Gross-Pitaevskii Equation as the Mean Field Limit of Weakly Coupled Bosons

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Abstract

We consider the dynamics of N boson systems interacting through a pair potential $N^{-1}V_a(x_i - x_j)$ where $V_a(x) = a^{-3}V(x/a)$. We denote the solution to the N-particle Schrödinger equation by $\psi_{N,t}$. Recall that the Gross-Pitaevskii (GP) equation is a nonlinear Schrödinger equation and the GP hierarchy is an infinite BBGKY hierarchy of equations so that if u_t solves the GP equation, then the family of k-particle density matrices $\{\otimes_k u_t, k \geq 1\}$ solves the GP hierarchy. Under the assumption that $a = N^{-\varepsilon}$ for $0 < \varepsilon < 3/5$, we prove that as $N \to \infty$ the limit points of the k-particle density matrices of $\psi_{N,t}$ are solutions of the GP hierarchy with the coupling constant in the nonlinear term of the GP equation given by $\int V(x)dx$. The uniqueness of the solutions to this hierarchy remains an open question.

1 Introduction

Consider N bosons in a three dimensional cube Λ with the periodic boundary condition and volume one. The bosons interact via a two body potential

$$V_a(x) = \frac{1}{a^3}V(x/a).$$

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We assume the potential V to be smooth, positive, and with compact support. The parameter a determines the range and the strength of the potential: a and N will be coupled so that $a \to 0$ as $N \to \infty$. Thus the potential V_a converges to a Dirac δ-function. The N-body Hamiltonian for the N weakly coupled bosons is thus given by

$$H_N = -\sum_{j=1}^{N} \Delta_j + \frac{1}{N} \sum_{i \neq j} V_a(x_i - x_j). \tag{1.1}$$

The density of the bosons in the cube, ρ, is clearly equal to N. Any given particle typically interacts via the potential V_a with $a^3 N$ other particles. If $a \gg N^{-1/3}$, there are a lot of interactions among the N bosons. In this case, the ground state of the system contains, to the leading order in N, no correlation among the particles. Thus the ground state wave function is a product function to the leading order. In fact, the same conclusion holds as long as $a \gg N^{-1}$. The correlations among the particles become important in the leading order only when $a \simeq N^{-1}$. This choice corresponds to the so called Gross-Pitaevskii scaling limit, as pointed out by Lieb, Seiringer and Yngvason [8] (see [7] for a review). For this choice of scaling, i.e., $a \simeq N^{-1}$, we study the dynamics of the Bose gas in [4]. In this paper, we consider the cases $a = N^{-\varepsilon}$ for $0 < \varepsilon < 3/5$.

In the following we denote by x a general variable in the box Λ. On the other hand $\mathbf{x} = (x_1, \dots x_N)$ denotes a point in Λ^N. We will also use the notations $\mathbf{x}_k = (x_1, \dots x_k) \in \Lambda^k$ and $\mathbf{x}_{N-k} = (x_{k+1}, \dots x_N) \in \Lambda^{N-k}$.

The dynamics of the Bose system is governed by the N-body Schrödinger Equation

$$i\partial_t \psi_{N,t} = H_N \psi_{N,t} \, . \tag{1.2}$$

Here the wave function $\psi_{N,t} \in L^2_s(\Lambda^N)$, the subspace of $L^2(\Lambda^N)$ consisting functions symmetric with respect to permutations of the N particles. More generally we can describe the N body system by its density matrix $\gamma_{N,t}$. A density matrix is a positive self-adjoint operator γ acting on $L^2_s(\Lambda^N)$, with $\operatorname{Tr} \gamma = 1$. The density matrix corresponding to the wave function $\psi_{N,t}$ is given by the orthogonal projection onto $\psi_{N,t}$, i.e., $\gamma_{N,t} = |\psi_{N,t}\rangle\langle\psi_{N,t}|$. Quantum mechanical states described by orthogonal projections are called pure states. In general a density matrix is a weighted average of orthogonal projection (mixed states). The time evolution of the density matrix $\gamma_{N,t}$ is given by

$$i\partial_t \gamma_{N,t} = [H_N, \gamma_{N,t}] \tag{1.3}$$

which is equivalent to the Schrödinger Equation (1.2).

