{\psi}(\boldsymbol{x}_0,T)}{T}) \subset B_{\delta_1 ab}$ for all $t \geq T$. Thus (3.42) holds in fact for *all* $t_2 > t_1 \geq T$ and $v^{\psi}_{\infty}(\boldsymbol{x}_0) = \lim_{t\to\infty} \frac{\boldsymbol{X}^{\psi}(\boldsymbol{x}_0,t)}{t}$ exists. Moreover, using (3.41) and (3.42),

$$\begin{aligned}&\Big|\boldsymbol{v}^{\psi}\left(\boldsymbol{X}^{\psi}(\boldsymbol{x}_0,t),t\right) - v^{\psi}_{\infty}(\boldsymbol{x}_0)\Big| \\ &\quad\leq \Big|\boldsymbol{v}^{\psi}\Big(\boldsymbol{X}^{\psi}(\boldsymbol{x}_0,t),t\Big) - \frac{\boldsymbol{X}^{\psi}(\boldsymbol{x}_0,t)}{t}\Big| + \lim_{s\to\infty}\Big|\frac{\boldsymbol{X}^{\psi}(\boldsymbol{x}_0,t)}{t} - \frac{\boldsymbol{X}^{\psi}(\boldsymbol{x}_0,s)}{s}\Big| \\ &\quad\leq 3Ct^{-\frac{1}{2}}\end{aligned} \tag{3.43}$$

for all $t \geq T$.

Now let $\boldsymbol{x}_0 \in G^{R}_{\delta_1\delta_2 ab}(T)$ (with the same T as before). Then $v^{\psi}_{\infty}(\boldsymbol{x}_0)$ exists and, since for $t \leq T^R(\boldsymbol{x}_0)$ $\boldsymbol{v}^{\psi^R_{\boldsymbol{x}_0}}(\boldsymbol{X}^R(\boldsymbol{x}_0,t),t) = \boldsymbol{v}^{\psi}(\boldsymbol{X}^{\psi}(\boldsymbol{x}_0,t),t)$, (3.43) already gives

$$\Big|\boldsymbol{v}^{\psi^R_{\boldsymbol{x}_0}}(\boldsymbol{X}^R(\boldsymbol{x}_0,t),t) - v^{\psi}_{\infty}(\boldsymbol{x}_0)\Big| \leq 3Ct^{-\frac{1}{2}}$$

for all $T \leq t \leq T^R(\boldsymbol{x}_0)$. Without loss of generality assume that $T^R(\boldsymbol{x}_0) = t_{\mathrm{ex}}^{B_{1,R}}(\boldsymbol{x}_0) < t_{\mathrm{ex}}^{B_{2,R}}(\boldsymbol{x}_0)$. Then $\boldsymbol{v}_2^{\psi^R_{\boldsymbol{x}_0}}(\boldsymbol{X}^R(\boldsymbol{x}_0,t),t) = \boldsymbol{v}^{\psi_{\boldsymbol{X}_1^{\psi}(\boldsymbol{x}_0,T^R(\boldsymbol{x}_0)),T^R(\boldsymbol{x}_0)}}(\boldsymbol{X}_2^R(\boldsymbol{x}_0,t),t)$ for $t \geq T^R(\boldsymbol{x}_0)$ and (3.41) (second equality) implies that $\left(\frac{\boldsymbol{X}_2^R(\boldsymbol{x}_0,t)}{t}\right)_{t\geq T^R(\boldsymbol{x}_0)}$ is Cauchy as long as $\left(\frac{\boldsymbol{X}_1^R\left(\boldsymbol{x}_0,T^R(\boldsymbol{x}_0)\right)}{T^R(\boldsymbol{x}_0)}, \frac{\boldsymbol{X}_2^R(\boldsymbol{x}_0,t)}{t}\right) = \left(\frac{\boldsymbol{X}_1^{\psi}(\boldsymbol{x}_0,T^R(\boldsymbol{x}_0))}{T^R(\boldsymbol{x}_0)}, \frac{\boldsymbol{X}_2^R(\boldsymbol{x}_0,t)}{t}\right)$ stays in $B_{\delta_1 ab}$: For $T \leq t_1 < t_2$ such that $\left(\frac{\boldsymbol{X}_1^R\left(\boldsymbol{x}_0,T^R(\boldsymbol{x}_0)\right)}{T^R(\boldsymbol{x}_0)}, \frac{\boldsymbol{X}_2^R(\boldsymbol{x}_0,t)}{t}\right) \in B_{\delta_1 ab}$ for all $t_1 \leq s < t_2$

$$\Big|\frac{\boldsymbol{X}_2^R(\boldsymbol{x}_0,t_1)}{t_1} - \frac{\boldsymbol{X}_2^R(\boldsymbol{x}_0,t_2)}{t_2}\Big| \leq 2Ct_1^{-\frac{1}{2}} \leq 2CT^{-\frac{1}{2}}\,. \tag{3.44}$$

But then (by(3.42) and (3.44))

$$
\begin{aligned}
&\Big|\Big(\frac{\boldsymbol{X}_1^{\psi}(\boldsymbol{x}_0,T^R(\boldsymbol{x}_0))}{T^R(\boldsymbol{x}_0)},\frac{\boldsymbol{X}_2^{R}(\boldsymbol{x}_0,t)}{t}\Big)-\frac{\boldsymbol{X}^{\psi}(\boldsymbol{x}_0,T)}{T}\Big|\\
&\qquad\qquad\le\Big|\frac{\boldsymbol{X}^{\psi}(\boldsymbol{x}_0,T^R(\boldsymbol{x}_0))}{T^R(\boldsymbol{x}_0)}-\frac{\boldsymbol{X}^{\psi}(\boldsymbol{x}_0,T)}{T}\Big|+\Big|\frac{\boldsymbol{X}_2^{R}(\boldsymbol{x}_0,t)}{t}-\frac{\boldsymbol{X}_2^{R}(\boldsymbol{x}_0,T^R(\boldsymbol{x}_0))}{T^R(\boldsymbol{x}_0)}\Big|\\
&\qquad\qquad\le 2CT^{-\frac{1}{2}}<\delta_2\,,
\end{aligned}
$$

i.e. also $\left(\frac{\boldsymbol{X}_1^{\psi}(\boldsymbol{x}_0,T^R(\boldsymbol{x}_0))}{T^R(\boldsymbol{x}_0)},\frac{\boldsymbol{X}_2^{R}(\boldsymbol{x}_0,t)}{t}\right)$ stays in $B_{\delta_2}(\frac{\boldsymbol{X}^{\psi}(\boldsymbol{x}_0,T)}{T})\subset B_{\delta_1\delta_2ab}$ and (3.44) holds in fact for *all* $t_2>t_1>T^R(\boldsymbol{x}_0)(\ge T)$. Thus by (3.41), (3.42) and (3.44)

$$
\begin{aligned}
&\Big|\boldsymbol{v}_2^{\psi^R_{\boldsymbol{x}_0}}(\boldsymbol{X}^R(\boldsymbol{x}_0,t),t)-\boldsymbol{v}^{\psi}_{\infty,2}(\boldsymbol{x}_0)\Big|\\
&\quad\le\Big|\boldsymbol{v}^{\psi_{\boldsymbol{X}_1^{\psi}(\boldsymbol{x}_0,T^R(\boldsymbol{x}_0)),T^R(\boldsymbol{x}_0)}}(\boldsymbol{X}_2^R(\boldsymbol{x}_0,t),t)-\frac{\boldsymbol{X}_2^{R}(\boldsymbol{x}_0,t)}{t}\Big|+\Big|\frac{\boldsymbol{X}_2^{R}(\boldsymbol{x}_0,t)}{t}-\frac{\boldsymbol{X}_2^{R}(\boldsymbol{x}_0,T^R(\boldsymbol{x}_0))}{T^R(\boldsymbol{x}_0)}\Big|\\
&\quad+\lim_{s\to\infty}\Big|\frac{\boldsymbol{X}_2^{R}(\boldsymbol{x}_0,T^R(\boldsymbol{x}_0))}{T^R(\boldsymbol{x}_0)}-\frac{\boldsymbol{X}_2^{R}(\boldsymbol{x}_0,s)}{s}\Big|\le 5C(T^R(\boldsymbol{x}_0))^{-\frac{1}{2}}
\end{aligned}
$$

for all $t>T^R(\boldsymbol{x}_0)$, i.e. $\boldsymbol{x}_0\in\mathcal{V}_{RTC}$.

So we get Theorem 2 (ii) (Theorem 4 (ii)), if we can adjust δ_1, δ_2, a, b and T (δ_1, δ_2, a, b, T and R) such that the set of "good" initial configurations $G^{\psi}_{\delta_1\delta_2ab}(T)$ ($G^{R}_{\delta_1\delta_2ab}(T)$) has (nearly) full measure. Let $\varepsilon>0$. By condition (II) and equivariance one easily sees that for any $T>0$ big enough

$$
\begin{aligned}
\mathbb{P}^{\psi}\left(\frac{\boldsymbol{X}^{\psi}(\boldsymbol{x}_0,T)}{T}\in A\right)&=\mathbb{P}^{\psi(\cdot,T)}\left(\frac{\boldsymbol{x}}{T}\in A\right)\ge\mathbb{P}^{\Phi(\cdot,T)}\left(\frac{\boldsymbol{x}}{T}\in A\right)-\varepsilon\\
&=\int_A|\widehat{\psi}_{\text{out}}(\boldsymbol{k})|^2d^{3N}k-\varepsilon
\end{aligned}
\tag{3.45}
$$

for any measurable $A\subset\mathbb{R}^{3N}$. Moreover, condition (III) guarantees

$$
\int_{B_{\delta_1\delta_2ab}}|\widehat{\psi}_{\text{out}}(\boldsymbol{k})|^2d^{3N}k>1-\varepsilon \tag{3.46}
$$

for δ_1, δ_2, a small and b big enough (cf. proof of Theorem 1 in [34])[17]. In particular, (3.45) and (3.46) show that there are $\delta_1>0$, $\delta_2>0$, $0<a<b<\infty$ and $T<\infty$ such that

$$
\mathbb{P}^{\psi}\left(G^{\psi}_{\delta_1\delta_2ab}(T)\right)=\mathbb{P}^{\psi}\Big(\frac{\boldsymbol{X}^{\psi}(\boldsymbol{x}_0,T)}{T}\in B_{\delta_1\delta_2ab}\Big)>1-2\varepsilon\,,
$$

i.e. Theorem 2 (ii) holds. Now note that global existence of Bohmian mechanics guarantees that $\mathbb{P}^{\psi}$-almost no trajectory reaches spatial infinity in finite time. Thus in particular there

[17] Note that the choice of δ_1, δ_2, a, b does evidently not depend on T. This is important since above we choose T such that $G^{\psi}_{\delta_1\delta_2ab}(T)$ and $G^{R}_{\delta_1\delta_2ab}(T)$ contained "good" initial configurations for *given* δ_1, δ_2, a, b. This is a point we failed to observe in the proof of Theorem 1 in [34].

is some $R_T < \infty$ such that

$$\mathbb{P}^\psi(\{\boldsymbol{x}_0 \mid T^R(\boldsymbol{x}_0) \geq T\}) \geq \mathbb{P}^\psi\left(\left\{\boldsymbol{x}_0 \mid \sup_{0\leq t\leq T}\left|\boldsymbol{X}^\psi(\boldsymbol{x}_0,t)\right| \leq R\right\}\right) > 1-\varepsilon$$

for all $R > R_T$. Since $G^R_{\delta_1\delta_2 ab}(T) = G^\psi_{\delta_1\delta_2 ab}(T) \cap \{\boldsymbol{x}_0 \mid T^R(\boldsymbol{x}_0) \geq T\}$ this gives

$$\mathbb{P}^\psi(G^R_{\delta_1\delta_2 ab}(T)) > 1-3\varepsilon$$

for all $R > R_T$, i.e. we get Theorem 4 (ii).

