Derivation of the Gross-Pitaevskii Equation for the Dynamics of Bose-Einstein Condensate

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Abstract

Consider a system of N bosons in three dimensions interacting via a repulsive short range pair potential $N^2V(N(x_i - x_j))$, where $\mathbf{x} = (x_1, \dots, x_N)$ denotes the positions of the particles. Let H_N denote the Hamiltonian of the system and let $\psi_{N,t}$ be the solution to the Schrödinger equation. Suppose that the initial data $\psi_{N,0}$ satisfies the energy condition

$$\langle \psi_{N,0}, H_N^k \psi_{N,0} \rangle \leq C^k N^k$$

for $k = 1, 2, \dots$. We also assume that the k-particle density matrices of the initial state are asymptotically factorized as $N \to \infty$. We prove that the k-particle density matrices of $\psi_{N,t}$ are also asymptotically factorized and the one particle orbital wave function solves the Gross-Pitaevskii equation, a cubic non-linear Schrödinger equation with the coupling constant given by the scattering length of the potential V. We also prove the same conclusion if the energy condition holds only for $k = 1$ but the factorization of $\psi_{N,0}$ is assumed in a stronger sense.

1 Introduction

Bose-Einstein condensation states that at a very low temperature Bose systems with a pair interaction exhibit a collective mode, the Bose-Einstein condensate. If one neglects the interaction and treats all bosons as independent particles, Bose-Einstein condensation is a simple exercise [15]. The many-body effects were traditionally treated by the Bogoliubov approximation, which postulates that the ratio between the non-condensate and the condensate is small. The coupling constant $\sigma/8\pi$ obtained by the Bogoliubov approximation is the semiclassical approximation of the the scattering length a_0 of the pair potential. To recover the scattering length, one needs to perform a higher order diagrammatic re-summation, a procedure that yet lacks mathematical rigor for interacting systems.

Gross [12, 13] and Pitaevskii [20] proposed to model the many-body effects by a nonlinear on-site self interaction of a complex order parameter (the "condensate wave function"). The strength of the

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nonlinear interaction in this model is given by the scattering length a_0. The *Gross-Pitaevskii (GP) equation* is given by

$$i\partial_t u_t = -\Delta u_t + \sigma |u_t|^2 u_t = \frac{\delta \mathcal{E}(u,\bar{u})}{\delta \bar{u}}\Big|_{u_t}, \quad \mathcal{E}(u,\bar{u}) = \int_{\mathbb{R}^3} \left[|\nabla u|^2 + \frac{\sigma}{2}|u|^4 \right], \tag{1.1}$$

where $\mathcal{E}$ is the *Gross-Pitaevskii energy functional* and $\sigma = 8\pi a_0$. The Gross-Pitaevskii equation is a phenomenological mean field type equation and its validity needs to be established from the Schrödinger equation with the Hamiltonian given by the pair interaction.

The first rigorous result concerning the many-body effects of the Bose gas was Dyson's estimate of the ground state energy. Dyson [5] proved the correct leading upper bound to the energy and a lower bound off by a factor around 10. Dyson's upper bound was obtained by using trial functions with short range two-body correlations. This short scale structure is crucial for the emergence of the scattering length and thus for the correct energy. The matching lower bound to the leading order in the low density regime was obtained by Lieb and Yngvason [19]. Lieb and Seiringer [16] later proved that the minimizer of the Gross-Pitaevskii energy functional correctly describes the ground state of an N-boson system in the limit $N \to \infty$ provided that the length scale of the pair potential is of order $1/N$. For a review on related results, see [17].

The experiments on the Bose-Einstein condensation were conducted by observing the dynamics of the condensate when the confining traps are removed. Since the ground state of the system with traps will no longer be the ground state without traps, the validity of the Gross-Pitaevskii equation for predicting the experimental outcomes asserts that the approximation of the many-body effects by a nonlinear on-site self interaction of the order parameter applies to a certain class of excited states and their subsequent time evolution as well.

In this paper, we shall prove that the Gross-Pitaevskii equation actually describes the dynamics of a large class of initial states. The allowed initial states include wave functions with the characteristic short scale two-body correlation structure of the ground state and also wave functions of product form. Notice that product wave functions do not have this characteristic short scale structure, nevertheless the GP evolution equation applies to them. It should be noted that our theorems concern only the evolution of the one particle density matrix but not its energy. In fact, for product initial states, the GP theory is correct on the level of density matrix, but not on the level of the energy. We shall discuss this surprising fact in more details in Section 3.

2 The Main Results

Recall that the Gross-Pitaevskii energy functional correctly describes the energy in the large N limit provided that the scattering length is of order $1/N$ [18]. We thus choose the interaction potential to be

$$V_N(x) := N^2 V(Nx) = \frac{1}{N} N^3 V(Nx).$$

This potential can also be viewed as an approximate delta function on scale $1/N$ with a prefactor $1/N$ which we will interpret as the mean field average. The Hamiltonian of the Bose system is given by

$$H_N := -\sum_{j=1}^{N} \Delta_j + \sum_{j<k}^{N} V_N(x_j - x_k), \quad V_N(x) := N^2 V(Nx). \tag{2.1}$$

The support of the initial state will not be scaled with N. Thus the density of the system is N and the typical inter-particle distance is $N^{-1/3}$, which is much bigger than the length scale of the

potential. The system is really a dilute gas scaled in such a way that the size of the total system is independent of N.

The dynamics of the system is governed by the Schrödinger equation

$$i\partial_t \psi_{N,t} = H_N \psi_{N,t} \tag{2.2}$$

for the wave function $\psi_{N,t} \in L^2_s(\mathbb{R}^{3N})$, the subspace of $L^2(\mathbb{R}^{3N})$ consisting of all functions symmetric with respect to any permutation of the N particles. We choose $\psi_{N,t}$ to have L^2-norm equal to one, $\|\psi_{N,t}\| = 1$.

Instead of describing the system through the wave function, we can describe it by a density matrix $\gamma_N \in \mathcal{L}^1(L^2_s(\mathbb{R}^{3N}))$, where $\mathcal{L}^1(L^2_s(\mathbb{R}^{3N}))$ denotes the space of trace class operators on the Hilbert space $L^2_s(\mathbb{R}^{3N})$. A density matrix is a non-negative trace class operator with trace equal to one. For the *pure* state described by the wave function ψ_N, the density matrix $\gamma_N = |\psi_N\rangle\langle\psi_N|$ is the orthogonal projection onto ψ_N. The time evolution of a density matrix γ_N is determined by the Heisenberg equation

$$i\partial_t \gamma_{N,t} = [H_N, \gamma_{N,t}]\,, \tag{2.3}$$

where $[A, B] = AB - BA$ is the commutator.

Introduce the shorthand notation

$$\mathbf{x} := (x_1, x_2, \ldots, x_N), \quad \mathbf{x}_k := (x_1, \ldots, x_k), \quad \mathbf{x}_{N-k} := (x_{k+1}, \ldots, x_N)$$

and similarly for the primed variables, $\mathbf{x}'_k := (x'_1, \ldots, x'_k)$. For $k = 1, \ldots, N$, the *k-particle reduced density matrix* (or *k-particle marginal*) associated with $\gamma_{N,t}$ is the non-negative operator in $\mathcal{L}^1(L^2_s(\mathbb{R}^{3k}))$ defined by taking the partial trace of $\gamma_{N,t}$ over $N-k$ variables. In other words, the kernel of $\gamma^{(k)}_{N,t}$ is given by

$$\gamma^{(k)}_{N,t}(\mathbf{x}_k; \mathbf{x}'_k) := \int \mathrm{d}\mathbf{x}_{N-k} \gamma_{N,t}\left(\mathbf{x}_k, \mathbf{x}_{N-k}; \mathbf{x}'_k, \mathbf{x}_{N-k}\right)\,. \tag{2.4}$$

Our normalization implies that $\operatorname{Tr} \gamma^{(k)}_{N,t} = 1$ for all $k = 1, \ldots, N$ and for every $t \in \mathbb{R}$.

We now define a topology on the density matrices. We denote by $\mathcal{L}^1_k = \mathcal{L}^1(L^2(\mathbb{R}^{3k}))$ the space of trace class operators acting on the Hilbert space $L^2(\mathbb{R}^{3k})$. Moreover, $\mathcal{K}_k = \mathcal{K}(L^2(\mathbb{R}^{3k}))$ will denote the space of compact operators acting on $L^2(\mathbb{R}^{3k})$ equipped with the operator norm, $\|\cdot\|_{\mathcal{K}_k} := \|\cdot\|$. Since $\mathcal{L}^1_k = \mathcal{K}^*_k$, we can define the weak* topology on $\mathcal{L}^1(L^2(\mathbb{R}^{3k}))$, i.e., $\omega_n \to \omega$ if and only if for every compact operator J on $L^2(\mathbb{R}^{3k})$ we have

$$\lim_{n\to\infty} \operatorname{Tr} J\,\omega_n = \operatorname{Tr} J\omega\,. \tag{2.5}$$

Throughout the paper we will assume that the unscaled interaction potential, $V(x)$, is a nonnegative, smooth, spherically symmetric function with a compact support in the ball of radius R,

$$\operatorname{supp} V \subset \{x \in \mathbb{R}^3 \;:\; |x| \leq R\}\,. \tag{2.6}$$

With the notation $r = |x|$, we will sometimes write $V(r)$ for $V(x)$. We define the following dimensionless quantity to measure the strength of V

$$\rho := \sup_{r\geq 0} r^2\, V(r) + \int_0^\infty \mathrm{d}r\, rV(r)\,. \tag{2.7}$$

Let f be the zero energy scattering solution associated with V with normalization $\lim_{|x|\to\infty} f(x) = 1$. We will write $f(x) = 1 - w_0(x)$. By definition, this function satisfies the equation

$$\Big[-\Delta + \frac{1}{2} V(x) \Big](1 - w_0(x)) = 0\,, \tag{2.8}$$

and $\lim_{|x|\to\infty} w_0(x) = 0$. The scattering length a_0 of V is defined by

$$a_0 := \lim_{|x|\to\infty} w_0(x)|x|\,. \tag{2.9}$$

Since V has a compact support (2.6), we have

$$f(x) = 1 - \frac{a_0}{|x|} \qquad |x| \geq R\,. \tag{2.10}$$

From the zero energy equation, we also have the identity

$$\int \mathrm{d}x\, V(x)(1 - w_0(x)) = 8\pi a_0\,. \tag{2.11}$$

By scaling, the scattering length of the potential $V_N(x)$ is $a := a_0/N$ and the zero energy scattering equation for the potential V_N is given by

$$\left(-\Delta + \frac{1}{2} V_N(x)\right)(1 - w(x)) = 0 \tag{2.12}$$

where $w(x) := w_0(Nx)$. Note that $w(x) = a/|x|$, for $|x| \geq R/N$.

We can now state our main theorems.

Theorem 2.1. *Suppose $V \geq 0$ is a smooth, compactly supported, spherically symmetric potential with scattering length a_0 and assume that ρ (defined in (2.7)) is small enough. We consider a family of systems described by initial wave functions $\psi_N \in L^2_s(\mathbb{R}^{3N})$ such that*

$$\langle \psi_N, H_N^k \psi_N \rangle \leq C^k N^k \tag{2.13}$$

for all $k \geq 1$. We assume that the marginal densities associated with ψ_N factorize in the limit $N \to \infty$, i.e. there is a function $\varphi \in L^2(\mathbb{R}^3)$ such that for every $k \geq 1$,

$$\gamma_N^{(k)} \to |\varphi\rangle\langle\varphi|^{\otimes k} \tag{2.14}$$

as $N \to \infty$ with respect to the weak topology of $\mathcal{L}^1(L^2(\mathbb{R}^{3k}))$. Then $\varphi \in H^1(\mathbb{R}^3)$, and for every fixed $k \geq 1$ and $t \in \mathbb{R}$, we have*

$$\gamma_{N,t}^{(k)} \to |\varphi_t\rangle\langle\varphi_t|^{\otimes k} \tag{2.15}$$

with respect to the same topology. Here $\varphi_t \in H^1(\mathbb{R}^3)$ is the solution of the nonlinear Gross-Pitaevskii equation

$$i\partial_t \varphi_t = -\Delta\varphi_t + 8\pi a_0 |\varphi_t|^2 \varphi_t \tag{2.16}$$

with initial condition $\varphi_{t=0} = \varphi$.

Using an approximation argument, we can relax the energy condition (2.13), and only assume that $\langle \psi_N, H_N \psi_N \rangle \leq CN$. However, in order to apply our approximation argument, we need to assume stronger asymptotic factorization properties on ψ_N.

Theorem 2.2. *Suppose $V \geq 0$ is a smooth, compactly supported, spherically symmetric potential with scattering length a_0 and assume that ρ (defined in (2.7)) is small enough. We consider a family of systems described by initial wave functions $\psi_N \in L^2_s(\mathbb{R}^{3N})$ such that*

$$\langle \psi_N, H_N \psi_N \rangle \leq CN\,. \tag{2.17}$$

We assume asymptotic factorization of ψ_N in the sense that there exists $\varphi \in L^2(\mathbb{R}^3)$ and, for every N, and every $1 \leq k \leq N$, there exists a $\xi_N^{(N-k)} \in L^2(\mathbb{R}^{3(N-k)})$ with $\|\xi_N^{(N-k)}\| = 1$ such that

$$\|\psi_N - \varphi^{\otimes k} \otimes \xi_N^{(N-k)}\| \to 0 \tag{2.18}$$

as $N \to \infty$. This implies, in particular that, for every $k \geq 1$,

$$\gamma_N^{(k)} \to |\varphi\rangle\langle\varphi|^{\otimes k} \tag{2.19}$$

as $N \to \infty$ with respect to the weak topology of $\mathcal{L}^1(L^2(\mathbb{R}^{3k}))$. Then $\varphi \in H^1(\mathbb{R}^3)$, and for every fixed $k \geq 1$ and $t \in \mathbb{R}$ we have*

$$\gamma_{N,t}^{(k)} \to |\varphi_t\rangle\langle\varphi_t|^{\otimes k} \tag{2.20}$$

with respect to the same topology. Here $\varphi_t \in H^1(\mathbb{R}^3)$ is the solution of the nonlinear Gross-Pitaevskii equation

$$i\partial_t \varphi_t = -\Delta\varphi_t + 8\pi a_0 |\varphi_t|^2 \varphi_t \tag{2.21}$$

with $\varphi_{t=0} = \varphi$.

Both theorems have analogous versions for initial data describing mixed states (that is γ_N is not an orthogonal projection). For example, suppose that γ_N is a family of density matrices satisfying

$$\mathrm{Tr}\; H_N^k \gamma_N \leq C^k N^k \qquad \text{and} \qquad \gamma_N^{(k)} \to \omega_0^{\otimes k} \tag{2.22}$$

where ω_0 is a one-particle density matrix and

$$\omega_0^{\otimes k}(\mathbf{x}_k; \mathbf{x}'_k) = \prod_{j=1}^k \omega_0(x_j; x'_j).$$

Then for every $t \in \mathbb{R}$ and $k \geq 1$ we have

$$\gamma_{N,t}^{(k)} \to \omega_t^{\otimes k} \tag{2.23}$$

where ω_t is the solution of the nonlinear Hartree equation

$$i\partial_t \omega_t = [-\Delta + 8\pi a_0 \varrho_t, \omega_t] \qquad \varrho_t(x) = \omega_t(x;x), \quad \omega_{t=0} = \omega_0 \tag{2.24}$$

The last equation is equivalent to (2.16) if $\omega_t = |\varphi_t\rangle\langle\varphi_t|$.

Lieb and Seiringer [16] have proved that, for pure states, the assumption

$$\gamma_N^{(1)} \to |\varphi\rangle\langle\varphi| \qquad \text{as } N \to \infty$$

implies automatically (2.14) for every $k \geq 1$ (see the argument after Theorem 1 in that paper)[1]. For mixed initial states we still need the second condition in (2.22) for all $k \geq 1$ in order to prove (2.23).

[1] We thank Robert Seiringer for pointing out this result to us.

Now we comment on the assumption of asymptotic factorization (2.18) for the initial data ψ_N. The most natural example that satisfies this condition is the factorized wave function $\psi_N(\mathbf{x}) = \prod_{j=1}^N \varphi(x_j)$. If, additionally, $\varphi \in H^1(\mathbb{R}^3)$, then (2.17) is also satisfied by the Schwarz and Sobolev inequalities. The evolution of ψ_N is therefore governed by the GP equation according to Theorem 2.2. This is, however, somewhat surprising because the emergence of the scattering length in the GP equation indicates that the wave function has a characteristic short scale correlation structure, which is clearly absent in the factorized initial data. We shall discuss this issue in more details in Section 3.

From the physical point of view, however, the product initial wave function is not the most relevant one. In real physical experiments, the initial state is prepared by cooling down a trapped Bose gas at extremely low temperatures. This state can be modelled by the ground state ψ_N^{trap} of the Hamiltonian

$$H_N^{\text{trap}} = \sum_{j=1}^N (-\Delta_j + V_{\text{ext}}(x_j)) + \sum_{i<j}^N V_N(x_i - x_j)$$

with a trapping potential $V_{\text{ext}}(x) \to \infty$ as $|x| \to \infty$. In Appendix C, we prove that assumptions (2.17) and (2.18) are satisfied for ψ_N^{trap}. In other words, Theorem 2.2 can be used to describe the evolution of the ground state of H_N^{trap}, after the traps are removed (see Corollary C.1). This provides a mathematically rigorous analysis of recent experiments in condensed matter physics, where the evolution of initially trapped Bose-Einstein condensates is observed.

In Appendix B, we show that Theorem 2.2 can also be applied to a general class of initial data, which are in some sense close to the ground state of the Hamiltonian H_N^{trap}. The ground state of a dilute Bose system with interaction potential V_N is believed to be very close to the form

$$W_N(\mathbf{x}) := \prod_{i<j} f(N(x_i - x_j)), \tag{2.25}$$

where $f = 1 - w_0$ is the zero-energy solution (2.8). We remark that Dyson [5] used a different function which was not symmetric, but the short distance behavior was the same as in W_N. An example of a family of initial wave functions which have local structure given by W is given by wave functions of the type

$$\psi_N(\mathbf{x}) = W_N(\mathbf{x}) \prod_{j=1}^N \varphi(x_j) \tag{2.26}$$

where $\varphi \in H^1(\mathbb{R}^3)$. Due to the factor W_N, this function carries the characteristic short scale structure of the ground state. We will prove in Lemma B.1 that wave functions of the form (2.26) (with correlations cutoff at length scales $\ell \gg N^{-1}$) satisfies the assumptions (2.17) and (2.18).

Part of Theorem 2.2 was proved in [8] for systems with the pair interaction cut off whenever three or more particles are much closer to each other than the mean particle distance, $N^{-1/3}$. For this model, it was proved that any limiting point of $\gamma_N^{(k)}$ satisfies the infinite BBGKY hierarchy (see Section 3) with coupling constant $8\pi a_0$. The uniqueness of the solution to the hierarchy was established in [9]. In the current paper we remove this cutoff and establish the apriori bounds needed for the uniqueness theorem in [9].

The Hamiltonian (2.1) is a special case of the Hamiltonian

$$H_{\beta,N} := -\sum_{j=1}^N \Delta_j + \frac{1}{N} \sum_{i<j}^N N^{3\beta} V(N^\beta (x_i - x_j)) \tag{2.27}$$

introduced in [6] and [9]. In [9] we have proved a version of Theorem 2.2 for $0 < \beta < 1/2$ provided the initial data is given by a product state $\psi_N(\mathbf{x}) = \prod_{j=1}^k \varphi(x_j)$ for some $\varphi \in H^1(\mathbb{R}^3)$. In this case the limiting macroscopic equation was given by

$$i\partial_t \varphi_t = -\Delta\varphi_t + b_0|\varphi_t|^2\varphi_t \,,$$

with $b_0 = \int \mathrm{d}x\, V(x)$. Note that $N^{3\beta}V(N^\beta x)$ is an approximate delta function on a scale much bigger than $O(1/N)$, the scattering length of $\frac{1}{N}V_N$. This explains why the strength of the on-site potential is given by the semiclassical approximation b_0 of the $8\pi a_0$. With the techniques used in this paper, it is straight-forward to extend the result of [9] to all $\beta < 1$ with the same coefficient b_0 in the limiting one-body equation provided that ρ (from (2.7)) is small enough. Combining this comment with Theorem 2.1 and 2.2, we have shown that the one particle density matrix for the N-body Schrödinger equation with Hamiltonian given by (2.27) converges to the Gross-Pitaevskii equation with coupling constant given by

$$\sigma = \begin{cases} b_0, & \text{if } \ 0 < \beta < 1 \\ 8\pi a_0, & \text{if } \ \beta = 1 \,. \end{cases} \tag{2.28}$$

The case $\beta = 0$ is the mean-field case and the limiting one-body equation is the Hartree equation:

$$i\partial_t \varphi_t = -\Delta\varphi_t + (V * |\varphi_t|^2)\varphi_t \,. \tag{2.29}$$

This was established by Hepp [14] for smooth potential. Ginibre and Velo [11] considered singular potentials but with a specific initial data based on second quantized formalism. Spohn [22] introduced a new approach to this problem using the BBGKY hierarchy. Recent progresses on mean-field limit of quantum dynamics have been based on the BBGKY hierarchy and we mention only a few: the Coulomb potential case [3, 10], the pseudo-relativistic Hamiltonian with Newtonian interaction [7], and the delta function interaction in one dimension by Adami, Bardos, Golse and Teta [1] [2]. In next section, we review the BBGKY hierarchy and the two-scale nature of the eigenfunctions of interacting Bose systems.

3 The BBGKY Hierarchy

The time evolution of the density matrices $\gamma_{N,t}^{(k)}$, for $k = 1, \ldots, N$, is given by a hierarchy of N equations, commonly known as the BBGKY hierarchy:

$$\begin{aligned} i\partial_t \gamma_{N,t}^{(k)} = &\sum_{j=1}^k \left[-\Delta_j, \gamma_{N,t}^{(k)}\right] + \sum_{i<j}^k \left[V_N(x_j - x_i), \gamma_{N,t}^{(k)}\right] \\ &+ (N-k)\sum_{j=1}^k \mathrm{Tr}_{k+1} \ \left[V_N(x_j - x_{k+1}), \gamma_{N,t}^{(k+1)}\right] \end{aligned} \tag{3.30}$$

for $k = 1, \ldots, N$ (we use the convention that $\gamma_{N,t}^{(k)} = 0$ if $k > N$). Here Tr_{k+1} denotes the partial trace over the $(k+1)$-th particle. In particular, the density matrix $\gamma_{N,t}^{(1)}(x_1; x_1')$ satisfies the equation

$$\begin{aligned} i\partial_t \gamma_{N,t}^{(1)}(x_1; x_1') = &(-\Delta_{x_1} + \Delta_{x_1'})\gamma_{N,t}^{(1)}(x_1; x_1') \\ &+ (N-1)\int \mathrm{d}x_2 \left(V_N(x_1 - x_2) - V_N(x_1' - x_2)\right) \gamma_{N,t}^{(2)}(x_1, x_2; x_1', x_2), \end{aligned} \tag{3.31}$$

To close this equation, one needs to assume some relation between $\gamma^{(2)}_{N,t}$ and $\gamma^{(1)}_{N,t}$. The simplest assumption would be the factorization property, i.e.,

$$\gamma^{(2)}_{N,t}(x_1, x_2; x_1', x_2') = \gamma^{(1)}_{N,t}(x_1; x_1')\gamma^{(1)}_{N,t}(x_2; x_2')\,. \tag{3.32}$$

This does not hold for finite N, but it may hold for a limit point $\gamma^{(k)}_t$ of $\gamma^{(k)}_{N,t}$ as $N \to \infty$, i.e.,

$$\gamma^{(2)}_{t}(x_1, x_2; x_1', x_2') = \gamma^{(1)}_{t}(x_1; x_1')\gamma^{(1)}_{t}(x_2; x_2')\,. \tag{3.33}$$

Under this assumption, $\gamma^{(1)}_t$ satisfies the limiting equation

$$i\partial_t\gamma^{(1)}_t(x_1; x_1') = \ (-\Delta_{x_1} + \Delta_{x_1'})\gamma^{(1)}_t(x_1; x_1') + \big(Q_t(x_1) - Q_t(x_1')\big)\,\gamma^{(1)}_t(x_1; x_1') \tag{3.34}$$

where

$$Q_t(x) := \lim_{N\to\infty} N\int \mathrm{d}y V_N(x-y)\rho_t(y), \quad \rho_t(x) = \gamma^{(1)}_t(x;x)\,. \tag{3.35}$$

If $\rho_t(x)$ is continuous, then Q_t is given by

$$Q_t(x) = b_0\rho_t(x).$$

Thus (3.34) gives the GP equation with a coupling constant $\sigma = b_0$ instead of $\sigma = 8\pi a_0$. This explains the case if $\beta < 1$. For $\beta = 1$, we note that $b_0/8\pi$ is the first Born approximation to the scattering length a_0 and the following inequality holds:

$$a_0 \le \frac{b_0}{8\pi} = \frac{1}{4\pi}\int_{\mathbb{R}^3} \frac{1}{2}\,V(x)\,dx\,. \tag{3.36}$$

Recall that the ground state of a dilute Bose system with interaction potential V_N is believed to be very close to $W(\mathbf{x})$ (see (2.25)). We assume, for the moment, that the ansatz, $\psi_t(\mathbf{x}) = W(\mathbf{x})\phi_t(\mathbf{x})$ with ϕ_t a product function, holds for all time. The reduced density matrices for $\psi_t(\mathbf{x})$ satisfy

$$\gamma^{(2)}_t(x_1, x_2; x_1', x_2') \sim f(N(x_1-x_2))f(N(x_1'-x_2'))\gamma^{(1)}_t(x_1; x_1')\gamma^{(1)}_t(x_2; x_2')\,. \tag{3.37}$$

Together with (2.11) and the assumption that ρ_t is smooth on scale $1/N$, we have

$$\lim_{N\to\infty} N\int \mathrm{d}x_2 V_N(x_1-x_2)\gamma^{(2)}_{N,t}(x_1, x_2; x_1', x_2) = 8\pi a_0\gamma^{(1)}_t(x_1; x_1')\rho_t(x_1)\,. \tag{3.38}$$

This formula is valid for $|x_1 - x_1'| \gg 1/N$. We have used that $\lim_{|x|\to\infty} f(x) = 1$. For pure states, this gives the GP equation with the correct dependence on the scattering length.

Notice that the correlation in $\gamma^{(2)}$ occurs at the scale $1/N$, which vanishes in a weak limit and the product relation (3.33) will hold. However, this short distance correlation shows up in the GP equation due to the singular potential $NV_N(x_1 - x_2)$. This phenomena occurs for the ground state as proved in [18]. Our task is to characterize wave functions with this short scale structure and establish it for the time evolved states. The key observation is the following Proposition. Recall the assumptions on V from Section 2 and that $1 - w(x)$ denotes the zero energy solution to $-\Delta + \frac{1}{2}V_N$ (2.12). We will use the short notation $w_{ij} := w(x_i - x_j)$, $\nabla w_{ij} = (\nabla w)(x_i - x_j)$ (note that $\nabla w_{ij} = -\nabla w_{ji}$).

Proposition 3.1 (H_N^2-energy estimate)**.** *Suppose that ρ (defined in (2.7)) is small enough. Then, there exists a universal constant $c > 0$ such that, for every $\psi \in L_s^2(\mathbb{R}^N)$, and for every fixed indices $i \neq j$, $i, j = 1, \ldots, N$, we have*

$$\langle \psi, H_N^2 \psi \rangle \geq (1 - c\rho) N(N-1) \int (1 - w_{ij})^2 \, |\nabla_i \nabla_j \, \phi_{ij}|^2 \tag{3.39}$$

where ϕ_{ij} defined by $\psi = (1 - w_{ij})\phi_{ij}$.

If ϕ_{ij} is singular when x_i approaches x_j, then $\nabla_i \nabla_j \phi_{ij}$ cannot be L^2-integrable. This Proposition thus shows that the short distance behavior of any function ψ with $\langle \psi, H_N^2 \psi \rangle \leq CN^2$ is given by $(1 - w(x_i - x_j))$ when x_i is near x_j.

We emphasized the importance of the local structure $(1 - w(x_i - x_j))$ for obtaining the scattering length a_0. While Theorem 2.2 concerns only the one particle density matrix in the weak limit and no statement on the local structure is made at all, the validity of the GP equation does suggest the existence of this structure. For the initial data (2.26) beginning with this local structure, it simply means its preservation by the dynamics. This is indeed the case if the local structure of the initial data ψ is precise enough so that $\langle \psi, H_N^2 \psi \rangle \leq CN^2$, see Proposition 3.1.

For the product initial state, there is no such structure to begin with. Theorem 2.2 thus indicates that on some short length scale a local structure similar to $(1 - w(x_i - x_j))$ forms in a very short time which approaches zero in the limit $N \to \infty$. Heuristically, notice that the two particle dynamics is described by the operator

$$i\partial_t - \Delta_{x_1} - \Delta_{x_2} - V_N(x_1 - x_2) = N^2 \left[i\partial_T - \Delta_{X_1} - \Delta_{X_2} - V(X_1 - X_2) \right]$$

where $X_i = Nx_i$ and $T = N^2 t$ are the microscopic coordinates. The small positive time behavior of the original wave function on the short length scale is the same as the long time behavior in the microscopic coordinates. Clearly, we expect the long time dynamics to be characterized by the relaxation to the zero energy solution. This picture, however, is far from rigorous as the true N-body dynamics develops higher order correlations as well.

On the other hand, the local structure $(1 - w(x_i - x_j))$ cannot be the only singular piece of the wave function in positive time for product initial states. A simple calculation shows that the energy per particle of a product initial state $\psi_N(\mathbf{x}) = \prod_{j=1}^N \varphi(x_j)$ is given by

$$\lim_{N \to \infty} N^{-1} \langle \psi_N, H_N \psi_N \rangle = \int_{\mathbb{R}^3} \mathrm{d}x \, |\nabla \varphi(x)|^2 + \frac{b_0}{2} \int_{\mathbb{R}^3} \mathrm{d}x \, |\varphi(x)|^4 \tag{3.40}$$

where $b_0 = \int V$. This is different from the GP energy functional (1.1) due to the coupling constant. Since the energy is a constant of the motion, this implies that the GP theory does not predict the evolution of the energy. If we grant that the local structure $(1 - w(x_i - x_j))$ does form for positive time $t > 0$, the discrepancy in energy suggests that there is some energy on intermediate length scales of order $N^{-\alpha}$, $0 < \alpha < 1$ which is not captured by the GP theory. This excess energy apparently does not participate in the evolution of the density matrix on length scale of order one which is the only scale that is visible by our weak limit. We do not know if such a picture can be established rigorously.

Notation. We will denote an arbitrary constant by C. In general C can depend on the choice of the unscaled potential V. Universal constants, *independent of* V, will be denoted by c. We write $f(N) = o(N^\alpha)$ if there is $\delta > 0$ such that $N^{-\alpha+\delta} f(N) \to 0$ as $N \to \infty$ (unless stated otherwise, this convergence does not need to be uniform in the other relevant parameters). We also write $f(N) \ll g(N)$ if $f(N)/g(N) = o(1)$. Integrations without specified domains are always understood on the whole space ($\mathbb{R}^3$, $\mathbb{R}^{3k}$ or $\mathbb{R}^{3N}$ according to the integrand) with the Lebesgue measure.

4 Proof of Theorem 2.1 and Theorem 2.2

In this section we present the main steps of the proofs and we reduce the argument to a sequence of key theorems and propositions. These will be proven in the rest of the paper.

We start with defining the space of density matrices that depend continuously on the time parameter with respect to the weak* topology. To use Arzela-Ascoli compactness argument, we will need to establish the concept of uniform continuity in this space, thus we have to metrize the weak* topology.

Since $\mathcal{K}_k$ is separable, we can fix a dense countable subset of the unit ball of $\mathcal{K}_k$: we denote it by $\{J_i^{(k)}\}_{i\geq 1} \in \mathcal{K}_k$, with $\|J_i^{(k)}\|_{\mathcal{K}_k} \leq 1$ for all $i \geq 1$. Using the operators $J_i^{(k)}$ we define the following metric on $\mathcal{L}_k^1$: for $\gamma^{(k)}, \bar{\gamma}^{(k)} \in \mathcal{L}_k^1$ we set

$$\eta_k(\gamma^{(k)}, \bar{\gamma}^{(k)}) := \sum_{i=1}^{\infty} 2^{-i} \left| \mathrm{Tr}\ J_i^{(k)} \left(\gamma^{(k)} - \bar{\gamma}^{(k)} \right) \right| . \tag{4.1}$$

Then the topology induced by the metric η_k and the weak* topology are equivalent on the unit ball of $\mathcal{L}_k^1$ (see [21], Theorem 3.16) and hence on any ball of finite radius as well. In other words, a uniformly bounded sequence $\gamma_N^{(k)} \in \mathcal{L}_k^1$ converges to $\gamma^{(k)} \in \mathcal{L}_k^1$ with respect to the weak* topology, if and only if $\eta_k(\gamma_N^{(k)}, \gamma^{(k)}) \to 0$ as $N \to \infty$.

For a fixed $T > 0$, let $C([0,T], \mathcal{L}_k^1)$ be the space of functions of $t \in [0,T]$ with values in $\mathcal{L}_k^1$ which are continuous with respect to the metric η_k. On $C([0,T], \mathcal{L}_k^1)$ we define the metric

$$\widehat{\eta}_k(\gamma^{(k)}(\cdot), \bar{\gamma}^{(k)}(\cdot)) := \sup_{t\in[0,T]} \eta_k(\gamma^{(k)}(t), \bar{\gamma}^{(k)}(t)) . \tag{4.2}$$

Finally, we denote by τ_{prod} the topology on the space $\bigoplus_{k\geq 1} C([0,T], \mathcal{L}_k^1)$ given by the product of the topologies generated by the metrics $\widehat{\eta}_k$ on $C([0,T], \mathcal{L}_k^1)$.

Proof of Theorem 2.1. The proof is divided in several steps.

Step 1. Compactness of $\Gamma_{N,t} = \{\gamma_{N,t}^{(k)}\}_{k\geq 1}$. We set $T > 0$ and work on the interval $t \in [0,T]$. Negative times can be handled analogously. We will prove in Theorem 6.1 that the sequence $\Gamma_{N,t}^{(k)} = \{\gamma_{N,t}^{(k)}\}_{k\geq 1} \in \bigoplus_{k\geq 1} C([0,T], \mathcal{L}_k^1)$ is compact with respect to the product topology τ_{prod} defined above (we use the convention that $\gamma_{N,t}^{(k)} = 0$ if $k > N$). Moreover, we also prove in Theorem 6.1, that any limit point $\Gamma_{\infty,t} = \{\gamma_{\infty,t}^{(k)}\}_{k\geq 1} \in \bigoplus_{k\geq 1} C([0,T], \mathcal{L}_k^1)$ is such that, for every $k \geq 1$, $\gamma_{\infty,t}^{(k)} \geq 0$, and $\gamma_{\infty,t}^{(k)}$ is symmetric w.r.t. permutations. In Proposition 6.3 we also show that

$$\mathrm{Tr}\ (1-\Delta_1)\dots(1-\Delta_k)\,\gamma_{\infty,t}^{(k)} \leq C^k \tag{4.3}$$

for every $t \in [0,T]$ and every $k \geq 1$. Note that, for finite N, the densities $\gamma_{N,t}^{(k)}$ do not satisfy estimates such as (4.3) (at least not uniformly in N), because they contain a short scale structure. Only after taking the weak limit, we can prove (4.3).