It is useful to introduce the marginal distributions corresponding to the density matrix $\gamma_{N,t}$. For $k = 1, \dots, N$, the k-particle marginal $\gamma^{(k)}_{N,t}$ is defined through its kernel by

$$\gamma^{(k)}_{N,t}(\mathbf{x}_k; \mathbf{x}'_k) = \int \mathrm{d}\mathbf{x}_{N-k} \, \gamma_{N,t}(\mathbf{x}_k, \mathbf{x}_{N-k}; \mathbf{x}'_k; \mathbf{x}_{N-k}) \tag{1.4}$$

where $\mathbf{x}'_k = (x'_1, \dots, x'_k)$ and where $\gamma_{N,t}(\mathbf{x};\mathbf{x}')$ denotes the kernel of the density matrix $\gamma_{N,t}$. From $\mathrm{Tr}\,\gamma_{N,t} = 1$, it immediately follows that

$$\mathrm{Tr}\gamma^{(k)}_{N,t} = 1 \tag{1.5}$$

for every $k = 1, \dots, N$.

Using (1.3) (and the symmetry of $\gamma_{N,t}$ with respect to permutations of the N particles) we find that the evolution of the marginal distributions of $\gamma_{N,t}$ is determined by the following hierarchy of N equations, commonly called the BBGKY Hierarchy:

$$\begin{aligned} i\partial_t \gamma^{(k)}_{N,t}(\mathbf{x}_k;\mathbf{x}'_k) &= \sum_{j=1}^{k} (-\Delta_{x_j} + \Delta_{x'_j})\gamma^{(k)}_{N,t}(\mathbf{x}_k;\mathbf{x}'_k) \\ &\quad + \frac{1}{N}\sum_{j\neq\ell}^{k} (V_a(x_j - x_\ell) - V_a(x'_j - x'_\ell))\gamma^{(k)}_{N,t}(\mathbf{x}_k;\mathbf{x}'_k) \\ &\quad + (1-\frac{k}{N})\sum_{j=1}^{k}\int \mathrm{d}x_{k+1}(V_a(x_j - x_{k+1}) - V_a(x'_j - x_{k+1}))\gamma^{(k+1)}_{N,t}(\mathbf{x}_k, x_{k+1};\mathbf{x}'_k, x_{k+1}). \end{aligned} \tag{1.6}$$

Rewriting this hierarchy in integral form yields

$$\begin{aligned} \gamma^{(k)}_{N,t}(\mathbf{x}_k;\mathbf{x}'_k) &= \gamma^{(k)}_{N,0}(\mathbf{x}_k;\mathbf{x}'_k) - i\sum_{j=1}^{k}\int_0^t \mathrm{d}s(-\Delta_{x_j} + \Delta_{x'_j})\gamma^{(k)}_{N,s}(\mathbf{x}_k;\mathbf{x}'_k) \\ &\quad - \frac{i}{N}\sum_{j\neq\ell}^{k}\int_0^t \mathrm{d}s\,(V_a(x_j - x_\ell) - V_a(x'_j - x'_\ell))\gamma^{(k)}_{N,s}(\mathbf{x}_k;\mathbf{x}'_k) \\ &\quad - i(1-\frac{k}{N})\sum_{j=1}^{k}\int_0^t \mathrm{d}s \int \mathrm{d}x_{k+1}\,(V_a(x_j - x_{k+1}) - V_a(x'_j - x_{k+1}))\gamma^{(k+1)}_{N,s}(\mathbf{x}_k, x_{k+1};\mathbf{x}'_k, x_{k+1}). \end{aligned} \tag{1.7}$$