Finally, looking once more at (3.45), we see that also Theorem 2 (iii) holds:

$$\mathbb{P}^\psi(v^\psi_\infty \in A) = \lim_{t\to\infty}\mathbb{P}^\psi\left(\frac{\boldsymbol{X}^\psi(\boldsymbol{x}_0,t)}{t} \in A\right) = \int\limits_A |\widehat{\psi}_{\mathrm{out}}(\boldsymbol{k})|^2 d^{3N}k$$

Now to the proof of conditions (I) to (III). Condition (I), i.e. Lemmas 5 and 6, will be proved in subsection 3.6.3. Condition (II) is a standard result, which follows from (3.10) (i.e.
$\lim_{t\to\infty}\|e^{-iHt}\psi - e^{-iH_0t}\psi_{\mathrm{out}}\| = 0$) and

$$\lim_{t\to\infty}\left\|e^{-iH_0t}\psi_{\mathrm{out}} - \Phi(\cdot,t)\right\| = 0$$

for all $\psi_{\mathrm{out}} \in L^2(\mathbb{R}^{3N})$ (see e.g. [14] or [32], Theorem IX.31). Finally, condition (III) is a consequence of $\psi \in \mathcal{G}^{(N)}$. For a proof see the mapping Lemma 10 at the end of subsection 3.6.3. □

3.6.2 Properties of generalized eigenfunctions

As explained in section 3.3 we shall use the method of expansion in generalized eigenfunctions to prove Lemmas 5 and 6, i.e. to get the pointwise estimates on $(\nabla)\psi$ needed to control the standard resp. the measured Bohmian velocity field $\boldsymbol{v}^\psi$ resp. $\boldsymbol{v}^{\psi^R_{\boldsymbol{x}_0}}$. In this Subsection we have collected the relevant properties of the generalized eigenfunctions. We first recall some standard [27] and some new [18, 37] results concerning generalized eigenfunctions in the single particle case. We then extend those results to the case of N particles.

Let $N = 1$. One looks for generalized eigenfunctions $\varphi_\pm$ that diagonalize (the single particle) Hamiltonian H (and thus the time evolution e^{-iHt}) on $\mathcal{H}_{\mathrm{a.c.}}(H)$:

$$(-\frac{1}{2}\Delta + V(\boldsymbol{x}))\varphi_\pm(\boldsymbol{x},\boldsymbol{k}) = \frac{k^2}{2}\varphi_\pm(\boldsymbol{x},\boldsymbol{k}) \tag{3.47}$$

Inverting $(-\frac{1}{2}\Delta - \frac{k^2}{2})$ one obtains the Lippmann-Schwinger equation. We recall the main parts of a result on this due to Ikebe [27]. In the present form it can be found in [37].

Proposition 4. *Let $V \in (V)_2$. Then for any $\boldsymbol{k} \in \mathbb{R}^3\backslash\{0\}$ there are unique solutions $\varphi_\pm(\cdot, \boldsymbol{k}) : \mathbb{R}^3 \to \mathbb{C}$ of the Lippmann-Schwinger equations*

$$\varphi_\pm(\boldsymbol{x}, \boldsymbol{k}) = e^{i\boldsymbol{k}\cdot\boldsymbol{x}} - \frac{1}{2\pi}\int \frac{e^{\mp ik|\boldsymbol{x}-\boldsymbol{x}'|}}{|\boldsymbol{x}-\boldsymbol{x}'|} V(\boldsymbol{x}')\varphi_\pm(\boldsymbol{x}', \boldsymbol{k}) d^3x' \,, \tag{3.48}$$

that satisfy the boundary conditions $\lim_{x\to\infty} |\varphi_\pm(\boldsymbol{x}, \boldsymbol{k}) - e^{i\boldsymbol{k}\cdot\boldsymbol{x}}| = 0$. They are also classical solutions of the stationary Schrödinger equation (3.47) *and such that:*

(i) For any $f \in L^2(\mathbb{R}^3)$ the generalized Fourier transforms

$$(\mathcal{F}_\pm f)(\boldsymbol{k}) = (2\pi)^{-\frac{3}{2}} \,\mathrm{l.\,i.\,m.} \int \varphi^*_\pm(\boldsymbol{x}, \boldsymbol{k}) f(\boldsymbol{x}) d^3x$$

exist in $L^2(\mathbb{R}^3)$.

(ii) Ran$(\mathcal{F}_\pm) = L^2(\mathbb{R}^3)$. Moreover, $\mathcal{F}_\pm : \mathcal{H}_{a.c.}(H) \to L^2(\mathbb{R}^3)$ are unitary and the inverses of these unitaries are given by

$$(\mathcal{F}^{-1}_\pm f)(\boldsymbol{x}) = (2\pi)^{-\frac{3}{2}} \,\mathrm{l.\,i.\,m.} \int \varphi_\pm(\boldsymbol{x}, \boldsymbol{k}) f(\boldsymbol{k}) d^3k.$$

(iii) For any $f \in L^2(\mathbb{R}^3)$ the relations $\Omega_\pm f = \mathcal{F}^{-1}_\pm \mathcal{F} f$ holds, where $\mathcal{F}$ is the ordinary Fourier transform in 3 *dimensions.*

(iv) For any $f \in \mathcal{H}_{a.c.}(H) \cap \mathrm{D}(H)$

$$Hf(\boldsymbol{x}) = \left(\mathcal{F}^{-1}_\pm \frac{k^2}{2} \mathcal{F}_\pm f\right)(\boldsymbol{x})$$

and therefore for any $f \in \mathcal{H}_{a.c.}(H)$

$$e^{-iHt} f(\boldsymbol{x}) = \left(\mathcal{F}^{-1}_\pm e^{-i\frac{k^2}{2}t} \mathcal{F}_\pm f\right)(\boldsymbol{x})\,.$$

In the next proposition we have collected results on the regularity of the generalized eigenfunctions (cf., e.g., Proposition 2 in [18]).

Proposition 5. *Let $V \in (V)_n$ for some $n \geq 3$. Then:*

(i) $\varphi_\pm(\boldsymbol{x}, \cdot) \in C^{n-2}(\mathbb{R}^3 \setminus \{0\})$ for all $\boldsymbol{x} \in \mathbb{R}^3$ and the partial derivatives $D^\alpha_{\boldsymbol{k}}\varphi_\pm(\boldsymbol{x}, \boldsymbol{k})$, $|\alpha| \leq n-2$, are continuous with respect to $\boldsymbol{x}$ and $\boldsymbol{k}$.

If, in addition, zero is neither an eigenvalue nor a resonance of H, then

(ii) $$\sup_{\boldsymbol{x}\in\mathbb{R}^3, \boldsymbol{k}\in\mathbb{R}^3} |\varphi_\pm(\boldsymbol{x}, \boldsymbol{k})| < \infty,$$

for any $|\alpha| \leq n-2$ there is a $c_\alpha < \infty$ such that ($\kappa := \frac{k}{\langle k\rangle}$)

(iii) $\sup_{\boldsymbol{k}\in\mathbb{R}^3\setminus\{0\}} \left|\kappa^{|\alpha|-1}D^\alpha_{\boldsymbol{k}}\varphi_\pm(\boldsymbol{x},\boldsymbol{k})\right| < c_\alpha\langle x\rangle^{|\alpha|}$

and for any $l\in\{1,\dots,n-2\}$ there is a $c_l<\infty$ such that

(iv) $\sup_{\boldsymbol{k}\in\mathbb{R}^3\setminus\{0\}} \left|\frac{\partial^l}{\partial k^l}\varphi_\pm(\boldsymbol{x},\boldsymbol{k})\right| < c_l\langle x\rangle^l,$

where $\frac{\partial}{\partial k}$ is the radial partial derivative in $\boldsymbol{k}$-space.

For a proof of (i), (ii) and (iv) see [37], for (iii) see [18].

Now let $N\geq 2$. For every $l\in\{1,2,\dots,N\}$ let $V_l\in(V)_2$ and let $\varphi_{\pm,l}$ denote the generalized eigenfunctions of H_l and $\mathcal{F}_{\pm,l}$ the generalized Fourier transform defined via $\varphi_{\pm,l}$. Define the $3N$-dimensional generalized (partial) Fourier transform(s) by

$$\mathcal{F}_{\pm,I} := \prod_{l\in I}\mathcal{F}_{\pm,l}\,,\qquad I\subset\{1,2,\dots,N\}\,, \tag{3.49}$$

and

$$\mathcal{F}^{(N)}_\pm := \mathcal{F}_{\pm,\{1,2,\dots,N\}} = \prod_{l=1}^N \mathcal{F}_{\pm,l}\,. \tag{3.50}$$

This is well defined, since the $\mathcal{F}_{\pm,l}$ obviously commute. By Proposition 4 $\mathcal{F}_{\pm,I}$ (and thus $\mathcal{F}^{(N)}_\pm$) got the following properties:

(i) For any $f\in L^2(\mathbb{R}^{3N})$

$$\begin{aligned}\left(\mathcal{F}_{\pm,I}f\right)(\boldsymbol{x}_{I^c},\boldsymbol{k}_I) &= (2\pi)^{-\frac{3|I|}{2}}\,\mathrm{l.i.m.}\int\left(\varphi_{\pm,I}\right)^*(\boldsymbol{x}_I,\boldsymbol{k}_I)f(\boldsymbol{x})d^{3|I|}x_I\\ \left(\left(\mathcal{F}^{(N)}_\pm f\right)(\boldsymbol{k}) \right.&= \left.(2\pi)^{-\frac{3N}{2}}\,\mathrm{l.i.m.}\int\left(\varphi^{(N)}_\pm\right)^*(\boldsymbol{x},\boldsymbol{k})f(\boldsymbol{x})d^{3N}x\right),\end{aligned} \tag{3.51}$$

where

$$\varphi_{\pm,I}(\boldsymbol{x}_I,\boldsymbol{k}_I) := \prod_{l\in I}\varphi_{\pm,l}(\boldsymbol{x}_l,\boldsymbol{k}_l)\qquad\left(\varphi^{(N)}_\pm(\boldsymbol{x},\boldsymbol{k}) := \prod_{l=1}^N\varphi_{\pm,l}(\boldsymbol{x}_l,\boldsymbol{k}_l)\right) \tag{3.52}$$

are generalized eigenfunctions of $H_I=\sum_{l\in I}H_l$ ($H=\sum_{l=1}^N H_l$) belonging to the eigenvalue $\frac{k_I^2}{2}=\sum_{l\in I}\frac{k_l^2}{2}$ ($\frac{k^2}{2}=\sum_{l=1}^N\frac{k_l^2}{2}$) and $(\boldsymbol{x}_{I^c},\boldsymbol{k}_I)_l := \begin{cases}\boldsymbol{x}_l & \text{if } l\in I^c,\\ \boldsymbol{k}_l & \text{if } l\in I\,.\end{cases}$