Step 2. Convergence to the infinite hierarchy. In Theorem 7.1 we prove that any limit point $\Gamma_{\infty,t} = \{\gamma_{\infty,t}^{(k)}\}_{k\geq 1} \in \bigoplus_{k\geq 1} C([0,T], \mathcal{L}_k^1)$ of $\Gamma_{N,t} = \{\gamma_{N,t}^{(k)}\}_{k\geq 1}$ with respect to the product topology τ_{prod} is a solution of the infinite hierarchy of integral equations ($k = 1, 2, \dots$)

$$\gamma_{\infty,t}^{(k)} = \mathcal{U}^{(k)}(t)\gamma_{\infty,0}^{(k)} - 8\pi i a_0 \sum_{j=1}^{k} \int_0^t \mathrm{d}s\, \mathcal{U}^{(k)}(t-s)\mathrm{Tr}_{k+1} \left[\delta(x_j - x_{k+1}), \gamma_{\infty,s}^{(k+1)} \right] \tag{4.4}$$

with initial data $\gamma^{(k)}_{\infty,0} = |\varphi\rangle\langle\varphi|^{\otimes k}$. Here Tr_{k+1} denotes the partial trace over the $(k+1)$-th particle, and $\mathcal{U}^{(k)}(t)$ is the free evolution, whose action on k-particle density matrices is given by

$$\mathcal{U}^{(k)}(t)\gamma^{(k)} := e^{it\sum_{j=1}^k \Delta_j}\gamma^{(k)} e^{-it\sum_{j=1}^k \Delta_j}\,.$$

Note that (4.4) is the (formal) limit of the N-particle BBGKY hierarchy (3.30) (written in integral form) if we replace the limit of $NV_N(x)$ with $8\pi a_0\delta(x)$ (see (3.38)).

The one-particle wave function φ was introduced in (2.14). From (2.13) and the positivity of the potential we note that

$$CN \geq \langle \psi_N, (H_N + N)\,\psi_N\rangle \geq N\mathrm{Tr}\,(1-\Delta)\,\gamma^{(1)}_N\,. \tag{4.5}$$

Since by (2.14), $\gamma^{(1)}_N \to |\varphi\rangle\langle\varphi|$ as $N\to\infty$, w.r.t. the weak * topology of $\mathcal{L}^1(L^2(\mathbb{R}^3))$, it follows from (4.5) that $\mathrm{Tr}\,(1-\Delta)|\varphi\rangle\langle\varphi| \leq C$, and therefore that $\varphi \in H^1(\mathbb{R}^3)$.

We remark here that the family of factorized densities,

$$\gamma^{(k)}_t = |\varphi_t\rangle\langle\varphi_t|^{\otimes k}, \tag{4.6}$$

is a solution of the infinite hierarchy (4.4) if φ_t is the solution of the nonlinear Gross-Pitaevskii equation (2.16) with initial data $\varphi_{t=0} = \varphi$. The nonlinear Schrödinger equation (2.16) is well posed in $H^1(\mathbb{R}^3)$ and it conserves the energy, $\mathcal{E}(\varphi) := \frac{1}{2}\int |\nabla\varphi|^2 + 4\pi a_0 \int |\varphi|^4$. From $\varphi \in H^1(\mathbb{R}^3)$, we thus obtain that $\varphi_t \in H^1(\mathbb{R}^3)$ for every $t\in\mathbb{R}$, with a uniformly bounded H^1-norm. Therefore

$$\mathrm{Tr}\,(1-\Delta_1)\dots(1-\Delta_k)|\varphi_t\rangle\langle\varphi_t|^{\otimes k} \leq \|\varphi_t\|^k_{H^1} \leq C^k \tag{4.7}$$

for all $t\in\mathbb{R}$, and a constant C only depending on the H^1-norm of φ.

Step 3. Uniqueness of the solution to the infinite hierarchy. In Section 9 of [9] we proved the following theorem, which states the uniqueness of solution to the infinite hierarchy (4.4) in the space of densities satisfying the a priori bound (4.3). The proof of this theorem is based on a diagrammatic expansion of the solution of (4.4).

Theorem 4.1. *[Theorem 9.1 of [9]] Suppose $\Gamma = \{\gamma^{(k)}\}_{k\geq 1} \in \bigoplus_{k\geq 1}\mathcal{L}^1_k$ is such that*

$$Tr\,(1-\Delta_1)\dots(1-\Delta_k)\gamma^{(k)} \leq C^k\,. \tag{4.8}$$

Then, for any fixed $T>0$, there exists at most one solution $\Gamma_t = \{\gamma^{(k)}_t\}_{k\geq 1} \in \bigoplus_{k\geq 1} C([0,T],\mathcal{L}^1_k)$ of (4.4) such that

$$Tr\,(1-\Delta_1)\dots(1-\Delta_k)\gamma^{(k)}_t \leq C^k \tag{4.9}$$

for all $t\in[0,T]$ and for all $k\geq 1$.

Step 4. Conclusion of the proof. From Step 2 and Step 3 it follows that the sequence $\Gamma_{N,t} = \{\gamma^{(k)}_{N,t}\}_{k\geq 1} \in \bigoplus_{k\geq 1} C([0,T],\mathcal{L}^1_k)$ is convergent with respect to the product topology τ_{prod}; in fact a compact sequence with only one limit point is always convergent. Since the family of densities $\Gamma_t = \{\gamma^{(k)}_t\}_{k\geq 1}$ defined in (4.6) satisfies (4.7) and it is a solution of (4.4), it follows that $\Gamma_{N,t} \to \Gamma_t$ w.r.t. the topology τ_{prod}. The estimates are uniform in $t\in[0,T]$, thus we can also conclude that $\widehat{\eta}_k(\gamma^{(k)}_{N,t},\gamma^{(k)}_t) \to 0$. In particular this implies that, for every fixed $k\geq 1$, and $t\in[0,T]$, $\gamma^{(k)}_{N,t} \to \gamma^{(k)}_t$ with respect to the weak* topology of $\mathcal{L}^1_k$. This completes the proof of Theorem 2.1. Actually, the estimates are uniform in $t\in[0,T]$, and thus we can also conclude that $\widehat{\eta}_k(\gamma^{(k)}_{N,t},\gamma^{(k)}_t) \to 0$. □

Next we prove Theorem 2.2; to this end we regularize the initial wave function, and then we apply the same arguments as in the proof of Theorem 2.1.

Proof of Theorem 2.2. Fix $\kappa > 0$ and $\chi \in C_0^\infty(\mathbb{R})$, with $0 \leq \chi \leq 1$, $\chi(s) = 1$, for $0 \leq s \leq 1$, and $\chi(s) = 0$ if $s \geq 2$. We define the regularized initial wave function

$$\widetilde{\psi}_N := \frac{\chi(\kappa H_N/N)\psi_N}{\|\chi(\kappa H_N/N)\psi_N\|},$$

and we denote by $\widetilde{\psi}_{N,t}$ the solution of the Schrödinger equation (2.2) with initial data $\widetilde{\psi}_N$. Denote by $\widetilde{\Gamma}_{N,t} = \{\widetilde{\gamma}_{N,t}^{(k)}\}_{k=1}^\infty$ the family of marginal densities associated with $\widetilde{\psi}_{N,t}$. By convention, we set $\widetilde{\gamma}_{N,t}^{(k)} := 0$ if $k > N$. The tilde in the notation indicates the dependence on the cutoff parameter κ. In Proposition 8.1, part i), we prove that

$$\langle \widetilde{\psi}_{N,t}, H_N^k \widetilde{\psi}_{N,t} \rangle \leq \widetilde{C}^k N^k \tag{4.10}$$

if $\kappa > 0$ is sufficiently small (the constant $\widetilde{C}$ depends on κ). Moreover, using the strong asymptotic factorization assumption (2.18), we prove in part iii) of Proposition 8.1 that for every $J^{(k)} \in \mathcal{K}_k$,

$$\text{Tr } J^{(k)} \left(\widetilde{\gamma}_N^{(k)} - |\varphi\rangle\langle\varphi|^{\otimes k} \right) \to 0 \tag{4.11}$$

as $N \to \infty$. From (4.10) and (4.11), we observe that the assumptions (2.13) and (2.14) of Theorem 2.1 are satisfied by the regularized wave function $\widetilde{\psi}_N$ and by the regularized marginal densities $\widetilde{\gamma}_{N,t}^{(k)}$. Therefore, applying Theorem 2.1, we obtain that, for every $t \in \mathbb{R}$ and $k \geq 1$,

$$\widetilde{\gamma}_{N,t}^{(k)} \to |\varphi_t\rangle\langle\varphi_t|^{\otimes k} \tag{4.12}$$

where φ_t is the solution of (2.16).

It remains to prove that the densities $\gamma_{N,t}^{(k)}$ associated with the original wave function $\psi_{N,t}$ (without cutoff κ) converge and have the same limit as the regularized densities $\widetilde{\gamma}_{N,t}^{(k)}$. This follows from Proposition 8.1, part ii), where we prove that

$$\|\psi_{N,t} - \widetilde{\psi}_{N,t}\| = \|\psi_N - \widetilde{\psi}_N\| \leq C\kappa^{1/2} \,,$$

where the constant C is independent of N and κ. This implies that, for every $J^{(k)} \in \mathcal{K}_k$, we have

$$\left| \text{Tr } J^{(k)} \left(\gamma_{N,t}^{(k)} - \widetilde{\gamma}_{N,t}^{(k)} \right) \right| \leq C\kappa^{1/2} \tag{4.13}$$

where the constant C depends on $J^{(k)}$, but is independent of N, k or κ. Therefore, for fixed $k \geq 1$, $t \in \mathbb{R}$, $J^{(k)} \in \mathcal{K}_k$, we have

$$\begin{aligned} \left| \text{Tr } J^{(k)} \left(\gamma_{N,t}^{(k)} - |\varphi_t\rangle\langle\varphi_t|^{\otimes k} \right) \right| &\leq \left| \text{Tr } J^{(k)} \left(\gamma_{N,t}^{(k)} - \widetilde{\gamma}_{N,t}^{(k)} \right) \right| + \left| \text{Tr } J^{(k)} \left(\widetilde{\gamma}_{N,t}^{(k)} - |\varphi_t\rangle\langle\varphi_t|^{\otimes k} \right) \right| \\ &\leq C\kappa^{1/2} + \left| \text{Tr } J^{(k)} \left(\widetilde{\gamma}_{N,t}^{(k)} - |\varphi_t\rangle\langle\varphi_t|^{\otimes k} \right) \right| . \end{aligned} \tag{4.14}$$

Since $\kappa > 0$ was arbitrary, it follows from (4.12) that the l.h.s. of (4.14) converges to zero as $N \to \infty$. This completes the proof of Theorem 2.2. □

5 Energy Estimates

In this section we prove two energy estimates that are the most important new tools used in the proof of the main theorem. Both estimates concern the smoothness of the solution $\psi_{N,t}(\mathbf{x})$ of the Schrödinger equation (2.2), uniformly in N (for N large enough) and in $t \in \mathbb{R}$. However, due to the short scale structure of the interaction, V_N, uniform smoothness, say in the x_1 variable, cannot be expected near the collision points $|x_1 - x_j| \sim 1/N$, $j = 2, 3, \ldots, N$. The key observation is that $x_1 \to \psi_{N,t}(\mathbf{x})$ will nevertheless be smooth away from these regimes, whose total volume is negligible. For technical reasons, the excluded regime will be somewhat larger, $|x_1 - x_j| \geq \ell$, but still with $N\ell^3 \ll 1$. The same statement holds for the smoothness in an arbitrary but fixed number of variables, $x_1, \ldots, x_k$. This is the content of our second energy estimate Proposition 5.3.

Our first energy estimate, Proposition 3.1, controls only two derivatives, but it is more refined: it establishes smoothness of $\psi_{N,t}(\mathbf{x})$ in the x_i and x_j variables (for any fixed pair i, j) after removing the explicit short scale factor $(1 - w(x_i - x_j))$. This factor represents the short scale effect of the two body interaction $V_N(x_i - x_j)$ on the wave function and it is responsible for the emergence of the scattering length (2.9).

5.1 H_N^2 Energy Estimate

In this section, we shall prove Proposition 3.1. We first collect some important properties of $w(x)$ (2.12) in the following lemma. This lemma is an improved version of Lemma A.2 from [8]. By defining ρ somewhat differently (see (2.7)), we also correct a minor error in (A.6) and (A.19) of [8].

Lemma 5.1. *Suppose $V \geq 0$ is smooth, spherical symmetric, compactly supported and with scattering length a_0. Let*

$$\rho = \sup_{r \geq 0} r^2 V(r) + \int_0^\infty \mathrm{d}r \, r \, V(r) \tag{5.1}$$

and let $a = a_0/N$ be the scattering length of the rescaled potential V_N. Then the following hold with constants uniform in N.

i) There exists a constant $C_0 > 0$, which depends on the unscaled potential V, such that

$$C_0 \leq 1 - w(x) \leq 1 \qquad \text{for all } x \in \mathbb{R}^3. \tag{5.2}$$

Moreover, there exists a universal constant c such that

$$1 - c\rho \leq 1 - w(x) \leq 1 \qquad \text{for all } x \in \mathbb{R}^3 \,. \tag{5.3}$$

ii) Let R be such that $\operatorname{supp} V \subset \{x \in \mathbb{R}^3 : |x| \leq R\}$. Then

$$w(x) = \frac{a}{|x|} \qquad \text{for all } x \quad \text{with } |x| > R/N \,.$$

iii) There exist constants C_1, C_2, depending on V, such that

$$|\nabla w(x)| \leq C_1 N, \qquad |\nabla^2 w(x)| \leq C_2 N^2 \,, \qquad \text{for all } x \in \mathbb{R}^3 \,. \tag{5.4}$$

Moreover, there exists a universal constant c such that

$$|\nabla w(x)| \leq c \frac{a}{|x|^2}, \qquad |\nabla w(x)| \leq c \, \frac{\rho}{|x|}, \qquad |\nabla^2 w(x)| \leq c \, \frac{\rho}{|x|^2} \qquad \text{for all } x \in \mathbb{R}^3. \tag{5.5}$$

iv) We have

$$8\pi a = \int \mathrm{d}x\, V_N(x)(1-w(x))\,. \tag{5.6}$$

Proof. We prove part i) and iii) in Appendix D. Part ii) follows trivially by the definition of the scattering length a and by the fact that the potential has compact support. As for part iv), note that, due to the spherical symmetry of V_N and $w(x)$, with the notation $r = |x|$, the function $g(r) := rf(r) = r(1-w(r))$ satisfies

$$-g''(r) + \frac{1}{2}V_N(r)g(r) = 0\,.$$

By ii) of this lemma, $g(r) = r - a$ for $r > Ra$. We thus obtain

$$\begin{aligned}\int \mathrm{d}x\, V_N(x)(1-w(x)) &= 4\pi\int_0^\infty \mathrm{d}r\, r^2 V_N(r)(1-w(r)) = 8\pi\int_0^\infty \mathrm{d}r\, r\, g''(r)\\ &= 8\pi \lim_{\varrho\to\infty}\big(r\,g'(r) - g(r)\big)\,|_0^\varrho = 8\pi a\,.\end{aligned} \tag{5.7}$$

□

Proof of Proposition 3.1. For $j = 1, \dots, N$, we define

$$\mathfrak{h}_j := -\Delta_j + \frac{1}{2}\sum_{i\neq j} V_N(x_j - x_i). \tag{5.8}$$

Then we clearly have

$$H_N = \sum_{j=1}^N \mathfrak{h}_j.$$

Since ψ is symmetric with respect to permutations, we have

$$\langle\psi, H_N^2\psi\rangle = \sum_{i,j}^N \langle\psi, \mathfrak{h}_i\mathfrak{h}_j\psi\rangle = N(N-1)\langle\psi, \mathfrak{h}_1\mathfrak{h}_2\psi\rangle + N\langle\psi, \mathfrak{h}_1^2\psi\rangle \geq N(N-1)\langle\psi, \mathfrak{h}_1\mathfrak{h}_2\psi\rangle\,. \tag{5.9}$$

Of course, instead of the indices $1, 2$ we could have chosen any $i \neq j$.

We have

$$\mathfrak{h}_1\psi = -\Delta_1\psi + \frac{1}{2}V_N(x_1 - x_2)\psi + \frac{1}{2}\sum_{j\geq 3} V_N(x_1 - x_j)\psi \tag{5.10}$$

Next we write $\psi = (1 - w_{12})\phi_{12}$ and we observe that

$$-\Delta_1[(1-w_{12})\phi_{12}] = (1-w_{12})(-\Delta_1\phi_{12}) + 2\nabla w_{12}\,\nabla_1\phi_{12} + \Delta w_{12}\,\phi_{12}. \tag{5.11}$$

Hence

$$\begin{aligned}(1-w_{12})^{-1}\mathfrak{h}_1\big[(1-w_{12})\phi_{12}\big] =& -\Delta_1\phi_{12} + 2\frac{\nabla w_{12}}{1-w_{12}}\nabla_1\phi_{12}\\ &+ \frac{(-\Delta_1 + (1/2)V_N(x_1-x_2))\,(1-w_{12})}{1-w_{12}}\phi_{12}\\ &+ \frac{1}{2}\sum_{j\geq 3} V_N(x_1 - x_j)\phi_{12}.\end{aligned} \tag{5.12}$$

Using the definition of $w(x)$ (see (2.12)), we obtain

$$(1-w_{12})^{-1}\mathfrak{h}_1\big[(1-w_{12})\phi_{12}\big] = L_1\phi_{12} + \frac{1}{2}\sum_{j\geq 3} V_N(x_1-x_j)\phi_{12} \tag{5.13}$$

where we defined

$$L_1 := -\Delta_1 + 2\frac{\nabla w_{12}}{1-w_{12}}\nabla_1 \,.$$

Note that this operator is symmetric with respect to the measure $(1-w_{12})^2 \mathrm{d}\mathbf{x}$, i.e.

$$\int (1-w_{12})^2 \overline{\phi}\,(L_1\chi) = \int (1-w_{12})^2\,(L_1\overline{\phi})\,\chi = \int (1-w_{12})^2\,\nabla_1\overline{\phi}\nabla_1\chi\,. \tag{5.14}$$

Analogously to (5.13), we have

$$(1-w_{12})^{-1}\mathfrak{h}_2\big[(1-w_{12})\phi_{12}\big] = L_2\phi_{12} + \frac{1}{2}\sum_{j\geq 3} V_N(x_2-x_j)\phi_{12} \tag{5.15}$$

with

$$L_2 = -\Delta_2 + 2\frac{\nabla w_{21}}{1-w_{12}}\nabla_2\,.$$

Therefore, from (5.9) we find

$$\begin{aligned}
\langle\psi, H_N^2\psi\rangle &\geq N(N-1)\int (1-w_{12})^2 \left(L_1 + \frac{1}{2}\sum_{j\geq 3} V_N(x_1-x_j)\right)\overline{\phi}_{12}\left(L_2 + \frac{1}{2}\sum_{j\geq 3} V_N(x_2-x_j)\right)\phi_{12} \\
&= N(N-1)\int (1-w_{12})^2\, L_1\overline{\phi}_{12}\, L_2\phi_{12} \\
&\quad + \frac{N(N-1)}{2}\sum_{j\geq 3}\int (1-w_{12})^2\,\left\{V_N(x_2-x_j)\; L_1\overline{\phi}_{12}\phi_{12} + V_N(x_1-x_j)\overline{\phi}_{12}L_2\phi_{12}\right\} \\
&\quad + \frac{N(N-1)}{4}\sum_{i,j\geq 3}\int (1-w_{12})^2\, V_N(x_1-x_j)V_N(x_2-x_i)|\phi_{12}|^2 \\
&= N(N-1)\int (1-w_{12})^2\, L_1\overline{\phi}_{12}\, L_2\phi_{12} \\
&\quad + \frac{N(N-1)}{2}\sum_{j\geq 3}\int (1-w_{12})^2\,\left\{V_N(x_1-x_j)|\nabla_2\phi_{12}|^2 + V_N(x_2-x_j)|\nabla_1\phi_{12}|^2\right\} \\
&\quad + \frac{N(N-1)}{4}\sum_{i,j\geq 3}\int (1-w_{12})^2\, V_N(x_1-x_j)V_N(x_2-x_i)|\phi_{12}|^2 \\
&\geq N(N-1)\int (1-w_{12})^2\, L_1\overline{\phi}_{12}\, L_2\phi_{12}.
\end{aligned} \tag{5.16}$$

Here we used that the potential is positive and that the sum $\sum_{j\geq 3} V_N(x_1-x_j)$ is independent of x_2 (and analogously $\sum_{j\geq 3} V_N(x_2-x_j)$ is independent of x_1).

From (5.16) we find

$$\begin{aligned}
\langle\psi, H_N^2\psi\rangle &\geq N(N-1)\int (1-w_{12})^2\,\nabla_1\overline{\phi}_{12}\nabla_1\, L_2\phi_{12} \\
&= N(N-1)\int (1-w_{12})^2\,|\nabla_1\nabla_2\,\phi_{12}|^2 + N(N-1)\int (1-w_{12})^2\,\nabla_1\,\overline{\phi}_{12}[\nabla_1, L_2]\phi_{12}\,.
\end{aligned} \tag{5.17}$$

To control the last term, we note that

$$\left|\left[\nabla_1, \frac{\nabla w_{21}}{1-w_{21}}\right]\right| \leq \frac{\left|\nabla^2 w_{21}\right|}{1-w_{12}} + \left(\frac{\nabla w_{12}}{1-w_{12}}\right)^2 \leq c\rho \frac{1}{|x_1-x_2|^2}$$

by (5.3) and (5.5), for ρ small enough. Therefore we have

$$\begin{aligned}\left|\int (1-w_{12})^2\, \nabla_1\phi_{12}[\nabla_1, L_2]\phi_{12}\right| &\leq c\rho \int (1-w_{12})^2\, \frac{1}{|x_1-x_2|^2}|\nabla_1\phi_{12}||\nabla_2\phi_{12}| \\ &\leq c\rho \int \frac{1}{|x_1-x_2|^2}|\nabla_1\phi_{12}|^2 \\ &\leq c\rho \int |\nabla_1\nabla_2\,\phi_{12}|^2 \\ &\leq c\rho \int (1-w_{12})^2\, |\nabla_1\nabla_2\phi_{12}|^2\end{aligned} \tag{5.18}$$

where we used (5.3) to remove and then reinsert the factor $(1-w_{12})^2$ (assuming ρ is small enough), and where we used the Hardy inequality to control the $1/|x|^2$ singularity. From (5.17) we have

$$\langle \psi, H_N^2 \psi\rangle \geq (1-c\rho)N(N-1)\int (1-w_{12})^2\, |\nabla_1\nabla_2\phi_{12}|^2. \tag{5.19}$$

This completes the proof of the Proposition 3.1. □

For fixed $2 \leq k \leq N$ and $i, j \leq k$, with $i \neq j$, we define the densities $\gamma^{(k)}_{N,i,j,t}$ by

$$\gamma^{(k)}_{N,i,j,t} := (1-w_{ij})^{-1}\gamma^{(k)}_{N,t}(1-w_{ij})^{-1}\,, \tag{5.20}$$

where $(1-w_{ij})^{-1} = (1-w(x_i-x_j))^{-1}$ is viewed as a multiplication operator. The kernel of $\gamma^{(k)}_{N,i,j,t}$ is given by

$$\gamma^{(k)}_{N,i,j,t}(\mathbf{x}_k;\mathbf{x}'_k) = (1-w(x_i-x_j))^{-1}\,(1-w(x'_i-x'_j))^{-1}\gamma^{(k)}_{N,t}(\mathbf{x}_k;\mathbf{x}'_k)\,. \tag{5.21}$$

Then, for every k, and every $i, j \leq k$, with $i \neq j$, $\gamma^{(k)}_{N,i,j,t}$ is a positive operator, with $\mathrm{Tr}\,\gamma^{(k)}_{N,i,j,t} \leq C$, uniformly in N, t.

Proposition 5.2 (A-priori bounds for $\gamma^{(k)}_{N,i,j,t}$)**.** *For any sufficiently small ρ, there exists a constant $C > 0$, such that*

$$Tr\,(1-\Delta_i)(1-\Delta_j)\,\gamma^{(k)}_{N,i,j,t} \leq C \tag{5.22}$$

for all $t \in \mathbb{R}$, $2 \leq k \leq N$, $i, j \leq k$, $i \neq j$, and for all N large enough.

Proof. For fixed $i \neq j$ we define the function $\phi_{i,j,t}$ by $\psi_{N,t} = (1-w_{ij})\phi_{i,j,t}$ (the N dependence of $\phi_{i,j,t}$ is omitted in the notation). Then we observe that

$$\mathrm{Tr}\,(1-\Delta_i)(1-\Delta_j)\,\gamma^{(k)}_{N,i,j,t} = \|S_iS_j\,\phi_{i,j,t}\|^2 = \|\phi_{i,j,t}\|^2 + 2\|\nabla_i\phi_{i,j,t}\|^2 + \|\nabla_i\nabla_j\phi_{i,j,t}\|^2 \tag{5.23}$$

with $S_n := (1-\Delta_n)^{1/2}$. Next we note that, by (5.3),

$$\|\phi_{i,j,t}\|^2 = \int \mathrm{d}\mathbf{x}\,|\phi_{i,j,t}(\mathbf{x})|^2 \leq C\int \mathrm{d}\mathbf{x}\,|\psi_{N,t}(\mathbf{x})|^2 \leq C \tag{5.24}$$

uniformly in N and t. Moreover

$$\begin{aligned}\|\nabla_i\phi_{i,j,t}\|^2 &= \int \mathrm{d}\mathbf{x}\, \left|\nabla_i \frac{\psi_{N,t}(\mathbf{x})}{1-w(x_i-x_j)}\right|^2 \\ &\leq \int \mathrm{d}\mathbf{x}\, \frac{1}{(1-w(x_i-x_j))^2}|\nabla_i\psi_{N,t}(\mathbf{x})|^2 + \int \mathrm{d}\mathbf{x}\, \left|\frac{\nabla_i w(x_i-x_j)}{(1-w(x_i-x_j))^2}\right|^2 |\psi_{N,t}(\mathbf{x})|^2 \\ &\leq C\int \mathrm{d}\mathbf{x}\, |\nabla_i\psi_{N,t}(\mathbf{x})|^2 + C\int \mathrm{d}\mathbf{x}\, \frac{1}{|x_i-x_j|^2}|\psi_{N,t}(\mathbf{x})|^2 \\ &\leq C\int \mathrm{d}\mathbf{x}\, |\nabla_i\psi_{N,t}(\mathbf{x})|^2\,.\end{aligned} \tag{5.25}$$

where we used (5.2), (5.5) and Hardy inequality. Next we note that, for every $i = 1, \dots, N$,

$$\langle \psi_{N,t}, H_N\, \psi_{N,t}\rangle \geq N\langle \psi_{N,t}, \Delta_i \psi_{N,t}\rangle = N\int |\nabla_i\psi_{N,t}|^2\,. \tag{5.26}$$

Therefore, from (5.25),

$$\|\nabla_i\phi_{i,j,t}\|^2 \leq\ CN^{-1}\langle \psi_{N,t}, H_N\, \psi_{N,t}\rangle = CN^{-1}\langle \psi_N, H_N\, \psi_N\rangle \leq C \tag{5.27}$$

by (2.13) and by conservation of energy. Finally, to bound the last term on the r.h.s. of (5.23), we note that, for a sufficiently small ρ,

$$\begin{aligned}\|\nabla_i\nabla_j\phi_{i,j,t}\|^2 &\leq C\int \mathrm{d}\mathbf{x}\, (1-w(x_i-x_j))^2\, |\nabla_i\nabla_j\phi_{i,j,t}(\mathbf{x})|^2 \\ &\leq \frac{C}{N(N-1)}\langle \psi_{N,t}, H_N^2\psi_{N,t}\rangle \\ &= \frac{C}{N(N-1)}\langle \psi_N, H_N^2\psi_N\rangle \leq C\end{aligned} \tag{5.28}$$

for all N large enough. Here we used (5.2) in the first line, Proposition 3.1 in the second line, the conservation of H_N^2 in the third line, and the assumption (2.13) in the last inequality. Proposition 5.2 now follows from (5.23), (5.24), (5.27), and (5.28). □

5.2 Higher Order Energy Estimates

We will choose a cutoff length scale ℓ. For technical reasons, we will have to work with exponentially decaying cutoff functions, so we set

$$h(x) := e^{-\frac{\sqrt{x^2+\ell^2}}{\ell}}. \tag{5.29}$$

Note that $h \simeq 0$ if $|x| \gg \ell$, and $h \simeq e^{-1}$ if $|x| \ll \ell$. For $i = 1, \dots, N$ we define the cutoff function

$$\theta_i(\mathbf{x}) := \exp\left(-\frac{1}{\ell^\varepsilon}\sum_{j\neq i} h(x_i - x_j)\right) \tag{5.30}$$

for some $\varepsilon > 0$. Note that $\theta_i(\mathbf{x})$ is exponentially small if there is at least one other particle at distance of order ℓ from x_i, while $\theta_i(\mathbf{x})$ is exponentially close to 1 if there is no other particle near x_i (on the length scale ℓ).

As for the choice of ℓ, to make sure that the presence of particles at distances smaller than ℓ from x_i is a rare event, we will need to assume $N\ell^3 \ll 1$. This condition is not used in Proposition

5.3 below, but if $N\ell^3 \gg 1$, then our estimates were empty in the limit $N \to \infty$ as the r.h.s. of the estimate (5.33) below tended to zero. On the other hand, choosing ℓ too small makes the price to pay for localizing the kinetic energy on the length scale ℓ too high. In Proposition 5.3 we will actually have to assume $N\ell^2 \gg 1$.

Next we define

$$\theta_i^{(n)}(\mathbf{x}) := \theta_i(\mathbf{x})^{2^n} = \exp\left(-\frac{2^n}{\ell^\varepsilon}\sum_{j\neq i} h(x_i - x_j)\right) \tag{5.31}$$

and their cumulative versions, for $n, k \in \mathbb{N}$,

$$\Theta_k^{(n)}(\mathbf{x}) := \theta_1^{(n)}(\mathbf{x}) \dots \theta_k^{(n)}(\mathbf{x}) = \exp\left(-\frac{2^n}{\ell^\varepsilon}\sum_{i\leq k}\sum_{j\neq i} h(x_i - x_j)\right) . \tag{5.32}$$

To cover all cases in one formula, we introduce the notation $\Theta_k^{(n)} = 1$ for any $k \leq 0$, $n \in \mathbb{Z}$. We will need to use the functions $\theta_i^{(n)}$ (instead of $\theta_i(\mathbf{x})$) to take into account the deterioration of the kinetic energy localization estimates. For example the bound $|\nabla_j \theta_i(\mathbf{x})| \leq C\ell^{-1}\theta_i(\mathbf{x})$ is wrong, while

$$|\nabla_j \theta_i^{(n)}(\mathbf{x})| \leq C\ell^{-1}\theta_i^{(n-1)}(\mathbf{x})$$

is correct and similar bounds hold for $\Theta_k^{(n)}$. This, and other important properties of the function $\Theta_k^{(n)}$, used throughout the proof of Proposition 5.3 are collected in Lemma A.1 of the Appendix.

Proposition 5.3 (H^k energy estimates)**.** *Suppose $\ell \gg N^{-1/2}$ and that ρ (from (2.7)) is small enough. Then for $C_0 > 0$ sufficiently small (depending on the constant $(1 - c\rho)$ in Proposition 3.1) and for every integer $k \geq 1$ there exists $N_0 = N_0(k, C_0)$ such that*

$$\begin{aligned}\langle \psi, (H_N + N)^k \psi\rangle \geq C_0^k N^k &\int \Theta_{k-1}^{(k)} |\nabla_1 \dots \nabla_k \psi|^2 \\ &+ C_0^k N^{k-1} \int \Theta_{k-1}^{(k)} |\nabla_1^2 \nabla_2 \dots \nabla_{k-1}\psi|^2 \\ &+ C_0^k N^{k+1} \int \Theta_{k-1}^{(k)}(\mathbf{x})\, V_N(x_k - x_{k+1})\, |\nabla_1 \dots \nabla_{k-1}\psi(\mathbf{x})|^2 \mathrm{d}\mathbf{x}\end{aligned} \tag{5.33}$$

for every wave function $\psi \in L^2_s(\mathbb{R}^{3N})$ and for every $N \geq N_0$.

In order to keep the exposition of the main ideas as clear as possible, we defer the proof of this proposition, which is quite long and technical, to Section 9, at the end of the paper.

6 Compactness of the Marginal Densities

In this section we prove the compactness of the sequence $\Gamma_{N,t} = \{\gamma_{N,t}^{(k)}\}_{k\geq 1}$ w.r.t. the topology τ_{prod}. (See Section 4 for the definition of τ_{prod} and recall the convention that $\gamma_{N,t}^{(k)} = 0$ if $k > N$.) Moreover, in Proposition 6.3, we prove important a-priori bounds on any limit point $\Gamma_{\infty,t}$ of the sequence $\Gamma_{N,t}$.

Theorem 6.1. *Assume that ρ is small enough and fix an arbitrary $T > 0$. Suppose that $\Gamma_{N,t} = \{\gamma_{N,t}^{(k)}\}_{k\geq 1}$ is the family of marginal density associated with the solution $\psi_{N,t}$ of the Schrödinger equation (2.2), and that (2.13) is satisfied. Then $\Gamma_{N,t} \in \bigoplus_{k\geq 1} C([0,T], \mathcal{L}^1_k)$ Moreover the sequence*

$\Gamma_{N,t} \in \bigoplus_{k\geq 1} C([0,T],\mathcal{L}^1_k)$ *is compact with respect to the product topology* τ_{prod} *generated by the metrics* $\widehat{\eta}_k$ *(defined in Section 4). For any limit point* $\Gamma_{\infty,t} = \{\gamma^{(k)}_{\infty,t}\}_{k\geq 1}$, $\gamma^{(k)}_{\infty,t}$ *is symmetric w.r.t. permutations,* $\gamma^{(k)}_{\infty,t} \geq 0$, *and*

$$Tr\, \gamma^{(k)}_{\infty,t} \leq 1 \tag{6.1}$$

for every $k \geq 1$.

Proof. By a standard "choice of the diagonal subsequence"-argument it is enough to prove the compactness of $\gamma^{(k)}_{N,t}$, for fixed $k \geq 1$, with respect to the metric $\widehat{\eta}_k$. In order to prove the compactness of $\gamma^{(k)}_{N,t}$ with respect to the metric $\widehat{\eta}_k$, we show the equicontinuity of $\gamma^{(k)}_{N,t}$ with respect to the metric η_k. The following lemma gives a useful criterium to prove the equicontinuity of a sequence in $C([0,T],\mathcal{L}^1_k)$. Its proof is very similar to the proof of Lemma 9.2 in [8]; the only difference is that here we keep k fixed and we consider sequences in $\mathcal{L}^1_k$, while in [8] we considered equicontinuity in the direct sum $C([0,T],\mathcal{H}) = \oplus_{k\geq 1} C([0,T],\mathcal{H}_k)$ over all $k \geq 1$, for some Sobolev space $\mathcal{H}_k$.