Letting $a = N^{-\varepsilon}$ and considering the limit $N \to \infty$, the BBGKY Hierarchy converges formally to the following infinite hierarchy of equations:

$$\begin{aligned} \gamma^{(k)}_t(\mathbf{x}_k;\mathbf{x}'_k) &= \gamma^{(k)}_0(\mathbf{x}_k;\mathbf{x}'_k) - i\sum_{j=1}^{k}\int_0^t \mathrm{d}s\,(-\Delta_{x_j} + \Delta_{x'_j})\gamma^{(k)}_s(\mathbf{x}_k;\mathbf{x}'_k) \\ &\quad - ib\sum_{j=1}^{k}\int_0^t \mathrm{d}s \int \mathrm{d}x_{k+1}(\delta(x_j - x_{k+1}) - \delta(x'_j - x_{k+1}))\gamma^{(k+1)}_s(\mathbf{x}_k, x_{k+1};\mathbf{x}'_k, x_{k+1}), \end{aligned} \tag{1.8}$$

where we defined

$$b = \int \mathrm{d}x V(x)$$

(recall that $V_a(x) = (1/a^3)V(x/a)$). We will call (1.8) the infinite BBGKY hierarchy, or the Gross-Pitaevskii (GP) hierarchy. Note that (1.8) has a factorized solution. The family of marginal distributions $\tilde{\gamma}_t^{(k)}(\mathbf{x}_k; \mathbf{x}'_k) = \prod_{j=1}^k \phi_t(x_j)\overline{\phi_t(x'_j)}$ is a solution of (1.8) if and only if the function ϕ_t satisfies the non-linear Schrödinger Equation

$$i\partial_t \phi_t(y) = -\Delta\phi_t(y) + b|\phi_t(y)|^2\phi_t(y)\,. \tag{1.9}$$

This is the Gross-Pitaevskii (GP) equation, except that the coupling constant in front of the non-linear interaction is given by b. In the standard GP equation, the coupling constant is $8\pi a_0$ where a_0 is the scattering length of the unscaled potential $V(x)$.

The aim of this paper is to prove the convergence of solutions of (1.6) to solutions of (1.8): more precisely we will prove that the sequence $\Gamma_{N,t} = \{\gamma_{N,t}^{(k)}\}_{k=1}^N$ has at least one limit point $\Gamma_{\infty,t} = \{\gamma_{\infty,t}^{(k)}\}_{k\geq 1}$ with respect to some weak topology, and that any weak limit point $\Gamma_{\infty,t}$ satisfies the infinite hierarchy (1.8). For dimension $d = 1$, the convergence to the GP hierarchy (1.8) for the delta potential was established by Adami, Bardos, Golse and Teta in [1]. If the potential has a weaker singularity, the convergence to the infinite BBGKY hierarchy was proved in [2].

In [4] we proved the convergence to the GP hierarchy with the coupling constant $8\pi a_0$ when $a \simeq N^{-1}$. Together with the result of the present paper, this means that the coupling constant changes from $8\pi a_0$ to b when a changes from N^{-1} to $N^{-\varepsilon}$, for $\varepsilon < 3/5$. In fact, the coupling constant should always be given by b, as long as $a = N^{-\varepsilon}$, with $\varepsilon < 1$. This fact follows from the observation that the potential $N^{-1}a^{-3}V(x/a)$ has scattering length of order $1/N$ for every choice of $a = N^{-\varepsilon}$, $\varepsilon > 0$. Hence the ground state correlations live on the scale $1/N$, for all $\varepsilon > 0$. As long as $\varepsilon < 1$, these correlations cannot affect the coupling constant because the potential live in the much larger scale $a = N^{-\varepsilon} \gg N^{-1}$. In other words, since the two-particles correlation function is of the form $1 - \text{const}/(N|x|)$, for $|x| > N^{-1}$, we have

$$\int \mathrm{d}x \frac{1}{a^3} V(x/a) \left(1 - \frac{\text{const}}{N|x|}\right) = b - \text{const}\,\frac{1}{Na} \tag{1.10}$$

which equals b in the limit $N \to \infty$, if $a \gg N^{-1}$. Thus, $a \simeq N^{-1}$ is the only scaling for which the coupling constant is given by the scattering length of the unscaled potential V.