(ii) $Ran(\mathcal{F}_{\pm,I})=L^2(\mathbb{R}^{3N})$. Moreover, $\mathcal{F}_{\pm,I}:\mathcal{H}_{\mathrm{s}}(H_I)\to L^2(\mathbb{R}^{3N})$ are unitary and the inverses of these unitaries are given by

$$\left(\mathcal{F}^{-1}_{\pm,I}f\right)(\boldsymbol{x}) = (2\pi)^{-\frac{3|I|}{2}}\,\mathrm{l.i.m.}\int\varphi_{\pm,I}(\boldsymbol{x}_I,\boldsymbol{k}_I)f(\boldsymbol{x}_{I^c},\boldsymbol{k}_I)d^{3|I|}k_I\,. \tag{3.53}$$

Here $\mathcal{H}_{\mathrm{s}}(H_I)\cong\bigoplus_{l=1}^N\mathcal{H}^{(I)}_{\mathrm{ac}}(H_l)$ with $\mathcal{H}^{(I)}_{\mathrm{ac}}(H_l) := \begin{cases}\mathcal{H}_{\mathrm{a.c.}}(H_l) & \text{if } l\in I\,,\\ L^2(\mathbb{R}^3) & \text{if } l\in I^c\,.\end{cases}$

(iii) For any $f \in L^2(\mathbb{R}^{3N})$

$$\Omega_{\pm}^{(N)} f = \left(\mathcal{F}_{\pm}^{(N)}\right)^{-1} \mathcal{F}^{(N)} f\,, \tag{3.54}$$

where $\mathcal{F}^{(N)}$ is the ordinary Fourier transform in $3N$ dimensions.

(iv) For any $f \in \mathcal{H}_{\mathrm{s}}(H_I) \cap \mathrm{D}(H_I)$

$$H_I f(\boldsymbol{x}) = \left(\mathcal{F}_{\pm,I}^{-1} \frac{k_I^2}{2} \mathcal{F}_{\pm,I} f\right)(\boldsymbol{x}) \tag{3.55}$$

and therefore for any $f \in \mathcal{H}_{\mathrm{s}}(H_I)$

$$\prod_{l\in I} e^{-iH_l t_l} f(\boldsymbol{x}) = \left[\mathcal{F}_{\pm,I}^{-1} \Big(\prod_{l\in I} e^{-i\frac{k_l^2}{2}t_l}\Big) \mathcal{F}_{\pm,I} f\right](\boldsymbol{x})\,. \tag{3.56}$$

3.6.3 Proof of Lemmas 5 and 6

Lemmas 5 and 6 are special cases of

Lemma 7. *Let $V_l \in (V)_4$ and let zero be neither a resonance nor an eigenvalue of H_l ($l = 1, 2, \ldots, N$). Let $\psi \in \mathcal{G}^{(N)}$. Then for all $0 < a < b < \infty$ there exist constants $T < \infty$ and $C < \infty$ such that for all subsets $I \subset \{1, 2, \ldots, N\}$ and for all $r \in I$*

$$|\psi(\boldsymbol{x};\boldsymbol{t}) - \Phi_I(\boldsymbol{x};\boldsymbol{t})| \leq C \left(\prod_{l=1}^{N} t_l\right)^{-\frac{3}{2}} (\min\{t_j \mid j \in I\})^{-\frac{1}{2}} \tag{3.57}$$

and

$$\left|\nabla_r \psi(\boldsymbol{x};\boldsymbol{t}) - i\frac{\boldsymbol{x}_r}{t_r} \Phi_I(\boldsymbol{x};\boldsymbol{t})\right| \leq C \left(\prod_{l=1}^{N} t_l\right)^{-\frac{3}{2}} (\min\{t_j \mid j \in I\})^{-\frac{1}{2}} \tag{3.58}$$

for all $\boldsymbol{x} \in \mathbb{R}^{3N}$, $\boldsymbol{t} \in \mathbb{R}^N$ with $t_j > T$ and $a < \frac{x_j}{t_j} < b$ for all $j \in \{1, 2, \ldots, N\}$. Here

$$\psi(\boldsymbol{x};\boldsymbol{t}) := \left(\prod_{l=1}^{N} e^{-iH_l t_l} \psi\right)(\boldsymbol{x})$$

and

$$\Phi_I(\boldsymbol{x};\boldsymbol{t}) := \left[\left(\prod_{j\in I} (it_j)^{-\frac{3}{2}} e^{i\frac{x_j^2}{2t_j}}\right) \mathcal{F}_{+,I}\psi\right] \left(\left(\frac{\boldsymbol{x}}{\boldsymbol{t}}\right)_I, \boldsymbol{x}_{I^c}; \boldsymbol{t}^{I^c}\right)$$

with $\left(\left(\frac{\boldsymbol{x}}{\boldsymbol{t}}\right)_I, \boldsymbol{x}_{I^c}\right)_l = \begin{cases} \frac{\boldsymbol{x}_l}{t_l} & \text{if } l \in I \\ \boldsymbol{x}_l & \text{if } l \in I^c \end{cases}$ *and* $t_l^{I^c} = \begin{cases} t_l & \text{if } l \in I^c \\ 0 & \text{if } l \in I \end{cases}.$

We first prove (3.57) and (3.58) under conditions on $\widehat{\psi}_{\text{out}}$ and then give a mapping lemma (Lemma 10) that allows us to transfer those conditions to corresponding ones on ψ.
To more concisely state the conditions on $\widehat{\psi}_{\text{out}}$, which consist of requirements regarding differentiability and decay, we introduce the following operators:
For $i \in \{1,2,\dots,5\}$ and $j \in \{1,2,\dots,N\}$ define $P_{i,j}^{(N)}$ acting on suitable functions $f : \mathbb{R}^{3N} \to \mathbb{C}$ by

$$\left(P_{i,j}^{(N)} f\right)(\boldsymbol{k}) := \begin{cases} f(\boldsymbol{k}) & \text{if } i = 1\,, \\ \frac{\partial}{\partial k_j} f(\boldsymbol{k}) & \text{if } i = 2\,, \\ \frac{\partial^2}{\partial k_j^2} f(\boldsymbol{k}) & \text{if } i = 3\,, \\ \sum\limits_{|\alpha|=1} D^{\alpha}_{\boldsymbol{k}_j} f(\boldsymbol{k}) & \text{if } i = 4\,, \\ \kappa_j \sum\limits_{|\alpha|=2} D^{\alpha}_{\boldsymbol{k}_j} f(\boldsymbol{k}) & \text{if } i = 5\,. \end{cases}$$

Here $\alpha = (\alpha_1, \alpha_2, \alpha_3) \in \mathbb{N}^3$, $\kappa_j := \frac{k_j}{\langle k_j \rangle}$ and $\langle \cdot \rangle = (1 + (\cdot)^2)^{\frac{1}{2}}$. In the case $N = 1$, where $\boldsymbol{k} = \boldsymbol{k}_1 \in \mathbb{R}^3$, we write P_i instead of $P_{i,1}^{(1)}$.
With that notation we define the set $\widehat{\mathcal{G}}^{(N)}$ of "good" $\widehat{\psi}_{\text{out}}$.

Definition 7. *Let $\boldsymbol{d} = (d_1, d_2, \dots, d_5) \in \mathbb{Z}^5$. A function $f : \mathbb{R}^{3N} \setminus \mathcal{N} \to \mathbb{C}$ is in $\widehat{\mathcal{G}}_{\boldsymbol{d}}^{(N)}$, if there is a constant $C < \infty$ such that for all $i_1, i_2, \dots, i_N \in \{1,2,\dots,5\}$*

$$\Big|\Big(\prod_{j=1}^{N} P_{i_j,j}^{(N)}\Big) f(\boldsymbol{k})\Big| \le C \prod_{j=1}^{N} \langle k_j \rangle^{-d_{i_j}}\,.$$

In particular, define

$$\widehat{\mathcal{G}}^{(N)} := \widehat{\mathcal{G}}^{(N)}_{(6,5,3,3,2)}\,.$$

Remark 7. To prove (3.13) and (3.14) we require $\widehat{\psi}_{\text{out}} \in \widehat{\mathcal{G}}^{(N)}$. In fact we could do with a slightly more general class (the decay could be a little weaker, $\widehat{\psi}_{\text{out}} \in \widehat{\mathcal{G}}^{(N)}_{(5,5,3,1,2)}$). However, $\widehat{\mathcal{G}}^{(N)}$ is the most general class of wave functions for which not only (3.13) and (3.14) can be established but which is also invariant under multiplication by $e^{-i\frac{k^2}{2}t}$. The latter means that it is invariant under the free time evolution in the sense that $\widehat{\psi}_{\text{out}} = \mathcal{F}^{(N)}(\psi_{\text{out}}) \in \widehat{\mathcal{G}}^{(N)}$ implies also $\mathcal{F}^{(N)}(e^{-iH_0 t}\psi_{\text{out}}) \in \widehat{\mathcal{G}}^{(N)}$. This corresponds to the invariance under full time evolution of $\mathcal{G}^{(N)}$ (cf. Definition 5) and will be needed in the proof of the mapping Lemma 10.