Lemma 6.2. *Fix* $k \in \mathbb{N}$ *and* $T > 0$. *A sequence* $\gamma^{(k)}_{N,t} \in \mathcal{L}^1_k$, $N = k, k+1, \ldots$, *with* $\gamma^{(k)}_{N,t} \geq 0$ *and* $Tr\, \gamma^{(k)}_{N,t} = 1$ *for all* $t \in [0,T]$ *and* $N \geq k$, *is equicontinuous in* $C([0,T],\mathcal{L}^1_k)$ *with respect to the metric* η_k, *if and only if there exists a dense subset* $\mathcal{J}_k$ *of* $\mathcal{K}_k$ *such that for any* $J^{(k)} \in \mathcal{J}_k$ *and for every* $\varepsilon > 0$ *there exists a* $\delta > 0$ *such that*

$$\sup_{N\geq 1} \left| Tr\, J^{(k)} \left(\gamma^{(k)}_{N,t} - \gamma^{(k)}_{N,s} \right) \right| \leq \varepsilon \tag{6.2}$$

for all $t, s \in [0,T]$ *with* $|t-s| \leq \delta$. $\square$

For the proof of the equicontinuity of $\gamma^{(k)}_{N,t}$ with respect to the metric η_k, we will choose the set $\mathcal{J}_k$ in Lemma 6.2 to consist of all $J^{(k)} \in \mathcal{K}_k$ such that $S_i S_j J^{(k)} S_i S_j$ is bounded, for all $i \neq j$, and $i, j \leq k$. We recall the notation $S_n = (1-\Delta_n)^{1/2}$.

Rewriting the BBGKY hierarchy (3.30) in integral form we obtain for any $s \leq t$

$$\begin{aligned} \gamma^{(k)}_{N,t} = \gamma^{(k)}_{N,s} &- i \sum_{j=1}^{k} \int_s^t \mathrm{d}r\, [-\Delta_j, \gamma^{(k)}_{N,r}] - i \sum_{i<j}^{k} \int_s^t \mathrm{d}r\, [V_N(x_i - x_j), \gamma^{(k)}_{N,r}] \\ &- i(N-k) \sum_{j=1}^{k} \int_s^t \mathrm{d}r\, \mathrm{Tr}_{k+1} [V_N(x_j - x_{k+1}), \gamma^{(k+1)}_{N,r}]\,. \end{aligned} \tag{6.3}$$

Multiplying the last equation with $J^{(k)} \in \mathcal{J}_k$ and taking the trace we get the bound (recall the

definition (5.20) of the densities $\gamma^{(k)}_{N,i,j,t}$)

$$\begin{aligned}
\left|\mathrm{Tr}\, J^{(k)}\left(\gamma^{(k)}_{N,t}-\gamma^{(k)}_{N,s}\right)\right| &\leq \sum_{j=1}^{k}\int_s^t \mathrm{d}r \left|\mathrm{Tr}\, \left(S_j^{-1}J^{(k)}S_j - S_jJ^{(k)}S_j^{-1}\right)\, S_j\gamma^{(k)}_{N,r}S_j\right| \\
&+ \sum_{i<j}^{k}\int_s^t \mathrm{d}r \left|\mathrm{Tr}\, \left(S_iS_jJ^{(k)}S_iS_j\right)\left(S_i^{-1}S_j^{-1}V_N(x_i-x_j)(1-w_{ij})S_i^{-1}S_j^{-1}\right)\right. \\
&\qquad \left.\times \left(S_iS_j\gamma^{(k)}_{N,i,j,r}S_iS_j\right)\left(S_i^{-1}S_j^{-1}(1-w_{ij})S_i^{-1}S_j^{-1}\right)\right| \\
&+ \sum_{i<j}^{k}\int_s^t \mathrm{d}r \left|\mathrm{Tr}\, \left(S_iS_jJ^{(k)}S_iS_j\right)\left(S_i^{-1}S_j^{-1}(1-w_{ij})S_i^{-1}S_j^{-1}\right)\right. \\
&\qquad \left.\times \left(S_iS_j\gamma^{(k)}_{N,i,j,r}S_iS_j\right)\left(S_i^{-1}S_j^{-1}V_N(x_i-x_j)(1-w_{ij})S_i^{-1}S_j^{-1}\right)\right| \\
&+ \left(1-\frac{k}{N}\right)\sum_{j=1}^{k}\int_s^t \mathrm{d}r \left|\mathrm{Tr}\, \left(S_jJ^{(k)}S_j\right)\, \left(S_j^{-1}S_{k+1}^{-1}NV_N(x_j-x_{k+1})(1-w_{j,k+1})S_{k+1}^{-1}S_j^{-1}\right)\right. \\
&\qquad \left.\times \left(S_{k+1}S_j\gamma^{(k+1)}_{N,j,k+1,r}S_jS_{k+1}\right)\left(S_j^{-1}S_{k+1}^{-1}(1-w_{j,k+1})S_{k+1}S_j^{-1}\right)\right| \\
&+ \left(1-\frac{k}{N}\right)\sum_{j=1}^{k}\int_s^t \mathrm{d}r \left|\mathrm{Tr}\, \left(S_jJ^{(k)}S_j\right)\left(S_j^{-1}S_{k+1}(1-w_{j,k+1})S_{k+1}^{-1}S_j^{-1}\right)\right. \\
&\qquad \left.\times \left(S_{k+1}S_j\gamma^{(k+1)}_{N,j,k+1,r}S_jS_{k+1}\right)\, \left(S_j^{-1}S_{k+1}^{-1}NV_N(x_j-x_{k+1})(1-w_{j,k+1})S_{k+1}^{-1}S_j^{-1}\right)\right| .
\end{aligned} \tag{6.4}$$

Here we used that S_{k+1} commutes with $J^{(k)}$. Next we observe that (see Lemma 6.4 below),

$$\|S_i^{-1}S_j^{-1}NV_N(x_i-x_j)(1-w_{ij})S_i^{-1}S_j^{-1}\| \leq CN\int V_N\,(1-w) \leq C\,, \tag{6.5}$$

by part iv) of Lemma 5.1. Moreover

$$\|S_i^{-1}S_j^{-1}(1-w_{ij})S_i^{-1}S_j^{-1}\| \leq C \tag{6.6}$$

and

$$\begin{aligned}
\|S_j^{-1}S_{k+1}^{-1}(1-w_{j,k+1})S_{k+1}S_j^{-1}\| &\leq \left\|S_j^{-1}S_{k+1}^{-1}(1-w_{j,k+1})S_{k+1}^2S_j^{-2}(1-w_{j,k+1})S_{k+1}^{-1}S_j^{-1}\right\|^{\frac12} \\
&\leq C + \left\|S_j^{-1}S_{k+1}^{-1}\nabla_{k+1}(1-w_{j,k+1})S_j^{-2}(1-w_{j,k+1})\nabla_{k+1}S_{k+1}^{-1}S_j^{-1}\right\|^{\frac12} \\
&\quad + \left\|S_j^{-1}S_{k+1}^{-1}(\nabla_{k+1}w_{j,k+1})S_j^{-2}(\nabla_{k+1}w_{j,k+1})S_{k+1}^{-1}S_j^{-1}\right\|^{\frac12} \\
&\leq C + \left\|S_j^{-1}S_{k+1}^{-1}(\nabla w_{j,k+1})^2S_{k+1}^{-1}S_j^{-1}\right\|^{\frac12} \leq C
\end{aligned} \tag{6.7}$$

In the last step we used the second bound in (5.5). Since $J^{(k)}\in\mathcal{J}_k$ is such that $\|S_iS_jJ^{(k)}S_iS_j\|\leq C$ for all $i,j=1,\ldots,k$, it follows from (6.4)–(6.7) that

$$\left|\mathrm{Tr}\, J^{(k)}\left(\gamma^{(k)}_{N,t}-\gamma^{(k)}_{N,s}\right)\right| \leq C_k(t-s)\max_{n=k,k+1}\max_{i\neq j,i,j\leq n}\sup_{r\in[s,t]}\mathrm{Tr}\, \left|S_iS_j\,\gamma^{(n)}_{N,i,j,r}S_iS_j\right| \tag{6.8}$$

for a constant C_k depending on k and on $J^{(k)}$, but independent of t, s, N. From Proposition 5.2, and from the fact that the subset $\mathcal{J}^{(k)}$ is dense in $\mathcal{K}_k$, it follows that the sequence $\gamma^{(k)}_{N,t} \in C([0,T], \mathcal{L}^1_k)$ is equicontinuous. Since, moreover, Tr $\gamma^{(k)}_{N,t} = 1$ uniformly in $t \in [0,T]$ and N, the compactness of the sequence $\gamma^{(k)}_{N,t}$ w.r.t. the metric $\widehat{\eta}_k$ follows from the Arzela-Ascoli theorem. This proves the compactness of $\Gamma_{N,t} = \{\gamma^{(k)}_{N,t}\}_{k\geq 1} \in \bigoplus_{k\geq 1} C([0,T], \mathcal{L}^1_k)$ with respect to the product topology τ_{prod}.

Now suppose that $\Gamma_{\infty,t} = \{\gamma^{(k)}_{\infty,t}\}_{k\geq 1} \in \bigoplus_{k\geq 1} C([0,T], \mathcal{L}^1_k)$ is a limit point of $\Gamma_{N,t}$ with respect to τ_{prod}. Then, for any $k \geq 1$, $\gamma^{(k)}_{\infty,t} \in C([0,T], \mathcal{L}^1_k)$ is a limit point of $\gamma^{(k)}_{N,t}$. The bound

$$\mathrm{Tr} \left| \gamma^{(k)}_{\infty,t} \right| \leq 1$$

follows because the norm can only drop in the weak limit.

To prove that $\gamma^{(k)}_{\infty,t}$ is non-negative, we observe that, for an arbitrary $\varphi \in L^2(\mathbb{R}^{3k})$ with $\|\varphi\| = 1$, the orthogonal projection $P_\varphi = |\varphi\rangle\langle\varphi|$ is in $\mathcal{K}_k$ and therefore we have

$$\langle \varphi, \gamma^{(k)}_{\infty,t} \varphi \rangle = \mathrm{Tr}\, P_\varphi \gamma^{(k)}_{\infty,t} = \lim_{j\to\infty} \mathrm{Tr}\, P_\varphi \gamma^{(k)}_{N_j,t} = \lim_{j\to\infty} \langle \varphi, \gamma^{(k)}_{N_j,t} \varphi \rangle \geq 0\,, \tag{6.9}$$

for an appropriate subsequence N_j with $N_j \to \infty$ as $j \to \infty$.

Similarly, the symmetry of $\gamma^{(k)}_{\infty,t}$ w.r.t. permutations is inherited from the symmetry of $\gamma^{(k)}_{N,t}$ for finite N. For a permutation $\pi \in \mathcal{S}_k$, we denote by Ξ_π the operator on $L^2(\mathbb{R}^{3k})$ defined by

$$\Xi_\pi \varphi(x_1, \dots x_k) = \varphi(x_{\pi 1}, \dots, x_{\pi k})\,.$$

Then the permutation symmetry of $\gamma^{(k)}_{\infty,t}$ is defined by

$$\Xi_\pi \gamma^{(k)}_{\infty,t} \Xi^{-1}_\pi = \gamma^{(k)}_{\infty,t} \tag{6.10}$$

for every $\pi \in \mathcal{S}_k$. To prove (6.10), we note that, for an arbitrary $J^{(k)} \in \mathcal{K}_k$ and a permutation $\pi \in \mathcal{S}_k$, we have, for an appropriate subsequence $N_j \to \infty$, as $j \to \infty$,

$$\begin{aligned} \mathrm{Tr}\, J^{(k)} \gamma^{(k)}_{\infty,t} &= \lim_{j\to\infty} J^{(k)} \gamma^{(k)}_{N_j,t} = \lim_{j\to\infty} \mathrm{Tr}\, J^{(k)} \Xi_\pi \gamma^{(k)}_{N_j,t} \Xi^{-1}_\pi = \lim_{j\to\infty} \mathrm{Tr}\, \Xi^{-1}_\pi J^{(k)} \Xi_\pi \gamma^{(k)}_{N_j,t} \\ &= \mathrm{Tr}\, \Xi^{-1}_\pi J^{(k)} \Xi_\pi \gamma^{(k)}_{\infty,t} = \mathrm{Tr}\, J^{(k)} \Xi_\pi \gamma^{(k)}_{\infty,t} \Xi^{-1}_\pi\,, \end{aligned} \tag{6.11}$$

where we used that, since $J^{(k)} \in \mathcal{K}_k$, also $\Xi^{-1}_\pi J^{(k)} \Xi_\pi \in \mathcal{K}_k$. □

In the next proposition we prove important a-priori bounds on the limit points $\Gamma_{\infty,t}$. These bounds are essential in the proof of the uniqueness of the solution to the infinite hierarchy (4.4), in Theorem 4.1.

Proposition 6.3. *Suppose that ρ is small enough, and assume that (2.13) is satisfied. Let $\Gamma_{\infty,t} = \{\gamma^{(k)}_{\infty,t}\}_{k\geq 1} \in \bigoplus_{k\geq 1} C([0,T], \mathcal{L}^1_k)$ is a limit point of the sequence $\Gamma_{N,t} = \{\gamma^{(k)}_{N,t}\}^N_{k=1}$ w.r.t. the product topology τ_{prod}. Then $\gamma^{(k)}_{\infty,t}$ (has a version which) satisfies*

$$Tr\,(1-\Delta_1)\dots(1-\Delta_k)\gamma^{(k)}_{\infty,t} \leq C_1^k \tag{6.12}$$

for a constant C_1 independent of $t \in [0,T]$ and $k \geq 1$.

Proof. We fix ℓ as a function of N, such that $N\ell^2 \gg 1$, and $N\ell^3 \ll 1$. Moreover we fix $\varepsilon > 0$ so small that $N\ell^{3-\varepsilon} \ll 1$. With this choice of ℓ and ε, we construct, for integer n, k the cutoff functions $\Theta_k^{(n)}(\mathbf{x})$ as in (5.32). For $k \in \mathbb{N}$, we will use the notation

$$D_k := \nabla_1 \dots \nabla_k, \qquad D'_k := \nabla'_1 \dots \nabla'_k, \qquad \text{with} \quad \nabla'_j = \nabla_{x'_j} .$$

We also set $D_k = I$ for $k \leq 0$ to cover all cases in a single formula. From Proposition 5.3, it follows that, for any fixed $k \geq 1$,

$$\begin{aligned} \int \Theta_{k-1}^{(k)} \, |D_k \psi_{N,t}|^2 &\leq \frac{1}{C_0^k N^k} \langle \psi_{N,t}, (H_N + N)^k \psi_{N,t} \rangle \\ &= \frac{1}{C_0^k N^k} \langle \psi_{N,0}, (H_N + N)^k \psi_{N,0} \rangle \leq C_2^k \end{aligned} \tag{6.13}$$

for any N large enough (depending only on k). In the last inequality we applied the assumption (2.13).

For $k = 1, \dots, N$, we define the densities $U_{N,t}^{(k)}$ by their kernels

$$U_{N,t}^{(k)}(\mathbf{x}_k; \mathbf{x}'_k) := \int \mathrm{d}\mathbf{x}_{N-k} \; \Theta_k^{(k)}(\mathbf{x}_k, \mathbf{x}_{N-k}) \Theta_k^{(k)}(\mathbf{x}'_k, \mathbf{x}_{N-k}) D_k \psi_{N,t}(\mathbf{x}_k, \mathbf{x}_{N-k}) \; D'_k \overline{\psi}_{N,t}(\mathbf{x}_k, \mathbf{x}_{N-k}). \tag{6.14}$$

Note that the operator $U_{N,t}^{(k)}$ is the k-particle marginal density associated with the N-body wave function $\Theta_k^{(k)}(\mathbf{x}) D_k \psi_{N,t}(\mathbf{x})$. Therefore $U_{N,t}^{(k)} \geq 0$. Moreover, it follows from (6.13) that, for N large enough,

$$\mathrm{Tr} \; U_{N,t}^{(k)} = \int \left[\Theta_k^{(k)}\right]^2 |D_k \, \psi_{N,t}|^2 \leq \int \Theta_{k-1}^{(k)} \, |D_k \psi_{N,t}|^2 \leq C_2^k \, . \tag{6.15}$$

It follows from (6.15) that for every fixed integer $k \geq 1$, and for every $t \in [0, T]$, the sequence $U_{N,t}^{(k)}$ is compact w.r.t. the weak* topology of $\mathcal{L}_k^1$. Moreover, if $U_{\infty,t}^{(k)}$ denotes an arbitrary limit point of $U_{N,t}^{(k)}$, then

$$\mathrm{Tr} \; U_{\infty,t}^{(k)} \leq C_2^k \, . \tag{6.16}$$

Next we assume that $\gamma_{\infty,t}^{(k)} \in C([0,T], \mathcal{L}_k^1)$ is a limit point of $\gamma_{N,t}^{(k)}$ w.r.t. to the topology $\widehat{\eta}_k$. It follows that for any fixed $t \in [0,T]$, $\gamma_{\infty,t}^{(k)}$ is a limit point of $\gamma_{N,t}^{(k)}$ w.r.t. the weak* topology of $\mathcal{L}_k^1$. Because of the compactness of the sequence $U_{N,t}^{(k)}$ w.r.t. the weak * topology of $\mathcal{L}_k^1$, we can assume, by passing to a common subsequence N_i, that there exists a limit point $U_{\infty,t}^{(k)} \in \mathcal{L}_k^1$ of $U_{N,t}^{(k)}$ such that,

$$\mathrm{Tr} \; J^{(k)} \, \gamma_{N_i,t}^{(k)} \to \mathrm{Tr} \; J^{(k)} \, \gamma_{\infty,t}^{(k)} \tag{6.17}$$

and

$$\mathrm{Tr} \; J^{(k)} \, U_{N_i,t}^{(k)} \to \mathrm{Tr} \; J^{(k)} \, U_{\infty,t}^{(k)} \tag{6.18}$$

for every $J^{(k)} \in \mathcal{K}_k$. For notational simplicity, we will drop the index i, but keep in mind that the limits hold only along a subsequence.

Next we fix $J^{(k)} \in \mathcal{K}_k$ such that $\nabla_1 \dots \nabla_k J^{(k)} \nabla_k^* \dots \nabla_1^*$ is compact and such that

$$\begin{aligned} \sup_{\mathbf{x}_k} \int \mathrm{d}\mathbf{x}'_k \, \sum_{b=0}^{4} |\nabla_{x'_n}^b \nabla_{i_1} \dots \nabla_{i_j} \nabla'_{r_1} \dots \nabla'_{r_m} J^{(k)}(\mathbf{x}_k; \mathbf{x}'_k)| < \infty \\ \sup_{\mathbf{x}'_k} \int \mathrm{d}\mathbf{x}_k \, \sum_{b=0}^{4} |\nabla_{x_n}^b \nabla_{i_1} \dots \nabla_{i_j} \nabla'_{r_1} \dots \nabla'_{r_m} J^{(k)}(\mathbf{x}_k; \mathbf{x}'_k)| < \infty \end{aligned} \tag{6.19}$$

for every $j, m, n \leq k$, and $(i_1, \dots i_j), (r_1, \dots, r_m) \subset \{1, 2, \dots, k\}$. Then we have, applying (6.17) to the derivatives of $J^{(k)}$,

$$\mathrm{Tr}\, \nabla_1 \dots \nabla_k J^{(k)} \nabla_k^* \dots \nabla_1^* \gamma_{N_i,t}^{(k)} \to \mathrm{Tr}\, \nabla_1 \dots \nabla_k J^{(k)} \nabla_k^* \dots \nabla_1^* \gamma_{\infty,t}^{(k)} \tag{6.20}$$

as $N_i \to \infty$. For such observable $J^{(k)}$ we rewrite the l.h.s. of (6.18), using (6.14), as

$$\begin{aligned} \mathrm{Tr}\, J^{(k)} \, U_{N,t}^{(k)} = \int \mathrm{d}\mathbf{x}_k \mathrm{d}\mathbf{x}'_k \mathrm{d}\mathbf{x}_{N-k} \; J^{(k)}(\mathbf{x}_k; \mathbf{x}'_k) \, \Theta_k^{(k)}(\mathbf{x}_k, \mathbf{x}_{N-k}) \Theta_k^{(k)}(\mathbf{x}'_k, \mathbf{x}_{N-k}) \\ \times D_k \psi_{N,t}(\mathbf{x}_k, \mathbf{x}_{N-k}) D'_k \overline{\psi}_{N,t}(\mathbf{x}'_k, \mathbf{x}_{N-k}) \, . \end{aligned} \tag{6.21}$$

From (6.21), we will show later that

$$\mathrm{Tr}\, J^{(k)} \, U_{N,t}^{(k)} = \int \mathrm{d}\mathbf{x}_k \mathrm{d}\mathbf{x}'_k \mathrm{d}\mathbf{x}_{N-k} \; \left(D_k \, D'_k \, J^{(k)} \right) (\mathbf{x}_k; \mathbf{x}'_k) \, \psi_{N,t}(\mathbf{x}_k, \mathbf{x}_{N-k}) \overline{\psi}_{N,t}(\mathbf{x}'_k, \mathbf{x}_{N-k}) + o(1) \tag{6.22}$$

as $N \to \infty$.

Before proving (6.22), let us show how Proposition 6.3 follows from it. Equation (6.22) implies that

$$\begin{aligned} \mathrm{Tr}\, J^{(k)} \, U_{N,t}^{(k)} &= \mathrm{Tr}\, \nabla_1 \dots \nabla_k J^{(k)} \nabla_k^* \dots \nabla_1^* \gamma_{N,t}^{(k)} + o(1) \\ &\to \mathrm{Tr}\, \nabla_1 \dots \nabla_k J^{(k)} \nabla_k^* \dots \nabla_1^* \gamma_{\infty,t}^{(k)} \end{aligned} \tag{6.23}$$

as $N \to \infty$ (using (6.20)). Comparing with (6.18), we obtain that

$$\mathrm{Tr}\, J^{(k)} \, U_{\infty,t}^{(k)} = \mathrm{Tr}\, \nabla_1 \dots \nabla_k J^{(k)} \nabla_k^* \dots \nabla_1^* \gamma_{\infty,t}^{(k)} \, . \tag{6.24}$$

Since the set of all $J^{(k)} \in \mathcal{K}_k$ with the property that $\nabla_1 \dots \nabla_k J^{(k)} \nabla_1^* \dots \nabla_k^* \in \mathcal{K}_k$ and such that (6.19) is satisfied is a dense subset of $\mathcal{K}_k$, it follows that

$$\nabla_1 \dots \nabla_k \gamma_{\infty,t}^{(k)} \nabla_k^* \dots \nabla_1^* = U_{\infty,t}^{(k)} \, . \tag{6.25}$$

From (6.16), we find

$$\mathrm{Tr}\, (-\Delta_1) \dots (-\Delta_k) \gamma_{\infty,t}^{(k)} \leq C_2^k \, . \tag{6.26}$$

Now suppose that $\Gamma_{\infty,t} = \{\gamma_{\infty,t}^{(k)}\}_{k \geq 1} \in C([0,T], \mathcal{L}_k^1)$ is a limit point of the sequence $\Gamma_{N,t}$. Then, for every fixed $k \geq 1$ and $t \in [0,T]$, $\gamma_{\infty,t}^{(k)}$ is a limit point of $\gamma_{N,t}^{(k)}$ and thus satisfies (6.26), for a constant C_2 independent of t and k. Moreover, for any $m \leq k$ we also have

$$\mathrm{Tr}\, (-\Delta_1) \dots (-\Delta_m) \gamma_{\infty,t}^{(k)} \leq \; C_2^m \, . \tag{6.27}$$

To prove the last equation, we repeat the same argument leading from (6.14) to (6.26), but with the densities $U^{(k)}_{N,t}$ replaced by

$$U^{(k)}_{m,N,t}(\mathbf{x}_k;\mathbf{x}'_k) = \int \mathrm{d}\mathbf{x}_{N-k}\ \Theta^{(k)}_k(\mathbf{x}_k,\mathbf{x}_{N-k})\Theta^{(k)}_k(\mathbf{x}'_k,\mathbf{x}_{N-k}) D_m\psi_{N,t}(\mathbf{x}_k,\mathbf{x}_{N-k})\ D'_m\overline{\psi}_{N,t}(\mathbf{x}_k,\mathbf{x}_{N-k})\,. \tag{6.28}$$

From (6.26), (6.27), and from the permutation symmetry of $\gamma^{(k)}_{\infty,t}$, we find

$$\mathrm{Tr}\ (1-\Delta_1)\dots(1-\Delta_k)\gamma^{(k)}_{\infty,t} = \sum_{m=0}^{k}\binom{k}{m}\mathrm{Tr}\ (-\Delta_1)\dots(-\Delta_m)\gamma^{(m)}_{\infty,t} \leq (C_2+1)^k \tag{6.29}$$

which completes the proof of Proposition 6.3.

It remains to prove (6.22). To this end, we rewrite the r.h.s. of (6.21) by using $\Theta^{(k)}_k = \theta^{(k)}_k\Theta^k_{k-1}$ as follows:

$$\mathrm{Tr}\ J^{(k)}\ U^{(k)}_{N,t} = (I) - (II) \tag{6.30}$$

with

$$\begin{aligned}(I) :=& \int \mathrm{d}\mathbf{x}_k\mathrm{d}\mathbf{x}'_k\mathrm{d}\mathbf{x}_{N-k}J^{(k)}(\mathbf{x}_k;\mathbf{x}'_k)\ \Theta^{(k)}_{k-1}(\mathbf{x}_k,\mathbf{x}_{N-k})\Theta^{(k)}_k(\mathbf{x}'_k,\mathbf{x}_{N-k})\\ &\qquad\times D_k\psi_{N,t}(\mathbf{x}_k,\mathbf{x}_{N-k})\ D'_k\overline{\psi}_{N,t}(\mathbf{x}'_k,\mathbf{x}_{N-k})\\ (II) :=& \int \mathrm{d}\mathbf{x}_k\mathrm{d}\mathbf{x}'_k\mathrm{d}\mathbf{x}_{N-k}J^{(k)}(\mathbf{x}_k;\mathbf{x}'_k)(1-\theta^{(k)}_k(\mathbf{x}_k,\mathbf{x}_{N-k}))\Theta^{(k)}_{k-1}(\mathbf{x}_k,\mathbf{x}_{N-k})\Theta^{(k)}_k(\mathbf{x}'_k,\mathbf{x}_{N-k})\\ &\qquad\times D_k\psi_{N,t}(\mathbf{x}_k,\mathbf{x}_{N-k})\ D'_k\overline{\psi}_{N,t}(\mathbf{x}'_k,\mathbf{x}_{N-k})\,.\end{aligned} \tag{6.31}$$

By integration by parts

$$(I) = (Ia) + (Ib) \tag{6.32}$$

with

$$\begin{aligned}(Ia) :=& -\int \mathrm{d}\mathbf{x}_k\mathrm{d}\mathbf{x}'_k\mathrm{d}\mathbf{x}_{N-k}\nabla_k J^{(k)}(\mathbf{x}_k;\mathbf{x}'_k)\ \Theta^{(k)}_{k-1}(\mathbf{x}_k,\mathbf{x}_{N-k})\ \Theta^{(k)}_k(\mathbf{x}'_k,\mathbf{x}_{N-k})\\ &\qquad\times D_{k-1}\psi_{N,t}(\mathbf{x}_k,\mathbf{x}_{N-k})\ D'_k\overline{\psi}_{N,t}(\mathbf{x}'_k,\mathbf{x}_{N-k})\\ (Ib) :=& -\int \mathrm{d}\mathbf{x}_k\mathrm{d}\mathbf{x}'_k\mathrm{d}\mathbf{x}_{N-k}J^{(k)}(\mathbf{x}_k;\mathbf{x}'_k)\ \nabla_k\Theta^{(k)}_{k-1}(\mathbf{x}_k,\mathbf{x}_{N-k})\Theta^{(k)}_k(\mathbf{x}'_k,\mathbf{x}_{N-k})\\ &\qquad\times D_{k-1}\psi_{N,t}(\mathbf{x}_k,\mathbf{x}_{N-k})\ D'_k\overline{\psi}_{N,t}(\mathbf{x}'_k,\mathbf{x}_{N-k})\end{aligned} \tag{6.33}$$

The main term is (Ia). To bound the term (Ib), we use Schwarz inequality with some $\alpha > 0$:

$$\begin{aligned}|(Ib)| \leq& \alpha\int \mathrm{d}\mathbf{x}_k\mathrm{d}\mathbf{x}'_k\mathrm{d}\mathbf{x}_{N-k}|J^{(k)}(\mathbf{x}_k;\mathbf{x}'_k)|\left|\nabla_k\Theta^{(k)}_{k-1}(\mathbf{x}_k,\mathbf{x}_{N-k})\right|^2|D_{k-1}\psi_{N,t}(\mathbf{x}_k,\mathbf{x}_{N-k})|^2\\ &+\alpha^{-1}\int \mathrm{d}\mathbf{x}_k\mathrm{d}\mathbf{x}'_k\mathrm{d}\mathbf{x}_{N-k}|J^{(k)}(\mathbf{x}_k;\mathbf{x}'_k)|\ \Theta^{(k+1)}_k(\mathbf{x}'_k,\mathbf{x}_{N-k})|D'_k\psi_{N,t}(\mathbf{x}'_k,\mathbf{x}_{N-k})|^2\\ \leq& \alpha\left(\sup_{\mathbf{x}_k}\int \mathrm{d}\mathbf{x}'_k|J^{(k)}(\mathbf{x}_k;\mathbf{x}'_k)|\right)\ \int \mathrm{d}\mathbf{x}\left|\nabla_k\Theta^{(k)}_{k-1}(\mathbf{x})\right|^2|D_{k-1}\psi_{N,t}(\mathbf{x})|^2\\ &+\alpha^{-1}\left(\sup_{\mathbf{x}'_k}\int \mathrm{d}\mathbf{x}_k|J^{(k)}(\mathbf{x}_k;\mathbf{x}'_k)|\right)\ \int \mathrm{d}\mathbf{x}'_k\mathrm{d}\mathbf{x}_{N-k}\ \Theta^{(k)}_{k-1}(\mathbf{x}'_k,\mathbf{x}_{N-k})|D'_k\psi_{N,t}(\mathbf{x}'_k,\mathbf{x}_{N-k})|^2.\end{aligned} \tag{6.34}$$

Using that

$$\left|\nabla_k \Theta_{k-1}^{(k)}(\mathbf{x})\right|^2 \leq C\ell^{-2} \left(\frac{2^k}{\ell^\varepsilon} \sum_{m=2}^{k} h(x_1 - x_m)\right)^2 \Theta_{k-1}^{(k+1)}(\mathbf{x}) \tag{6.35}$$

we obtain that

$$\begin{aligned}
&\int \mathrm{d}\mathbf{x} \left|\nabla_k \Theta_{k-1}^{(k)}(\mathbf{x})\right|^2 |D_{k-1}\psi_{N,t}(\mathbf{x})|^2 \\
&\qquad \leq C\ell^{-2} \int \mathrm{d}\mathbf{x} \left(\frac{2^k}{\ell^\varepsilon} \sum_{m=2}^{k} h(x_1 - x_m)\right)^2 \Theta_{k-1}^{(k+1)}(\mathbf{x}) |D_{k-1}\psi_{N,t}(\mathbf{x})|^2 \\
&\qquad \leq C(N-k)^{-1}\ell^{-2} \sum_{i \geq k} \int \mathrm{d}\mathbf{x} \left(\frac{2^k}{\ell^\varepsilon} \sum_{m=2}^{k} h(x_i - x_m)\right)^2 \Theta_{k-1}^{(k+1)}(\mathbf{x}) |D_{k-1}\psi_{N,t}(\mathbf{x})|^2,
\end{aligned} \tag{6.36}$$

where we used the symmetry of the $D_{k-1}\psi_{N,t}$ w.r.t. permutations of the last $N-k$ variables. Since

$$\sum_{i \geq k} \left(\frac{2^k}{\ell^\varepsilon} \sum_{m=2}^{k} h(x_i - x_m)\right)^2 \Theta_{k-1}^{(k+1)}(\mathbf{x}) \leq \left(\frac{2^k}{\ell^\varepsilon} \sum_{i \geq k} \sum_{m=2}^{k} h(x_i - x_m)\right)^2 \Theta_{k-1}^{(k+1)}(\mathbf{x}) \leq C\Theta_{k-1}^{(k)}(\mathbf{x}) \tag{6.37}$$

(see part ii) of Lemma A.1), it follows from (6.36) that

$$\begin{aligned}
\int \left|\nabla_k \Theta_{k-1}^{(k)}\right|^2 |D_{k-1}\psi_{N,t}|^2 &\leq C\ell^{-2}(N-k)^{-1} \int \Theta_{k-1}^{(k)} \, |D_{k-1}\psi_{N,t}|^2 \\
&\leq C\ell^{-2}(N-k)^{-1} \int \Theta_{k-2}^{(k-1)} \, |D_{k-1}\psi_{N,t}|^2 \\
&\leq C_k \, \ell^{-2}(N-k)^{-1}
\end{aligned} \tag{6.38}$$

by (6.13) (here the constant C_k depends on k and on the observable $J^{(k)}$). From (6.34), from the assumptions (6.19), and again using (6.13), it follows that

$$|(Ib)| \leq \; C_k \left(\alpha(N-k)^{-1}\ell^{-2} + \alpha^{-1}\right) = o(1) \tag{6.39}$$

because $N\ell^2 \gg 1$.

Next we consider the term (II) in (6.31). By Schwarz inequality, we have

$$\begin{aligned}
|(II)| &\leq \alpha \int \mathrm{d}\mathbf{x}_k \mathrm{d}\mathbf{x}'_k \mathrm{d}\mathbf{x}_{N-k} \, |J^{(k)}(\mathbf{x}_k;\mathbf{x}'_k)| \Theta_{k-1}^{(k+1)}(\mathbf{x}_k, \mathbf{x}_{N-k}) |D_k \psi_{N,t}(\mathbf{x}_k, \mathbf{x}_{N-k})|^2 \\
&\quad + \alpha^{-1} \int \mathrm{d}\mathbf{x}_k \mathrm{d}\mathbf{x}'_k \mathrm{d}\mathbf{x}_{N-k} \, |J^{(k)}(\mathbf{x}_k;\mathbf{x}'_k)| (1 - \theta_k^{(k)}(\mathbf{x}_k, \mathbf{x}_{N-k})) \Theta_k^{(k+1)}(\mathbf{x}'_k, \mathbf{x}_{N-k}) \\
&\qquad\qquad \times |D'_k \psi_{N,t}(\mathbf{x}'_k, \mathbf{x}_{N-k})|^2 \\
&\leq \alpha \left(\sup_{\mathbf{x}_k} \int \mathrm{d}\mathbf{x}'_k \, |J^{(k)}(\mathbf{x}_k;\mathbf{x}'_k)|\right) \int \mathrm{d}\mathbf{x} \, \Theta_{k-1}^{(k+1)}(\mathbf{x}) |D_k \psi_{N,t}(\mathbf{x})|^2 \\
&\quad + \alpha^{-1} \left(\sup_{\mathbf{x}'_k, \mathbf{x}_{N-k}} \int \mathrm{d}\mathbf{x}_k \, |J^{(k)}(\mathbf{x}_k;\mathbf{x}'_k)| (1 - \theta_k^{(k)}(\mathbf{x}_k, \mathbf{x}_{N-k}))\right) \\
&\qquad\qquad \times \int \mathrm{d}\mathbf{x}'_k \mathrm{d}\mathbf{x}_{N-k} \, \Theta_k^{(k+1)}(\mathbf{x}'_k, \mathbf{x}_{N-k}) |D'_k \psi_{N,t}(\mathbf{x}'_k, \mathbf{x}_{N-k})|^2 \\
&\leq C_k \left(\alpha + \alpha^{-1} \sup_{\mathbf{x}'_k, \mathbf{x}_{N-k}} \int \mathrm{d}\mathbf{x}_k \, |J^{(k)}(\mathbf{x}_k;\mathbf{x}'_k)| (1 - \theta_k^{(k)}(\mathbf{x}_k, \mathbf{x}_{N-k}))\right) ,
\end{aligned} \tag{6.40}$$

where we used (6.13). Next we note that

$$\begin{aligned}\int \mathrm{d}\mathbf{x}_k \, |J^{(k)}(\mathbf{x}_k;\mathbf{x}'_k)|(1-\theta_k^{(k)}(\mathbf{x}_k,\mathbf{x}_{N-k})) &\leq \frac{2^k}{\ell^\varepsilon}\sum_{m\neq k}\int \mathrm{d}\mathbf{x}_k \, |J^{(k)}(\mathbf{x}_k;\mathbf{x}'_k)|h(x_k-x_m) \\ &\leq C^k N\ell^{3-\varepsilon}\int \mathrm{d}\mathbf{x}_k \, |\nabla_k^4 J^{(k)}(\mathbf{x}_k;\mathbf{x}'_k)| + |J^{(k)}(\mathbf{x}_k;\mathbf{x}'_k)|\end{aligned} \tag{6.41}$$

because, with $h(x)=\exp(-(x^2+\ell^2)^{1/2}/\ell)$, we have, by the Sobolev inequality,

$$\int \mathrm{d}x \, h(x)|f(x)| \leq \|h\|_1\|f\|_\infty \leq C\ell^3\int\sum_{b=0}^4 |\nabla^b f| \, . \tag{6.42}$$

From (6.40), (6.41), and from the assumptions (6.19) we find

$$|(II)| \leq C_k \, \left(\alpha+\alpha^{-1}N\ell^{3-\varepsilon}\right) \to 0 \tag{6.43}$$

as $N\to\infty$, because $N\ell^{3-\varepsilon}\ll 1$.