For $\widehat{\psi}_{\text{out}} \in \widehat{\mathcal{G}}^{(N)}$ we shall prove (3.13) and (3.14) using the corresponding one-particle result (derived in [18, 37]) and induction: By (3.56)

$$\begin{aligned} \psi(\boldsymbol{x};\boldsymbol{t}) &= \Big(\prod_{j\in I} e^{-iH_j t_j}\psi\Big)(\boldsymbol{x};\boldsymbol{t}^{I^c}) = \Big[\mathcal{F}_{+,I}^{-1}\Big(\prod_{j\in I} e^{-i\frac{k_j^2}{2}t_j}\Big)\mathcal{F}_{+,I}\psi\Big](\boldsymbol{x};\boldsymbol{t}^{I^c}) \\ &= \Big[\Big(\prod_{j\in I} \mathcal{F}_{+,j}^{-1} e^{-i\frac{k_j^2}{2}t_j}\Big)\mathcal{F}_{+,I}\psi\Big](\boldsymbol{x};\boldsymbol{t}^{I^c}) \end{aligned}$$

resp.

$$\nabla_r \psi(\boldsymbol{x};\boldsymbol{t}) = \Big[\nabla_r \mathcal{F}^{-1}_{+,r} e^{-i\frac{k_r^2}{2}t_r} \Big(\prod_{j\in I\setminus\{r\}} \mathcal{F}^{-1}_{+,j} e^{-i\frac{k_j^2}{2}t_j}\Big)\mathcal{F}_{+,I}\psi\Big](\boldsymbol{x};\boldsymbol{t}^{I^c}).$$

For $N=1$ this reduces to ($\mathcal{F}_+\psi = \mathcal{F}\Omega_+^{-1}\psi = \widehat{\psi}_{\mathrm{out}}$ by Proposition 4 (iii))

$$\psi(\boldsymbol{x},t) = \Big(\mathcal{F}_+^{-1} e^{-i\frac{k^2}{2}t}\mathcal{F}_+\psi\Big)(\boldsymbol{x}) = \Big(\mathcal{F}_+^{-1} e^{-i\frac{k^2}{2}t}\widehat{\psi}_{\mathrm{out}}\Big)(\boldsymbol{x})$$

resp.

$$\nabla\psi(\boldsymbol{x},t) = \Big(\nabla\mathcal{F}_+^{-1} e^{-i\frac{k^2}{2}t}\widehat{\psi}_{\mathrm{out}}\Big)(\boldsymbol{x}).$$

So the one-particle result will give us the action of each factor $\mathcal{F}^{-1}_{+,j} e^{-i\frac{k_j^2}{2}t_j}$ resp. $\nabla_r\mathcal{F}^{-1}_{+,r} e^{-i\frac{k_r^2}{2}t_r}$ on functions in $\widehat{\mathcal{G}}^{(1)}$ and our first task will be to show that $\widehat{\psi}_{\mathrm{out}} \in \widehat{\mathcal{G}}^{(N)}$ guarantees that ($I_1 \cup I_2 = I$)

$$\Big[\Big(\prod_{j\in I_2} \mathcal{F}^{-1}_{+,j} e^{-i\frac{k_j^2}{2}t_j}\Big)\mathcal{F}_{+,I}\psi\Big](\boldsymbol{x}_{I_1^c},\boldsymbol{k}_{I_1};\boldsymbol{t}^{I^c})$$

viewed as a function of $\boldsymbol{k}_j$ with $j \in I_1$ is in $\widehat{\mathcal{G}}^{(1)}$, i.e. that – when doing induction on the length of I – we stay in the regime where the one-particle result is applicable. Since, however,

$$\begin{aligned}
&\Big(\mathcal{F}_{+,I}\psi\Big)(\boldsymbol{x}_{I^c},\boldsymbol{k}_I;\boldsymbol{t}^{I^c})\\
&= \Big[\mathcal{F}_{+,I}\Big(\prod_{j\in I^c} e^{-iH_jt_j}\Big)\psi\Big](\boldsymbol{x}_{I^c},\boldsymbol{k}_I) = \Big[\mathcal{F}_{+,I}\Big(\prod_{j\in I^c}\mathcal{F}^{-1}_{+,j} e^{-i\frac{k_j^2}{2}t_j}\Big)\mathcal{F}_{+,I^c}\psi\Big](\boldsymbol{x}_{I^c},\boldsymbol{k}_I)\\
&= \Big[\Big(\prod_{j\in I^c}\mathcal{F}^{-1}_{+,j} e^{-i\frac{k_j^2}{2}t_j}\Big)\mathcal{F}_{+,I}\mathcal{F}_{+,I^c}\psi\Big](\boldsymbol{x}_{I^c},\boldsymbol{k}_I) = \Big[\Big(\prod_{j\in I^c}\mathcal{F}^{-1}_{+,j} e^{-i\frac{k_j^2}{2}t_j}\Big)\widehat{\psi}_{\mathrm{out}}\Big](\boldsymbol{x}_{I^c},\boldsymbol{k}_I)
\end{aligned}$$

and thus

$$\Big[\Big(\prod_{j\in I_2}\mathcal{F}^{-1}_{+,j} e^{-i\frac{k_j^2}{2}t_j}\Big)\mathcal{F}_{+,I}\psi\Big](\boldsymbol{x}_{I_1^c},\boldsymbol{k}_{I_1};\boldsymbol{t}^{I^c}) = \Big[\Big(\prod_{j\in I_1^c}\mathcal{F}^{-1}_{+,j} e^{-i\frac{k_j^2}{2}t_j}\Big)\widehat{\psi}_{\mathrm{out}}\Big](\boldsymbol{x}_{I_1^c},\boldsymbol{k}_{I_1}),$$

this can again be done using the one-particle result and induction (this time on the length of I_1^c).

The one-particle result is collected in the following

Lemma 8. *Let $V \in (V)_4$ and let zero be neither a resonance nor an eigenvalue of H. Let $\chi \in \widehat{\mathcal{G}}^{(1)}_{(5,5,3,1,2)}$. Then for all $0 < a < \infty$ there exists some $T < \infty$ such that*

$$\Big(\mathcal{F}_+^{-1} e^{-i\frac{k^2}{2}t}\chi\Big)(\boldsymbol{x}) = \Big[\Big(t^{-\frac{3}{2}}P_{\leftrightarrow}(t) + t^{-2}P_f(t)\Big)\chi\Big](\boldsymbol{x}) \tag{3.59}$$

and

$$\left(\nabla\mathcal{F}_+^{-1}e^{-i\frac{k^2}{2}t}\chi\right)(\boldsymbol{x}) = \left[\left(t^{-\frac{3}{2}}i\frac{\boldsymbol{x}}{t}P_{\leftrightarrow}(t) + t^{-2}P_{\widetilde{f}}(t)\right)\chi\right](\boldsymbol{x}) \tag{3.60}$$

for all $t \geq T$, $a < \frac{x}{t}$. *Here*

$$[P_{\leftrightarrow}(t)\chi](\boldsymbol{x}) := i^{-\frac{3}{2}}e^{i\frac{x^2}{2t}}\chi\left(\frac{\boldsymbol{x}}{t}\right)$$

and

$$[P_F(t)\chi](\boldsymbol{x}) := \sum_{j=1}^{5}\int_{\mathbb{R}^3} F_j(\boldsymbol{k},\boldsymbol{x},t)P_i\chi(\boldsymbol{k})\frac{d^3k}{k^2}$$

for any quintuple of (possibly vector-valued) functions $F = (F_1,\dots,F_5) : \mathbb{R}^{6N+1} \to (\mathbb{C}^{(3)},\dots,\mathbb{C}^{(3)})$. *Further,* $f := g + [\frac{x}{t}(1+\frac{x}{t})]^{-1}h = (g_1,\dots,g_5) + [\frac{x}{t}(1+\frac{x}{t})]^{-1}(h_1,h_2,0,0,0)$ *and* $\widetilde{f} := i\boldsymbol{k}g + [\frac{x}{t}(1+\frac{x}{t})]^{-1}\widetilde{h} = i\boldsymbol{k}(g_1,\dots,g_5) + [\frac{x}{t}(1+\frac{x}{t})]^{-1}(\widetilde{h}_1,\widetilde{h}_2,0,0,0)$ *are independent of* χ *and satisfy*

$$\begin{aligned} &\sup_{t\in\mathbb{R},\boldsymbol{x}\in\mathbb{R}^3}|g_j(\boldsymbol{k},\boldsymbol{x},t)| \leq C\langle k\rangle^{-\widetilde{d}_j} && (j=1,\dots,5)\\ &\sup_{t\geq T,\boldsymbol{x}\in\mathbb{R}^3}|h_j(\boldsymbol{k},\boldsymbol{x},t)| \leq C\langle k\rangle^2, \quad \sup_{t\geq T,x\geq aT}|\widetilde{h}_j(\boldsymbol{k},\boldsymbol{x},t)| \leq C\langle k\rangle^3, && (j=1,2)\end{aligned} \tag{3.61}$$

for some $C < \infty$ *and* $\widetilde{\boldsymbol{d}} = (-2,1,0,2,1)$. *Moreover,* g *does not depend on the potential* V.

For the proof of Lemma 8 see Lemma 4 (resp. equations (17) and (18)) in [18] and equations (15) and (16) in [37]: The proofs in [18, 37] use the splitting[18]

$$\begin{aligned}\psi(\boldsymbol{x},t) &= \left(\mathcal{F}_+^{-1}e^{-i\frac{k^2}{2}t}\widehat{\psi}_{\text{out}}\right)(\boldsymbol{x}) = (2\pi)^{-\frac{3}{2}}\int e^{-i\frac{k^2}{2}t}\varphi_+(\boldsymbol{x},\boldsymbol{k})\widehat{\psi}_{\text{out}}(\boldsymbol{k})d^3k\\ &= (2\pi)^{-\frac{3}{2}}\int e^{-i\frac{k^2}{2}t}e^{i\boldsymbol{k}\cdot\boldsymbol{x}}\widehat{\psi}_{\text{out}}(\boldsymbol{k})d^3k + (2\pi)^{-\frac{3}{2}}\int e^{-i\frac{k^2}{2}t}\eta_+(\boldsymbol{x},\boldsymbol{k})\widehat{\psi}_{\text{out}}(\boldsymbol{k})d^3k\\ &=: \alpha(\boldsymbol{x},t) + \beta(\boldsymbol{x},t)\end{aligned}$$

with $\eta_+(\boldsymbol{x},\boldsymbol{k}) := \varphi_+(\boldsymbol{x},\boldsymbol{k}) - e^{i\boldsymbol{k}\cdot\boldsymbol{x}}$. Then α resp. $\nabla\alpha$ corresponds to the free time evolution and gives the leading order term $t^{-\frac{3}{2}}P_{\leftrightarrow}(t)\widehat{\psi}_{\text{out}}$ resp. $t^{-\frac{3}{2}}i\frac{\boldsymbol{x}}{t}P_{\leftrightarrow}(t)\widehat{\psi}_{\text{out}}$ and the error term $t^{-2}P_g(t)\widehat{\psi}_{\text{out}}$ resp. $t^{-2}P_{i\boldsymbol{k}g}(t)\widehat{\psi}_{\text{out}}$ ([18], Lemma 4) while β resp. $\nabla\beta$ gives the error term $t^{-2}P_h(t)\widehat{\psi}_{\text{out}}$ resp. $t^{-2}P_{\widetilde{h}}(t)\widehat{\psi}_{\text{out}}$ ([37], equation (15) resp. (16)). Both parts of the proof rely on stationary phase methods, where one uses partial integration with respect to $\boldsymbol{k}$ at most twice. This is why one needs bounds on $\widehat{\psi}_{\text{out}}$ up to its second order derivatives, i.e. $\widehat{\psi}_{\text{out}} \in \mathcal{G}^{(1)}$. However, in [18, 37] the explicit form of $P_f(t)\widehat{\psi}_{\text{out}} = (P_g(t) + P_h(t))\widehat{\psi}_{\text{out}}$

[18] Cf. Proposition 4 (i): Since the $\varphi_+(\boldsymbol{x},\boldsymbol{k})$ are bounded by Proposition 5 (ii) and $\widehat{\psi}_{\text{out}} \in \widehat{\mathcal{G}}^{(1)} \subset L^1(\mathbb{R}^3)$ one can omit the l. i. m..

resp. $P_{\widetilde{f}}(t)\widehat{\psi}_{\text{out}} = (P_{i\boldsymbol{k}g}(t) + P_{\widetilde{h}}(t))\widehat{\psi}_{\text{out}}$ was not needed and thus not stated, so one has to go through the corresponding proofs to verify that the error terms are indeed of the form given in Lemma 8. Note also that the results in [18, 37] were formulated in the regime $t \geq T_0$, $x \geq R_0$ for some appropriate $T_0 < \infty$, $R_0 < \infty$. Since for T big enough $t \geq T$ and $a < \frac{x}{t}$ imply $x > at \geq aT \geq R_0$, this of course includes our regime.