From (6.30), (6.39) and last equation we find

$$\begin{aligned}\mathrm{Tr}\; J^{(k)}\, U_{N,t}^{(k)} = \int \mathrm{d}\mathbf{x}_k\mathrm{d}\mathbf{x}'_k\mathrm{d}\mathbf{x}_{N-k}\nabla_k J^{(k)}(\mathbf{x}_k;\mathbf{x}'_k)\,\Theta_{k-1}^{(k)}(\mathbf{x}_k,\mathbf{x}_{N-k})\,\Theta_k^{(k)}(\mathbf{x}'_k,\mathbf{x}_{N-k}) \\ \times D_{k-1}\psi_{N,t}(\mathbf{x}_k,\mathbf{x}_{N-k})\,D'_k\overline{\psi}_{N,t}(\mathbf{x}'_k,\mathbf{x}_{N-k}) + o(1)\end{aligned} \tag{6.44}$$

Repeating the same arguments to move the derivative ∇'_k from $\psi_{N,t}$ to $J^{(k)}$, we obtain

$$\begin{aligned}\mathrm{Tr}\; J^{(k)}\, U_{N,t}^{(k)} = \int \mathrm{d}\mathbf{x}_k\mathrm{d}\mathbf{x}'_k\mathrm{d}\mathbf{x}_{N-k}\nabla_k\nabla'_k J^{(k)}(\mathbf{x}_k;\mathbf{x}'_k)\,\Theta_{k-1}^{(k)}(\mathbf{x}_k,\mathbf{x}_{N-k})\,\Theta_{k-1}^{(k)}(\mathbf{x}'_k,\mathbf{x}_{N-k}) \\ \times D_{k-1}\psi_{N,t}(\mathbf{x}_k,\mathbf{x}_{N-k})\,D'_{k-1}\overline{\psi}_{N,t}(\mathbf{x}'_k,\mathbf{x}_{N-k}) + o(1)\end{aligned} \tag{6.45}$$

Iterating this argument $k-1$ more times to move all derivatives to the observable, we prove (6.22). □

The following lemma was used in the proof of Theorem 6.1, and will also be used in the next sections, in order to bound potentials by the action of derivatives.

Lemma 6.4. *i) Suppose $V\in L^{3/2}(\mathbb{R}^3)$. Then*

$$\int \mathrm{d}x \, V(x)|\varphi(x)|^2 \leq C\|V\|_{L^{3/2}}\int \mathrm{d}x \, \left(|\nabla\varphi(x)|^2+|\varphi(x)|^2\right) \tag{6.46}$$

ii) Suppose $V\in L^1(\mathbb{R}^3)$. Then the operator $V(x_1-x_2)$, viewed as a multiplication operator on $L^2(\mathbb{R}^3\times\mathbb{R}^3,\mathrm{d}x_1\,\mathrm{d}x_2)$, satisfies the following operator inequalities

$$V(x_1-x_2)\leq C\|V\|_{L^1}\,(1-\Delta_1)(1-\Delta_2), \quad \textit{and} \quad V(x_1-x_2)\leq C\|V\|_{L^1}(1-\Delta_1)^2. \tag{6.47}$$

The proof of (6.46) is given in Lemma 5.2 of [8], the proof of the first inequality of (6.47) is found in Lemma 5.3 of [10]. The last inequality follows from the usual Sobolev imbedding. □

7 Convergence to the infinite hierarchy

The aim of this section is to prove that any limit point $\Gamma_{\infty,t} \in \bigoplus_{k\geq 1} C([0,T],\mathcal{L}^1_k)$ of the sequence $\Gamma_{N,t}$ satisfies the infinite hierarchy (4.4).

Theorem 7.1. *Suppose the assumptions of Theorem 2.1 are satisfied and fix $T > 0$. Suppose $\Gamma_{\infty,t} = \{\gamma^{(k)}_{\infty,t}\}_{k\geq 1} \in \bigoplus_{k\geq 1} C([0,T],\mathcal{L}^1_k)$ is a limit point of $\Gamma_{N,t} = \{\gamma^{(k)}_{N,t}\}^N_{k=1}$ with respect to the topology τ_{prod}. Then $\Gamma_{\infty,t}$ is a solution of the infinite BBGKY hierarchy*

$$\gamma^{(k)}_{\infty,t} = \mathcal{U}^{(k)}(t)\,\gamma^{(k)}_{\infty,0} - 8\pi i a_0 \sum_{j=1}^{k} \int_0^t \mathrm{d}s\, \mathcal{U}^{(k)}(t-s)\, Tr_{k+1}\, \Big[\delta(x_j - x_{k+1}), \gamma^{(k+1)}_{\infty,s}\Big] \tag{7.1}$$

with initial data $\gamma^{(k)}_{\infty,0} = |\varphi\rangle\langle\varphi|^{\otimes k}$.

Remark. Note that in terms of kernels

$$\Big(\mathrm{Tr}_{k+1}\,\delta(x_j - x_{k+1})\gamma^{(k+1)}_{\infty,s}\Big)\,(\mathbf{x}_k;\mathbf{x}'_k) = \gamma^{(k+1)}_{\infty,s}(\mathbf{x}_k, x_j; \mathbf{x}'_k, x_j)\,.$$

To define this kernel properly, we choose a function $g \in C^\infty_0(\mathbb{R}^3)$, $g \geq 0$, $\int g = 1$, and we let $g_r(x) = r^{-3}g(x/r)$. Then the definition is given by the limit

$$\begin{aligned}\lim_{r,r'\to 0} \int \mathrm{d}x'_{k+1}\mathrm{d}x_{k+1}\, g_r(x'_{k+1} - x_{k+1}) g_{r'}(x_{k+1} - x_j)\gamma^{(k+1)}_{\infty,s}(\mathbf{x}_k, x_{k+1}; \mathbf{x}'_k, x'_{k+1}) \\ =: \gamma^{(k+1)}_{\infty,s}(\mathbf{x}_k, x_j; \mathbf{x}'_k, x_j).\end{aligned} \tag{7.2}$$

The existence of this limit in a weak sense (tested against a sufficiently smooth observable) follows from the apriori estimate (6.12) and from the following lemma (whose proof was given in Lemma 8.2 in [9]).

Lemma 7.2. *Suppose that $\delta_\alpha(x)$ is a function satisfying $0 \leq \delta_\alpha(x) \leq C\alpha^{-3}\mathbf{1}(|x| \leq \alpha)$ and $\int \delta_\alpha(x)\mathrm{d}x = 1$ (for example $\delta_\alpha(x) = \alpha^{-3}g(x/\alpha)$, for a bounded probability density $g(x)$ supported in $\{x : |x| \leq 1\}$). Moreover, for $J^{(k)} \in \mathcal{K}_k$, and for $j = 1,\ldots,k$, we define the norm*

$$|\!|\!| J^{(k)} |\!|\!|_j := \sup_{\mathbf{x}_k,\mathbf{x}'_k} \langle x_1\rangle^4 \ldots \langle x_k\rangle^4 \langle x'_1\rangle^4 \ldots \langle x'_k\rangle^4 \Big(|J^{(k)}(\mathbf{x}_k;\mathbf{x}'_k)| + |\nabla_{x_j} J^{(k)}(\mathbf{x}_k;\mathbf{x}'_k)| + |\nabla_{x'_j} J^{(k)}(\mathbf{x}_k;\mathbf{x}'_k)|\Big) \tag{7.3}$$

for any $j \leq k$ and for any function $J^{(k)}(\mathbf{x}_k;\mathbf{x}'_k)$ (here $\langle x\rangle^2 := 1 + x^2$). Then if $\gamma^{(k+1)}(\mathbf{x}_{k+1};\mathbf{x}'_{k+1})$ is the kernel of a density matrix on $L^2(\mathbb{R}^{3(k+1)})$, we have, for any $j \leq k$,

$$\begin{aligned}\Big| \int \mathrm{d}\mathbf{x}_{k+1}\mathrm{d}\mathbf{x}'_{k+1}\, J^{(k)}(\mathbf{x}_k;\mathbf{x}'_k) \big(\delta_{\alpha_1}(x_{k+1} - x'_{k+1})\delta_{\alpha_2}(x_j - x_{k+1}) - \delta(x_{k+1} - x'_{k+1})\delta(x_j - x_{k+1})\big) \\ \times \gamma^{(k+1)}(\mathbf{x}_{k+1};\mathbf{x}'_{k+1})\Big| \\ \leq (\text{const.})^k\, |\!|\!| J^{(k)} |\!|\!|_j\, (\alpha_1 + \sqrt{\alpha_2})\; Tr|S_j S_{k+1}\gamma^{(k+1)} S_j S_{k+1}|\,.\end{aligned} \tag{7.4}$$

Recall that $S_\ell = (1 - \Delta_{x_\ell})^{1/2}$. The same bound holds if x_j is replaced with x'_j in (7.4) by symmetry.

Proof of Theorem 7.1. For every integer $k \geq 1$, and every $J^{(k)} \in \mathcal{K}_k$, we have

$$\sup_{t\in[0,T]} \mathrm{Tr}\; J^{(k)} \Big(\gamma^{(k)}_{N_i,t} - \gamma^{(k)}_{\infty,t}\Big) \to 0 \tag{7.5}$$

along a subsequence $N_i \to \infty$. For an arbitrary integer $k \geq 1$, we define

$$\Omega_k := \prod_{j=1}^{k} \left(\langle x_j \rangle + S_j \right) \ .$$

In the following we assume that the observable $J^{(k)} \in \mathcal{K}_k$ is such that

$$\left\| \Omega_k^7 J^{(k)} \Omega_k^7 \right\|_{\mathrm{HS}} < \infty, \tag{7.6}$$

where $\|A\|_{\mathrm{HS}}$ denotes the Hilbert-Schmidt norm of the operator A, that is $\|A\|_{\mathrm{HS}}^2 = \mathrm{Tr} A^* A$. Note that the set of observables $J^{(k)}$ satisfying the condition (7.6) is a dense subset of $\mathcal{K}_k$.

It is straightforward to check that

$$\| S_1 \dots S_k \, J^{(k)} S_1 \dots S_k \| \leq \left\| \Omega_k^7 J^{(k)} \Omega_k^7 \right\|_{\mathrm{HS}}. \tag{7.7}$$

Moreover, for any $j \leq k$

$$|\!|\!| J^{(k)} |\!|\!|_j \leq (\text{const.})^k \left\| \Omega_k^7 J^{(k)} \Omega_k^7 \right\|_{\mathrm{HS}}, \tag{7.8}$$

where the norm $|\!|\!| . |\!|\!|_j$ is defined in (7.3). This follows from the standard Sobolev inequality $\|f\|_\infty \leq (\text{const.}) \, \|f\|_{W^{2,2}}$ in three dimensions applied to each variable separately in the form

$$\begin{aligned} \Big(\sup_{x,x'} \langle x \rangle^4 \langle x' \rangle^4 |\nabla_x J(x,x')| \Big)^2 &\leq (\text{const.}) \int \mathrm{d}x \mathrm{d}x' \Big| (1-\Delta_x) \Big[\langle x \rangle^4 \big(\nabla_x J(x,x') \big) \langle x' \rangle^4 \Big] \Big|^2 \\ &\leq (\text{const.}) \ \mathrm{Tr} \ (1-\Delta) \langle x \rangle^4 \nabla \ J \, \langle x \rangle^8 \, J^* \ \nabla^* \ \langle x \rangle^4 \, (1-\Delta) \\ &\leq (\text{const.}) \ \mathrm{Tr} \ \Omega^7 J \Omega^{14} J^* \Omega^7 \end{aligned}$$

with $\Omega = \langle x \rangle + (1-\Delta)^{1/2}$. Similar estimates are valid for each term in the definition of $|\!|\!| \cdot |\!|\!|_j$, for $j \leq k$. Here we commuted derivatives and the weights $\langle x \rangle$; the commutators can be estimated using Schwarz inequalities.

For $J^{(k)} \in \mathcal{K}_k$ satisfying (7.6), we prove that

$$\mathrm{Tr} \, J^{(k)} \gamma_{\infty,0}^{(k)} = \mathrm{Tr} \, J^{(k)} |\varphi\rangle\langle\varphi|^{\otimes k} \tag{7.9}$$

and that, for $t \in [0,T]$,

$$\mathrm{Tr} \ J^{(k)} \gamma_{\infty,t}^{(k)} = \mathrm{Tr} \ J^{(k)} \mathcal{U}^{(k)}(t) \gamma_{\infty,0}^{(k)} - 8\pi a_0 i \sum_{j=1}^{k} \int_0^t \mathrm{d}s \mathrm{Tr} \, J^{(k)} \mathcal{U}^{(k)}(t-s) \left[\delta(x_j - x_{k+1}), \gamma_{\infty,s}^{(k+1)} \right] \ . \tag{7.10}$$

Note that the trace in the last term of (7.10) is over $k+1$ variables. The theorem then follows from (7.9) and (7.10), because the set of $J^{(k)} \in \mathcal{K}_k$ satisfying (7.6) is dense in $\mathcal{K}_k$.

The relation (7.9) follows from the assumption (2.14) and (7.5).

In order to prove (7.10), we fix $t \in [0,T]$, we rewrite the BBGKY hierarchy (3.30) in integral form and we test it against the observable $J^{(k)}$. We obtain

$$\begin{aligned} \mathrm{Tr} \ J^{(k)} \, \gamma_{N,t}^{(k)} = \mathrm{Tr} \ J^{(k)} \, \mathcal{U}^{(k)}(t) \gamma_{N,0}^{(k)} - i \sum_{i<j}^{k} \int_0^t \mathrm{d}s \, \mathrm{Tr} \ J^{(k)} \, \mathcal{U}^{(k)}(t-s) [V_N(x_i - x_j), \gamma_{N,s}^{(k)}] \\ - i(N-k) \sum_{j=1}^{k} \int_0^t \mathrm{d}s \, \mathrm{Tr} J^{(k)} \mathcal{U}^{(k)}(t-s) [V_N(x_j - x_{k+1}), \gamma_{N,s}^{(k+1)}] \, . \end{aligned} \tag{7.11}$$

From (7.5) it follows immediately that

$$\text{Tr } J^{(k)}\, \gamma^{(k)}_{N,t} \to \text{Tr } J^{(k)} \gamma^{(k)}_{\infty,t} \tag{7.12}$$

and also that

$$\begin{aligned}\text{Tr } J^{(k)}\, \mathcal{U}^{(k)}(t)\gamma^{(k)}_{N,0} &= \text{Tr } \left(\mathcal{U}^{(k)}(-t)J^{(k)}\right)\, \gamma^{(k)}_{N,0} \\ &\to \text{Tr } \left(\mathcal{U}^{(k)}(-t)J^{(k)}\right) \gamma^{(k)}_{\infty,0} = \text{Tr } J^{(k)}\, \mathcal{U}^{(k)}(t)\gamma^{(k)}_{\infty,0}\end{aligned} \tag{7.13}$$

as $N \to \infty$. Here we used that, if $J^{(k)} \in \mathcal{K}_k$, then also $\mathcal{U}^{(k)}(-t)J^{(k)} \in \mathcal{K}_k$.

Next we consider the second term on the r.h.s. of (7.11) and we prove that it converges to zero, as $N \to \infty$. To this end, we recall the definition (5.21)

$$\gamma^{(k)}_{N,i,j,t}(\mathbf{x}_k;\mathbf{x}'_k) = (1-w(x_i-x_j))^{-1}(1-w(x'_i-x'_j))^{-1}\gamma^{(k)}_{N,t}(\mathbf{x}_k;\mathbf{x}'_k)$$

for every $i \neq j$, $i,j \leq k$. Then we obtain

$$\begin{aligned}&\left|\text{Tr } J^{(k)}\, \mathcal{U}^{(k)}(t-s)[V_N(x_i-x_j), \gamma^{(k)}_{N,s}]\right| \\ &\quad\leq \left|\text{Tr } \left(S_iS_j(\mathcal{U}^{(k)}(s-t)J^{(k)})S_iS_j\right)\left(S_i^{-1}S_j^{-1}V_N(x_i-x_j)(1-w_{ij})S_i^{-1}S_j^{-1}\right)\right. \\ &\qquad\qquad \left.\times \left(S_iS_j\gamma^{(k)}_{N,i,j,s}S_iS_j\right)\left(S_i^{-1}S_j^{-1}(1-w_{ij})S_i^{-1}S_j^{-1}\right)\right| \\ &\qquad + \left|\text{Tr } \left(S_iS_j(\mathcal{U}^{(k)}(s-t)J^{(k)})S_iS_j\right)\left(S_i^{-1}S_j^{-1}(1-w_{ij})S_i^{-1}S_j^{-1}\right)\right. \\ &\qquad\qquad \left.\times \left(S_iS_j\gamma^{(k)}_{N,i,j,s}S_iS_j\right)\left(S_i^{-1}S_j^{-1}V_N(x_i-x_j)(1-w_{ij})S_i^{-1}S_j^{-1}\right)\right|.\end{aligned} \tag{7.14}$$

Since, by part iv) of Lemma 5.1,

$$\|S_i^{-1}S_j^{-1}V_N(x_i-x_j)(1-w_{ij})S_i^{-1}S_j^{-1}\| \leq C\int \mathrm{d}x V_N(x)(1-w(x)) \leq CN^{-1} \tag{7.15}$$

and

$$\|S_i^{-1}S_j^{-1}(1-w(x_i-x_j))S_i^{-1}S_j^{-1}\| \leq 1 \tag{7.16}$$

we find

$$\left|\text{Tr } J^{(k)}\ \mathcal{U}^{(k)}(t-s)[V_N(x_i-x_j), \gamma^{(k)}_{N,s}]\right| \leq\ CN^{-1}\|S_iS_j\left(\mathcal{U}^{(k)}(s-t)J^{(k)}\right)S_iS_j\|\ \text{Tr } S_i^2S_j^2\gamma^{(k)}_{N,i,j,s}\,.$$

From $\|S_iS_j\left(\mathcal{U}^{(k)}(s-t)J^{(k)}\right)S_iS_j\| = \|S_iS_jJ^{(k)}S_iS_j\| < \infty$, and from Proposition 5.2 it follows immediately that, for any $t \in [0,T]$,

$$\sum_{i<j}^{k}\int_0^t \mathrm{d}s\, \text{Tr } J^{(k)}\, \mathcal{U}^{(k)}(t-s)[V_N(x_i-x_j), \gamma^{(k)}_{N,s}] \to 0 \tag{7.17}$$

as $N \to \infty$ (the convergence is not uniform in k).

Finally we consider the last term on the r.h.s. of (7.11). First of all, we note that

$$k\sum_{j=1}^{k}\int_0^t \mathrm{d}s\, \text{Tr } J^{(k)}\mathcal{U}^{(k)}(t-s)[V_N(x_j-x_{k+1}), \gamma^{(k+1)}_{N,s}] \to 0 \tag{7.18}$$

as $N \to \infty$. In fact

$$\begin{aligned}
&\left|\mathrm{Tr}\, J^{(k)}\mathcal{U}^{(k)}(t-s)[V_N(x_j - x_{k+1}), \gamma_{N,s}^{(k+1)}]\right| \\
&\quad \leq \left|\mathrm{Tr}\, \left(S_j \mathcal{U}^{(k)}(s-t) J^{(k)} S_j\right) \left(S_j^{-1} S_{k+1}^{-1} V_N(x_j - x_{k+1})(1 - w_{j,k+1}) S_{k+1}^{-1} S_j^{-1}\right)\right. \\
&\qquad\qquad \left. \times \left(S_{k+1} S_j \gamma_{N,j,k+1,s}^{(k+1)} S_j S_{k+1}\right) \left(S_j^{-1} S_{k+1}^{-1}(1 - w_{j,k+1}) S_{k+1} S_j^{-1}\right)\right| \\
&\qquad + \left|\mathrm{Tr}\, \left(S_j J^{(k)} S_j\right) \left(S_j^{-1} S_{k+1}(1 - w_{j,k+1}) S_{k+1}^{-1} S_j^{-1}\right)\right. \\
&\qquad\qquad \left. \times \left(S_{k+1} S_j \gamma_{N,j,k+1,s}^{(k+1)} S_j S_{k+1}\right) \left(S_j^{-1} S_{k+1}^{-1} N V_N(x_j - x_{k+1})(1 - w_{j,k+1}) S_{k+1}^{-1} S_j^{-1}\right)\right|.
\end{aligned} \tag{7.19}$$

As in (7.15) we have $\|S_j^{-1} S_{k+1}^{-1} V_N(x_j - x_{k+1})(1 - w_{j,k+1}) S_j^{-1} S_{k+1}^{-1}\| \leq C N^{-1}$. Moreover (see (6.7)),

$$\|S_j^{-1} S_{k+1}(1 - w_{j,k+1}) S_{k+1}^{-1} S_j^{-1}\| \leq C. \tag{7.20}$$

By an argument very similar to (7.14)–(7.17) and by Proposition 5.2 we obtain (7.18).

It remains to consider

$$\begin{aligned}
&N \sum_{j=1}^{k} \int_0^t \mathrm{d}s\, \mathrm{Tr}\, J^{(k)}\mathcal{U}^{(k)}(t-s)[V_N(x_j - x_{k+1}), \gamma_{N,s}^{(k+1)}] \\
&\quad = \sum_{j=1}^{k} \int_0^t \mathrm{d}s\, \mathrm{Tr}\, \left(\mathcal{U}^{(k)}(s-t) J^{(k)}\right) \left[N V_N(x_j - x_{k+1})(1 - w_{j,k+1}), \gamma_{N,j,k+1,s}^{(k+1)}\right] \\
&\qquad - \sum_{j=1}^{k} \int_0^t \mathrm{d}s\, \mathrm{Tr}\, \left(\mathcal{U}^{(k)}(s-t) J^{(k)}\right) N V_N(x_j - x_{k+1})(1 - w_{j,k+1}) \gamma_{N,j,k+1,s}^{(k+1)} w_{j,k+1} \\
&\qquad + \sum_{j=1}^{k} \int_0^t \mathrm{d}s\, \mathrm{Tr}\, \left(\mathcal{U}^{(k)}(s-t) J^{(k)}\right) w_{j,k+1} \gamma_{N,j,k+1,s}^{(k+1)} (1 - w_{j,k+1}) N V_N(x_j - x_{k+1}).
\end{aligned} \tag{7.21}$$

The terms on the third and fourth lines converge to zero, as $N \to \infty$. For example, the contributions on the third line can be bounded by

$$\begin{aligned}
&\left|\mathrm{Tr}\, \left(\mathcal{U}^{(k)}(s-t) J^{(k)}\right) N V_N(x_j - x_{k+1})(1 - w_{j,k+1}) \gamma_{N,j,k+1,s}^{(k+1)} w_{j,k+1}\right| \\
&\leq \|S_j \left(\mathcal{U}^{(k)}(s-t) J^{(k)}\right) S_j\| \|S_j^{-1} S_{k+1}^{-1} \left(N V_N(x_j - x_{k+1})(1 - w_{j,k+1})\right) S_j^{-1} S_{k+1}^{-1}\| \\
&\quad \times \|S_j^{-1} S_{k+1} w_{j,k+1} S_j^{-1} S_{k+1}^{-1}\|\, \mathrm{Tr}\, S_j^2 S_{k+1}^2\, \gamma_{N,j,k+1,s}^{(k+1)}.
\end{aligned} \tag{7.22}$$

Then we use

$$\|S_j^{-1} S_{k+1}^{-1} N V_N(x_j - x_{k+1})(1 - w_{j,k+1}) S_j^{-1} S_{k+1}^{-1}\| \leq C \tag{7.23}$$

and

$$\begin{aligned}
\|S_j^{-1} S_{k+1} w_{j,k+1} S_j^{-1} S_{k+1}^{-1}\| &\leq \left\| S_{k+1}^{-1} S_j^{-1} w_{j,k+1} S_{k+1}^2 w_{j,k+1} S_j^{-1} S_{k+1}^{-1} \right\|^{1/2} \\
&\leq \|S_j^{-1} w_{j,k+1}^2 S_j^{-1}\|^{1/2} + \|S_{k+1}^{-1} S_j^{-1} (\nabla w_{j,k+1})^2 S_j^{-1} S_{k+1}^{-1}\|^{1/2} \\
&\leq C N^{-1} + C N^{-1/4}.
\end{aligned} \tag{7.24}$$

To prove (7.24), we applied Lemma 6.4 and the fact that, by Lemma 5.1, with R such that $\mathrm{supp}\, V \subset \{x \in \mathbb{R}^3 : |x| \leq R\}$,

$$w(x) \leq C\chi(|x| < R/N) + a\frac{\chi(|x| > R/N)}{|x|} \leq \frac{C}{N|x|},$$

and

$$|\nabla w(x)|^2 \leq C\frac{a}{|x|^2}\,|\nabla w(x)| \leq C\frac{1}{N^{1/2}|x|^{5/2}}$$

(the last bound is obtained interpolating the first bound in (5.4) and the second bound in (5.5)). It follows that

$$\begin{aligned}\Big|\sum_{j=1}^{k}\int_0^t \mathrm{d}s\,\mathrm{Tr}\,\Big(\mathcal{U}^{(k)}(s-t)J^{(k)}\Big)NV_N(x_j-x_{k+1})(1-w_{j,k+1})\gamma^{(k+1)}_{N,j,k+1,s}w_{j,k+1}\Big| \\ \leq Ctk N^{-1/4}\max_{j\leq k}\sup_{s\in[0,t]}\mathrm{Tr}\; S_jS_{k+1}\gamma^{(k+1)}_{N,j,k+1,s}S_jS_{k+1}\end{aligned} \tag{7.25}$$

which converges to zero, as $N \to \infty$, by using Proposition 5.2. The fourth line of (7.21) can be handled analogously. Hence, from (7.21),

$$\begin{aligned}N\sum_{j=1}^{k}\int_0^t \mathrm{d}s\,\mathrm{Tr}\,J^{(k)}\mathcal{U}^{(k)}(t-s)[V_N(x_j-x_{k+1}),\gamma^{(k+1)}_{N,s}] \\ = \sum_{j=1}^{k}\int_0^t \mathrm{d}s\,\mathrm{Tr}\,\Big(\mathcal{U}^{(k)}(s-t)J^{(k)}\Big)\Big[NV_N(x_j-x_{k+1})(1-w_{j,k+1}),\gamma^{(k+1)}_{N,j,k+1,s}\Big] \\ + C_{k,T}\,o_N(1)\end{aligned} \tag{7.26}$$

where $o_N(1) \to 0$ as $N \to \infty$ and $C_{k,T}$ is a constant depending on k and on T.

To handle the r.h.s. of (7.26), we choose a compactly supported positive function $h \in C_0^\infty(\mathbb{R}^3)$ with $\int \mathrm{d}x\, h(x) = 1$. For $\beta > 0$, we define $\delta_\beta(x) = \beta^{-3}h(x/\beta)$, i.e. δ_β is an approximate delta-function on the scale β. Then we have

$$\begin{aligned}&\sum_{j=1}^{k}\int_0^t \mathrm{d}s\,\mathrm{Tr}\,\Big(\mathcal{U}^{(k)}(s-t)J^{(k)}\Big)\Big[NV_N(x_j-x_{k+1})(1-w_{j,k+1}),\gamma^{(k+1)}_{N,j,k+1,s}\Big] \\ &= \sum_{j=1}^{k}\int_0^t \mathrm{d}s\,\mathrm{Tr}\,\Big(\mathcal{U}^{(k)}(s-t)J^{(k)}\Big)\Big[NV_N(x_j-x_{k+1})(1-w_{j,k+1}) - 8\pi a_0\delta_\beta(x_j-x_{k+1}),\gamma^{(k+1)}_{N,j,k+1,s}\Big] \\ &\quad + \sum_{j=1}^{k}\int_0^t \mathrm{d}s\,\mathrm{Tr}\,\Big(\mathcal{U}^{(k)}(s-t)J^{(k)}\Big)\Big[8\pi a_0\delta_\beta(x_j-x_{k+1}),\gamma^{(k+1)}_{N,j,k+1,s}\Big] \\ &= \sum_{j=1}^{k}\int_0^t \mathrm{d}s\,\mathrm{Tr}\,\Big(\mathcal{U}^{(k)}(s-t)J^{(k)}\Big)\Big[8\pi a_0\delta_\beta(x_j-x_{k+1}),\gamma^{(k+1)}_{N,j,k+1,s}\Big] \\ &\quad + C_{k,T}\Big(O(N^{-1/2}) + O(\beta^{1/2})\Big)\end{aligned} \tag{7.27}$$

for some constant $C_{k,T}$ which depends on $k \geq 1$, on T, and on $J^{(k)}$ ($O(\beta^{1/2})$ is independent of N). Here we used that, by (5.6),

$$\int \mathrm{d}x NV_N(x)(1-w(x)) = 8\pi a_0\,, \tag{7.28}$$

and we applied Lemma 7.2. To apply Lemma 7.2, we used Proposition 5.2 and that, by (7.8),

$$\|\!|\mathcal{U}_0^{(k)}(s-t)J^{(k)}|\!\|_j \leq C \left\|\Omega_k^7\, \mathcal{U}_0^{(k)}(s-t)J^{(k)}\, \Omega_k^7\right\|_{\mathrm{HS}}$$

with a k-dependent constant C. Since $e^{-i(s-t)\Delta_j}\langle x_j\rangle^m e^{i(s-t)\Delta_j} = \langle x_j + 2(s-t)p_j\rangle^m$, for any $j = 1,\dots,k$, $m \in \mathbb{N}$, we obtain that

$$\|\!|\mathcal{U}_0^{(k)}(s-t)J^{(k)}|\!\|_j \leq C(1+|t-s|^7)\left\|\Omega_k^7\, J^{(k)}\, \Omega_k^7\right\|_{\mathrm{HS}}\,.$$

To control the first term on the r.h.s. of (7.27) we go back to $\gamma_{N,t}^{(k+1)}$. We write

$$\gamma_{N,j,k+1,s}^{(k+1)} = \gamma_{N,s}^{(k+1)} + \Big(\frac{1}{1-w_{j,k+1}} - 1\Big)\gamma_{N,s}^{(k+1)} + \frac{1}{1-w_{j,k+1}}\gamma_{N,s}^{(k+1)}\Big(\frac{1}{1-w_{j,k+1}} - 1\Big)\,. \tag{7.29}$$

When we insert (7.29) in the r.h.s. of (7.27), the contributions arising from the last two terms in (7.29) converge to zero, as $N \to \infty$, for any fixed $\beta > 0$. For example, to bound the contribution of the second term on the r.h.s. of (7.29), we use that

$$\begin{aligned}
&\Big|\mathrm{Tr}\,\Big(\mathcal{U}^{(k)}(s-t)J^{(k)}\Big)\left[8\pi a_0\delta_\beta(x_j-x_{k+1}), \left(\frac{1}{1-w_{j,k+1}}-1\right)\gamma_{N,s}^{(k+1)}\right]\Big| \\
&\leq C\Big|\mathrm{Tr}\,\Big(\mathcal{U}^{(k)}(s-t)J^{(k)}\Big)\left(S_{k+1}^{-1}\delta_\beta(x_j-x_{k+1})S_{k+1}\right)\left(S_{k+1}^{-1}\frac{w_{j,k+1}}{1-w_{j,k+1}}S_{k+1}^{-1}\right)\left(S_{k+1}\gamma_{N,s}^{(k+1)}S_{k+1}\right)\Big| \\
&\quad + C\Big|\mathrm{Tr}\,\Big(\mathcal{U}^{(k)}(s-t)J^{(k)}\Big)\left(S_{k+1}^{-1}\frac{w_{j,k+1}}{1-w_{j,k+1}}S_{k+1}^{-1}\right)\left(S_{k+1}\gamma_{N,s}^{(k+1)}S_{k+1}\right)\left(S_{k+1}^{-1}\delta_\beta(x_j-x_{k+1})S_{k+1}\right)\Big| \\
&\leq C\|S_{k+1}^{-1}\delta_\beta(x_j-x_{k+1})S_{k+1}\|\,\left\|S_{k+1}^{-1}\frac{w_{j,k+1}}{1-w_{j,k+1}}S_{k+1}^{-1}\right\|\,\mathrm{Tr}\;S_{k+1}^2\gamma_{N,s}^{(k+1)}\,.
\end{aligned} \tag{7.30}$$

Now we have

$$\left\|S_{k+1}^{-1}\frac{w_{j,k+1}}{1-w_{j,k+1}}S_{k+1}^{-1}\right\| \leq CN^{-1} \tag{7.31}$$

because $w(x) \leq Ca|x|^{-1}$ and thus, as an operator inequality, $w_{j,k+1} \leq CaS_{k+1}^2$ (and $a \simeq N^{-1}$). Moreover

$$\begin{aligned}
\mathrm{Tr}\;S_{k+1}^2\gamma_{N,s}^{(k)} &= \langle\psi_{N,s}, (1-\Delta_{k+1})\psi_{N,s}\rangle \\
&\leq N^{-1}\langle\psi_{N,s}, (H_N+N)\psi_{N,s}\rangle \\
&= N^{-1}\langle\psi_N, (H_N+N)\psi_N\rangle \leq C
\end{aligned} \tag{7.32}$$

by the assumption (2.13). It is also easy to see that

$$\|S_{k+1}^{-1}\delta_\beta(x_j-x_{k+1})S_{k+1}\| \leq C\beta^{-4} \tag{7.33}$$

for $\beta < 1$. The contribution arising from the last term on the r.h.s. of (7.29) can also be controlled

similarly. Therefore, it follows from (7.26), (7.27), (7.29), and (7.30) that

$$\begin{aligned} N\sum_{j=1}^{k}\int_0^t \mathrm{d}s\,\mathrm{Tr}\,J^{(k)}\mathcal{U}^{(k)}(t-s)\left[V_N(x_j-x_{k+1}),\gamma_{N,s}^{(k+1)}\right] \\ = 8\pi a_0\sum_{j=1}^{k}\int_0^t \mathrm{d}s\,\mathrm{Tr}\,\left(\mathcal{U}^{(k)}(s-t)J^{(k)}\right)\left[\delta_\beta(x_j-x_{k+1}),\gamma_{\infty,s}^{(k+1)}\right] \\ + 8\pi a_0\sum_{j=1}^{k}\int_0^t \mathrm{d}s\,\mathrm{Tr}\,\left(\mathcal{U}^{(k)}(s-t)J^{(k)}\right)\left[\delta_\beta(x_j-x_{k+1}),\gamma_{N,s}^{(k+1)}-\gamma_{\infty,s}^{(k+1)}\right] \\ + C_{k,T}\left(O(\beta^{1/2})+o_N(1)\right), \end{aligned} \tag{7.34}$$

where $o_N(1)\to 0$ as $N\to\infty$ (for any fixed $\beta>0$). The first term is the main term. To control the second term, we rewrite it, for $\varepsilon>0$, as

$$\begin{aligned} \sum_{j=1}^{k}\int_0^t \mathrm{d}s\,\mathrm{Tr}\,\left(\mathcal{U}^{(k)}(s-t)J^{(k)}\right)\left[\delta_\beta(x_j-x_{k+1}),\gamma_{N,s}^{(k+1)}-\gamma_{\infty,s}^{(k+1)}\right] \\ = \sum_{j=1}^{k}\int_0^t \mathrm{d}s\,\mathrm{Tr}\,\left(\mathcal{U}^{(k)}(s-t)J^{(k)}\right)\delta_\beta(x_j-x_{k+1})\frac{1}{1+\varepsilon S_{k+1}}\left(\gamma_{N,s}^{(k+1)}-\gamma_{\infty,s}^{(k+1)}\right) \\ + \sum_{j=1}^{k}\int_0^t \mathrm{d}s\,\mathrm{Tr}\,\left(\mathcal{U}^{(k)}(s-t)J^{(k)}\right)\delta_\beta(x_j-x_{k+1})\left(1-\frac{1}{1+\varepsilon S_{k+1}}\right)\left(\gamma_{N,s}^{(k+1)}-\gamma_{\infty,s}^{(k+1)}\right) \\ - \sum_{j=1}^{k}\int_0^t \mathrm{d}s\,\mathrm{Tr}\,\delta_\beta(x_j-x_{k+1})\frac{1}{1+\varepsilon S_{k+1}}\left(\mathcal{U}^{(k)}(s-t)J^{(k)}\right)\left(\gamma_{N,s}^{(k+1)}-\gamma_{\infty,s}^{(k+1)}\right) \\ - \sum_{j=1}^{k}\int_0^t \mathrm{d}s\,\mathrm{Tr}\,\delta_\beta(x_j-x_{k+1})\left(1-\frac{1}{1+\varepsilon S_{k+1}}\right)\left(\mathcal{U}^{(k)}(s-t)J^{(k)}\right)\left(\gamma_{N,s}^{(k+1)}-\gamma_{\infty,s}^{(k+1)}\right). \end{aligned} \tag{7.35}$$

The second term on the r.h.s. of (7.35) can be bounded by using that

$$\begin{aligned} \left|\mathrm{Tr}\,\left(\mathcal{U}^{(k)}(s-t)J^{(k)}\right)\delta_\beta(x_j-x_{k+1})\left(1-\frac{1}{1+\varepsilon S_{k+1}}\right)\left(\gamma_{N,s}^{(k+1)}-\gamma_{\infty,s}^{(k+1)}\right)\right| \\ \leq \varepsilon\left\|\left(\mathcal{U}^{(k)}(s-t)J^{(k)}\right)\delta_\beta(x_j-x_{k+1})\right\|\left(\mathrm{Tr}\;S_{k+1}\gamma_{N,s}^{(k+1)}S_{k+1}+\mathrm{Tr}S_{k+1}\gamma_{\infty,s}^{(k+1)}S_{k+1}\right) \\ \leq C\beta^{-3}\varepsilon\left(\mathrm{Tr}\;S_{k+1}^2\gamma_{N,s}^{(k+1)}+\mathrm{Tr}S_{k+1}^2\gamma_{\infty,s}^{(k+1)}\right) \\ \leq C\beta^{-3}\varepsilon \end{aligned} \tag{7.36}$$

where we used (7.32) and Proposition 6.3. Also the fourth term on the r.h.s. of (7.35) can be controlled analogously. As for the first and third term on the r.h.s. of (7.35), we note that for every fixed $\varepsilon>0$, $\beta>0$ and $s\in[0,t]$, the integrand converges to zero, as $N\to\infty$, by (7.5), and because

$$\left(\mathcal{U}^{(k)}(s-t)J^{(k)}\right)\delta_\beta(x_j-x_{k+1})\frac{1}{1+\varepsilon S_{k+1}},\quad \delta_\beta(x_j-x_{k+1})\frac{1}{1+\varepsilon S_{k+1}}\left(\mathcal{U}^{(k)}(s-t)J^{(k)}\right)\in\mathcal{K}_{k+1}\,. \tag{7.37}$$

Since, moreover, the integrand is bounded uniformly in $s \in [0,t]$ (because for fixed $\varepsilon, \beta > 0$ the norm of the operators (7.37) is bounded uniformly in s), it follows from Lebesgue dominated convergence theorem and from (7.34) that

$$\begin{aligned} N \sum_{j=1}^{k} \int_0^t \mathrm{d}s \, \mathrm{Tr}\, J^{(k)} \mathcal{U}^{(k)}(t-s) \left[V_N(x_j - x_{k+1}), \gamma_{N,s}^{(k+1)} \right] \\ = \sum_{j=1}^{k} \int_0^t \mathrm{d}s \, \mathrm{Tr} \left(\mathcal{U}^{(k)}(s-t) J^{(k)} \right) \left[8\pi a_0 \delta_\beta(x_j - x_{k+1}), \gamma_{\infty,s}^{(k+1)} \right] \\ + C_{k,T} \left(O(\beta^{1/2}) + \beta^{-3} O(\varepsilon) + o_N(1) \right) \end{aligned} \tag{7.38}$$

where the convergence $o_N(1) \to 0$ as $N \to \infty$ depends on ε and β. By applying Lemma 7.2 again and by using that, by Proposition 6.3,

$$\max_{j=1,\dots,k} \sup_{t \in [0,T]} \mathrm{Tr}(1-\Delta_j)(1-\Delta_{k+1}) \, \gamma_{\infty,t}^{(k+1)} \leq C \, .$$

we can replace $\delta_\beta(x_j - x_{k+1})$ with $\delta(x_j - x_{k+1})$ in (7.38) at the expense of an error $O(\beta^{-1/2})$.

From (7.11), (7.12), (7.13), (7.17), (7.18), and (7.38) with $\delta(x_j - x_{k+1})$ it follows, letting $N \to \infty$ with fixed $\beta > 0$ and $\varepsilon > 0$, that

$$\begin{aligned} \mathrm{Tr}\, J^{(k)} \gamma_{\infty,t}^{(k)} = \mathrm{Tr}\, J^{(k)} \mathcal{U}^{(k)}(t) \, \gamma_{\infty,0}^{(k)} \\ - i \sum_{j=1}^{k} \int_0^t \mathrm{d}s \, \mathrm{Tr} \left(\mathcal{U}^{(k)}(s-t) J^{(k)} \right) \left[8\pi a_0 \delta(x_j - x_{k+1}), \gamma_{\infty,s}^{(k+1)} \right] + O(\beta^{1/2}) + \beta^{-4} O(\varepsilon) \, . \end{aligned}$$

Eq. (7.10) now follows from the last equation letting first $\varepsilon \to 0$ and then $\beta \to 0$. □

8 Regularization of the Initial Wave Function

In this section we show how to regularize the initial wave function ψ_N given in Theorem 2.2.

Proposition 8.1. *Suppose that (2.17) is satisfied. For $\kappa > 0$ we define*

$$\widetilde{\psi}_N := \frac{\chi(\kappa H_N / N) \psi_N}{\| \chi(\kappa H_N / N) \psi_N \|} \, . \tag{8.1}$$

Here $\chi \in C_0^\infty(\mathbb{R})$ is a cutoff function such that $0 \leq \chi \leq 1$, $\chi(s) = 1$ for $0 \leq s \leq 1$ and $\chi(s) = 0$ for $s \geq 2$. We denote by $\widetilde{\gamma}_N^{(k)}$, for $k = 1, \dots, N$, the marginal densities associated with $\widetilde{\psi}_N$.

i) For every integer $k \geq 1$ we have

$$\langle \widetilde{\psi}_N, H_N^k \, \widetilde{\psi}_N \rangle \leq \frac{2^k N^k}{\kappa^k} \, . \tag{8.2}$$

ii) We have

$$\sup_N \| \psi_N - \widetilde{\psi}_N \| \leq C \kappa^{1/2} \, .$$

iii) Suppose, moreover, that the assumption (2.18) is satisfied, that is, suppose that there exists $\varphi \in L^2(\mathbb{R}^3)$ and, for every $N \in \mathbb{N}$ and $k = 1, \dots, N$, there exists $\xi_N^{(N-k)} \in L^2_s(\mathbb{R}^{3(N-k)})$ with $\|\xi_N^{(N-k)}\| = 1$ such that

$$\lim_{N\to\infty} \|\psi_N - \varphi^{\otimes k} \otimes \xi_N^{(N-k)}\| = 0 \,. \tag{8.3}$$

Then, for $\kappa > 0$ small enough, and for every fixed $k \geq 1$ and $J^{(k)} \in \mathcal{K}_k$, we have

$$\lim_{N\to\infty} Tr\, J^{(k)} \left(\widetilde{\gamma}_N^{(k)} - |\varphi\rangle\langle\varphi|^{\otimes k}\right) = 0 \,. \tag{8.4}$$

Proof. The proof of part i) and ii) is analogous to the proof of part i) and ii) of Proposition 5.1 in [9]. Introduce the shorthand notation $\Xi := \chi(\kappa H_N/N)$. In order to prove i), we note that $\mathbf{1}(H_N \leq 2N/\kappa)\Xi = \Xi$, where $\mathbf{1}(s \leq \lambda)$ is the characteristic function of $[0, \lambda]$. Therefore

$$\begin{aligned} \langle \widetilde{\psi}_N, H_N^k\, \widetilde{\psi}_N\rangle &= \left\langle \frac{\Xi\psi_N}{\|\Xi\psi_N\|}, H_N^k \frac{\Xi\psi_N}{\|\Xi\psi_N\|} \right\rangle = \left\langle \frac{\Xi\psi_N}{\|\Xi\psi_N\|}, \mathbf{1}(H_N \leq 2N/\kappa) H_N^k \frac{\Xi\psi_N}{\|\Xi\psi_N\|} \right\rangle \\ &\leq \|\mathbf{1}(H_N \leq 2N/\kappa) H_N^k\| \leq \frac{2^k N^k}{\kappa^k} \,. \end{aligned} \tag{8.5}$$

To prove ii), we compute

$$\|\Xi\psi_N - \psi_N\|^2 = \left\langle \psi_N, (1-\Xi)^2 \psi_N \right\rangle \leq \left\langle \psi_N, \mathbf{1}(\kappa H_N \geq N)\psi_N \right\rangle \,. \tag{8.6}$$

Next we use that $\mathbf{1}(s \geq 1) \leq s$, for all $s \geq 0$. Therefore

$$\|\Xi\psi_N - \psi_N\|^2 \leq \frac{\kappa}{N} \langle \psi_N, H_N \psi_N\rangle \leq C\kappa \tag{8.7}$$

by the assumption (2.17). Hence

$$\|\Xi\psi_N - \psi_N\| \leq C\kappa^{1/2}. \tag{8.8}$$

Since $\|\psi_N\| = 1$, part ii) follows by (8.8), because

$$\begin{aligned} \left\|\psi_N - \frac{\Xi\psi_N}{\|\Xi\psi_N\|}\right\| &\leq \|\psi_N - \Xi\psi_N\| + \left\|\Xi\psi_N - \frac{\Xi\psi_N}{\|\Xi\psi_N\|}\right\| = \|\psi_N - \Xi\psi_N\| + |1 - \|\Xi\psi_N\|| \\ &\leq 2\|\psi_N - \Xi\psi_N\| \,. \end{aligned} \tag{8.9}$$

Finally, we prove iii). For any sufficiently small κ we will prove that for any fixed $k \geq 1$, $J^{(k)} \in \mathcal{K}_k$ and $\varepsilon > 0$ (small enough)

$$\left|\mathrm{Tr}\; J^{(k)} \left(\widetilde{\gamma}_N^{(k)} - |\varphi\rangle\langle\varphi|^{\otimes k}\right)\right| \leq \varepsilon \tag{8.10}$$

holds if $N \geq N_0(k, \varepsilon)$ is large enough. To this end, we choose $\varphi_* \in H^2(\mathbb{R}^3)$ with $\|\varphi_*\| = 1$, such that $\|\varphi - \varphi_*\| \leq \varepsilon/(32k\|J^{(k)}\|)$. Then we have

$$\|\varphi^{\otimes k} \otimes \xi_N^{(N-k)} - \varphi_*^{\otimes k} \otimes \xi_N^{(N-k)}\| \leq k\|\varphi - \varphi_*\| \leq \frac{\varepsilon}{32\|J^{(k)}\|} \,. \tag{8.11}$$

Therefore

$$\left\|\frac{\Xi\psi_N}{\|\Xi\psi_N\|} - \frac{\Xi\left(\varphi_*^{\otimes k} \otimes \xi_N^{(N-k)}\right)}{\|\Xi\left(\varphi_*^{\otimes k} \otimes \xi_N^{(N-k)}\right)\|}\right\| \leq \frac{2}{\|\Xi\psi_N\|} \left\|\Xi\left(\psi_N - \varphi_*^{\otimes k} \otimes \xi_N^{(N-k)}\right)\right\| \leq 4\left\|\psi_N - \varphi_*^{\otimes k} \otimes \xi_N^{(N-k)}\right\| \tag{8.12}$$

for $\kappa > 0$ small enough (by (8.8) and because $\|\Xi\| \leq 1$). Hence

$$\Big\| \frac{\Xi\psi_N}{\|\Xi\psi_N\|} - \frac{\Xi\left(\varphi_*^{\otimes k} \otimes \xi_N^{(N-k)}\right)}{\|\Xi\left(\varphi_*^{\otimes k} \otimes \xi_N^{(N-k)}\right)\|} \Big\| \leq 4\|\psi_N - \varphi^{\otimes k} \otimes \xi_N^{(N-k)}\| + 4\|\varphi^{\otimes k} \otimes \xi_N^{(N-k)} - \varphi_*^{\otimes k} \otimes \xi_N^{(N-k)}\| \\ \leq \frac{\varepsilon}{6\|J^{(k)}\|} \tag{8.13}$$

for N large enough. Here we used (8.11) and the assumption (8.3). Next we define the Hamiltonian

$$\widehat{H}_N := -\sum_{j=k+1}^{N} \Delta_j + \sum_{k<i<j}^{N} V_N(x_i - x_j)\,. \tag{8.14}$$

Note that $\widehat{H}_N$ acts only on the last $N-k$ variables. We set $\widehat{\Xi} := \chi(\kappa\widehat{H}_N/N)$. Then, from (8.13), we will obtain

$$\Big\| \frac{\Xi\psi_N}{\|\Xi\psi_N\|} - \frac{\widehat{\Xi}\left(\varphi_*^{\otimes k} \otimes \xi_N^{(N-k)}\right)}{\|\widehat{\Xi}\left(\varphi_*^{\otimes k} \otimes \xi_N^{(N-k)}\right)\|} \Big\| \leq \frac{\varepsilon}{3\|J^{(k)}\|} \tag{8.15}$$

for N sufficiently large (if $\kappa > 0$ and $\varepsilon > 0$ are small enough).

Before proving (8.15), let us show how (8.10) follows from it. Let

$$\widehat{\psi}_N := \frac{\widehat{\Xi}\left(\varphi_*^{\otimes k} \otimes \xi_N^{(N-k)}\right)}{\|\widehat{\Xi}\left(\varphi_*^{\otimes k} \otimes \xi_N^{(N-k)}\right)\|} = \varphi_*^{\otimes k} \otimes \frac{\widehat{\Xi}\xi_N^{(N-k)}}{\|\widehat{\Xi}\xi_N^{(N-k)}\|}$$

since $\widehat{\Xi}$ acts only on the last $N-k$ variables and since $\|\varphi_*\| = 1$. Moreover, we define

$$\widehat{\gamma}_N^{(k)}(\mathbf{x}_k; \mathbf{x}_k') := \int \mathrm{d}\mathbf{x}_{N-k}\, \widehat{\psi}_N(\mathbf{x}_k, \mathbf{x}_{N-k})\overline{\widehat{\psi}}_N(\mathbf{x}_k', \mathbf{x}_{N-k})\,.$$

Note that $\widehat{\psi}_N$ is not symmetric in all variables, but it is symmetric in the first k and the last $N-k$ variables. In particular, $\widehat{\gamma}_N^{(k)}$ is a density matrix and clearly

$$\widehat{\gamma}_N^{(k)} = |\varphi_*\rangle\langle\varphi_*|^{\otimes k} \quad \text{i.e.} \quad \widehat{\gamma}_N^{(k)}(\mathbf{x}_k; \mathbf{x}_k') = \prod_{j=1}^{k} \varphi_*(x_j)\overline{\varphi}_*(x_j')\,.$$

Therefore, since $\|\widetilde{\psi}_N - \widehat{\psi}_N\| \leq \varepsilon/(3\|J^{(k)}\|)$ by (8.15) and since $\|\varphi - \varphi_*\| \leq \varepsilon/(32k\|J^{(k)}\|)$, we have

$$\Big|\mathrm{Tr}\, J^{(k)}\left(\widetilde{\gamma}_N^{(k)} - |\varphi\rangle\langle\varphi|^{\otimes k}\right)\Big| \leq \Big|\mathrm{Tr}\, J^{(k)}\left(\widetilde{\gamma}_N^{(k)} - |\varphi_*\rangle\langle\varphi_*|^{\otimes k}\right)\Big| + \Big|\mathrm{Tr}\, J^{(k)}\left(|\varphi_*\rangle\langle\varphi_*|^{\otimes k} - |\varphi\rangle\langle\varphi|^{\otimes k}\right)\Big| \\ \leq 2\|J^{(k)}\|\,\|\widetilde{\psi}_N - \widehat{\psi}_N\| + 2k\|J^{(k)}\|\,\|\varphi - \varphi_*\| \leq \varepsilon \tag{8.16}$$

for N sufficiently large (for arbitrary $\kappa, \varepsilon > 0$ small enough). This proves (8.10).

It remains to prove (8.15). To this end, we set $\psi_{N,*} := \varphi_*^{\otimes k} \otimes \xi_N^{(N-k)}$, and we expand the operator $\Xi - \widehat{\Xi} = \chi(\kappa H_N/N) - \chi(\kappa\widehat{H}_N/N)$ using the Helffer-Sjöstrand functional calculus (see,

for example, [4]). Let $\widetilde{\chi}$ be an almost analytic extension of the smooth function χ of order three (that is $|\partial_{\bar{z}}\widetilde{\chi}(z)| \leq C|y|^3$, for $y = \mathrm{Im} z$ near zero): for example we can take $\widetilde{\chi}(z = x + iy) := [\chi(x)+iy\chi'(x)+\chi''(x)(iy)^2/2+\chi'''(x)(iy)^3/6]\theta(x,y)$, where $\theta \in C_0^\infty(\mathbb{R}^2)$ and $\theta(x,y) = 1$ for $z = x+iy$ in some complex neighborhood of the support of χ. Then

$$\begin{aligned}(\Xi - \widehat{\Xi})\psi_{N,*} &= -\frac{1}{\pi}\int \mathrm{d}x\,\mathrm{d}y\,\partial_{\bar{z}}\widetilde{\chi}(z)\left(\frac{1}{z-(\kappa H_N/N)} - \frac{1}{z-(\kappa\widehat{H}_N/N)}\right)\psi_{N,*} \\ &= -\frac{\kappa}{N\pi}\int \mathrm{d}x\,\mathrm{d}y\,\partial_{\bar{z}}\widetilde{\chi}(z)\,\frac{1}{z-(\kappa H_N/N)}(H_N - \widehat{H}_N)\frac{1}{z-(\kappa\widehat{H}_N/N)}\psi_{N,*}\,.\end{aligned} \tag{8.17}$$

Taking the norm we obtain

$$\|(\Xi - \widehat{\Xi})\psi_{N,*}\| \leq \frac{C\kappa}{N}\int \mathrm{d}x\,\mathrm{d}y\,\frac{|\partial_{\bar{z}}\widetilde{\chi}(z)|}{|y|}\left\|\frac{1}{z-(\kappa H_N/N)}(H_N - \widehat{H}_N)\frac{1}{z-(\kappa\widehat{H}_N/N)}\psi_{N,*}\right\|. \tag{8.18}$$

Notice that the operator

$$H_N - \widehat{H}_N = -\sum_{j=1}^{k}\Delta_j + \sum_{i\leq k, i<j\leq N} V_N(x_i - x_j) \tag{8.19}$$

is positive hence $(H_N - \widehat{H}_N)^{1/2}$ exists. By using $\|AB\psi\|^2 \leq \|A\|^2\langle\psi, B^*B\psi\rangle$, we obtain

$$\begin{aligned}&\left\|\frac{1}{z-(\kappa H_N/N)}(H_N - \widehat{H}_N)\frac{1}{z-(\kappa\widehat{H}_N/N)}\psi_{N,*}\right\|^2 \\ &\qquad\leq \left\|(H_N - \widehat{H}_N)^{1/2}\frac{1}{|z-(\kappa H_N/N)|^2}(H_N - \widehat{H}_N)^{1/2}\right\| \\ &\qquad\qquad\times\left\langle\psi_{N,*}, \frac{1}{\bar{z}-(\kappa\widehat{H}_N/N)}(H_N - \widehat{H}_N)\frac{1}{z-(\kappa\widehat{H}_N/N)}\psi_{N,*}\right\rangle.\end{aligned} \tag{8.20}$$

Moreover (since $\|BA^2B\| = \|AB^2A\| \leq \|AC^2A\|$ for positive operators A, B, C with $B^2 \leq C^2$),

$$\begin{aligned}\left\|(H_N - \widehat{H}_N)^{1/2}\frac{1}{|z-(\kappa H_N/N)|^2}(H_N - \widehat{H}_N)^{1/2}\right\| &= \left\|\frac{1}{|z-(\kappa H_N/N)|}(H_N - \widehat{H}_N)\frac{1}{|z-(\kappa H_N/N)|}\right\| \\ &\leq \left\|\frac{1}{|z-(\kappa H_N/N)|}H_N\frac{1}{|z-(\kappa H_N/N)|}\right\| \\ &\leq \frac{CN}{|y|^2\kappa}\end{aligned} \tag{8.21}$$

for z in the support of $\widetilde{\chi}$, where we used the spectral theorem in the last step. On the other hand, the second factor on the r.h.s. of (8.20) can be bounded by

$$\begin{aligned}&\left\langle\psi_{N,*}, \frac{1}{\bar{z}-(\kappa\widehat{H}_N/N)}(H_N - \widehat{H}_N)\frac{1}{z-(\kappa\widehat{H}_N/N)}\psi_{N,*}\right\rangle \\ &\qquad\leq k\left\langle\psi_{N,*}, \frac{1}{\bar{z}-(\kappa\widehat{H}_N/N)}\left(-\Delta_1 + kV_N(x_1-x_2) + NV_N(x_1-x_{k+1})\right)\frac{1}{z-(\kappa\widehat{H}_N/N)}\psi_{N,*}\right\rangle.\end{aligned}$$

Here we used the fact that $\psi_{N,*}$ is symmetric w.r.t. permutations of the first k and the last $N-k$ variables, and that the operator $\widehat{H}_N$ preserves this property. Since $NV_N(x_1-x_{k+1}) \leq C\|V\|_{L^1}(1-\Delta_1)^2$, and $kV_N(x_1-x_2) \leq C\|V\|_{L^1}(1-\Delta_1)^2$ (see (6.47)) we find

$$\begin{aligned}\Big\langle \psi_{N,*}, \frac{1}{\bar{z}-(\kappa\widehat{H}_N/N)}(H_N-\widehat{H}_N)\frac{1}{z-(\kappa\widehat{H}_N/N)}\psi_{N,*}\Big\rangle \\ \leq k\Big\langle \psi_{N,*}\frac{1}{\bar{z}-(\kappa H_N/N)}\left(-\Delta_1+(1-\Delta_1)^2\right)\frac{1}{z-(\kappa H_N/N)}\psi_{N,*}\Big\rangle \leq C\,k\,|y|^{-2}\|\varphi_*\|^2_{H_2}\end{aligned} \tag{8.22}$$

because Δ_1 commutes with $\widehat{H}_N$ (recall that $\psi_{N,*}=\varphi_*^{\otimes k}\otimes\xi_N^{(N-k)}$). From (8.18), (8.20), (8.21) and (8.22) we find that

$$\|(\Xi-\widehat{\Xi})\psi_{N,*}\| \leq C_{k,\varepsilon}N^{-1/2}$$

for a constant $C_{k,\varepsilon}$ depending on k and ε (through the norm $\|\varphi^*\|_{H^2}$) but independent of κ, for κ small enough. This implies that

$$\begin{aligned}\left\|\frac{\Xi\left(\varphi_*^{\otimes k}\otimes\xi_N^{(N-k)}\right)}{\|\Xi\left(\varphi_*^{\otimes k}\otimes\xi_N^{(N-k)}\right)\|}-\frac{\widehat{\Xi}\left(\varphi_*^{\otimes k}\otimes\xi_N^{(N-k)}\right)}{\|\widehat{\Xi}\left(\varphi_*^{\otimes k}\otimes\xi_N^{(N-k)}\right)\|}\right\| &\leq \frac{2}{\|\Xi\left(\varphi_*^{\otimes k}\otimes\xi_N^{(N-k)}\right)\|}\,\|(\Xi-\widehat{\Xi})\psi_{N,*}\| \\ &\leq 4\,\|(\Xi-\widehat{\Xi})\psi_{N,*}\| \leq \frac{\varepsilon}{6\|J^{(k)}\|}\end{aligned} \tag{8.23}$$

for N large enough (and assuming that $\varepsilon>0$ and $\kappa>0$ are small enough, independently of N). Here we used that (by (8.3), (8.8), and (8.11))

$$\begin{aligned}\|\Xi\left(\varphi_*^{\otimes k}\otimes\xi_N^{(N-k)}\right)\| &\geq \|\psi_N\|-\|\Xi\psi_N-\psi_N\|-\|\Xi\left(\psi_N-\varphi^{\otimes k}\otimes\xi_N^{(N-k)}\right)\| \\ &\quad -\|\Xi\left(\varphi^{\otimes k}\otimes\xi_N^{(N-k)}-\varphi_*^{\otimes k}\otimes\xi_N^{(N-k)}\right)\| \\ &\geq 1-C\kappa^{1/2}-o(1)-\frac{\varepsilon}{32\|J^{(k)}\|} \geq 1/2\end{aligned} \tag{8.24}$$

for κ,ε small enough and for N large enough. From (8.23) and (8.13) we obtain (8.15). This completes the proof of part iii). □

9 Proof of Proposition 5.3

This section is devoted to the proof the Proposition 5.3. Let us recall the definition of the cutoff functions

$$\Theta_k^{(n)}=\Theta_k^{(n)}(\mathbf{x})=\exp\left(-\frac{2^n}{\ell^\varepsilon}\sum_{i\leq k}\sum_{j\neq i}h(x_i-x_j)\right)$$

from (5.32) with the function h defined in (5.29). We introduce the notation $h_{ij}=h(x_i-x_j)$ and we also adopt the convention that $h_{ii}=0$ for any $i\in\mathbb{N}$. Moreover we recall that $D_k:=\nabla_1\dots\nabla_k$.

Proof of Proposition 5.3. We prove (5.33) by induction over k. For $k=1$ we clearly have

$$\langle\psi,(H_N+N)\psi\rangle \geq N\int|\nabla_1\psi|^2+\frac{N(N-1)}{2}\int V_N(x_1-x_2)|\psi|^2. \tag{9.1}$$

For $k=2$ we have, from (5.9), (5.16) (but keeping the term on the sixth line, which was neglected, because of its positivity, in the last inequality in (5.16)), (5.17), and (5.18) we find, for ρ small enough (recall the definition of ρ in (2.7)),

$$\begin{aligned}\langle\psi,(H_N+N)^2\psi\rangle &\geq \langle\psi,H_N^2\psi\rangle\\ &\geq N(N-1)\langle\psi,\mathfrak{h}_1\mathfrak{h}_2\psi\rangle+N\langle\psi,\mathfrak{h}_1^2\psi\rangle\\ &\geq N(N-1)(1-c\rho)\int(1-w_{12})^2|\nabla_1\nabla_2\phi_{12}|^2\\ &\quad+\frac{N(N-1)(N-2)}{2}\int(1-w_{12})^2\,V_N(x_2-x_3)|\nabla_1\phi_{12}|^2+N\int|\mathfrak{h}_1\psi|^2\end{aligned}\tag{9.2}$$

where $\mathfrak{h}_i$, for $i=1,\dots,N$, was defined in (5.8). From the last term we get

$$\int|\mathfrak{h}_1\psi|^2\geq\int\theta_1^{(2)}|\mathfrak{h}_1\psi|^2\geq\int\theta_1^{(2)}\Delta_1\overline{\psi}\Delta_1\psi+\frac{1}{2}\sum_{j\geq2}\int\theta_1^{(2)}\left(\Delta_1\overline{\psi}\,V_N(x_1-x_j)\psi+\text{h.c.}\right)\tag{9.3}$$

where h.c. denotes the hermitian conjugate. The last term is exponentially small in N because on the support of the potential $V_N(x_1-x_j)$ the point x_1 is close to x_j (on the length scale N^{-1}) and this makes the factor $\theta_1^{(2)}$ exponentially small. Hence we find (with the notation $\nabla_1^j:=\partial_{x_1^{(j)}}$ where $x_1=(x_1^{(1)},x_1^{(2)},x_1^{(3)})\in\mathbb{R}^3$),

$$\begin{aligned}\int\theta_1^{(2)}|\mathfrak{h}_1\psi|^2\geq{}&\int\theta_1^{(2)}|\nabla_1^2\psi|^2+\int\sum_{i,j=1}^3\left\{(\nabla_1^i\theta_1^{(2)})(\nabla_1^j\overline{\psi})\nabla_1^i\nabla_1^j\psi+\text{h.c.}\right\}+\int\sum_{i,j=1}^3\nabla_1^i\nabla_1^j\theta_1^{(2)}\nabla_1^i\overline{\psi}\nabla_1^j\psi\\&-o(N)\left\{\int\theta_1^{(1)}|\nabla_1\psi|^2+\int|\psi|^2\right\}\end{aligned}\tag{9.4}$$

by using $|\nabla_1\theta_1^{(2)}|\leq C\ell^{-1}\theta_1^{(1)}$ from Lemma A.1, part iii). From part ii) and iv) of the same lemma we also have

$$\frac{\left|\nabla_1\theta_1^{(2)}\right|^2}{\theta_1^{(2)}}\leq C\ell^{-2}\theta_1^{(1)}\quad\text{and}\quad\left|\nabla_1^2\theta_1^{(2)}\right|\leq C\ell^{-2}\theta_1^{(1)}\,,\tag{9.5}$$

and therefore we obtain

$$\begin{aligned}\sum_{i,j=1}^3\left|\int(\nabla_1^i\theta_1^{(2)})(\nabla_1^j\overline{\psi})\nabla_1^i\nabla_1^j\psi\right|&\leq\alpha\int\theta_1^{(2)}|\nabla_1^2\psi|^2+\alpha^{-1}\int\frac{|\nabla_1\theta_1^{(2)}|^2}{\theta_1^{(2)}}|\nabla_1\psi|^2\\&\leq o(1)\int\theta_1^{(2)}|\nabla_1^2\psi|^2+o(N)\int\theta_1^{(1)}|\nabla_1\psi|^2\,,\end{aligned}\tag{9.6}$$

where we used that $N\ell^2\gg1$ (and an appropriate choice of the parameter α). Analogously

$$\sum_{i,j=1}^3\int\left|\nabla_1^i\nabla_1^j\theta_1^{(2)}\nabla_1^i\overline{\psi}\nabla_1^j\psi\right|\leq o(N)\int\theta_1^{(1)}|\nabla_1\psi|^2\,.\tag{9.7}$$

From (9.2)–(9.7), we find

$$\begin{aligned}\langle\psi,(H_N+N)^2\psi\rangle \geq N^2(1-c\rho-o(1))\int(1-w_{12})^2|\nabla_1\nabla_2\phi_{12}|^2\\ +\frac{N^3}{2}(1-o(1))\int(1-w_{12})^2\,V_N(x_2-x_3)|\nabla_1\phi_{12}|^2\\ +N(1-o(1))\int\theta_1^{(2)}|\nabla_1^2\psi|^2-o(N^2)\left\{\int\theta_1^{(1)}|\nabla_1\psi|^2+\int\theta_1^{(1)}|\psi|^2\right\}.\end{aligned}\tag{9.8}$$

Next we apply Lemma 9.4 (with $n=0$) to replace, in the first and second term on the r.h.s. of the last equation, ϕ_{12} by ψ. We find

$$\begin{aligned}\langle\psi,(H_N+N)^2\psi\rangle \geq N^2(1-c\rho-o(1))\int\theta_1^{(2)}|\nabla_1\nabla_2\psi|^2\\ +\frac{N^3}{2}(1-o(1))\int\theta_1^{(2)}\,V_N(x_2-x_3)|\nabla_1\psi|^2+N(1-o(1))\int\theta_1^{(2)}|\nabla_1^2\psi|^2\\ -o(N^2)\int\left\{\theta_1^{(1)}|\nabla_1\psi|^2+\theta_1^{(1)}|\psi|^2+NV_N(x_1-x_2)|\psi|^2\right\}.\end{aligned}\tag{9.9}$$

By (9.1) we have

$$\begin{aligned}o(N^2)\int\left\{\theta_1^{(1)}|\nabla_1\psi|^2+\theta_1^{(1)}|\psi|^2+NV_N(x_1-x_2)|\psi|^2\right\}&\leq o(N)\langle\psi,(H_N+N)\psi\rangle\\ &\leq o(1)\langle\psi,(H_N+N)^2\psi\rangle\,.\end{aligned}\tag{9.10}$$

Hence, from (9.9), we obtain

$$\begin{aligned}(1+o(1))\langle\psi,(H_N+N)^2\psi\rangle \geq N^2(1-c\rho-o(1))\int\theta_1^{(2)}|\nabla_1\nabla_2\psi|^2\\ +\frac{N^3}{2}(1-o(1))\int\theta_1^{(2)}\,V_N(x_2-x_3)|\nabla_1\psi|^2\\ +N(1-o(1))\int\theta_1^{(2)}|\nabla_1^2\psi|^2\,.\end{aligned}\tag{9.11}$$

It follows that, for ρ small enough, there exists $C_0>0$ such that we have

$$\begin{aligned}\langle\psi,(H_N+N)^2\psi\rangle \geq C_0^2N^2\int\theta_1^{(2)}|\nabla_1\nabla_2\psi|^2+C_0^2N^3\int\theta_1^{(2)}\,V_N(x_2-x_3)|\nabla_1\psi|^2\\ +C_0^2N\int\theta_1^{(2)}|\nabla_1^2\psi|^2\end{aligned}\tag{9.12}$$

if N is large enough.