We return to general N and extend Lemma 8 to

Lemma 9. *Let $V_l \in (V)_4$ and let zero be neither a resonance nor an eigenvalue of H_l $(l = 1, 2, \dots, N)$. Let $\chi \in \mathcal{G}^{(N)}_{(5,5,3,1,2)}$. Then for all $0 < a < \infty$ there exist $T < \infty$, $C < \infty$ such that for all subsets $I \subset \{1, 2, \dots, N\}$ and all $r \in I$*

$$\Big[\mathcal{F}^{-1}_{+,I}\Big(\prod_{j\in I} e^{-i\frac{k_j^2}{2}t_j}\Big)\chi\Big](\boldsymbol{x}_I, \boldsymbol{k}_{I^c}) = \Big[\prod_{j\in I}\Big(t_j^{-\frac{3}{2}}P^{(N)}_{\leftrightarrow,j}(t_j) + t_j^{-2}P^{(N)}_{f^{(j)},j}(t_j)\Big)\chi\Big](\boldsymbol{x}_I, \boldsymbol{k}_{I^c}) \tag{3.62}$$

and

$$\begin{aligned}&\Big[\nabla_r\mathcal{F}^{-1}_{+,I}\Big(\prod_{j\in I} e^{-i\frac{k_j^2}{2}t_j}\Big)\chi\Big](\boldsymbol{x}_I, \boldsymbol{k}_{I^c})\\ &= \Big[\Big(t_r^{-\frac{3}{2}} i\frac{\boldsymbol{x}_r}{t_r}P^{(N)}_{\leftrightarrow,r}(t_r) + t_r^{-2}P^{(N)}_{\widetilde{f}^{(r)},r}(t_r)\Big)\prod_{j\in I\setminus\{r\}}\Big(t_j^{-\frac{3}{2}}P^{(N)}_{\leftrightarrow,j}(t_j) + t_j^{-2}P^{(N)}_{f^{(j)},j}(t_j)\Big)\chi\Big](\boldsymbol{x}_I, \boldsymbol{k}_{I^c})\end{aligned} \tag{3.63}$$

for all $\boldsymbol{x} \in \mathbb{R}^{3N}$, $\boldsymbol{t} \in \mathbb{R}^N$ with $t_j \geq T$ and $a < \frac{x_j}{t_j}$ for $j \in I$. Here

$$\Big[P^{(N)}_{\leftrightarrow,j}(t_j)\varphi\Big](\boldsymbol{x}_{\{j\}}, \boldsymbol{y}_{\{j\}^c}) := i^{-\frac{3}{2}} e^{i\frac{x_j^2}{2t_j}}\varphi\Big(\Big(\frac{\boldsymbol{x}}{\boldsymbol{t}}\Big)_{\{j\}}, \boldsymbol{y}_{\{j\}^c}\Big),$$

$$\Big[P^{(N)}_{F,j}(t_j)\varphi\Big](\boldsymbol{x}_{\{j\}}, \boldsymbol{y}_{\{j\}^c}) := \sum_{i=1}^{5}\int_{\mathbb{R}^3} F_i(\boldsymbol{k}_j, \boldsymbol{x}_j, t_j)P^{(N)}_{i,j}\varphi(\boldsymbol{k}_{\{j\}}, \boldsymbol{y}_{\{j\}^c})\frac{d^3k_j}{k_j^2}$$

and, for $j \in I$, $f^{(j)} = g + [\frac{x_j}{t_j}(1 + \frac{x_j}{t_j})]^{-1}h^{(j)}$, $\widetilde{f}^{(j)} = i\boldsymbol{k}_j g + [\frac{x_j}{t_j}(1 + \frac{x_j}{t_j})]^{-1}\widetilde{h}^{(j)}$ with g as in Lemma 8 and $h^{(j)} = (h^{(j)}_1, h^{(j)}_2, 0, 0, 0)$, $\widetilde{h}^{(j)} = (\widetilde{h}^{(j)}_1, \widetilde{h}^{(j)}_2, 0, 0, 0)$ independent of χ and such that (3.61) holds.
Further, for $\boldsymbol{d} = (5, 5, 3, 1, 2)$ and all $I_1 \cup I_2 = I$, $r \in I_2$ and $i_j \in \{1, 2, \dots, 5\}$ $(j \in I^c)$

$$\begin{aligned}\Big|\Big[\Big(\prod_{j\in I^c} P^{(N)}_{i_j,j}\Big)\Big(\prod_{l\in I_1} t_l^{-\frac{3}{2}}P^{(N)}_{\leftrightarrow,l}(t_l)\Big)\Big(\prod_{m\in I_2} t_m^{-2}P^{(N)}_{f^{(m)},m}(t_m)\Big)\chi\Big](\boldsymbol{x}_I, \boldsymbol{k}_{I^c})\Big|&\\ \leq C\Big(\prod_{l\in I_1} t_l^{-\frac{3}{2}}\Big)\Big(\prod_{m\in I_2} t_m^{-2}\Big)\Big(\prod_{j\in I^c}\langle k_j\rangle^{-d_{i_j}}\Big)&\end{aligned} \tag{3.64}$$

and

$$\begin{aligned}\Big|\Big[\Big(\prod_{j\in I^c} P^{(N)}_{i_j,j}\Big)\Big(\prod_{l\in I_1} t_l^{-\frac{3}{2}}P^{(N)}_{\leftrightarrow,l}(t_l)\Big)\Big(t_r^{-2}P^{(N)}_{\widetilde{f}^{(r)},r}(t_r)\Big)\Big(\prod_{m\in I_2\setminus\{r\}} t_m^{-2}P^{(N)}_{f^{(m)},m}(t_m)\Big)\chi\Big](\boldsymbol{x}_I, \boldsymbol{k}_{I^c})\Big|&\\ \leq C\Big(\prod_{l\in I_1} t_l^{-\frac{3}{2}}\Big)\Big(\prod_{m\in I_2} t_m^{-2}\Big)\Big(\prod_{j\in I^c}\langle k_j\rangle^{-d_{i_j}}\Big)&\end{aligned} \tag{3.65}$$

for all $\boldsymbol{x} \in \mathbb{R}^{3N}$, $\boldsymbol{t} \in \mathbb{R}^N$ with $t_j \geq T$ and $a < \frac{x_j}{t_j}$ for $j \in I$.

Proof of Lemma 9. We first prove (3.64) and (3.65). By the definition of $P^{(N)}_{\leftrightarrow,j}$ and $P^{(N)}_{f^{(j)},j}$ we have

$$\begin{aligned}
&\Big|\Big[\Big(\prod_{j\in I^c} P^{(N)}_{i_j,j}\Big)\Big(\prod_{l\in I_1} t_l^{-\frac{3}{2}} P^{(N)}_{\leftrightarrow,l}(t_l)\Big)\Big(\prod_{m\in I_2} t_m^{-2} P^{(N)}_{f^{(m)},m}(t_m)\Big)\chi\Big](\boldsymbol{x}_I,\boldsymbol{k}_{I^c})\Big| \\
&\quad\le \sum_{\substack{i_m=1\\(m\in I_2)}}^{5}\ \int_{\mathbb{R}^{3|I_2|}} \frac{d^{3|I_2|}k_{I_2}}{k_{I_2}^2}\Bigg[\Big(\prod_{m\in I_2} t_m^{-2}|f^{(m)}_{i_m}(\boldsymbol{x}_m,\boldsymbol{k}_m,t_m)|\Big) \\
&\qquad\qquad \Big(\prod_{l\in I_1} t_l^{-\frac{3}{2}}\Big)\Big|\Big(\prod_{j\in I^c} P^{(N)}_{i_j,j}\Big)\Big(\prod_{m\in I_2} P^{(N)}_{i_m,m}\Big)\chi\Big(\big(\frac{\boldsymbol{x}}{\boldsymbol{t}}\big)_{I_1},\boldsymbol{k}_{I_2\cup I^c}\Big)\Big|\Bigg] \qquad (3.66)\\
&\quad= \Big(\prod_{l\in I_1} t_l^{-\frac{3}{2}}\Big)\Big(\prod_{m\in I_2} t_m^{-2}\Big) \\
&\qquad \sum_{\substack{i_m=1\\(m\in I_2)}}^{5}\ \int_{\mathbb{R}^{3|I_2|}} \frac{d^{3|I_2|}k_{I_2}}{k_{I_2}^2}\Big(\prod_{m\in I_2}|f^{(m)}_{i_m}(\boldsymbol{x}_m,\boldsymbol{k}_m,t_m)|\Big)\Big|\Big(\prod_{j\in I_1^c} P^{(N)}_{i_j,j}\Big)\chi\Big(\big(\frac{\boldsymbol{x}}{\boldsymbol{t}}\big)_{I_1},\boldsymbol{k}_{I_1^c}\Big)\Big|
\end{aligned}$$

where $k_{I_2}^2 := \prod_{m\in I_2} k_m^2$ and exchange of differentiation and integration (i.e. that we put all the differential operators $P^{(N)}_{i,j}$ inside the innermost integral) will be justified below. Remember that the $f^{(m)}$ fulfill (3.61) (with $\widetilde{\boldsymbol{d}} = (-2,1,0,2,1),$) resp. that $\chi \in \mathcal{G}^{(N)}_{\boldsymbol{d}}$ with $\boldsymbol{d} = (5,5,3,1,2)$. Then we have

$$\begin{aligned}
&\Big(\prod_{m\in I_2}|f^{(m)}_{i_m}(\boldsymbol{x}_m,\boldsymbol{k}_m,t_m)|\Big) \\
&\quad\le C\prod_{m\in I_2}\Big[\langle k_m\rangle^{-\widetilde{d}_{i_m}} + \frac{\langle k_m\rangle^2(\delta_{i_m1}+\delta_{i_m2})}{\frac{x_m}{t_m}(1+\frac{x_m}{t_m})}\Big] \le C\prod_{m\in I_2}\Big[\langle k_m\rangle^{-\widetilde{d}_{i_m}} + \frac{\langle k_m\rangle^2(\delta_{i_m1}+\delta_{i_m2})}{a(1+a)}\Big]
\end{aligned}$$

resp. (cf. Definition 7)

$$\Big|\Big(\prod_{j\in I_1^c} P^{(N)}_{i_j,j}\Big)\chi\Big(\big(\frac{\boldsymbol{x}}{\boldsymbol{t}}\big)_{I_1},\boldsymbol{k}_{I_1^c}\Big)\Big| \le C\Big(\prod_{j\in I_1^c}\langle k_j\rangle^{-d_{i_j}}\Big)$$

and thus

$$\begin{aligned}
&\Big(\prod_{m\in I_2}|f^{(m)}_{i_m}(\boldsymbol{x}_m,\boldsymbol{k}_m,t_m)|\Big)\Big|\Big(\prod_{j\in I_1^c} P^{(N)}_{i_j,j}\Big)\chi\Big(\big(\frac{\boldsymbol{x}}{\boldsymbol{t}}\big)_{I_1},\boldsymbol{k}_{I_1^c}\Big)\Big| \\
&\qquad\le C\prod_{m\in I_2}\Big[\langle k_m\rangle^{-\widetilde{d}_{i_m}} + \frac{\langle k_m\rangle^2(\delta_{i_m1}+\delta_{i_m2})}{a(1+a)}\Big]\Big(\prod_{j\in I_1^c}\langle k_j\rangle^{-d_{i_j}}\Big) \qquad (3.67)\\
&\qquad\le C\Big(\prod_{m\in I_2}\langle k_m\rangle^{-3}\Big)\Big(\prod_{j\in I^c}\langle k_j\rangle^{-d_{i_j}}\Big)
\end{aligned}$$

for some constant $C<\infty$ (depending on a and T). In particular, (3.67) is integrable with respect to $\frac{d^{3|I_2|}k_{I_2}}{k_{I_2}^2}$. Thus exchange of differentiation and integration in (3.66) is justified and putting (3.67) into it gives (3.64). The proof of (3.65) is completely analogous, we just need to replace $t_r^{-2}P^{(N)}_{f^{(r)},r}$ by $t_r^{-2}P^{(N)}_{\widetilde{f}^{(r)},r}$ for some $r \in I_2$. Then the bound in (3.67) will be proportional to $\langle k_r\rangle^{-2}\Big(\prod_{m\in I_2\setminus\{r\}}\langle k_m\rangle^{-3}\Big)$ instead of $\Big(\prod_{m\in I_2}\langle k_m\rangle^{-3}\Big)$, which, however, still suffices to get integrability with respect to $\frac{d^{3|I_2|}k_{I_2}}{k_{I_2}^2}$ and thus (3.65).

With (3.64) established, the proof of (3.62) and (3.63) is a straightforward induction on the length of the subsets I. First, let $I = \{j\}$. Since $\chi \in \mathcal{G}^{(N)}_{(5,5,3,1,2)}$ implies $\chi(\cdot_{\{j\}}, \boldsymbol{k}_{\{j\}^c}) \in \mathcal{G}^{(1)}_{(5,5,3,1,2)}$ for all $\boldsymbol{k}_{\{j\}^c} \in \mathbb{R}^{3(N-1)}$, (3.62) and (3.63) follow immediately from Lemma 8. Now let $I \subset \{1,2,\dots N\}$ with $1 \le |I| \le N-1$. Then by the induction hypothesis

$$\begin{aligned}
&\Big[\mathcal{F}^{-1}_{+,I\cup\{r\}}\Big(\prod_{j\in I\cup\{r\}} e^{-i\frac{k_j^2}{2}t_j}\Big)\chi\Big](\boldsymbol{x}_{I\cup\{r\}}, \boldsymbol{k}_{I^c\setminus\{r\}}) \\
&\quad= \Big[\Big(\mathcal{F}^{-1}_{+,r}e^{-i\frac{k_r^2}{2}t_r}\Big)\mathcal{F}^{-1}_{+,I}\Big(\prod_{j\in I} e^{-i\frac{k_j^2}{2}t_j}\Big)\chi\Big](\boldsymbol{x}_{I\cup\{r\}}, \boldsymbol{k}_{I^c\setminus\{r\}}) \\
&\quad= \Big[\Big(\mathcal{F}^{-1}_{+,r}e^{-i\frac{k_r^2}{2}t_r}\Big)\prod_{j\in I}\Big(t_j^{-\frac{3}{2}}P^{(N)}_{\leftrightarrow,j}(t_j) + t_j^{-2}P^{(N)}_{f^{(j)},j}(t_j)\Big)\chi\Big](\boldsymbol{x}_{I\cup\{r\}}, \boldsymbol{k}_{I^c\setminus\{r\}})
\end{aligned} \tag{3.68}$$

and

$$\begin{aligned}
&\Big[\nabla_r\mathcal{F}^{-1}_{+,I\cup\{r\}}\Big(\prod_{j\in I\cup\{r\}} e^{-i\frac{k_j^2}{2}t_j}\Big)\chi\Big](\boldsymbol{x}_{I\cup\{r\}}, \boldsymbol{k}_{I^c\setminus\{r\}}) \\
&\quad= \Big[\nabla_r\Big(\mathcal{F}^{-1}_{+,r}e^{-i\frac{k_r^2}{2}t_r}\Big)\prod_{j\in I}\Big(t_j^{-\frac{3}{2}}P^{(N)}_{\leftrightarrow,j}(t_j) + t_j^{-2}P^{(N)}_{f^{(j)},j}(t_j)\Big)\chi\Big](\boldsymbol{x}_{I\cup\{r\}}, \boldsymbol{k}_{I^c\setminus\{r\}})
\end{aligned} \tag{3.69}$$

for any $r \in I^c$. Since

$$\begin{aligned}
&\Big[\prod_{j\in I}\Big(t_j^{-\frac{3}{2}}P^{(N)}_{\leftrightarrow,j}(t_j) + t_j^{-2}P^{(N)}_{f^{(j)},j}(t_j)\Big)\chi\Big](\boldsymbol{x}_I, \boldsymbol{k}_{I^c}) \\
&\qquad= \sum_{I_1\cup I_2 = I}\Big[\Big(\prod_{j\in I_1}\Big(t_j^{-\frac{3}{2}}P^{(N)}_{\leftrightarrow,j}(t_j)\Big)\Big(\prod_{l\in I_2} t_l^{-2}P^{(N)}_{f^{(l)},l}(t_l)\Big)\chi\Big](\boldsymbol{x}_I, \boldsymbol{k}_{I^c}),
\end{aligned}$$

(3.64) in particular implies

$$\Big[\prod_{j\in I}\Big(t_j^{-\frac{3}{2}}P^{(N)}_{\leftrightarrow,j}(t_j) + t_j^{-2}P^{(N)}_{f^{(j)},j}(t_j)\Big)\chi\Big](\boldsymbol{x}_I, \boldsymbol{k}_{I^c\setminus\{r\}}, \cdot_{\{r\}}) \in \widehat{\mathcal{G}}^{(1)}_{(5,5,3,1,2)}$$

for all $\boldsymbol{k}_{I^c\setminus\{r\}} \in \mathbb{R}^{3(|I^c|-1)}$ and all $\boldsymbol{x} \in \mathbb{R}^{3N}$, $\boldsymbol{t} \in \mathbb{R}^N$ with $t_j \ge T$ and $a < \frac{x_j}{t_j}$ for $j \in I$. Thus (3.68), (3.69) and Lemma 8 already give (3.62) and (3.63). □

With Lemma 9 we can now prove (3.57) and (3.58) for $\widehat{\psi}_{\text{out}} \in \widehat{\mathcal{G}}^{(N)}_{(5,5,3,1,2)}$. Let $0 < a < b < \infty$ and $T < \infty$, $C < \infty$ as in Lemma 9. Further let $I \subset \{1,2,\dots,N\}$ and $\boldsymbol{x} \in \mathbb{R}^{3N}$,

$\boldsymbol{t} \in \mathbb{R}^N$ such that $t_j \geq T$ and $a < \frac{x_j}{t_j} < b$ for all $j \in \{1, 2, \dots, N\}$. First, note that

$$\begin{aligned}
&\Big(\mathcal{F}_{+,I}\psi\Big)\big(\boldsymbol{x}_{I^c}, \boldsymbol{k}_I; \boldsymbol{t}^{I^c}\big) \\
&= \Big[\mathcal{F}_{+,I}\Big(\prod_{j\in I^c} e^{-iH_j t_j}\Big)\psi\Big]\big(\boldsymbol{x}_{I^c}, \boldsymbol{k}_I\big) \overset{(3.56)}{=} \Big[\mathcal{F}_{+,I}\mathcal{F}_{+,I^c}^{-1}\Big(\prod_{j\in I^c} e^{-i\frac{k_j^2}{2}t_j}\Big)\mathcal{F}_{+,I^c}\psi\Big]\big(\boldsymbol{x}_{I^c}, \boldsymbol{k}_I\big) \\
&= \Big[\mathcal{F}_{+,I^c}^{-1}\Big(\prod_{j\in I^c} e^{-i\frac{k_j^2}{2}t_j}\Big)\mathcal{F}_{+,I}\mathcal{F}_{+,I^c}\psi\Big]\big(\boldsymbol{x}_{I^c}, \boldsymbol{k}_I\big) \\
&= \Big[\mathcal{F}_{+,I^c}^{-1}\Big(\prod_{j\in I^c} e^{-i\frac{k_j^2}{2}t_j}\Big)\mathcal{F}_{+}^{(N)}\psi\Big]\big(\boldsymbol{x}_{I^c}, \boldsymbol{k}_I\big) \\
&\overset{(3.54)}{=} \Big[\mathcal{F}_{+,I^c}^{-1}\Big(\prod_{j\in I^c} e^{-i\frac{k_j^2}{2}t_j}\Big)\widehat{\psi}_{\mathrm{out}}\Big]\big(\boldsymbol{x}_{I^c}, \boldsymbol{k}_I\big) \\
&\overset{(3.62)}{=} \Big[\prod_{j\in I^c}\Big(t_j^{-\frac{3}{2}}P_{\leftrightarrow,j}^{(N)}(t_j) + t_j^{-2}P_{f^{(j)},j}^{(N)}(t_j)\Big)\widehat{\psi}_{\mathrm{out}}\Big]\big(\boldsymbol{x}_{I^c}, \boldsymbol{k}_I\big) \\
&= \sum_{I_1\cup I_2 = I^c}\Big[\Big(\prod_{j\in I_1} t_j^{-\frac{3}{2}}P_{\leftrightarrow,j}^{(N)}(t_j)\Big)\Big(\prod_{l\in I_2} t_l^{-2}P_{f^{(l)},l}^{(N)}(t_l)\Big)\widehat{\psi}_{\mathrm{out}}\Big]\big(\boldsymbol{x}_{I^c}, \boldsymbol{k}_I\big)\,,
\end{aligned} \tag{3.70}$$

so in particular we have by (3.64)

$$\Big(\mathcal{F}_{+,I}\psi\Big)\big(\boldsymbol{x}_{I^c}, \boldsymbol{k}_I; \boldsymbol{t}^{I^c}\big) \in \widehat{\mathcal{G}}_{(5,5,3,1,2)}^{(|I|)}\,.$$

Thus by (3.56) and (3.62) resp. (3.63)

$$\begin{aligned}
\psi(\boldsymbol{x}; \boldsymbol{t}) &= \Big[\mathcal{F}_{+,I}^{-1}\Big(\prod_{j\in I} e^{-i\frac{k_j^2}{2}t_j}\Big)\mathcal{F}_{+,I}\psi\Big]\big(\boldsymbol{x}; \boldsymbol{t}^{I^c}\big) \\
&= \Big[\prod_{j\in I}\Big(t_j^{-\frac{3}{2}}P_{\leftrightarrow,j}^{(N)}(t_j) + t_j^{-2}P_{f^{(j)},j}^{(N)}(t_j)\Big)\mathcal{F}_{+,I}\psi\Big]\big(\boldsymbol{x}; \boldsymbol{t}^{I^c}\big)
\end{aligned} \tag{3.71}$$

resp.