We assume now that (5.33) is correct for all $k\leq n+1$ and we prove if for $k=n+2$, assuming $n\geq 1$. To this end we note that, for $N\geq N_0(n)$, using the induction hypothesis we have

$$\begin{aligned}\langle\psi,(H_N+N)^{n+2}\psi\rangle &\geq \langle H_N\psi,(H_N+N)^nH_N\psi\rangle\\ &\geq C_0^nN^n\int\Theta_{n-1}^{(n)}\,|D_nH_N\psi|^2\\ &\geq C_0^nN^n\int\Theta_n^{(n+2)}\,|D_nH_N\psi|^2\end{aligned}\tag{9.13}$$

where we used that $1 \geq \theta_i^{(n)} \geq \theta_i^{(n+2)}$ for every $i = 1, \ldots, n$. We write $H_N = \sum_{j=1}^N \mathfrak{h}_j^{(n)}$, with

$$\mathfrak{h}_j^{(n)} = \begin{cases} -\Delta_j + \frac{1}{2}\sum_{i>n, i\neq j} V_N(x_i - x_j) & \text{if } j > n \\ -\Delta_j + \frac{1}{2}\sum_{i\leq n} V_N(x_i - x_j) + \sum_{i>n} V_N(x_i - x_j) & \text{if } j \leq n\,. \end{cases} \tag{9.14}$$

Then we have

$$\begin{aligned} \langle \psi, (H_N + N)^{n+2}\psi\rangle \geq C_0^n N^n \sum_{i,j>n} \int \Theta_n^{(n+2)}\; D_n \mathfrak{h}_i^{(n)}\, \overline{\psi}\, D_n \mathfrak{h}_j^{(n)} \psi \\ + C_0^n N^n \left\{ \sum_{i\leq n<j} \int \Theta_n^{(n+2)}\; D_n \mathfrak{h}_i^{(n)}\, \overline{\psi}\, D_n \mathfrak{h}_j^{(n)} \psi + \text{h.c.} \right\} \\ + C_0^n N^n \sum_{i,j\leq n} \int \Theta_n^{(n+2)}\; D_n \mathfrak{h}_i^{(n)}\, \overline{\psi}\, D_n \mathfrak{h}_j^{(n)} \psi\,. \end{aligned} \tag{9.15}$$

The last term on the r.h.s. (where $i, j \leq n$) is positive and therefore it can be neglected. In the first term on the r.h.s. we can neglect all terms where $i = j$ (because they are all positive). Therefore we obtain

$$\begin{aligned} \langle \psi, (H_N + N)^{n+2}\psi\rangle \geq C_0^n N^n \sum_{i,j>n, i\neq j} \int \Theta_n^{(n+2)}\; D_n\, \mathfrak{h}_i^{(n)}\, \overline{\psi}\; D_n\, \mathfrak{h}_j^{(n)}\; \psi \\ + C_0^n N^n \sum_{i\leq n<j} \int \Theta_n^{(n+2)}\; \left\{ D_n \mathfrak{h}_i^{(n)}\, \overline{\psi}\; D_n \mathfrak{h}_j^{(n)}\; \psi + \text{h.c.} \right\}\,. \end{aligned} \tag{9.16}$$

In Proposition 9.1 below we give a lower bound for the first term in (9.16), while Proposition 9.5 estimates the second term. Combining these two estimates, we find that, for ρ small enough (independently of N and n) and for N large enough,

$$\begin{aligned} \langle \psi, (H_N + N)^{n+2}\psi\rangle \geq C_0^n N^{n+2}(1 - c\rho - o(1)) \int\; \Theta_{n+1}^{(n+2)}\; |D_{n+2}\psi|^2 \\ + C_0^n N^{n+1}(1 - o(1)) \int \Theta_{n+1}^{(n+2)}\; |\nabla_1 D_{n+1}\,\psi|^2 \\ + \frac{C_0^n N^{n+3}}{2}(1 - o(1)) \int \Theta_{n+1}^{(n+2)}\, V_N(x_{n+2} - x_{n+3})\; |D_{n+1}\psi|^2 \\ - \Omega_n(\psi) \end{aligned} \tag{9.17}$$

where the error $\Omega_n(\psi)$ is given by

$$\begin{aligned} \Omega_n(\psi) = o(N^{n+3}) \int \Theta_n^{(n+1)}\, V_N(x_{n+1} - x_{n+2})\, |D_n\,\psi|^2 \\ + o(N^{n+1}) \left\{ \int \Theta_n^{(n+1)} |\nabla_1 D_n \psi|^2 + \int \Theta_{n-1}^{(n)} |\nabla_1 D_{n-1}\psi|^2 \right\} \\ + o(N^{n+2}) \left\{ \int \Theta_n^{(n+1)} |D_{n+1}\psi|^2 + \int \Theta_{n-1}^{(n)} |D_n \psi|^2 \right. \\ \left. + \int \Theta_{n-2}^{(n-1)} |D_{n-1}\psi|^2 + \int \Theta_{n-3}^{(n-2)} |D_{n-2}\psi|^2 \right\}. \end{aligned} \tag{9.18}$$

Now we use the induction hypothesis, Eq. (5.33), with $k = n-1, n, n+1$ to bound the negative contributions. For example, (5.33) with $k = n+1$ implies that

$$o(N^{n+3}) \int \Theta_n^{(n+1)}\, V_N(x_{n+1} - x_{n+2})\, |D_n\, \psi|^2 \leq o(N) \langle \psi, (H_N + N)^{n+1} \psi \rangle \leq o(1) \langle \psi, (H_N + N)^{n+2} \psi \rangle$$

because $H_N \geq 0$. The other terms in (9.18) are treated similarly. It follows that

$$\begin{aligned} (1 + o(1))\, \langle \psi,\, (H_N + N)^{n+2} \psi \rangle \geq C_0^n N^{n+2} (1 - c\rho - o(1)) \int\, \Theta_{n+1}^{(n+2)}\, |D_{n+2} \psi|^2 \\ + C_0^n N^{n+1} (1 - o(1)) \int \Theta_{n+1}^{(n+2)}\, |\nabla_1 D_{n+1}\, \psi|^2 \\ + \frac{C_0^n N^{n+3}}{2} (1 - o(1)) \int \Theta_{n+1}^{(n+2)}\, V_N(x_{n+2} - x_{n+3})\, |D_{n+1} \psi|^2 \,. \end{aligned}$$

Thus, if ρ and C_0 are small enough (independently of n), we can find $N_0(n+2, C_0) > N_0(n, C_0)$ such that

$$\begin{aligned} \langle \psi,\, (H_N + N)^{n+2} \psi \rangle \geq C_0^{n+2} N^{n+2} \int\, \Theta_{n+1}^{(n+2)}\, |D_{n+2} \psi|^2 + C_0^{n+2} N^{n+1} \int \Theta_{n+1}^{(n+2)}\, |\nabla_1 D_{n+1}\, \psi|^2 \\ + C_0^{n+2} N^{n+3} \int \Theta_{n+1}^{(n+2)}\, V_N(x_{n+2} - x_{n+3})\, |D_{n+1} \psi|^2. \end{aligned} \tag{9.19}$$

□

In the rest of this section we will state and prove Propositions 9.1 and 9.5 used in (9.16). Both proofs will be divided into several Lemmas.

Similarly to the H_N^2-energy estimate from Proposition 3.1, the key idea in Proposition 9.1 is that $\mathfrak{h}_i^{(n)} \psi$ can be conveniently estimated by the derivatives of ϕ_{ij}, where ϕ_{ij} is given by the relation $\psi = (1 - w_{ij}) \phi_{ij}$. The estimates of all errors are done in terms of ϕ_{ij} and its derivatives. Finally, Lemma 9.4 will show how to go back from the estimates on ϕ_{ij} to estimates involving ψ with a cutoff supported on a bigger set.

Proposition 9.1. *Suppose ρ is small enough and $\ell \gg N^{-1/2}$. For $i = 1, \ldots, N$, let $\mathfrak{h}_i^{(n)}$ be defined as in (9.14). Then*

$$\begin{aligned} C_0^n N^n \sum_{i,j>n, i \neq j} \int \Theta_n^{(n+2)}\, D_n\, \mathfrak{h}_i^{(n)}\, \overline{\psi}\, D_n\, \mathfrak{h}_j^{(n)}\, \psi \\ \geq C_0^n N^{n+2} (1 - c\rho - o(1)) \int\, \Theta_{n+1}^{(n+2)}\, |D_{n+2} \psi|^2 \\ + \frac{C_0^n N^{n+3}}{2} (1 - o(1)) \int \Theta_{n+1}^{(n+2)}\, V_N(x_{n+2} - x_{n+3})\, |D_{n+1} \psi|^2 - \Omega_n(\psi) \end{aligned} \tag{9.20}$$

where the error term $\Omega_n(\psi)$ has been defined in (9.18).

Proof. For any $i \neq j$, $i, j > n$, we write $\psi = (1 - w_{ij}) \phi_{ij}$. Then we have, similarly to (5.13),

$$\begin{aligned} (1 - w_{ij})^{-1} \mathfrak{h}_i^{(n)} \big[(1 - w_{ij}) \phi_{ij} \big] &= -\Delta_i \phi_{ij} + 2 \frac{\nabla w_{ij}}{1 - w_{ij}} \nabla_i \phi_{ij} + \frac{1}{2} \sum_{m>n,\, m \neq i,j} V_N(x_i - x_m) \phi_{ij} \\ &= L_i \phi_{ij} + \frac{1}{2} \sum_{m>n,\, m \neq i,j} V_N(x_i - x_m) \phi_{ij} \end{aligned} \tag{9.21}$$

where the differential operator $L_i := -\Delta_i + 2\frac{\nabla w_{ij}}{1-w_{ij}}\nabla_i$ is such that

$$\int (1-w_{ij})^2 (L_i\overline{\phi})\chi = \int (1-w_{ij})^2 \overline{\phi}(L_i\chi) = \int (1-w_{ij})^2 \nabla_i\overline{\phi}\nabla_i\chi. \tag{9.22}$$

Note that the operator L_i also depends on the choice of the index j. Analogously, we have

$$(1-w_{ij})^{-1}\mathfrak{h}_j^{(n)}\big[(1-w_{ij})\phi_{ij}\big] = L_j\phi_{ij} + \frac{1}{2}\sum_{m>n,\, m\neq i,j} V_N(x_j-x_m)\phi_{ij}$$

with $L_j = -\Delta_j + 2\frac{\nabla w_{ji}}{1-w_{ij}}\nabla_j$. Note that D_n commutes with L_i, L_j and $1-w_{ij}$ if $i,j>n$. The l.h.s of (9.20) is thus given by

$$\begin{aligned}
C_0^n N^n \sum_{i,j>n, i\neq j} \int (1-w_{ij})^2\, \Theta_n^{(n+2)}\, D_n \left[\left(L_i + \frac{1}{2}\sum_{m>n, m\neq i,j} V_N(x_m-x_i)\right)\overline{\phi}_{ij}\right] \\
\times D_n\left[\left(L_j + \frac{1}{2}\sum_{r>n, r\neq i,j} V_N(x_j-x_r)\right)\phi_{ij}\right] \\
\geq C_0^n N^n \sum_{i,j>n,i\neq j}\int (1-w_{ij})^2\, \Theta_n^{(n+2)}\, L_iD_n\,\overline{\phi}_{ij}\, L_jD_n\,\phi_{ij} \\
+ \frac{C_0^n N^n}{2}\sum_{i,j>n,i\neq j}\ \sum_{r>n,\, r\neq i,j}\int (1-w_{ij})^2\, \Theta_n^{(n+2)}\, V_N(x_j-x_r)\, L_iD_n\,\overline{\phi}_{ij}\, D_n\phi_{ij} + \text{h.c.}\,,
\end{aligned}$$

because of the positivity of the potential. Proposition 9.1 now follows from Lemma 9.2 and Lemma 9.3, where we consider separately the two terms on the r.h.s. of the last equation. □

Lemma 9.2. *Suppose the assumptions of Lemma 9.1 are satisfied. Then we have*

$$\begin{aligned}
C_0^n N^n \sum_{i,j>n,i\neq j}\int (1-w_{ij})^2\, \Theta_n^{(n+2)}\, L_i\, D_n\,\overline{\phi}_{ij}\, L_j\, D_n\,\phi_{ij} \\
\geq C_0^n N^{n+2}\,(1-c\rho-o(1))\int \Theta_{n+1}^{(n+2)}\,|D_{n+2}\psi|^2 \\
- o(N^{n+2})\left(\int \Theta_n^{(n+1)}\,|D_{n+1}\,\psi|^2 + \int \Theta_{n-1}^{(n)}\,|D_n\psi|^2\right).
\end{aligned}\tag{9.23}$$

Proof. By the symmetry (9.22) we have

$$\begin{aligned}
&C_0^n N^n \sum_{i,j>n,i\neq j}\int (1-w_{ij})^2\, \Theta_n^{(n+2)}\, L_iD_n\,\overline{\phi}_{ij}\, L_jD_n\,\phi_{ij} \\
&= C_0^n N^n \sum_{i,j>n,i\neq j}\int (1-w_{ij})^2\,\Big\{\Theta_n^{(n+2)}\,\nabla_iD_n\,\overline{\phi}_{ij}\,\nabla_iL_jD_n\,\phi_{ij} + \nabla_i\Theta_n^{(n+2)}\,\nabla_iD_n\,\overline{\phi}_{ij}\,L_jD_n\,\phi_{ij}\Big\} \\
&= C_0^n N^n \sum_{i,j>n,i\neq j}\int (1-w_{ij})^2\,\Big\{\Theta_n^{(n+2)}\,|\nabla_j\nabla_iD_n\,\phi_{ij}|^2 + \nabla_j\Theta_n^{(n+2)}\,\nabla_iD_n\,\overline{\phi}_{ij}\,\nabla_j\nabla_iD_n\,\phi_{ij} \\
&\qquad + \nabla_i\Theta_n^{(n+2)}\,\nabla_j\nabla_iD_n\,\overline{\phi}_{ij}\,\nabla_jD_n\,\phi_{ij} + \nabla_i\nabla_j\Theta_n^{(n+2)}\,\nabla_iD_n\,\overline{\phi}_{ij}\,\nabla_jD_n\,\phi_{ij} \\
&\qquad + \Theta_n^{(n+2)}\,\nabla_iD_n\,\overline{\phi}_{ij}\,[\nabla_i,L_j]D_n\,\phi_{ij}\Big\}
\end{aligned}\tag{9.24}$$

To bound the second and third term on the r.h.s. of (9.24), we note that, by part iii) of Lemma A.1,

$$\left|\nabla_j \Theta_n^{(n+2)}\right| \leq C\ell^{-1}\left(\frac{2^{n+2}}{\ell^\varepsilon}\sum_{m=1}^n h_{mj}\right)\Theta_n^{(n+2)}\,. \tag{9.25}$$

Therefore the second term on the r.h.s. of (9.24) can be bounded by

$$\begin{aligned}
&\sum_{i,j>n,i\neq j}\left|\int (1-w_{ij})^2\,\nabla_j\Theta_n^{(n+2)}\,\nabla_i D_n\,\overline{\phi}_{ij}\,\nabla_j\nabla_i D_n\,\phi_{ij}\right| \\
&\qquad\leq \alpha\sum_{i,j>n,i\neq j}\int (1-w_{ij})^2\,\Theta_n^{(n+2)}|\nabla_j\nabla_i D_n\,\phi_{ij}|^2 \\
&\qquad\quad + C\ell^{-2}\alpha^{-1}\sum_{i,j>n,i\neq j}\int (1-w_{ij})^2\,\left(\frac{2^{n+2}}{\ell^\varepsilon}\sum_{m=1}^n h_{mj}\right)^2\Theta_n^{(n+2)}\,|\nabla_i D_n\,\phi_{ij}|^2
\end{aligned} \tag{9.26}$$

for some $\alpha>0$. Next we use that $\phi_{ij}=\psi(1-w_{ij})^{-1}$. Since $i,j>n$, we have

$$\nabla_i D_n\left(\psi(1-w_{ij})^{-1}\right) = \nabla_i w_{ij}(1-w_{ij})^{-2}D_n\psi + (1-w_{ij})^{-1}\nabla_i D_n\psi$$

and thus

$$(1-w_{ij})^2\,|\nabla_i D_n\phi_{ij}|^2 \leq 2\left(\frac{\nabla w_{ij}}{1-w_{ij}}\right)^2|D_n\psi|^2 + 2|\nabla_i D_n\psi|^2 \leq \frac{C}{|x_i-x_j|^2}|D_n\psi|^2 + 2|\nabla_i D_n\psi|^2\,. \tag{9.27}$$

Therefore the second term on the r.h.s. of (9.26) is bounded by

$$\begin{aligned}
&\sum_{i,j>n,i\neq j}\int (1-w_{ij})^2\,\left(\frac{2^{n+2}}{\ell^\varepsilon}\sum_{m=1}^n h_{mj}\right)^2\Theta_n^{(n+2)}\,|\nabla_i D_n\,\phi_{ij}|^2 \\
&\qquad\leq C\sum_{i,j>n,i\neq j}\int\left(\frac{2^{n+2}}{\ell^\varepsilon}\sum_{m=1}^n h_{mj}\right)^2\Theta_n^{(n+2)}\left\{|\nabla_i D_n\psi|^2 + \frac{1}{|x_i-x_j|^2}|D_n\psi|^2\right\} \\
&\qquad\leq C\sum_{i,j>n,i\neq j}\int\left(\frac{2^{n+2}}{\ell^\varepsilon}\sum_{m=1}^n h_{mj}\right)^2\left\{\Theta_n^{(n+2)}\,|\nabla_i D_n\psi|^2 + \left|\nabla_i\left(\Theta_n^{(n+2)}\right)^{\frac{1}{2}}\right|^2\,|D_n\psi|^2\right\}
\end{aligned} \tag{9.28}$$

where we used Hardy inequality and the fact that $i\neq j$ and $i>n$. Using a bound similar to (9.25),

and part ii) of Lemma A.1, we can continue this estimate

$$\begin{aligned}
&\sum_{i,j>n,i\neq j}\int (1-w_{ij})^2\,\left(\frac{2^{n+2}}{\ell^\varepsilon}\sum_{m=1}^n h_{mj}\right)^2\,\Theta_n^{(n+2)}\,|\nabla_i D_n\,\phi_{ij}|^2\\
&\qquad\le C\sum_{i,j>n,i\neq j}\int\left(\frac{2^{n+2}}{\ell^\varepsilon}\sum_{m=1}^n h_{mj}\right)^2\Theta_n^{(n+2)}\left\{|\nabla_i D_n\psi|^2+\ell^{-2}\left(\frac{2^{n+1}}{\ell^\varepsilon}\sum_{m=1}^n h_{mi}\right)^2\,|D_n\psi|^2\right\}\\
&\qquad\le C\sum_{i>n}\int\left(\frac{2^{n+2}}{\ell^\varepsilon}\sum_{j>n}\sum_{m=1}^n h_{mj}\right)^2\,\Theta_n^{(n+2)}\,|\nabla_i D_n\psi|^2\\
&\qquad\quad+C\ell^{-2}\int\left(\frac{2^{n+2}}{\ell^\varepsilon}\sum_{j>n}\sum_{m=1}^n h_{mj}\right)^2\left(\frac{2^{n+1}}{\ell^\varepsilon}\sum_{i>n}\sum_{m=1}^n h_{mi}\right)^2\,\Theta_n^{(n+2)}\,|D_n\psi|^2\\
&\qquad\le C\sum_{i>n}\int\Theta_n^{(n+1)}\,|\nabla_i D_n\psi|^2+C\ell^{-2}\int\Theta_n^{(n)}\,|D_n\psi|^2\\
&\qquad\le CN\int\Theta_n^{(n+1)}\,|D_{n+1}\psi|^2+C\ell^{-2}\int\Theta_n^{(n)}\,|D_n\psi|^2\,,
\end{aligned}\tag{9.29}$$

because of the permutation symmetry of ψ. From (9.26) we find

$$\begin{aligned}
&\sum_{i,j>n,i\neq j}\left|\int(1-w_{ij})^2\,\nabla_j\Theta_n^{(n+2)}\,\nabla_i D_n\,\overline{\phi}_{ij}\,\nabla_j\nabla_i D_n\,\phi_{ij}\right|\\
&\qquad\le\alpha N^2\int(1-w_{n+1,n+2})^2\,\Theta_n^{(n+2)}|D_{n+2}\,\phi_{n+1,n+2}|^2\\
&\qquad\quad+\alpha^{-1}C\ell^{-2}N\int\Theta_n^{(n+1)}\,|D_{n+1}\psi|^2+\alpha^{-1}C\ell^{-4}\int\Theta_n^{(n)}\,|D_n\psi|^2\\
&\qquad\le o(N^2)\left(\int(1-w_{n+1,n+2})^2\,\Theta_n^{(n+2)}|D_{n+2}\,\phi_{n+1,n+2}|^2+\int\Theta_n^{(n+1)}\,|D_{n+1}\psi|^2+\int\Theta_{n-1}^{(n)}\,|D_n\psi|^2\right)
\end{aligned}\tag{9.30}$$

for an appropriate choice of α (using that $N\ell^2\gg 1$). In the last term we also used that $\theta_n^{(n)}\le 1$.

The third term on the r.h.s. of (9.24), being the hermitian conjugate of the second term can be bounded exactly in the same way.

Now we consider the fourth term on the r.h.s. of (9.24). To this end we use that, since $i\neq j$, and $i,j>n$, we have, by Lemma A.1, part v),

$$\left|\nabla_i\nabla_j\,\Theta_n^{(n+2)}\right|\le C\ell^{-2}\left(\frac{2^{n+2}}{\ell^\varepsilon}\sum_{m=1}^n h_{mj}\right)\left(\frac{2^{n+2}}{\ell^\varepsilon}\sum_{m=1}^n h_{mi}\right)\Theta_n^{(n+2)}\,.\tag{9.31}$$

Therefore

$$\begin{aligned}
&\sum_{i,j>n,i\neq j} \Big| \int (1-w_{ij})^2\, \nabla_i\nabla_j\Theta_n^{(n+2)}\, \nabla_i D_n\, \overline{\phi}_{ij}\, \nabla_j D_n\, \phi_{ij}\Big| \\
&\qquad\qquad \leq C\ell^{-2} \sum_{i,j>n,i\neq j} \int (1-w_{ij})^2 \left(\frac{2^{n+2}}{\ell^\varepsilon}\sum_{m=1}^n h_{mj}\right)^2 \Theta_n^{(n+2)}\, |\nabla_i D_n\phi_{ij}|^2 \\
&\qquad\qquad \leq C\ell^{-2}N \int \Theta_n^{(n+1)}\, |D_{n+1}\psi|^2 + C\ell^{-4}\int \Theta_n^{(n)}\, |D_n\psi|^2 \\
&\qquad\qquad \leq o(N^2)\left(\int \Theta_n^{(n+1)}\, |D_{n+1}\psi|^2 + \int \Theta_{n-1}^{(n)}\, |D_n\psi|^2\right)\,,
\end{aligned} \tag{9.32}$$

where in the second line we used (2.51) and a Schwarz inequality, in the third line we used the bound (9.29), while in the last line we used $N\ell^2 \gg 1$.

Next we consider the last term on the r.h.s. of (9.24). To this end we note that, by (5.3) and (5.5),

$$\left|\left[\nabla_i, \frac{\nabla w_{ji}}{1-w_{ij}}\right]\right| \leq \frac{\left|\nabla^2 w_{ji}\right|}{1-w_{ij}} + \left(\frac{\nabla w_{ji}}{1-w_{ij}}\right)^2 \leq c\rho \frac{1}{|x_i-x_j|^2}$$

assuming that ρ is small enough. Therefore, the terms in the sum on the last line of (9.24) can be bounded by using Hardy inequality as

$$\begin{aligned}
&\left|\int (1-w_{ij})^2\, \Theta_n^{(n+2)}\, \nabla_i D_n\, \overline{\phi}_{ij}\, [\nabla_i, L_j] D_n\, \phi_{ij}\right| \\
&\qquad\qquad \leq c\rho \int (1-w_{ij})^2 \Theta_n^{(n+2)}\, \frac{1}{|x_i-x_j|^2} |\nabla_i D_n\phi_{ij}|^2 \\
&\qquad\qquad \leq c\rho \int \Theta_n^{(n+2)}\, \frac{1}{|x_i-x_j|^2} |\nabla_i D_n\phi_{ij}|^2 \\
&\qquad\qquad \leq c\rho \int \Theta_n^{(n+2)}\, |\nabla_j\nabla_i D_n\phi_{ij}|^2 + C\int \left|\nabla_j \left(\Theta_n^{(n+2)}\right)^{\frac{1}{2}}\right|^2 |\nabla_i D_n\phi_{ij}|^2 \\
&\qquad\qquad \overset{(9.25)}{\leq} c\rho \int (1-w_{ij})^2\, \Theta_n^{(n+2)}\, |\nabla_j\nabla_i D_n\phi_{ij}|^2 \\
&\qquad\qquad\quad + C\ell^{-2}\int (1-w_{ij})^2 \left(\frac{2^{n+1}}{\ell^\varepsilon}\sum_{m=1}^n h_{jm}\right)^2 \Theta_n^{(n+2)}\, |\nabla_i D_n\phi_{ij}|^2\,.
\end{aligned} \tag{9.33}$$

Next we sum over $i,j>n$ $(i\neq j)$; to control the contribution originating from the second term on

the r.h.s. of the last equation we use (9.29). We obtain

$$\begin{aligned}
\sum_{i,j>n,i\neq j} \Big| \int (1-w_{ij})^2\, \Theta_n^{(n+2)}\, \nabla_i D_n\, \overline{\phi}_{ij}\, [\nabla_i, L_j] D_n\, \phi_{ij} \Big| & \\
&\leq c\rho \sum_{i,j>n,i\neq j} \int (1-w_{ij})^2\, \Theta_n^{(n+2)}\, |\nabla_j \nabla_i D_n \phi_{ij}|^2 \\
&\quad + C\ell^{-2} N \int \Theta_n^{(n+1)}\, |D_{n+1}\psi|^2 + C\ell^{-4} \int \Theta_n^{(n)}\, |D_n\psi|^2 \qquad (9.34)\\
&\leq c\rho \sum_{i,j>n,i\neq j} \int (1-w_{ij})^2\, \Theta_n^{(n+2)}\, |\nabla_j \nabla_i D_n \phi_{ij}|^2 \\
&\quad + o(N^2) \left(\int \Theta_n^{(n+1)}\, |D_{n+1}\psi|^2 + \int \Theta_{n-1}^{(n)}\, |D_n\psi|^2 \right) .
\end{aligned}$$

Inserting (9.30), (9.32), and (9.34) into the right side of (9.24) it follows that

$$\begin{aligned}
& C_0^n N^n \sum_{i,j>n,i\neq j} \int (1-w_{ij})^2\, \Theta_n^{(n+2)}\, L_i D_n\, \overline{\phi}_{ij}\, L_j D_n\, \phi_{ij} \\
&\quad \geq C_0^n N^{n+2} (1 - c\rho - o(1)) \int (1-w_{n+1,n+2})^2\, \Theta_n^{(n+2)}\, |D_{n+2}\phi_{n+1,n+2}|^2 \qquad (9.35)\\
&\quad\quad - o(N^{n+2}) \left(\int \Theta_n^{(n+1)}\, |D_{n+1}\,\psi|^2 + \int \Theta_{n-1}^{(n)}\, |D_n\psi|^2 \right) .
\end{aligned}$$

Lemma 9.2 now follows from (9.41) in Lemma 9.4 below that shows how to replace estimates involving the function $\phi_{ij} = (1-w_{ij})^{-1}\psi$ with estimates on ψ. □

Lemma 9.3. *Suppose the assumptions of Lemma 9.1 are satisfied. Then we have*

$$\begin{aligned}
& \frac{C_0^n N^n}{2} \sum_{i,j>n,i\neq j} \sum_{r>n,\, r\neq i,j} \int (1-w_{ij})^2\, \Theta_n^{(n+2)}\, V_N(x_j - x_r)\, L_i\, D_n\, \overline{\phi}_{ij}\, D_n\, \phi_{ij} + h.c. \\
&\quad \geq \frac{C_0^n N^{n+3}}{2} (1 - o(1)) \int \Theta_{n+1}^{(n+2)}\, V_N(x_{n+2} - x_{n+3})\, |D_{n+1}\psi|^2 \qquad (9.36)\\
&\quad\quad - o(N^{n+3}) \int \Theta_n^{(n+1)}\, V_N(x_{n+1} - x_{n+2}) |D_n\psi|^2 .
\end{aligned}$$

Proof. Using (9.22), we find

$$\begin{aligned}
& \frac{C_0^n N^n}{2} \sum_{i,j>n,i\neq j} \sum_{r>n,\, r\neq i,j} \int (1-w_{ij})^2\, \Theta_n^{(n+2)}\, V_N(x_j - x_r)\, L_i D_n\, \overline{\phi}_{ij} D_n\, \phi_{ij} \\
&= \frac{C_0^n N^n}{2} \sum_{i,j>n,i\neq j} \sum_{r>n,\, r\neq i,j} \int (1-w_{ij})^2\, V_N(x_j - x_r) \qquad (9.37)\\
&\quad\quad \times \Big\{ \Theta_n^{(n+2)}\, |\nabla_i D_n \phi_{ij}|^2 + \nabla_i \Theta_n^{(n+2)}\, \nabla_i D_n\, \overline{\phi}_{ij}\, D_n \phi_{ij} \Big\} .
\end{aligned}$$

Using (9.25) (with j replaced by i) the second term in the curly bracket can be bounded by

$$\begin{aligned}
&\sum_{i,j>n,i\neq j}\sum_{r>n,\,r\neq i,j}\left|\int (1-w_{ij})^2\,V_N(x_j-x_r)\,\nabla_i\Theta_n^{(n+2)}\,\nabla_i D_n\,\overline{\phi}_{ij}D_n\phi_{ij}\right| \\
&\quad\le\ C\alpha\sum_{i,j>n,i\neq j}\sum_{r\neq i,j}^{N}\int (1-w_{ij})^2\,\Theta_n^{(n+2)}\,V_N(x_j-x_r)\,|\nabla_i D_n\phi_{ij}|^2 \\
&\quad\quad + C\ell^{-2}\alpha^{-1}\sum_{i,j>n,i\neq j}\sum_{r\neq i,j}^{N}\int (1-w_{ij})^2\left(\frac{2^{n+2}}{\ell^{\varepsilon}}\sum_{m=1}^{n}h_{im}\right)^2\Theta_n^{(n+2)}\,V_N(x_j-x_r)\,|D_n\phi_{ij}|^2.
\end{aligned}\tag{9.38}$$

Since $i,j>n$, and $\psi=(1-w_{ij})\phi_{ij}$, the second term can be estimated as

$$\begin{aligned}
&C\ell^{-2}\alpha^{-1}\sum_{i,j>n,i\neq j}\sum_{r>n,r\neq i,j}\int\left(\frac{2^{n+2}}{\ell^{\varepsilon}}\sum_{m=1}^{n}h_{im}\right)^2\Theta_n^{(n+2)}\,V_N(x_j-x_r)\,|D_n\psi|^2 \\
&\quad\le C\ell^{-2}\alpha^{-1}\sum_{j>n}\sum_{r>n,r\neq j}\int\left(\frac{2^{n+2}}{\ell^{\varepsilon}}\sum_{i>n}\sum_{m=1}^{n}h_{im}\right)^2\Theta_n^{(n+2)}\,V_N(x_j-x_r)\,|D_n\psi|^2 \\
&\quad\le C\ell^{-2}\alpha^{-1}\sum_{j>n}\sum_{r>n,\,r\neq j}\int\Theta_n^{(n+1)}\,V_N(x_j-x_r)\,|D_n\psi|^2 \\
&\quad= C\ell^{-2}\alpha^{-1}(N-n)(N-n-1)\int\Theta_n^{(n+1)}\,V_N(x_{n+1}-x_{n+2})|D_n\psi|^2\,,
\end{aligned}\tag{9.39}$$

because of the permutation symmetry of ψ and $\Theta_n^{(n+1)}$. From (9.39) and (9.38), it follows that

$$\begin{aligned}
&\sum_{i,j>n,i\neq j}\sum_{r>n,r\neq i,j}\left|\int (1-w_{ij})^2\,\nabla_i\Theta_n^{(n+2)}\,V_N(x_j-x_r)\,\nabla_i D_n\,\overline{\phi}_{ij}D_n\phi_{ij}\right| \\
&\qquad\le o(1)\sum_{i,j>n,i\neq j}\sum_{r\neq i,j}^{N}\int (1-w_{ij})^2\,\Theta_n^{(n+2)}\,V_N(x_j-x_r)\,|\nabla_i D_n\phi_{ij}|^2 \\
&\qquad\quad + o(N^3)\int\Theta_n^{(n+1)}\,V_N(x_{n+1}-x_{n+2})|D_n\psi|^2
\end{aligned}\tag{9.40}$$

where we used that $N\ell^2\gg 1$ and we made a suitable choice of the parameter α. Inserting this bound into (9.37), using the permutation symmetry, and (9.42) from Lemma 9.4, the lemma follows easily. □

The next lemma, showing how to replace estimates on ϕ_{ij} with estimates on ψ, has already been used in the previous proofs.