$$\begin{aligned}
&\nabla_r\psi(\boldsymbol{x}; \boldsymbol{t}) \\
&\quad = \Big[\Big(t_r^{-\frac{3}{2}} i\frac{\boldsymbol{x}_r}{t_r}P_{\leftrightarrow,j}^{(N)}(t_r) + t_r^{-2}P_{\widetilde{f}^{(r)},r}^{(N)}(t_r)\Big) \\
&\qquad\qquad \prod_{j\in I\setminus\{r\}}\Big(t_j^{-\frac{3}{2}}P_{\leftrightarrow,j}^{(N)}(t_j) + t_j^{-2}P_{f^{(j)},j}^{(N)}(t_j)\Big)\mathcal{F}_{+,I}\psi\Big]\big(\boldsymbol{x}; \boldsymbol{t}^{I^c}\big).
\end{aligned} \tag{3.72}$$

Since

$$\Phi_I(\boldsymbol{x}; \boldsymbol{t}) = \Big[\prod_{j\in I}\Big((it_j)^{-\frac{3}{2}} e^{i\frac{x_j^2}{2t_j}}\Big)\mathcal{F}_{+,I}\psi\Big]\Big(\big(\frac{\boldsymbol{x}}{\boldsymbol{t}}\big)_I, \boldsymbol{x}_{I^c}; \boldsymbol{t}^{I^c}\Big) = \Big[\prod_{j\in I}\Big(t_j^{-\frac{3}{2}}P_{\leftrightarrow,j}^{(N)}(t_j)\Big)\mathcal{F}_{+,I}\psi\Big]\big(\boldsymbol{x}; \boldsymbol{t}^{I^c}\big)$$

extracting the leading order term in (3.71) gives

$$
\begin{aligned}
&|\psi(\boldsymbol{x};\boldsymbol{t}) - \Phi_I(\boldsymbol{x};\boldsymbol{t})| \\
&\quad \leq \sum_{\substack{I_1 \cup I_2 = I \\ I_2 \neq \emptyset}} \Big| \Big[\Big(\prod_{j\in I_1} \Big(t_j^{-\frac{3}{2}} P^{(N)}_{\leftrightarrow,j}(t_j)\Big)\Big(\prod_{l\in I_2} t_l^{-2} P^{(N)}_{f^{(l)},l}(t_l)\Big) \mathcal{F}_{+,I}\psi \Big] (\boldsymbol{x}; \boldsymbol{t}^{I^c}) \Big| \\
&\quad \overset{(3.70)}{\leq} \sum_{\substack{I_1 \cup I_2 = I \\ I_2 \neq \emptyset \\ I_3\cup I_4 = I^c}} \Big| \Big[\Big(\prod_{j\in I_1\cup I_3} \Big(t_j^{-\frac{3}{2}} P^{(N)}_{\leftrightarrow,j}(t_j)\Big)\Big(\prod_{l\in I_2\cup I_4} t_l^{-2} P^{(N)}_{f^{(l)},l}(t_l)\Big) \widehat{\psi}_{\text{out}} \Big] (\boldsymbol{x}; \boldsymbol{t}^{I^c}) \Big| \\
&\quad \overset{(3.64)}{\leq} C \sum_{\substack{I_1 \cup I_2 = I \\ I_2 \neq \emptyset \\ I_3\cup I_4 = I^c}} \Big(\prod_{j\in I_1\cup I_3} t_j^{-\frac{3}{2}}\Big)\Big(\prod_{l\in I_2\cup I_4} t_l^{-2}\Big) \leq C \Big(\prod_{j=1}^{N} t_j^{-\frac{3}{2}}\Big) \Big(\min\{t_j | j\in I\}\Big)^{-\frac{1}{2}},
\end{aligned}
$$

i.e. (3.57). In the same way extracting the leading order term in (3.71) gives (3.58):

$$
\begin{aligned}
&|\nabla_r \psi(\boldsymbol{x};\boldsymbol{t}) - i\frac{\boldsymbol{x}_r}{t_r}\Phi_I(\boldsymbol{x};\boldsymbol{t})| \\
&\quad \overset{(3.70)}{\leq} \frac{x_r}{t_r} \sum_{\substack{I_1 \cup I_2 = I \\ r\notin I_2 \neq \emptyset \\ I_3\cup I_4 = I^c}} \Big| \Big[\Big(\prod_{j\in I_1\cup I_3} \Big(t_j^{-\frac{3}{2}} P^{(N)}_{\leftrightarrow,j}(t_j)\Big)\Big(\prod_{l\in I_2\cup I_4} t_l^{-2} P^{(N)}_{f^{(l)},l}(t_l)\Big) \widehat{\psi}_{\text{out}} \Big] (\boldsymbol{x}; \boldsymbol{t}^{I^c}) \Big| \\
&\quad\quad + \sum_{\substack{I_1 \cup I_2 = I\setminus\{r\} \\ I_3\cup I_4 = I^c}} \Big| \Big[\Big(\prod_{j\in I_1\cup I_3} \Big(t_j^{-\frac{3}{2}} P^{(N)}_{\leftrightarrow,j}(t_j)\Big)\Big(\prod_{l\in I_2\cup I_4} t_l^{-2} P^{(N)}_{f^{(l)},l}(t_l)\Big) t_r^{-2} P^{(N)}_{\widehat{f}^{(r)},r}(t_r) \widehat{\psi}_{\text{out}} \Big] (\boldsymbol{x}; \boldsymbol{t}^{I^c}) \Big| \\
&\quad \overset{(3.64),(3.65)}{\leq} C \Big(\prod_{j=1}^{N} t_j^{-\frac{3}{2}}\Big) \Big[b\Big(\min\{t_j | j\in I\setminus\{r\}\}\Big)^{-\frac{1}{2}} + t_r^{-\frac{1}{2}} \Big] \\
&\quad \leq C \Big(\prod_{j=1}^{N} t_j^{-\frac{3}{2}}\Big) \Big(\min\{t_j | j\in I\}\Big)^{-\frac{1}{2}}.
\end{aligned}
$$

Thus, to finish the proof of Lemma 7 it suffices to show that $\widehat{\psi}_{\text{out}} \in \widehat{\mathcal{G}}^{(N)} \subset \widehat{\mathcal{G}}^{(N)}_{(5,5,3,1,2)}$ if $\psi \in \mathcal{G}^{(N)}$. That is the content of the following mapping

Lemma 10. *Let $V_l \in (V)_4$ and let zero be neither a resonance nor an eigenvalue of H_l $(l = 1, \ldots, N)$. Then*

$$\psi \in \mathcal{G}^{(N)} \Rightarrow \widehat{\psi}_{out} \in \widehat{\mathcal{G}}^{(N)}.$$

Remark 8. $\psi \in \mathcal{G}^{(N)}$ contains the requirement $\psi \in C^\infty(H)$. This is necessary to get almost sure global existence of Bohmian mechanics and the main Theorems 3 and 5. For the mapping Lemma 10 $\psi \in C^{3N}(H) := \bigcap_{n=1}^{3N} \mathrm{D}(H^n)$ would be sufficient.

Proof of Lemma 10. The proof is adapted from that of Lemma 1 in [17] (an analogous mapping lemma for $N = 1$).

Let $\psi \in \mathcal{G}^{(N)}$. Then there is a $\chi \in \mathcal{G}_0^{(N)}$ and a $t \in \mathbb{R}$ such that

$$\psi = e^{-iHt}\chi\,.$$

Using (3.54) and (3.56) (or alternatively the intertwining property $\Omega_+^{-1}H = H_0\Omega_+^{-1}$) we get

$$\widehat{\psi}_{\rm out} = \mathcal{F}_+^{(N)}\psi = \mathcal{F}_+^{(N)}e^{-iHt}\left(\mathcal{F}_+^{(N)}\right)^{-1}\mathcal{F}_+^{(N)}\chi = e^{-i\frac{k^2}{2}t}\widehat{\chi}_{\rm out}\,.$$

Since $\widehat{\mathcal{G}}^{(N)}$ is invariant under multiplication by $e^{-i\frac{k^2}{2}t}$ (this is easy to check), it suffices to show that $\widehat{\chi}_{\rm out}$ is in $\widehat{\mathcal{G}}_0^{(N)}$.

Since

$$\begin{aligned}&\langle x\rangle^{\frac{3N+1}{2}+\beta}H^n\chi \in L^2(\mathbb{R}^{3N}), \quad \beta\in\{N+1,\dots,2N\},\ n\in\{0,1,\dots,4N-\beta\}\,,\\ &\langle x\rangle^{\frac{3N+1}{2}+N}H^n\chi \in L^2(\mathbb{R}^{3N}), \quad n\in\{2N,\dots,3N\}\,,\end{aligned}$$

we have

$$\begin{aligned}&\langle x\rangle^{\beta}H^n\chi \in L^1(\mathbb{R}^{3N})\cap L^2(\mathbb{R}^{3N}), \quad \beta\in\{N+1,\dots,2N\},\ n\in\{0,1,\dots,4N-\beta\}\,,\\ &\langle x\rangle^{N}H^n\chi \in L^1(\mathbb{R}^{3N})\cap L^2(\mathbb{R}^{3N}), \quad n\in\{2N,\dots,3N\}\,.\end{aligned} \tag{3.73}$$

Let $\boldsymbol{d} := (6,5,3,3,2)$ and $\boldsymbol{\beta} := (0,1,2,1,2)$. For $\boldsymbol{i} = (i_1,i_2,\dots,i_N)\in\{1,2,\dots,5\}^N$ define[19]

$$\boldsymbol{d_i} := (d_{i_1},d_{i_2},\dots,d_{i_N}), \qquad d_{\boldsymbol{i}} := \sum_{j=1}^N\left\lceil\frac{d_{i_j}}{2}\right\rceil\,,$$

$$\boldsymbol{\beta_i} := (\beta_{i_1},\beta_{i_2},\dots,\beta_{i_N}), \qquad \beta_{\boldsymbol{i}} := \sum_{j=1}^N\beta_{i_j}\,,$$

$$P_{\boldsymbol{i}} := \prod_{j=1}^N P_{i_j,j}^{(N)}$$

and note that, with the usual multi-index notation, $\langle\boldsymbol{k}\rangle^{\boldsymbol{d_i}} = \prod_{j=1}^N\langle k_j\rangle^{d_{i_j}}$. We shall show that there is some $C<\infty$ such that

$$\left|\langle\boldsymbol{k}\rangle^{\boldsymbol{d_i}}P_{\boldsymbol{i}}\widehat{\chi}_{\rm out}(\boldsymbol{k})\right| \le C\max_{n=0,1,\dots,d_{\boldsymbol{i}}}\left\|\langle x\rangle^{\beta_{\boldsymbol{i}}}H^n\chi\right\|_{L^1(\mathbb{R}^{3N})} \tag{3.74}$$

for all $\boldsymbol{i}\in\{1,2,\dots,5\}^N$ and $\boldsymbol{k}\in\mathbb{R}^{3N}\setminus\mathcal{N}$ and that (3.73) in fact implies

$$\langle x\rangle^{\beta_{\boldsymbol{i}}}H^n \in L^1(\mathbb{R}^{3N}), \qquad n\in\{0,1,\dots,d_{\boldsymbol{i}}\}\,. \tag{3.75}$$

Then

$$|P_{\boldsymbol{i}}\widehat{\chi}_{\rm out}(\boldsymbol{k})| \le \widetilde{C}\langle\boldsymbol{k}\rangle^{-\boldsymbol{d_i}}\,,$$

[19] $\lceil\ \rceil$ denotes the ceiling function.

i.e. $\widehat{\chi}_{\text{out}} \in \widehat{\mathcal{G}}^{(N)}$.