Lemma 9.4. *Suppose the assumptions of Proposition 5.3 are satisfied. Recall that ϕ_{ij} is defined by $\psi=(1-w_{ij})\phi_{ij}$.*

i) For $n\ge 0$, we have

$$\begin{aligned}
&\int(1-w_{n+1,n+2})^2\,\Theta_n^{(n+2)}\,|D_{n+2}\phi_{n+1,n+2}|^2 \\
&\quad\ge(1-o(1))\int\Theta_{n+1}^{(n+2)}\,|D_{n+2}\psi|^2-o(1)\left\{\int\Theta_n^{(n+1)}\,|D_{n+1}\psi|^2+\int\Theta_{n-1}^{(n)}\,|D_n\psi|^2\right\}.
\end{aligned}\tag{9.41}$$

ii) For $n \geq 0$, we have

$$\int (1-w_{n+1,n+2})^2\, \Theta_n^{(n+2)}\, V_N(x_{n+2}-x_{n+3})\, |D_{n+1}\phi_{n+1,n+2}|^2$$
$$\geq (1-o(1)) \int \Theta_{n+1}^{(n+2)}\, V_N(x_{n+2}-x_{n+3})\, |D_{n+1}\psi|^2 - o(1) \int \Theta_n^{(n+1)}\, V_N(x_{n+1}-x_{n+2})\, |D_n\psi|^2 \,. \tag{9.42}$$

Proof. In order to prove part i) we start by noticing that

$$\int (1-w_{n+1,n+2})^2\, \Theta_n^{(n+2)}\, |D_{n+2}\phi_{n+1,n+2}|^2 \geq \int (1-w_{n+1,n+2})^2\, \Theta_{n+1}^{(n+2)}\, |D_{n+2}\phi_{n+1,n+2}|^2. \tag{9.43}$$

Using that $\phi_{n+1,n+2} = (1-w_{n+1,n+2})^{-1}\,\psi$ we find

$$D_{n+2}\phi_{n+1,n+2} = \frac{1}{1-w_{n+1,n+2}} D_{n+2}\,\psi + \frac{\nabla w_{n+1,n+2}}{(1-w_{n+1,n+2})^2} D_n \nabla_{n+2}\,\psi$$
$$+ \frac{\nabla w_{n+2,n+1}}{(1-w_{n+1,n+2})^2} D_{n+1}\,\psi + \left(\frac{\nabla^2 w_{n+1,n+2}}{(1-w_{n+1,n+2})^2} + 2\frac{(\nabla w_{n+1,n+2})^2}{(1-w_{n+1,n+2})^3} \right) D_n\,\psi$$

and thus, from (5.3) bounds]

$$\int (1-w_{n+1,n+2})^2\, \Theta_n^{(n+2)}\, |D_{n+2}\phi_{n+1,n+2}|^2$$
$$\geq \int \Theta_{n+1}^{(n+2)}\, |D_{n+2}\psi|^2 - C\int \Theta_{n+1}^{(n+2)}\, |\nabla w_{n+1,n+2}|\, |D_{n+2}\psi|\, |D_{n+1}\psi| \tag{9.44}$$
$$- C\int \Theta_{n+1}^{(n+2)}\, \left(|\nabla w_{n+1,n+2}|^2 + |\nabla^2 w_{n+1,n+2}|\right)\, |D_{n+2}\psi|\, |D_n\psi| \,.$$

The second term can be bounded by

$$\int \Theta_{n+1}^{(n+2)}\, |\nabla w_{n+1,n+2}|\, |D_{n+2}\psi|\, |D_{n+1}\psi|$$
$$\leq \alpha \int \Theta_{n+1}^{(n+2)}\, |D_{n+2}\psi|^2 + \alpha^{-1} \int \Theta_{n+1}^{(n+2)} |\nabla w_{n+1,n+2}|^2\, |D_{n+1}\psi|^2$$
$$\leq \alpha \int \Theta_{n+1}^{(n+2)}\, |D_{n+2}\psi|^2 + \alpha^{-1} \int \Theta_{n+1}^{(n+2)}\, \chi(|x_{n+1}-x_{n+2}| \geq \ell)\, |\nabla w_{n+1,n+2}|^2\, |D_{n+1}\psi|^2$$
$$+ \alpha^{-1} \int \Theta_{n+1}^{(n+2)}\, \chi(|x_{n+1}-x_{n+2}| \leq \ell) |\nabla w_{n+1,n+2}|^2\, |D_{n+1}\psi|^2 \tag{9.45}$$
$$\leq \alpha \int \Theta_{n+1}^{(n+2)}\, |D_{n+2}\psi|^2 + C\alpha^{-1}a^2 \int \Theta_{n+1}^{(n+2)}\, \frac{\chi(|x_{n+1}-x_{n+2}| \geq \ell)}{|x_{n+1}-x_{n+2}|^4}\, |D_{n+1}\psi|^2$$
$$+ C\alpha^{-1}N^2 \int \Theta_{n+1}^{(n+2)}\, \chi(|x_{n+1}-x_{n+2}| \leq \ell)\, |D_{n+1}\psi|^2,$$

where in the last inequality we used that, by Lemma 5.1, $|\nabla w_{n+1,n+2}| \leq CN$. Moreover we used that $\nabla w(x) = a/|x|$ for $|x| > R/N$ (with R such that $\operatorname{supp} V \subset \{x \in \mathbb{R}^3 : |x| \leq R\}$), and that $R/N \leq \ell$ for N large enough. Using that

$$\theta_{n+1}^{(n+2)} \chi(|x_{n+1}-x_{n+2}| \leq \ell) \leq Ce^{-C\ell^{-\varepsilon}} \tag{9.46}$$

we have (recall that $a = a_0/N$)

$$\begin{aligned}
&\int \Theta_{n+1}^{(n+2)} \, |\nabla w_{n+1,n+2}| \, |D_{n+2}\psi| \, |D_{n+1}\psi| \\
&\quad \leq \alpha \int \Theta_{n+1}^{(n+2)} \, |D_{n+2}\psi|^2 + C\alpha^{-1} a^2 \ell^{-4} \int \Theta_n^{(n+2)} \, |D_{n+1}\psi|^2 + C\alpha^{-1} N^2 e^{-C\ell^{-\varepsilon}} \int \Theta_n^{(n+2)} \, |D_{n+1}\psi|^2 .
\end{aligned}$$

Since $N\ell^2 \gg 1$, we find

$$\int \Theta_{n+1}^{(n+2)} |\nabla w_{n+1,n+2}| \, |D_{n+2}\psi| |D_{n+1}\psi| \leq o(1) \left\{ \int \Theta_{n+1}^{(n+2)} \, |D_{n+2}\psi|^2 + \int \Theta_n^{(n+1)} \, |D_{n+1}\psi|^2 \right\}. \quad (9.47)$$

As for the third term on the r.h.s. of (9.44), we proceed as follows.

$$\begin{aligned}
&\int \Theta_{n+1}^{(n+2)} \, \left(|\nabla w_{n+1,n+2}|^2 + |\nabla^2 w_{n+1,n+2}| \right) \, |D_{n+2}\psi| \, |D_n \psi| \\
&\qquad \leq \alpha \int \Theta_{n+1}^{(n+2)} \, |D_{n+2}\psi|^2 \, + \alpha^{-1} \int \Theta_{n+1}^{(n+2)} \, \left(|\nabla w_{n+1,n+2}|^2 + |\nabla^2 w_{n+1,n+2}| \right)^2 \, |D_n \psi|^2 \\
&\qquad \leq \alpha \int \Theta_{n+1}^{(n+2)} \, |D_{n+2}\psi|^2 \, + C\alpha^{-1} a^2 \int \Theta_{n+1}^{(n+2)} \, \frac{\chi(|x_{n+1} - x_{n+2}| \geq \ell)}{|x_{n+1} - x_{n+2}|^6} \, |D_n \psi|^2 \\
&\qquad\quad + C\alpha^{-1} N^4 \int \Theta_{n+1}^{(n+2)} \, \chi(|x_{n+1} - x_{n+2}| \leq \ell) \, |D_n \psi|^2
\end{aligned} \quad (9.48)$$

where we used the bounds for $|\nabla w|$ and $|\nabla^2 w|$ from (5.4) and that $w(x) = a/|x|$ for $|x| \geq \ell$ since $\ell \gg R/N$. Using (9.46) to bound the last term, we obtain

$$\begin{aligned}
&\int \Theta_{n+1}^{(n+2)} \, \left(|\nabla w_{n+1,n+2}|^2 + |\nabla^2 w_{n+1,n+2}| \right) \, |D_{n+2}\psi| \, |D_n \psi| \\
&\qquad \leq \alpha \int \Theta_{n+1}^{(n+2)} \, |D_{n+2}\psi|^2 \, + C\alpha^{-1} a^2 \ell^{-4} \int \Theta_n^{(n+2)} \, \frac{1}{|x_{n+1} - x_{n+2}|^2} \, |D_n \psi|^2 \\
&\qquad\quad + C\alpha^{-1} N^4 e^{-C\ell^{-\varepsilon}} \int \Theta_{n-1}^{(n)} \, |D_n \psi|^2 .
\end{aligned} \quad (9.49)$$

To bound the second term on the r.h.s., we apply Hardy inequality. We have

$$\begin{aligned}
&\int \Theta_n^{(n+2)} \, \frac{1}{|x_{n+1} - x_{n+2}|^2} \, |D_n \psi|^2 \\
&\qquad \leq C \int \Theta_n^{(n+2)} \, |D_{n+1}\psi|^2 + C \int \left| \nabla_{n+1} \left(\Theta_n^{(n+2)} \right)^{\frac{1}{2}} \right|^2 \, |D_n \psi|^2 \\
&\qquad \leq C \int \Theta_n^{(n+2)} \, |D_{n+1}\psi|^2 + C\ell^{-2} \int \left(\frac{2^{n+1}}{\ell^\varepsilon} \sum_{i=1}^{n} h_{i,n+1} \right)^2 \Theta_n^{(n+2)} \, |D_n \psi|^2 \\
&\qquad \leq C \int \Theta_n^{(n+2)} \, |D_{n+1}\psi|^2 + C(N-n)^{-1} \ell^{-2} \int \left(\frac{2^{n+1}}{\ell^\varepsilon} \sum_{j \geq n+1} \sum_{i=1}^{n} h_{ij} \right)^2 \Theta_n^{(n+2)} \, |D_n \psi|^2 \\
&\qquad \leq C \int \Theta_n^{(n+1)} \, |D_{n+1}\psi|^2 + C(N-n)^{-1} \ell^{-2} \int \Theta_{n-1}^{(n)} \, |D_n \psi|^2 .
\end{aligned} \quad (9.50)$$

Since $N\ell^2 \gg 1$, it follows from (9.49) that

$$\begin{aligned}
&\int \Theta_{n+1}^{(n+2)} \, \left(|\nabla w_{n+1,n+2}|^2 + |\nabla^2 w_{n+1,n+2}| \right) \, |D_{n+2}\psi| \, |D_n \psi| \\
&\qquad \leq o(1) \left\{ \int \Theta_{n+1}^{(n+2)} \, |D_{n+2}\psi|^2 + \int \Theta_n^{(n+1)} \, |D_{n+1}\psi|^2 + \int \Theta_{n-1}^{(n)} \, |D_n \psi|^2 \right\} .
\end{aligned}$$

Part i) of Lemma 9.4 follows now from (9.44), (9.47) and from last equation.

In order to prove part ii) we rewrite the l.h.s. of (9.42) as follows.

$$\begin{aligned}\int (1-w_{n+1,n+2})^2 \Theta_n^{(n+2)}\, V_N(x_{n+2}-x_{n+3})\, |D_{n+1}\phi_{n+1,n+2}|^2 \\ \geq \int (1-w_{n+1,n+2})^2 \Theta_{n+1}^{(n+2)}\, V_N(x_{n+2}-x_{n+3})\, |D_{n+1}\phi_{n+1,n+2}|^2 \,.\end{aligned} \tag{9.51}$$

Using

$$D_{n+1}\phi_{n+1,n+2} = \frac{1}{1-w_{n+1,n+2}} D_{n+1}\psi + \frac{\nabla w_{n+1,n+2}}{(1-w_{n+1,n+2})^2} D_n\psi$$

we find

$$\begin{aligned}\int (1-w_{n+1,n+2})^2 \Theta_n^{(n+2)}\, V_N(x_{n+2}-x_{n+3})\, |D_{n+1}\phi_{n+1,n+2}|^2 \\ \geq (1-\alpha)\int \Theta_{n+1}^{(n+2)}\, V_N(x_{n+2}-x_{n+3})\, |D_{n+1}\psi|^2 \\ - C\alpha^{-1}\int \Theta_{n+1}^{(n+2)}\, |\nabla w_{n+1,n+2}|^2\, V_N(x_{n+2}-x_{n+3})\, |D_n\psi|^2 \,.\end{aligned} \tag{9.52}$$

The last term can be controlled by using (5.4) and that $w(x) = a/|x|$ for $|x| > \ell \gg R/N$ by

$$\begin{aligned}&\int \Theta_{n+1}^{(n+2)} |\nabla w_{n+1,n+2}|^2\, V_N(x_{n+2}-x_{n+3})\, |D_n\psi|^2 \\ &\leq CN^2 \int \Theta_{n+1}^{(n+2)} \chi(|x_{n+1}-x_{n+2}|\leq \ell)\, V_N(x_{n+2}-x_{n+3})\, |D_n\psi|^2 \\ &\quad + Ca^2 \int \Theta_{n+1}^{(n+2)} \frac{\chi(|x_{n+1}-x_{n+2}|\geq \ell)}{|x_{n+1}-x_{n+2}|^4}\, V_N(x_{n+2}-x_{n+3})\, |D_n\psi|^2 \\ &\leq CN^2 e^{-C\ell^{-\varepsilon}} \int \Theta_{n+1}^{(n+1)}\, V_N(x_{n+2}-x_{n+3})\, |D_n\psi|^2 + Ca^2\ell^{-4}\int \Theta_{n+1}^{(n+2)}\, V_N(x_{n+2}-x_{n+3})\, |D_n\psi|^2 \\ &\leq o(1)\int \Theta_{n+1}^{(n+1)}\, V_N(x_{n+2}-x_{n+3})\, |D_n\psi|^2 \,.\end{aligned} \tag{9.53}$$

From (9.51), we have

$$\begin{aligned}\int (1-w_{n+1,n+2})^2 \Theta_n^{(n+2)}\, V_N(x_{n+2}-x_{n+3})\, |D_{n+1}\phi_{n+1,n+2}|^2 \\ \geq (1-o(1))\int \Theta_{n+1}^{(n+2)}\, V_N(x_{n+2}-x_{n+3})\, |D_{n+1}\psi|^2 \\ - o(1)\int \Theta_n^{(n+1)}\, V_N(x_{n+1}-x_{n+2})\, |D_n\psi|^2 \,.\end{aligned} \tag{9.54}$$

In the last term we used $\Theta_{n+1}^{(n+1)} \leq \Theta_n^{(n+1)}$, the permutation symmetry of ψ and we shifted the indices $n+2, n+3 \to n+1, n+2$ □

Proposition 9.5. *Suppose $N\ell^2 \gg 1$. Let $\mathfrak{h}_i^{(n)}$ be defined as in (9.14). Then, if N is large enough (depending on n),*

$$\begin{aligned}C_0^n N^n \sum_{i\leq n<j} \int \Theta_n^{(n+2)}\, D_n\mathfrak{h}_i^{(n)}\, \overline{\psi}\, D_n\mathfrak{h}_j^{(n)}\, \psi + h.c. \geq C_0^n N^{n+1}(1-o(1))\int \Theta_{n+1}^{(n+2)}\, |\nabla_1\, D_{n+1}\, \psi|^2 \\ - \Omega_n(\psi)\end{aligned} \tag{9.55}$$

where the error term $\Omega_n(\psi)$ has been defined in (9.18).

Proof. We rewrite the l.h.s. of (9.55) as

$$\begin{aligned}
&C_0^n N^n \sum_{i\le n<j} \int \Theta_n^{(n+2)}\; D_n \mathfrak{h}_i^{(n)}\, \overline{\psi}\; D_n \mathfrak{h}_j^{(n)}\, \psi + \text{h.c.} \\
&\quad = C_0^n N^n \sum_{i\le n<j} \int \Theta_n^{(n+2)}\; D_n \Delta_i\, \overline{\psi}\; D_n \Delta_j\, \psi \\
&\qquad - \frac{C_0^n N^n}{2} \sum_{i\le n<j} \sum_{m>n,\, m\neq j} \int \Theta_n^{(n+2)}\; V_N(x_j - x_m)\; D_n \Delta_i\, \overline{\psi}\; D_n\, \psi \\
&\qquad - C_0^n N^n \sum_{i\le n<j} \sum_{r\neq i} \lambda_r \int \Theta_n^{(n+2)}\; D_n (V_N(x_i - x_r)\, \overline{\psi})\; D_n \Delta_j\, \psi \\
&\qquad + \frac{C_0^n N^n}{4} \sum_{i\le n<j} \sum_{r\neq i} \lambda_r \sum_{m>n,\, m\neq j} \int \Theta_n^{(n+2)}\; D_n \left(V_N(x_i - x_r)\, \overline{\psi}\right)\; D_n (V_N(x_j - x_m)\, \psi) + \text{h.c.}
\end{aligned} \tag{9.56}$$

with $\lambda_r = 1$ if $r > n$, and $\lambda_r = 1/2$ if $r \le n$ (recall the definition of $\mathfrak{h}_i^{(n)}$, for $i \le n$, in (9.14)). The terms on the last two lines are easy to bound because the potential $V_N(x_i - x_r)$ forces the particle i to be close (on the length scale N^{-1}) to the particle r. But then the factor $\theta_i^{(n+2)}$ in $\Theta_n^{(n+2)}$ makes this contribution exponentially small. More precisely, for $i \le n$, we have the bound

$$\left(\nabla^\alpha \Theta_n^{(n+2)}\right)\; |\nabla^\beta V_N(x_i - x_r)| \le e^{-C\ell^{-\varepsilon}} \Theta_n^{(n+1)} \tag{9.57}$$

for $\alpha = 0, 1$, $\beta = 0, 1, 2$, and for all N large enough. It is therefore easy to prove that

$$\begin{aligned}
&C_0^n N^n \sum_{i\le n<j} \int \Theta_n^{(n+2)}\; D_n \mathfrak{h}_i^{(n)}\, \overline{\psi}\; D_n \mathfrak{h}_j^{(n)}\, \psi + \text{h.c.} \\
&= C_0^n N^n \sum_{i\le n<j} \int \Theta_n^{(n+2)}\; D_n \Delta_i\, \overline{\psi}\; D_n \Delta_j\, \psi \\
&\quad - \frac{C_0^n N^n}{2} \sum_{i\le n<j} \sum_{m>n,\, m\neq j} \int \Theta_n^{(n+2)}\; V_N(x_j - x_m)\; D_n \Delta_i\, \overline{\psi}\; D_n\, \psi + \text{h.c.} \\
&\quad - O\left(e^{-C\ell^{-\varepsilon}}\right) \int \left\{ \Theta_n^{(n+1)} |D_{n+1}\psi|^2 + \Theta_{n-1}^{(n)} |D_n \psi|^2 + \Theta_{n-2}^{(n-1)} |D_{n-1}\psi|^2 + \Theta_{n-3}^{(n-2)} |D_{n-2}\psi|^2 \right\}.
\end{aligned}$$

Lemma 9.5 now follows from Lemma 9.6 and Lemma 9.7 below, where we handle the first and, respectively, the second term on the r.h.s. of the last equation. □

Lemma 9.6. *Suppose the assumptions of Lemma 9.5 are satisfied. Then we have*

$$\begin{aligned}
&C_0^n N^n \sum_{i\le n<j} \int \Theta_n^{(n+2)}\; D_n \Delta_i\, \overline{\psi}\; D_n \Delta_j\, \psi + h.c. \\
&\qquad\qquad \ge C_0^n N^{n+1} (1 - o(1)) \int \Theta_{n+1}^{(n+2)}\; |\nabla_1 D_{n+1}\, \psi|^2 \\
&\qquad\qquad\quad - o(N^{n+2}) \int \Theta_n^{(n+1)} |D_{n+1}\psi|^2 - o(N^{n+1}) \int \Theta_n^{(n+1)} |\nabla_1 D_n \psi|^2 .
\end{aligned} \tag{9.58}$$

Proof. Integration by parts leads to

$$\begin{aligned}
&\sum_{i\le n<j}\int \Theta_n^{(n+2)}\; D_n\Delta_i\,\overline{\psi}\; D_n\Delta_j\,\psi + \text{h.c.}\\
&\quad=\sum_{i\le n<j}\int \Theta_n^{(n+2)}\;|\nabla_i\nabla_j D_n\,\psi|^2+\sum_{i\le n<j}\int \nabla_i\Theta_n^{(n+2)}\;\nabla_i\nabla_j D_n\,\overline{\psi}\;\nabla_j D_n\,\psi\\
&\qquad+\sum_{i\le n<j}\int \nabla_j\Theta_n^{(n+2)}\;\nabla_i D_n\,\overline{\psi}\;\nabla_i\nabla_j D_n\,\psi\\
&\qquad+\sum_{i\le n<j}\int \nabla_i\nabla_j\Theta_n^{(n+2)}\;\nabla_i D_n\,\overline{\psi}\;\nabla_j D_n\,\psi+\text{h.c.}
\end{aligned}\tag{9.59}$$

The second term on the r.h.s. of the last equation can be bounded by

$$\begin{aligned}
&\sum_{i\le n<j}\Big|\int \nabla_i\Theta_n^{(n+2)}\;\nabla_i\nabla_j D_n\,\overline{\psi}\;\nabla_j D_n\,\psi\Big|\\
&\qquad\le\alpha\sum_{i\le n<j}\int\frac{|\nabla_i\Theta_n^{(n+2)}|^2}{\Theta_n^{(n+2)}}\;|\nabla_j D_n\,\psi|^2+\alpha^{-1}\sum_{i\le n<j}\int\Theta_n^{(n+2)}\;|\nabla_i\nabla_j D_n\,\psi|^2
\end{aligned}\tag{9.60}$$

for some $\alpha>0$. Next we use that, by Lemma A.1, part iv),

$$\sum_{i\le n}\frac{|\nabla_i\Theta_n^{(n+2)}|^2}{\Theta_n^{(n+2)}}\le C\ell^{-2}\Theta_n^{(n+1)}$$

and therefore, since $N\ell^2\gg 1$,

$$\begin{aligned}
&\sum_{i\le n<j}\Big|\int \nabla_i\Theta_n^{(n+2)}\;\nabla_i\nabla_j D_n\,\overline{\psi}\;\nabla_j D_n\,\psi\Big|\\
&\qquad\le\alpha C\ell^{-2}\sum_{j>n}\int\Theta_n^{(n+1)}\;|\nabla_j D_n\,\psi|^2+\alpha^{-1}\sum_{i\le n<j}\int\Theta_n^{(n+2)}\;|\nabla_i\nabla_j D_n\,\psi|^2\\
&\qquad\le o(N^2)\int\Theta_n^{(n+1)}\;|D_{n+1}\,\psi|^2+o(1)\sum_{i\le n<j}\int\Theta_n^{(n+2)}\;|\nabla_i\nabla_j D_n\,\psi|^2\,.
\end{aligned}\tag{9.61}$$

The estimate of the third term on the r.h.s. of (9.59) is almost identical to the second term;

$$\begin{aligned}
&\sum_{i\le n<j}\Big|\int \nabla_j\;\Theta_n^{(n+2)}\;\nabla_i D_n\,\overline{\psi}\;\nabla_i\nabla_j D_n\,\psi\Big|\\
&\qquad\le\alpha\sum_{i\le n<j}\int\frac{|\nabla_j\,\Theta_n^{(n+2)}|^2}{\Theta_n^{(n+2)}}|\nabla_i D_n\psi|^2+\alpha^{-1}\sum_{i\le n<j}\int\Theta_n^{(n+2)}\;|\nabla_i\nabla_j D_n\,\psi|^2\\
&\qquad\le C\alpha\ell^{-2}\sum_{i\le n}\int\Theta_n^{(n+1)}|\nabla_i D_n\psi|^2+\alpha^{-1}\sum_{i\le n<j}\int\Theta_n^{(n+2)}\;|\nabla_i\nabla_j D_n\,\psi|^2\\
&\qquad\le o(N)\int\Theta_n^{(n+1)}\;|\nabla_1 D_n\psi|^2+o(1)\sum_{i\le n<j}\int\Theta_n^{(n+2)}\;|\nabla_i\nabla_j D_n\,\psi|^2\,.
\end{aligned}\tag{9.62}$$

Finally, to bound the fourth term on the r.h.s. of (9.59), we use that, by Lemma A.1, part vi),

$$\sum_{j>n} |\nabla_j \nabla_i \, \Theta_n^{(n+2)}| \leq C\ell^{-2}\Theta_n^{(n+1)} \quad \text{and} \qquad \sum_{i\leq n} |\nabla_j \nabla_i \, \Theta_n^{(n+2)}| \leq C\ell^{-2}\Theta_n^{(n+1)}. \tag{9.63}$$

This implies that

$$\begin{aligned}
&\sum_{i\leq n<j} \Big| \int \nabla_j \nabla_i \, \Theta_n^{(n+2)} \; \nabla_i D_n \, \overline{\psi} \; \nabla_j D_n \, \psi \Big| \\
&\qquad \leq C \sum_{i\leq n} \int \sum_{j>n} |\nabla_i \nabla_j \Theta_n^{(n+2)}| |\nabla_i D_n \psi|^2 + \sum_{j>n} \int \sum_{i\leq n} |\nabla_i \nabla_j (\Theta_n^{(n+2)})| \; |\nabla_j \, D_n \, \psi|^2 \\
&\qquad \leq o(N) \int \Theta_n^{(n+1)} |\nabla_1 D_n \psi|^2 + o(N^2) \int \Theta_n^{(n+1)} |D_{n+1} \psi|^2 \, .
\end{aligned} \tag{9.64}$$

Lemma 9.6 now follows from (9.59), (9.61), (9.62) and (9.64). □

Lemma 9.7. *Suppose the assumptions of Lemma 9.5 are satisfied. Then we have, for N large enough (depending on n),*

$$\begin{aligned}
-\frac{C_0^n N^n}{2} \sum_{i\leq n<j} \sum_{m>n,\, m\neq j} \int \Theta_n^{(n+2)} \; V_N(x_j - x_m) \; D_n \Delta_i \, \overline{\psi} \; D_n \, \psi + h.c. \\
\geq \; - o(N^{n+3}) \int \Theta_n^{(n+1)} \, V_N(x_{n+1} - x_{n+2}) \, |D_n \, \psi|^2 \, .
\end{aligned} \tag{9.65}$$

Proof. We have

$$\begin{aligned}
&- \sum_{i\leq n<j} \sum_{m>n,\, m\neq j} \int \Theta_n^{(n+2)} \; V_N(x_j - x_m) \; D_n \Delta_i \, \overline{\psi} \; D_n \, \psi + \text{h.c.} \\
&\qquad = \sum_{i\leq n<j} \sum_{m>n,\, m\neq j} \int \Theta_n^{(n+2)} \; V_N(x_m - x_j) |\nabla_i D_n \, \psi|^2 \\
&\qquad\quad + \sum_{i\leq n<j} \sum_{m>n,\, m\neq j} \int \nabla_i \, \Theta_n^{(n+2)} \; V_N(x_j - x_m) \, \nabla_i D_n \, \overline{\psi} \; D_n \, \psi + \text{h.c.} \, .
\end{aligned} \tag{9.66}$$

The second term can be bounded by

$$\begin{aligned}
&\Big| \sum_{i\leq n<j} \sum_{m>n,\, m\neq j} \int \nabla_i \, \Theta_n^{(n+2)} \; V_N(x_j - x_m) \, \nabla_i D_n \, \overline{\psi} \; D_n \, \psi + \text{h.c.} \Big| \\
&\qquad \leq \alpha \sum_{i\leq n<j} \sum_{m>n,\, m\neq j} \int \frac{|\nabla_i \Theta_n^{(n+2)}|^2}{\Theta_n^{(n+2)}} \; V_N(x_j - x_m) \, |D_n \, \psi|^2 \\
&\qquad\quad + \alpha^{-1} \sum_{i\leq n<j} \sum_{m>n,\, m\neq j} \int \Theta_n^{(n+2)} \; V_N(x_j - x_m) \, |\nabla_i D_n \, \psi|^2 \, .
\end{aligned} \tag{9.67}$$

Since, by Lemma A.1, part iv),

$$\sum_{i\leq n} \frac{|\nabla_i \, \Theta_n^{(n+2)}|^2}{\Theta_n^{(n+2)}} \leq C\ell^{-2}\Theta_n^{(n+1)} \, , \tag{9.68}$$

using the permutation symmetry and optimizing α, we obtain

$$\begin{aligned}\Big| \sum_{i\leq n<j} \sum_{m>n, m\neq j} \int \nabla_i \, \Theta_n^{(n+2)} \, V_N(x_j - x_m) \, \nabla_i D_n \, \overline{\psi} \, D_n \, \psi + \text{h.c.} \Big| \\ \leq o(N^3) \int \Theta_n^{(n+1)} \, V_N(x_{n+1} - x_{n+2}) \, |D_n \, \psi|^2 \\ + o(1) \sum_{i\leq n<j} \sum_{m>n,\, m\neq j} \int \Theta_n^{(n+2)} \, V_N(x_j - x_m) \, |\nabla_i D_n \, \psi|^2 \, .\end{aligned} \tag{9.69}$$

Inserting the last bound in (9.66), we conclude the proof of Lemma 9.7. □

A Properties of the cutoff function $\theta_i^{(n)}$

Recall that the cutoff functions $\Theta_k^{(n)} = \Theta_k^{(n)}(\mathbf{x})$ defined for $k = 1, \ldots, N$ and $n \in \mathbb{N}$, in Eq. (5.32). In the following lemma we collect some of their important properties which were used in the energy estimate, Proposition 5.3.

Lemma A.1. *i) The functions $\Theta_k^{(n)}$ are monotonic in both parameters, that is for any $n, k \in \mathbb{N}$,*

$$\Theta_{k+1}^{(n)} \leq \Theta_k^{(n)} \leq 1 \, , \qquad \Theta_k^{(n+1)} \leq \Theta_k^{(n)} \leq 1 \, .$$

Moreover, $\Theta_k^{(n)}$ is permutation symmetric in the first k and the last $N - k$ variables.

ii) We have, for any $n \in \mathbb{N}$, $k = 1, \ldots, N$,

$$\left(\frac{2^n}{\ell^\varepsilon} \sum_{i=1}^{k} \sum_{j\neq i}^{N} h_{ij} \right)^m \Theta_k^{(n)} \leq C_m \, \Theta_k^{(n-1)} \, . \tag{A.1}$$

iii) For every $k = 1, \ldots, N$, $n \in \mathbb{N}$, we have

$$\begin{aligned} |\nabla_i \Theta_k^{(n)}| &\leq C\ell^{-1} \left(\frac{2^n}{\ell^\varepsilon} \sum_{r=1}^{N} h_{ri} \right) \Theta_k^{(n)} \leq C\ell^{-1} \Theta_k^{(n-1)} \qquad \text{if } i \leq k \\ |\nabla_i \Theta_k^{(n)}| &\leq C\ell^{-1} \left(\frac{2^n}{\ell^\varepsilon} \sum_{r=1}^{k} h_{ri} \right) \Theta_k^{(n)} \leq C\ell^{-1} \Theta_k^{(n-1)} \qquad \text{if } i > k \end{aligned} \tag{A.2}$$

iv) For every $k = 1, \ldots, N$, $n \in \mathbb{N}$ we have

$$\sum_{j=1}^{N} \frac{\left| \nabla_j \Theta_k^{(n)} \right|^2}{\Theta_k^{(n)}} \leq C\ell^{-2} \Theta_k^{(n-1)} \tag{A.3}$$

v) For every fixed $k = 1, \ldots, N$ and $n \in \mathbb{N}$ we have

$$\begin{aligned} &\left| \nabla_i \nabla_j \Theta_k^{(n)} \right| \leq C\ell^{-2} \left(\frac{2^n}{\ell^\varepsilon} \sum_{m=1}^{k} h_{mj} \right) \left(\frac{2^n}{\ell^\varepsilon} \sum_{r=1}^{k} h_{ri} \right) \Theta_k^{(n)} \leq C\ell^{-2} \, \Theta_k^{(n-1)}, \quad \text{if} \quad i \neq j \text{ and } i, j > k \\ &\left| \nabla_i \nabla_j \Theta_k^{(n)} \right| \leq C\ell^{-2} \, \Theta_k^{(n-1)}, \quad \text{for any} \quad i, j \end{aligned} \tag{A.4}$$

vi) For every fixed $k = 1, \dots, N$ and $n \in \mathbb{N}$ we have

$$\sum_{i,j} \left| \nabla_i \nabla_j \Theta_k^{(n)} \right| \leq C\ell^{-2} \Theta_k^{(n-1)} \,. \tag{A.5}$$

Proof. Part i) follows trivially from the definition of $\theta_i^{(n)}$. Part ii) follows from $x^m e^{-x} \leq C_m e^{-x/2}$ for every real x. To prove part iii), we observe that, for $i > k$

$$\nabla_i \Theta_k^{(n)} = -\Big(\frac{2^n}{\ell^\varepsilon} \sum_{r=1}^{k} \nabla h_{ir} \Big) \exp\left(-\frac{2^n}{\ell^\varepsilon} \sum_{r=1}^{k} \sum_{j \neq r} h_{jr} \right) \,. \tag{A.6}$$

Since $|\nabla h(x)| \leq C\ell^{-1} h(x)$, we obtain

$$\left| \nabla_i \Theta_k^{(n)} \right| \leq C\ell^{-1} \left(\frac{2^n}{\ell^\varepsilon} \sum_{r=1}^{k} h_{ir} \right) \exp\left(-\frac{2^n}{\ell^\varepsilon} \sum_{r=1}^{k} \sum_{j \neq r} h_{jr} \right) \,. \tag{A.7}$$

Similarly, for $i \leq k$, we have

$$\nabla_i \Theta_k^{(n)} = -\left(\frac{2^n}{\ell^\varepsilon} \sum_{r=1}^{N} \nabla h_{ir} (1 + \eta_r) \right) \exp\left(-\frac{2^n}{\ell^\varepsilon} \sum_{r=1}^{k} \sum_{j \neq r} h_{jr} \right) \tag{A.8}$$

with $\eta_r = 0$ if $r > k$ and $\eta_r = 1$ if $r \leq k$. Therefore, in this case

$$\left| \nabla_i \Theta_k^{(n)} \right| \leq C\ell^{-1} \left(\frac{2^n}{\ell^\varepsilon} \sum_{r=1}^{N} h_{ir} \right) \exp\left(-\frac{2^n}{\ell^\varepsilon} \sum_{r=1}^{N} \sum_{j \neq r} h_{jr} \right) \,. \tag{A.9}$$

Eqs. (A.7) and (A.9), together with part ii), prove (A.2).

As for part iv), we have, from (A.7),

$$\begin{aligned} \sum_{j=k+1}^{N} \frac{\left| \nabla_j \Theta_k^{(n)} \right|^2}{\Theta_k^{(n)}} &\leq C\ell^{-2} \sum_{j=k+1}^{N} \left(\frac{2^n}{\ell^\varepsilon} \sum_{r=1}^{k} h_{jr} \right)^2 \exp\left(-\frac{2^n}{\ell^\varepsilon} \sum_{r=1}^{k} \sum_{j \neq r} h_{jr} \right) \\ &\leq C\ell^{-2} \left(\frac{2^n}{\ell^\varepsilon} \sum_{j=k+1}^{N} \sum_{r=1}^{k} h_{jr} \right)^2 \exp\left(-\frac{2^n}{\ell^\varepsilon} \sum_{r=1}^{k} \sum_{j \neq r} h_{jr} \right) \\ &\leq C\ell^{-2} \Theta_k^{(n-1)} \end{aligned} \tag{A.10}$$

by part ii) of this lemma. The contribution to (A.3) from terms with $j \leq k$ can be controlled similarly, using (A.9). The proof of part v) and vi) is based on simple explicit computations and the same bounds used for part iii) and iv). □

B Example of an Initial Data

In this section, we denote by $(1 - \omega(x))$ the ground state solution of the Neumann problem

$$\left(-\Delta + \frac{1}{2} V_N(x) \right) (1 - \omega(x)) = e_\ell (1 - \omega(x))$$

on the ball $\{x : |x| \leq \ell\}$ with the normalization condition $\omega(x) = 0$ if $|x| = \ell$. We extend $\omega(x) = 0$ for all $x \in \mathbb{R}^3$ with $|x| > \ell$. We will choose ℓ such that $a \ll \ell \ll 1$. Recall that $a = a_0/N$ is the scattering length of the potential $V_N(x) = N^2 V(Nx)$. Assuming that $V \geq 0$ is smooth spherical symmetric and compactly supported, we have, from Lemma A.2 in [8], the following properties of e_ℓ and $\omega(x)$.

i) If a/ℓ is small enough, then

$$e_\ell = 3a\ell^{-3}(1 + o(a/\ell)) \tag{B.1}$$

ii) There exists $c_0 > 0$ such that

$$c_0 \leq 1 - \omega(x) \leq 1$$

for all $x \in \mathbb{R}^3$. Moreover

$$|\omega(x)| \leq Ca\frac{\mathbf{1}(|x| \leq \ell)}{|x| + a} \qquad \text{and} \qquad |\nabla\omega(x)| \leq Ca\frac{\mathbf{1}(|x| \leq \ell)}{(|x| + a)^2}\,. \tag{B.2}$$

We define the N-body wave function

$$W_N(\mathbf{x}) := \prod_{i<j}^{N}(1 - \omega(x_i - x_j))\,.$$

For $m = 1, \ldots, N$, we also define

$$W_N^{[m]}(x_{m+1}, \ldots, x_N) := \prod_{m<i<j}^{N}(1 - \omega(x_i - x_j)).$$

Lemma B.1. *Define*

$$\psi_N(\mathbf{x}) = \frac{W_N(\mathbf{x})\prod_{j=1}^{N}\varphi(x_j)}{\|W_N(\mathbf{x})\prod_{j=1}^{N}\varphi(x_j)\|}$$

for any $\varphi \in H^1(\mathbb{R}^3)$ with $\|\varphi\|_{L^2} = 1$. Then, if $a \ll \ell \ll 1$, we have

$$\langle\psi_N, H_N\psi_N\rangle \leq CN \tag{B.3}$$

and, for any fixed k,

$$\lim_{N\to\infty}\|\psi_N - \varphi^{\otimes k} \otimes \xi_N^{(N-k)}\| = 0\,, \tag{B.4}$$

where

$$\xi_N^{(N-k)}(x_{k+1}, \ldots, x_N) := \frac{\prod_{k<i<j}(1 - \omega(x_i - x_j))\prod_{j=k+1}^{N}\varphi(x_j)}{\|\prod_{k<i<j}(1 - \omega(x_i - x_j))\prod_{j=k+1}^{N}\varphi(x_j)\|}\,.$$

Proof. Let $\phi_N(\mathbf{x}) := \prod_{j=1}^{N}\varphi(x_j)$, and, for $m = 1, \ldots, N$, $\phi_N^{[m]}(x_{m+1}, \ldots, x_N) := \prod_{j>m}^{N}\varphi(x_j)$. We start by noticing that

$$(1 - o(1))\left\|W_N^{[1]}\,\phi_N^{[1]}\right\|^2 \leq \left\|W_N\,\phi_N\right\|^2 \leq \left\|W_N^{[1]}\,\phi_N^{[1]}\right\|^2. \tag{B.5}$$

Here $\|W_N^{[1]}\phi_N^{[1]}\|$ is the norm on $L^2(\mathbb{R}^{3(N-1)})$. The upper bound in (B.5) is clear since $1-\omega \leq 1$ and $\|\varphi\| = 1$. To prove the lower bound, we note that, by (B.2), and using the notation $\omega_{ij} = \omega(x_i - x_j)$,

$$\begin{aligned}
\|W_N\,\phi_N\|^2 &= \int \mathrm{d}\mathbf{x} \prod_{i<j}^{N} (1-\omega_{ij})^2\,|\phi_N(\mathbf{x})|^2 \\
&= \int \mathrm{d}\mathbf{x} \prod_{1<i<j}^{N} (1-\omega_{ij})^2\,|\phi_N(\mathbf{x})|^2 - \int \mathrm{d}\mathbf{x} \left(1 - \prod_{j=2}^{N}(1-\omega_{1,j})^2\right) \prod_{1<i<j}^{N} (1-\omega_{ij})^2\,|\phi_N(\mathbf{x})|^2 \\
&\geq \|\varphi\|^2 \|W_N^{[1]}\phi_N^{[1]}\|^2 - 2\sum_{j=1}^{N} \int \mathrm{d}\mathbf{x}\,\omega_{1,j} \Big[W_N^{[1]}(x_2,\ldots,x_N)\Big]^2\,|\phi_N(\mathbf{x})|^2 \\
&\geq \|W_N^{[1]}\phi_N^{[1]}\|^2 - CNa \int \mathrm{d}\mathbf{x}\,\frac{\mathbf{1}(|x_1-x_j|\leq \ell)}{|x_1-x_j|} \Big[W_N^{[1]}(x_2,\ldots,x_N)\Big]^2\,|\phi_N(\mathbf{x})|^2 \\
&\geq (1 - CNa\ell\|\varphi\|_{H^1}^2)\|W_N^{[1]}\phi_N^{[1]}\|^2
\end{aligned}$$

using that $\mathbf{1}(|x_1-x_j|\leq \ell) \leq \ell |x_1-x_j|^{-1}$, and then applying a Hardy inequality in the variable x_1. This proves (B.5), because $\ell \ll 1$. Analogously, we can prove that

$$(1-o_k(1))\Big\|W_N^{[k]}\,\phi_N^{[k]}\Big\|^2 \leq \Big\|W_N\,\phi_N\Big\|^2 \leq \Big\|W_N^{[k]}\,\phi_N^{[k]}\Big\|^2 \tag{B.6}$$

where $o_k(1) \to 0$ as $N\to\infty$, for every fixed $k \geq 1$, and where $\|W_N^{[k]}\phi_N^{[k]}\|$ is the norm on $L^2(\mathbb{R}^{3(N-k)})$.

Next we prove (B.4). To this end we remark that, by (B.6),

$$\Big\|\frac{W_N\phi_N}{\|W_N\phi_N\|} - \frac{W_N\phi_N}{\|W_N^{[k]}\phi^{[k]}\|}\Big\| \leq \Big|\frac{\|W_N\phi_N\|}{\|W_N^{[k]}\phi^{[k]}\|} - 1\Big| \to 0 \tag{B.7}$$

as $N\to\infty$. Moreover, since

$$\varphi^{\otimes k} \otimes \xi_N^{(N-k)} = \frac{W_N^{[k]}\phi_N}{\|W_N^{[k]}\phi_N^{[k]}\|}\,,$$

we observe from (B.7) and (B.6) that

$$\limsup_{N\to\infty} \|\psi_N - \varphi^{\otimes k}\otimes\xi_N^{(N-k)}\|^2 \leq \limsup_{N\to\infty} \frac{\Big\|(W_N - W_N^{[k]})\phi_N\Big\|^2}{\|W_N^{[k]}\phi_N^{[k]}\|^2} \tag{B.8}$$

Now we have

$$\begin{aligned}
\Big\|(W_N - W_N^{[k]})\phi_N\Big\|^2 &= \int \mathrm{d}\mathbf{x} \left(1 - \prod_{i<j<k, i<k<j} (1-\omega_{ij})^2\right) \big[W_N^{[k]}(x_{k+1},\ldots,x_N)\big]^2 \prod_{j=1}^{N} |\varphi(x_j)|^2 \\
&\leq C\sum_{i<k}\sum_{j=1}^{N} \int \mathrm{d}\mathbf{x}\,\omega_{ij}\big[W_N^{[k]}(x_{k+1},\ldots,x_N)\big]^2 \prod_{j=1}^{N} |\varphi(x_j)|^2 \\
&\leq CNka\ell\|\varphi\|_{H^1}^2 \|W_N^{[k]}\phi_N^{[k]}\|^2
\end{aligned}$$

by using (B.2) and Sobolev inequality in x_i (see Lemma 6.4, part i)). By (B.8) and $\ell \ll 1$, this proves (B.4).

Finally, we prove (B.3). To this end we observe that

$$\frac{1}{W_N} H_N(W_N\phi_N) = \sum_{j=1}^N L_j\phi_N + e_\ell \sum_{j\neq m}^N \mathbf{1}(|x_m - x_j| \leq \ell)\phi_N - \sum_{i=1}^N \sum_{j,m\neq i, j\neq m}^N \frac{\nabla\omega_{ij}}{1-\omega_{ij}} \cdot \frac{\nabla\omega_{im}}{1-\omega_{im}}\phi_N \quad \text{(B.9)}$$

where

$$L_j = -\Delta_j + 2\sum_{m\neq j} \frac{\nabla\omega_{jm}}{1-\omega_{jm}} \cdot \nabla_j \,.$$

Note that

$$\int W_N^2\, \overline{\phi}_N\, L_j\psi_N = \int W_N^2\, L_j\overline{\phi}_N\, \psi_N = \int W_N^2\, \nabla_j\overline{\phi}_N\, \nabla_j\psi_N \,.$$

From (B.9) we find, by using (B.1), $W_N \leq W_N^{[k]}$ and by applying the Sobolev type inequalities of Lemma 6.4 and the permutational symmetries,

$$\begin{aligned}
&\langle W_N\phi_N, H_N W_N\phi_N\rangle \\
&= \sum_{j=1}^N \int W_N^2 |\nabla_j\phi_N|^2 + e_\ell \sum_{j\neq m}^N \int \mathrm{d}\mathbf{x}\, W_N^2(\mathbf{x})\mathbf{1}(|x_j - x_m| \leq \ell)|\phi_N(\mathbf{x})|^2 \\
&\quad - \sum_{i=1}^N \sum_{j,m\neq i, j\neq m}^N \int W_N^2 \frac{\nabla\omega_{ij}}{1-\omega_{ij}} \cdot \frac{\nabla\omega_{im}}{1-\omega_{im}} |\phi_N|^2 \qquad \text{(B.10)} \\
&\leq N\|\varphi\|_{H^1}^2 \left\| W_N^{[1]}\phi_N^{[1]} \right\|^2 + CN(N-1)a\|\varphi\|_{H^1}^4 \left\| W_N^{[2]}\phi^{[2]} \right\|^2 \\
&\quad + CN(N-1)(N-2)a^2\, \|\varphi\|_{H^1}^4 \left\| W_N^{[3]}\phi^{[3]} \right\|^2
\end{aligned}$$

for any $\varepsilon > 0$. From (B.6), and since $\ell \ll 1$, we have

$$\left\langle \frac{W_N\phi_N}{\|W_N\phi_N\|}, H_N \frac{W_N\phi_N}{\|W_N\phi_N\|} \right\rangle \leq CN \qquad \text{(B.11)}$$

which completes the proof of (B.3). □

C Trapped condensates

In this Appendix we show that Theorem 2.2 can be applied to the ground state of interacting Bose Hamiltonians with a trap. Recall the definition of the Hamiltonian H_N without a trap from (2.1), and define

$$H_N^{\mathrm{trap}} = H_N + \sum_{j=1}^N V_{\mathrm{ext}}(x_j) = \sum_{j=1}^N (-\Delta_j + V_{\mathrm{ext}}(x_j)) + \sum_{i<j}^N V_N(x_i - x_j)$$

with a smooth trapping potential $V_{\mathrm{ext}} \geq 0$ satisfying $\lim_{|x|\to\infty} V_{\mathrm{ext}}(x) = \infty$. Denote by ψ_N^{trap} the positive normalized ground state vector of H_N^{trap}. The corresponding Gross-Pitaevskii energy functional is given by

$$\mathcal{E}_{\mathrm{GP}}^{\mathrm{trap}}(\phi) = \int \mathrm{d}x\, \left(|\nabla\phi(x)|^2 + V_{\mathrm{ext}}(x)|\phi(x)|^2 + 4\pi a_0|\phi(x)|^4\right)$$

and we denote by $\phi_{\rm GP}^{\rm trap}$ the L^2-normalized, positive minimizer of $\mathcal{E}_{\rm GP}^{\rm trap}$. As proven in [16], the ground state energy per particle is given by minimum value of $\mathcal{E}_{\rm GP}^{\rm trap}$ as $N \to \infty$,

$$\frac{1}{N}\langle \psi_N^{\rm trap}, H_N^{\rm trap}\psi_N^{\rm trap}\rangle \to \mathcal{E}_{\rm GP}^{\rm trap}(\phi_{\rm GP}^{\rm trap}), \tag{C.12}$$

and the one-particle marginal density $\gamma_{N,\rm trap}^{(1)}$ associated with $\psi_N^{\rm trap}$ satisfies $\gamma_{N,\rm trap}^{(1)} \to |\phi_{\rm GP}^{\rm trap}\rangle\langle\phi_{\rm GP}^{\rm trap}|$ (with convergence in the trace-norm). From (C.12), $\langle \psi_N^{\rm trap}, H_N^{\rm trap}\psi_N^{\rm trap}\rangle \leq CN$ and since $H_N \leq H_N^{\rm trap}$, we obtain that $\psi_N^{\rm trap}$ satisfies (2.17). The goal of this section is to prove in Proposition C.2 below that $\psi_N^{\rm trap}$ satisfies the asymptotic factorization property (2.18). From Theorem 2.2 we therefore immediately obtain the following corollary:

Corollary C.1. *Suppose V satisfies the same conditions as in Theorem 2.2. Let $\psi_{N,t}$ be the solution of the Schrödinger equation without a trap, $i\partial_t\psi_{N,t} = H_N\psi_{N,t}$, but with initial data given by the trapped ground state, $\psi_{N,0} := \psi_N^{trap}$. For $k = 1, \ldots, N$, let $\gamma_{N,t}^{(k)}$ be the one-particle marginal density associated with $\psi_{N,t}$. Then, for every $t \in \mathbb{R}$, and $k \geq 1$,*

$$\gamma_{N,t}^{(k)} \to |\varphi_t\rangle\langle\varphi_t|^{\otimes k} \qquad \text{as } N \to \infty \tag{C.13}$$

in the weak topology of $\mathcal{L}^1(L^2(\mathbb{R}^{3k}))$. Here φ_t is the solution to the Gross-Pitaevskii equation*

$$i\partial_t\varphi_t = -\Delta\varphi_t + 8\pi a_0|\varphi_t|^2\varphi_t$$

with initial data $\varphi_{t=0} = \phi_{GP}^{trap}$. □

Proposition C.2. *For any fixed $k = 1, 2, \ldots$, there exists a sequence of normalized wave functions, $\xi_N^{(N-k)} \in L^2(\mathbb{R}^{3(N-k)})$, $N > k$, such that*

$$\left\|\psi_N^{trap} - [\phi_{GP}^{trap}]^{\otimes k} \otimes \xi_N^{(N-k)}\right\| \to 0$$

as $N \to \infty$.

We will prove this proposition only for $k = 1$, the proof for arbitrary $k \geq 1$ can be obtained similarly. For brevity, we set $\xi_N = \xi_N^{N-1}$. For the proof, we make use of the following three lemmas.

Lemma C.3. *There exists a constant $C > 0$ independent of R, N such that*

$$\|\mathbf{1}(|x_1| > R)\psi_N^{trap}\| \leq Ce^{-R} \tag{C.14}$$

where $\mathbf{1}(s > \lambda)$ denotes the characteristic function of the interval $[\lambda, \infty)$.

Lemma C.4. *We have $\phi_{GP}^{trap}(x) > 0$ for all $x \in \mathbb{R}^3$. Moreover*

$$\|(1-\Delta)\phi_{GP}^{trap}\| < \infty, \qquad \langle \phi_{GP}^{trap}, V_{ext}(x)\phi_{GP}^{trap}\rangle < \infty$$

and there exists a constant $C > 0$ such that

$$\|\mathbf{1}(|x| > R)\phi_{GP}^{trap}\| \leq Ce^{-R}$$

for all $R > 0$.

Lemma C.5. *For fixed $R > 0$, $N \in \mathbb{N}$ define $\widetilde{\xi}_{R,N} \in L^2(\mathbb{R}^{3(N-1)})$ by*

$$\widetilde{\xi}_{R,N}(\mathbf{x}_{N-1}) = \frac{1}{\int_{|x_1|<R} \mathrm{d}x_1 \, |\phi_{GP}^{trap}(x_1)|^2} \int_{|x_1|<R} \mathrm{d}x_1 \, |\phi_{GP}^{trap}(x_1)|^2 \, \frac{\psi_N^{trap}(x_1, \mathbf{x}_{N-1})}{\phi_{GP}^{trap}(x_1)}$$

where $\mathbf{x}_{N-1} = (x_2, \ldots, x_N)$. Then we have

$$\int \mathrm{d}\mathbf{x}_{N-1} \int_{|x_1|<R} \mathrm{d}x_1 \, \left| \psi_N^{trap}(x_1, \mathbf{x}_{N-1}) - \phi_{GP}^{trap}(x_1) \, \widetilde{\xi}_{R,N}(\mathbf{x}_{N-1}) \right|^2 \leq c_R \, d_N \tag{C.15}$$

where $c_R < \infty$ is independent of N and d_N is independent of R and satisfies $d_N \to 0$ as $N \to \infty$.

Using these three lemmas we can prove Proposition C.2.

Proof of Proposition C.2 for $k = 1$. Using the notation introduced in Lemma C.5 we have

$$\begin{aligned} \|\psi_N^{\mathrm{trap}} - \phi_{\mathrm{GP}}^{\mathrm{trap}} \otimes \widetilde{\xi}_{R,N}\|^2 &= \int \mathrm{d}\mathbf{x}_{N-1} \int \mathrm{d}x_1 \, |\psi_N^{\mathrm{trap}}(x_1, \mathbf{x}_{N-1}) - \phi_{\mathrm{GP}}^{\mathrm{trap}}(x_1) \widetilde{\xi}_{R,N}(\mathbf{x}_{N-1})|^2 \\ &= \int \mathrm{d}\mathbf{x}_{N-1} \int_{|x_1|<R} \mathrm{d}x_1 \, |\psi_N^{\mathrm{trap}}(\mathbf{x}) - \phi_{\mathrm{GP}}^{\mathrm{trap}}(x_1) \widetilde{\xi}_{R,N}(\mathbf{x}_{N-1})|^2 \\ &\quad + \int \mathrm{d}\mathbf{x}_{N-1} \int_{|x_1|\geq R} \mathrm{d}x_1 \, |\psi_N^{\mathrm{trap}}(\mathbf{x}) - \phi_{\mathrm{GP}}^{\mathrm{trap}}(x_1) \widetilde{\xi}_{R,N}(\mathbf{x}_{N-1})|^2 \\ &\leq c_R \, d_N + C e^{-R} \end{aligned} \tag{C.16}$$

where we used Lemma C.5 to bound the term on the second line, and Lemmas C.3 and C.4 to bound the term on the third line. Eq. (C.16) implies that

$$\begin{aligned} \left\| \psi_N^{\mathrm{trap}} - \phi_{\mathrm{GP}}^{\mathrm{trap}} \otimes \frac{\widetilde{\xi}_{R,N}}{\|\widetilde{\xi}_{R,N}\|} \right\| &= \left\| \psi_N^{\mathrm{trap}} - \frac{\phi_{\mathrm{GP}}^{\mathrm{trap}} \otimes \widetilde{\xi}_{R,N}}{\|\phi_{\mathrm{GP}}^{\mathrm{trap}} \otimes \widetilde{\xi}_{R,N}\|} \right\| \\ &\leq \frac{2 \, \|\psi_N^{\mathrm{trap}} - \phi_{\mathrm{GP}}^{\mathrm{trap}} \otimes \widetilde{\xi}_{R,N}\|}{1 - \|\psi_N^{\mathrm{trap}} - \phi_{\mathrm{GP}}^{\mathrm{trap}} \otimes \widetilde{\xi}_{R,N}\|} \, . \end{aligned} \tag{C.17}$$

Now choose a sequence R_N such that $R_N \to \infty$ and $c_{R_N} d_N \to 0$ as $N \to \infty$. Then, taking $\xi_N = \widetilde{\xi}_{R_N,N} / \|\widetilde{\xi}_{R_N,N}\|$, we clearly have $\|\xi_N\| = 1$ for all N, and, by (C.16) and (C.17),

$$\|\psi_N^{\mathrm{trap}} - \phi_{\mathrm{GP}}^{\mathrm{trap}} \otimes \xi_N\| \to 0 \qquad \text{as } N \to \infty \, .$$

□

We still have to prove Lemmas C.3, C.4 and C.5. Lemma C.4 is a standard result which follows from the fact that $\phi_{\mathrm{GP}}^{\mathrm{trap}}$ is the solution of the elliptic non-linear eigenvalue equation

$$-\Delta \phi_{\mathrm{GP}}^{\mathrm{trap}} + V_{\mathrm{ext}} \phi_{\mathrm{GP}}^{\mathrm{trap}} + 8\pi a_0 |\phi_{\mathrm{GP}}^{\mathrm{trap}}|^2 \phi_{\mathrm{GP}}^{\mathrm{trap}} = \mu \phi_{\mathrm{GP}}^{\mathrm{trap}} \tag{C.18}$$

with some constant μ. Lemma C.5 has been proven in [16], more precisely, it follows from Eq. (13) of [16] by noticing that the two terms in the parenthesis in this equation converge to zero, uniformly in R, because of Eq. (7) and Lemma 1 in [16]. It only remains to prove Lemma C.3. To this end we use the following two lemmas.

Lemma C.6. *Let $\chi \in C^\infty(\mathbb{R})$ with $\chi(s) = 0$ if $s < 1$ and $\chi(s) = 1$ if $s > 2$, and let $f \in C^1(\mathbb{R})$ be a monotonically increasing function with $\sup_x |f'(x)| < \infty$. Then we have, for $R > 0$ large enough,*

$$\chi(|x_1|/R)\left(H_N^{trap} - |f'(|x_1|)|^2 - E_N\right)\chi(|x_1|/R) \geq \chi(|x_1|/R)^2,$$

where E_N denotes the ground state energy of H_N^{trap}.

Proof. Define

$$\widetilde{H}_{N-1}^{\mathrm{trap}} = \sum_{j=2}^{N}(-\Delta_j + V_{\mathrm{ext}}(x_j)) + \sum_{2\leq i<j}^{N} V_N(x_i - x_j)$$

and let $\widetilde{E}_{N-1} = \inf\sigma(\widetilde{H}_{N-1}^{\mathrm{trap}})$. Moreover, we define $\widetilde{\psi}_{N-1}^{\mathrm{trap}} \in L^2(\mathbb{R}^{3(N-1)})$ to be the positive normalized ground state of $\widetilde{H}_{N-1}^{\mathrm{trap}}$. Then we have, since $-\Delta_1 \geq 0$ and $V_N(x) \geq 0$,

$$\begin{aligned}
\chi(|x_1|/R)\Big(H_N^{\mathrm{trap}} - |f'(|x_1|)|^2 - E_N\Big)\chi(|x_1|/R) & \\
&\geq \chi(|x_1|/R)\left(\widetilde{H}_{N-1}^{\mathrm{trap}} + V_{\mathrm{ext}}(x_1) - |f'(|x_1|)|^2 - E_N\right)\chi(|x_1|/R) \\
&\geq \chi(|x_1|/R)^2\left(V_{\mathrm{ext}}(x_1) - C - (E_N - \widetilde{E}_{N-1})\right)
\end{aligned} \tag{C.19}$$

where we used the assumption $|f'| \leq C$. Next we remark that there exists a constant $C > 0$ such that

$$E_N \leq \widetilde{E}_{N-1} + C \qquad \text{for all } N\,.$$

In fact (using the symmetry of the wave function)

$$\begin{aligned}
E_N \leq \langle \phi_{\mathrm{GP}}^{\mathrm{trap}} \otimes \widetilde{\psi}_{N-1}^{\mathrm{trap}}, H_N\, \phi_{\mathrm{GP}}^{\mathrm{trap}} \otimes \widetilde{\psi}_{N-1}^{\mathrm{trap}}\rangle &= \widetilde{E}_{N-1} + \langle \phi_{\mathrm{GP}}^{\mathrm{trap}}, (-\Delta_1 + V_{\mathrm{ext}}(x_1))\,\phi_{\mathrm{GP}}^{\mathrm{trap}}\rangle \\
&\quad + \langle \phi_{\mathrm{GP}}^{\mathrm{trap}} \otimes \widetilde{\psi}_{N-1}^{\mathrm{trap}}, (N-1)N^2 V(N(x_1 - x_2))\phi_{\mathrm{GP}}^{\mathrm{trap}} \otimes \widetilde{\psi}_{N-1}^{\mathrm{trap}}\rangle \\
&\leq \widetilde{E}_{N-1} + C\,\|(1-\Delta)\phi_{\mathrm{GP}}^{\mathrm{trap}}\|^2 + C\langle \phi_{\mathrm{GP}}^{\mathrm{trap}}, V_{\mathrm{ext}}(x_1)\phi_{\mathrm{GP}}^{\mathrm{trap}}\rangle \\
&\leq \widetilde{E}_{N-1} + C
\end{aligned} \tag{C.20}$$

where we used the operator inequality $W(x_1 - x_2) \leq C\|W\|_{L^1}(1 - \Delta_1)^2$ and Lemma C.4. Since $\lim_{|x|\to\infty} V_{\mathrm{ext}}(x) = \infty$, the lemma now follows from (C.19). □

Lemma C.7. *Suppose that f, χ are as in Lemma C.6. Then we have, for R large enough,*

$$\|e^{f(|x_1|)}\chi(|x_1|/R)\psi_N^{trap}\| \leq C_R \tag{C.21}$$

for some constant C_R depending on R but not on N.

Proof. We compute

$$e^{f(|x_1|}(H_N^{\mathrm{trap}} - E_N)e^{-f(|x_1|)} = H_N^{\mathrm{trap}} - |f'(|x_1|)|^2 - E_N + i\left(p_1 \cdot \frac{x_1}{|x_1|}f'(|x_1|) + f'(|x_1|)\frac{x_1}{|x_1|}\cdot p_1\right),$$

with $p_1 = -i\nabla_1$. Therefore, for R large enough,

$$\begin{aligned}
\mathrm{Re}\left\langle e^{f(|x_1|)}\chi(|x_1|/R)\psi_N^{\mathrm{trap}}, e^{f(|x_1|)}\left(H_N^{\mathrm{trap}} - E_N\right)e^{-f(|x_1|)}e^{f(|x_1|)}\chi(|x_1|/R)\psi_N^{\mathrm{trap}}\right\rangle & \\
&= \left\langle e^{f(|x_1|)}\psi_N^{\mathrm{trap}}\chi(|x_1|/R), \left(H_N^{\mathrm{trap}} - |f'(|x_1|)|^2 - E_N\right)\chi(|x_1|/R)e^{f(|x_1|)}\psi_N^{\mathrm{trap}}\right\rangle \\
&\geq \|e^{f(|x_1|)}\chi(|x_1|/R)\psi_N^{\mathrm{trap}}\|^2
\end{aligned} \tag{C.22}$$

where we used Lemma C.6. On the other hand

$$\begin{aligned}\mathrm{Re}\left\langle e^{f(|x_1|)}\chi(|x_1|/R)\psi_N^{\mathrm{trap}},\, e^{f(|x_1|)}\left(H_N^{\mathrm{trap}}-E_N\right)e^{-f(|x_1|)}e^{f(|x_1|)}\chi(|x_1|/R)\psi_N^{\mathrm{trap}}\right\rangle \\ \leq \|e^{f(|x_1|)}\chi(|x_1|/R)\psi_N^{\mathrm{trap}}\|\left\|e^{f(|x_1|)}\left(H_N^{\mathrm{trap}}-E_N\right)\chi(|x_1|/R)\psi_N^{\mathrm{trap}}\right\| \\ \leq \|e^{f(|x_1|)}\chi(|x_1|/R)\psi_N^{\mathrm{trap}}\|\left\|e^{f(|x_1|)}\left[H_N^{\mathrm{trap}},\chi(|x_1|/R)\right]\psi_N^{\mathrm{trap}}\right\|\end{aligned} \tag{C.23}$$

because $(H_N^{\mathrm{trap}}-E_N)\psi_N^{\mathrm{trap}}=0$. Combining (C.22) and (C.23) we obtain that, for R large enough,

$$\|e^{f(|x_1|)}\chi(|x_1|/R)\psi_N^{\mathrm{trap}}\| \leq \left\|e^{f(|x_1|)}\Big[H_N,\chi(|x_1|/R)\Big]\psi_N^{\mathrm{trap}}\right\|.$$

Next we note that

$$[H_N,\chi(|x_1|/R)] = -2iR^{-1}\chi'(|x_1|/R)\frac{x_1}{|x_1|}\cdot\nabla_1 + R^{-2}\chi''(|x_1|/R) + R^{-1}\frac{\chi'(|x_1|/R)}{|x_1|}\,.$$

Since f is monotone increasing, we see that

$$\begin{aligned}&\left\|e^{f(|x_1|)}\chi'(|x_1|/R)\frac{x_1}{|x_1|}\right\| \leq Ce^{f(2R)}, \quad \left\|e^{f(|x_1|)}\frac{\chi'(|x_1|/R)}{|x_1|}\right\| \leq CR^{-1}e^{f(2R)} \quad \text{and} \\ &\left\|e^{f(|x_1|)}\chi''(|x_1|/R)\right\| \leq Ce^{f(2R)}.\end{aligned} \tag{C.24}$$

The energy estimate (C.12) and $V_N \geq 0$ imply that $\|\nabla_1\psi_N^{\mathrm{trap}}\| \leq C$ uniformly in N. From these estimates the lemma follows. □

Proof of Lemma C.3. Suppose χ is as in Lemmas C.6 and C.7. For a fixed R_0 large enough, we have, by Lemma C.7,

$$\|e^{|x_1|}\psi_N^{\mathrm{trap}}\| \leq \|e^{|x_1|}\chi(|x_1|/R_0)\psi_N^{\mathrm{trap}}\| + \|e^{|x_1|}\left(1-\chi(|x_1|/R_0)\right)\psi_N^{\mathrm{trap}}\| \leq C.$$

Therefore

$$\|\mathbf{1}(|x_1|>R)\psi_N^{\mathrm{trap}}\| \leq \|e^{-|x_1|}\mathbf{1}(|x_1|>R)e^{|x_1|}\psi_N^{\mathrm{trap}}\| \leq Ce^{-R}.$$

□

D Properties of the one-body scattering solution $1-w(x)$

In this section we prove part i) and iii) of Lemma 5.1.

Lemma D.1. *Suppose that $V \geq 0$ is smooth, spherical symmetric with compact support and with scattering length a_0. Let*

$$\rho = \sup_{r\geq 0} r^2 V(r) + \int_0^\infty \mathrm{d}r\, r\, V(r), \tag{D.1}$$

and suppose $\varphi_0(x)$ is the solution of

$$\left(-\Delta+\frac{1}{2}V\right)\varphi_0 = 0 \qquad \textit{with} \quad \varphi_0 \to 1 \quad \textit{as } |x|\to\infty\,. \tag{D.2}$$

i) There exists $C_0 > 0$, depending on V, such that $C_0 \leq \varphi_0(x) \leq 1$ for all $x \in \mathbb{R}^3$. Moreover there exists a universal constant c such that

$$1 - c\rho \leq \varphi_0(x) \leq 1 \qquad \text{for all } x \in \mathbb{R}^3 \,. \tag{D.3}$$

ii) There exists a universal constant $c > 0$ such that

$$|\nabla\varphi_0(x)| \leq c\frac{a_0}{|x|^2}, \qquad |\nabla\varphi_0(x)| \leq c\frac{\rho}{|x|} \qquad \text{and} \qquad |\nabla^2\varphi_0(x)| \leq c\frac{\rho}{|x|^2} \,. \tag{D.4}$$

Moreover there are constant C_1, C_2, depending on the potential V, such that

$$|\nabla\varphi_0(x)| \leq C_1 \qquad |\nabla^2\varphi_0| \leq C_2. \tag{D.5}$$

Proof. Let R be such that $\operatorname{supp} V \subset \{x \in \mathbb{R}^3 : |x| \leq R\}$, and let a_0 denote the scattering length of V. Then we fix $\widetilde{R} > R$ such that $a_0/\widetilde{R} \leq \min(\rho, 1/2)$, with ρ defined in (D.1).

In order to prove part i), we observe that, for $|x| \geq \widetilde{R}$, $\varphi_0(x) = 1 - a_0/|x|$. Hence

$$\frac{1}{2} \leq \varphi_0(x) \leq 1, \qquad \text{and} \qquad 1 - \rho \leq \varphi_0(x) \leq 1 \,, \qquad \text{for } |x| \geq \widetilde{R} \,. \tag{D.6}$$

Next, by Harnack principle the ratio between the supremum and the infimum of φ_0 in a given ball is bounded: therefore φ_0 is bounded away from zero in the ball $|x| \leq \widetilde{R}$ and thus there exists $C_0 > 0$ such that $\varphi_0(x) \geq C_0$ for all $x \in \mathbb{R}^3$. Moreover by the maximum principle, and since, from (D.2), $-\Delta\varphi_0 \leq 0$, it follows that $\varphi_0(x) \leq 1$, for all $x \in \mathbb{R}^3$. To prove (D.3) for $|x| \leq \widetilde{R}$, we write $\varphi_0(x) = m(r)/r$, with $r = |x|$. Then $m'(\widetilde{R}) = 1$, and, from (D.2),

$$-m''(r) + \frac{1}{2}V(r)m(r) = 0 \,. \tag{D.7}$$

Since $0 < \varphi_0(x) \leq 1$, it follows that $m(0) = 0$ and $0 < m(r)/r \leq 1$. Therefore, for $r < \widetilde{R}$,

$$m'(r) = m'(\widetilde{R}) - \int_r^{\widetilde{R}} \mathrm{d}s\, m''(s) = 1 - \frac{1}{2}\int_r^{\widetilde{R}} \mathrm{d}s\, s\, V(s)\frac{m(s)}{s} \geq 1 - c\int_0^{\infty} \mathrm{d}s\, s\, V(s) \geq 1 - c\rho \tag{D.8}$$

and

$$m(r) = \int_0^r \mathrm{d}s\, m'(s) \geq r(1 - c\rho) \qquad \Rightarrow \quad \varphi_0(r) = \frac{m(r)}{r} \geq 1 - c\rho \qquad \text{for all } r < \widetilde{R} \,. \tag{D.9}$$

The last equation, together with (D.6), implies (D.3).

Next we prove ii). For $|x| \geq \widetilde{R}$, we have $\varphi_0(x) = 1 - a_0/|x|$ and thus

$$|\nabla\varphi_0(x)| \leq \frac{a_0}{|x|^2} \leq \frac{a_0}{\widetilde{R}|x|} \leq \frac{\rho}{|x|}, \qquad \text{for } |x| \geq \widetilde{R}, \tag{D.10}$$

by definition of $\widetilde{R}$. Next, for $|x| < \widetilde{R}$, we write $\varphi_0(x) = m(r)/r$, with $r = |x|$. Then

$$\begin{aligned} |\nabla\varphi_0(x)| &= \Big|\frac{m'(r)r - m(r)}{r^2}\Big| \\ &= \Big|\frac{1}{r}\int_0^r \mathrm{d}s\, m''(s) - \frac{1}{r^2}\int_0^r \mathrm{d}s \int_0^s \mathrm{d}\kappa\, m''(\kappa)\Big| \\ &= \frac{1}{r^2}\int_0^r \mathrm{d}\kappa\, \kappa\, m''(\kappa) \,, \end{aligned} \tag{D.11}$$

because $m''(\kappa) \geq 0$. From (D.7) we obtain

$$|\nabla\varphi_0(x)| \leq \frac{1}{2r^2}\int_0^r \mathrm{d}\kappa\,\kappa^2 V(\kappa)\,\frac{m(\kappa)}{\kappa} \leq c\frac{a_0}{|x|^2}\,, \tag{D.12}$$

because $8\pi a_0 = \int V(x)\varphi_0(x)$ (see Lemma 5.1), part iv). Moreover, again from (D.11) and (D.7), we have

$$|\nabla\varphi_0(x)| \leq \frac{1}{2r^2}\int_0^r \mathrm{d}\kappa\,\kappa^2 V(\kappa)\,\frac{m(\kappa)}{\kappa} \leq c\frac{\sup_{\kappa\geq 0}\kappa^2\,V(\kappa)}{r} \leq c\frac{\rho}{r}\,. \tag{D.13}$$

Together with (D.10) we obtain the first two inequalities in (D.4). From (D.10) and from the first inequality in (D.13), it also follows that there exists C_1, depending on the bounded potential V, such that $|\nabla\varphi_0(x)| \leq C_1$. To prove the second bounds in (D.4) and (D.5), we note that

$$|\nabla^2\varphi_0(x)| \leq \frac{a_0}{|x|^3} \leq \frac{\rho}{|x|^2} \qquad \text{for } |x| > \widetilde{R}, \tag{D.14}$$

by the definition of $\widetilde{R}$. For $|x| \leq \widetilde{R}$, we have (expanding $m(r)$ and $m'(r)$ and using that $m(0) = 0$)

$$\begin{aligned} |\nabla^2\varphi_0(x)| &\leq \Big|\frac{m''(r)}{r} - 2\frac{m'(r)}{r^2} + 2\frac{m(r)}{r^3}\Big| \\ &= \Big|\frac{1}{2}V(r)\frac{m(r)}{r} + \frac{2}{r^3}\int_0^r \mathrm{d}s\,s^2\,V(s)\frac{m(s)}{s}\Big| \\ &\leq c\frac{\big(\sup_{s\geq 0}\,s^2V(s)\big)}{r^2} \leq c\frac{\rho}{r^2} \end{aligned} \tag{D.15}$$

Last equation, together with (D.14), implies the third bound in (D.4). Moreover, from (D.14) and the second line in (D.15), it also follows that there exists C_2, depending on the bounded potential V, such that $|\nabla^2\varphi_0(x)| \leq C_2$. □

Proof of Lemma 5.1, part i) and iii). By scaling $1-w(x) = \varphi_0(Nx)$, with φ_0 defined in Lemma D.1. Therefore part i) of Lemma 5.1 follows immediately by part i) of Lemma D.1, and part iii) of Lemma 5.1 follows from (D.4) and (D.5). □

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