Let $\boldsymbol{i} \in \{1, 2, \ldots, 5\}^N$. Then

$$\begin{aligned} \left|\langle \boldsymbol{k}\rangle^{\boldsymbol{d_i}} P_{\boldsymbol{i}}\widehat{\chi}_{\text{out}}(\boldsymbol{k})\right| &\leq \left|(1+k^2)^{\sum_{j=1}^{N}\frac{d_{i_j}}{2}} P_{\boldsymbol{i}}\widehat{\chi}_{\text{out}}(\boldsymbol{k})\right| \\ &\leq \left|(1+k^2)^{d_{\boldsymbol{i}}} P_{\boldsymbol{i}}\widehat{\chi}_{\text{out}}(\boldsymbol{k})\right| \leq C\sum_{n=0}^{d_{\boldsymbol{i}}}\left|\left(\frac{k^2}{2}\right)^n P_{\boldsymbol{i}}\widehat{\chi}_{\text{out}}(\boldsymbol{k})\right|. \end{aligned} \tag{3.76}$$

Since the $P_{i_j,j}^{(N)}$s are differential operators of at most order two, the commutator $\left[\left(\frac{k^2}{2}\right)^n, P_{\boldsymbol{i}}\right]$ can be easily calculated and we find

$$\left|\left(\frac{k^2}{2}\right)^n P_{\boldsymbol{i}}\widehat{\chi}_{\text{out}}(\boldsymbol{k})\right| \leq C_n \max_{\substack{n'=0,1,\ldots,n \\ \boldsymbol{i'}\in M_{\boldsymbol{i}}}}\left|P_{\boldsymbol{i'}}\left(\frac{k^2}{2}\right)^{n'}\widehat{\chi}_{\text{out}}(\boldsymbol{k})\right|$$

with $M_{\boldsymbol{i}} := \{\boldsymbol{i'} \in \{1, 2, \ldots, 5\}^N \mid i'_j \in \{1, i_j\}$ if $i_j = 1, 2, 4$ and $i'_j \in \{1, i_j, i_j - 1\}$ if $i_j = 3, 5$. Since $\left(\frac{k^2}{2}\right)^{n'}\widehat{\chi}_{\text{out}} = \left(\frac{k^2}{2}\right)^{n'}\mathcal{F}_+^{(N)}\chi = \mathcal{F}_+^{(N)}H^{n'}\chi$ by (3.55), this gives

$$\left|\left(\frac{k^2}{2}\right)^n P_{\boldsymbol{i}}\widehat{\chi}_{\text{out}}(\boldsymbol{k})\right| \leq C_n \max_{\substack{n'=0,1,\ldots,n \\ \boldsymbol{i'}\in M_{\boldsymbol{i}}}}\left|P_{\boldsymbol{i'}}\left(\mathcal{F}_+^{(N)}H^{n'}\chi\right)(\boldsymbol{k})\right|. \tag{3.77}$$

We claim that there is some $C < \infty$ such that

$$\left|P_{\boldsymbol{i'}}\widehat{f}_{\text{out}}(\boldsymbol{k})\right| \leq C\left\|\langle x\rangle^{\beta_{\boldsymbol{i'}}} f\right\|_{L^1(\mathbb{R}^{3N})} \tag{3.78}$$

for all $\boldsymbol{i'} \in \{1, 2, \ldots, 5\}^N$, $\boldsymbol{k} \in \mathbb{R}^{3N}\setminus\mathcal{N}$ and $f \in L^2(\mathbb{R}^{3N})$ with $\langle x\rangle^{\beta_{\boldsymbol{i'}}} f \in L^1(\mathbb{R}^{3N})$. Then (3.77) yields

$$\left|\left(\frac{k^2}{2}\right)^n P_{\boldsymbol{i}}\widehat{\chi}_{\text{out}}(\boldsymbol{k})\right| \leq C_n \max_{\substack{n'=0,1,\ldots,n \\ \boldsymbol{i'}\in M_{\boldsymbol{i}}}}\left\|\langle x\rangle^{\beta_{\boldsymbol{i'}}} H^{n'}\chi\right\|_{L^1(\mathbb{R}^{3N})}$$

which together with (3.76) gives

$$\left|\langle \boldsymbol{k}\rangle^{\boldsymbol{i}} P_{\boldsymbol{i}}\widehat{\chi}_{\text{out}}(\boldsymbol{k})\right| \leq C \max_{\substack{n=0,1,\ldots,d_{\boldsymbol{i}} \\ \boldsymbol{i'}\in M_{\boldsymbol{i}}}}\left\|\langle x\rangle^{\beta_{\boldsymbol{i'}}} H^n\chi\right\|_{L^1(\mathbb{R}^{3N})}.$$

Since $\beta_{i'_j} \leq \beta_{i_j}$ and thus $\beta_{\boldsymbol{i'}} \leq \beta_{\boldsymbol{i}}$ for all $\boldsymbol{i'} \in M_{\boldsymbol{i}}$, we obtain

$$\max_{\substack{n=0,1,\ldots,d_{\boldsymbol{i}} \\ \boldsymbol{i'}\in M_{\boldsymbol{i}}}}\left\|\langle x\rangle^{\beta_{\boldsymbol{i'}}} H^n\chi\right\|_{L^1(\mathbb{R}^{3N})} \leq \max_{n=0,1,\ldots,d_{\boldsymbol{i}}}\left\|\langle x\rangle^{\beta_{\boldsymbol{i}}} H^n\chi\right\|_{L^1(\mathbb{R}^{3N})}$$

and thus (3.74).

To prove (3.78) note that by Proposition 5

$$\left|P_{\boldsymbol{i'}}\left(\varphi_+^{(N)}\right)^*(\boldsymbol{x},\boldsymbol{k})\right| = \left|P_{\boldsymbol{i'}}\prod_{j=1}^N\varphi_{+,j}^*(\boldsymbol{x}_j,\boldsymbol{k}_j)\right| \leq C\prod_{j=1}^N\langle x_j\rangle^{\beta_{i'_j}} \leq C\langle x\rangle^{\beta_{\boldsymbol{i'}}}$$

for all $\boldsymbol{k} \in \mathbb{R}^{3N} \setminus \mathcal{N}$. Thus

$$\int\limits_{\mathbb{R}^{3N}} \left| P_{\boldsymbol{i}'} \left(\varphi_+^{(N)}\right)^* (\boldsymbol{x}, \boldsymbol{k}) f(\boldsymbol{x}) \right| d^{3N}x \leq C \left\| \langle k \rangle^{\beta_{\boldsymbol{i}'}} f \right\|_{L^1(\mathbb{R}^{3N})} < \infty$$

which justifies the omission of the l. i. m. and the exchange of integration and differentiation in

$$\begin{aligned} \left| P_{\boldsymbol{i}'} \widehat{f}_{\text{out}}(\boldsymbol{k}) \right| &\overset{(3.51)}{=} \left| P_{\boldsymbol{i}'} (2\pi)^{-\frac{3N}{2}} \,\text{l. i. m.} \int\limits_{\mathbb{R}^{3N}} \left(\varphi_+^{(N)}\right)^* (\boldsymbol{x}, \boldsymbol{k}) f(\boldsymbol{x}) d^{3N}x \right| \\ &= \left| (2\pi)^{-\frac{3N}{2}} \int\limits_{\mathbb{R}^{3N}} P_{\boldsymbol{i}'} \left(\varphi_+^{(N)}\right)^* (\boldsymbol{x}, \boldsymbol{k}) f(\boldsymbol{x}) d^{3N}x \right| \leq (2\pi)^{-\frac{3N}{2}} C \left\| \langle k \rangle^{\beta_{\boldsymbol{i}'}} f \right\|_{L^1(\mathbb{R}^{3N})} \end{aligned}$$

and gives us (3.78).

Finally, to prove (3.75) note that

$$\begin{aligned} \beta_{\boldsymbol{i}} &= \sum_{j=1}^{N} \beta_{i_j} = \sum_{j=1}^{N} \left(\delta_{i_j 2} + 2\delta_{i_j 3} + \delta_{i_j 4} + 2\delta_{i_j 5}\right) && \in \{0, 1, \ldots, 2N\}, \\ d_{\boldsymbol{i}} &= \sum_{j=1}^{N} \left\lceil \frac{d_{i_j}}{2} \right\rceil = \sum_{j=1}^{N} \left(3\delta_{i_j 1} + 3\delta_{i_j 2} + 2\delta_{i_j 3} + 2\delta_{i_j 4} + \delta_{i_j 5}\right) && \in \{N, N+1, \ldots, 3N\}, \\ \beta_{\boldsymbol{i}} + d_{\boldsymbol{i}} &= \sum_{j=1}^{N} \left(3\delta_{i_j 1} + 4\delta_{i_j 2} + 4\delta_{i_j 3} + 3\delta_{i_j 4} + 3\delta_{i_j 5}\right) && \in \{3N, 3N+1, \ldots, 4N\}. \end{aligned}$$

Thus

$$d_{\boldsymbol{i}} \in \{\max\{N, 3N - \beta_{\boldsymbol{i}}\}, \max\{N, 3N - \beta_{\boldsymbol{i}}\} + 1, \ldots, \min\{3N, 4N - \beta_{\boldsymbol{i}}\}\}$$

and hence (3.75) follows if

$$\langle x \rangle^{\beta_{\boldsymbol{i}}} H^n \chi \in L^1(\mathbb{R}^{3N}), \qquad n \in \{0, 1, \ldots, \min\{3N, 4N - \beta_{\boldsymbol{i}}\}\} .$$

For $\beta_{\boldsymbol{i}} \in \{N+1, N+2, \ldots, 2N\}$ this is exactly the first part of (3.73), while for $\beta_{\boldsymbol{i}} \in \{0, 1, \ldots, N\}$ (3.73) implies

$$\begin{aligned} &\left\| \langle x \rangle^{\beta_{\boldsymbol{i}}} H^n \chi \right\|_{\in L^1(\mathbb{R}^{3N})} \leq \left\| \langle x \rangle^{\beta} H^n \right\|_{\in L^1(\mathbb{R}^{3N})} < \infty, \quad \beta = 2N,\ n \in \{0, 1, \ldots, 4N - \beta = 2N\}, \\ &\left\| \langle x \rangle^{\beta_{\boldsymbol{i}}} H^n \chi \right\|_{\in L^1(\mathbb{R}^{3N})} \leq \left\| \langle x \rangle^{N} H^n \right\|_{\in L^1(\mathbb{R}^{3N})} < \infty, \quad n \in \{2N, 2N+1, \ldots, 3N\}. \end{aligned}$$

□

Bibliography

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