We remark that in [4], we need to use a modified version of the Hamiltonian (1.1), in which two-body interactions are removed, whenever too many particles come into a small region. In the present paper, this assumption is not needed. Moreover, we prove a much stronger a-priori estimate on the limiting density matrices, see (2.16).

Since the δ-function cannot be bounded by the Laplace operator, we are unable to prove the uniqueness of the solutions of (1.8). Hence we cannot conclude the *propagation of chaos*. The best known result in this direction is [3], which covers the case of a Coulomb singularity in the potential in $d = 3$. Previously, uniqueness was proved by Hepp [6] and Spohn [9] for bounded potential; Ginibre and Velo [5] had a completely different approach for quasifree states.

2 The Main Result

Since our main result states properties of limit points of the sequence $\gamma_{N,t}^{(k)}$ for $N \to \infty$, in order to formulate it, we need to specify a topology on the space of density matrices.

Quantum mechanical states of a k-boson system can be described by a density matrices $\gamma^{(k)}$: $\gamma^{(k)}$ is a positive, trace class operator, with trace normalized to one. We can also identify $\gamma^{(k)}$ with its kernel and consider it as a distribution in $L^2(\Lambda^k \times \Lambda^k)$: in fact, since $\gamma^{(k)}$ is a positive operator with trace equal to one, its Hilbert Schmidt norm is also bounded by one, and

$$\|\gamma^{(k)}\|_2 := \int \mathrm{d}\mathbf{x}_k \mathrm{d}\mathbf{x}'_k \, |\gamma^{(k)}(\mathbf{x}_k; \mathbf{x}'_k)|^2 \leq 1 \, . \tag{2.11}$$

For $\Gamma = \{\gamma^{(k)}\}_{k\geq 1} \in \oplus_{k\geq 1} L^2(\Lambda^k \times \Lambda^k)$ we define the norm

$$\|\Gamma\|_{H_-} := \sum_{k=1}^{\infty} 2^{-k} \|\gamma^{(k)}\|_2, \tag{2.12}$$

and we put

$$H_- := \{\Gamma \in \bigoplus_{k\geq 1} L^2(\Lambda^k \times \Lambda^k) : \|\Gamma\|_{H_-} < \infty\}.$$

Analogously, we define

$$H_+ = \{\Gamma \in \bigoplus_{k\geq 1} L^2(\Lambda^k \times \Lambda^k) : \lim_{k\to\infty} 2^k \|\gamma^{(k)}\|_2 = 0\},$$

and we equip H_+ with the norm

$$\|\Gamma\|_{H_+} = \sup_{k\geq 1} 2^k \|\gamma^{(k)}\|_2.$$

The Banach space H_- is the dual space to H_+. A sequence $\Gamma_N = \{\gamma_N^{(k)}\}_{k\geq 1} \in H_-$ converges to $\Gamma_\infty = \{\gamma_\infty^{(k)}\}_{k\geq 1} \in H_-$ in the weak$*$ topology if and only if

$$\lim_{N\to\infty} \sum_{k\geq 1} \int \mathrm{d}\mathbf{x}_k \mathrm{d}\mathbf{x}'_k \, J^{(k)}(\mathbf{x}_k, \mathbf{x}'_k) \left(\gamma_N^{(k)}(\mathbf{x}_k, \mathbf{x}'_k) - \gamma_\infty^{(k)}(\mathbf{x}_k, \mathbf{x}'_k) \right) = 0 \tag{2.13}$$

for all $J = \{J^{(k)}\}_{k\geq 1} \in H_+$ (this is actually equivalent to convergence for each fixed k). We will denote by $C([0, T], H_-)$ the space of functions of $t \in [0, T]$ with values in H_- which are continuous with respect to the weak star topology on H_-. Since the space H_+ is separable, we can fix a dense countable subset in the unit ball of H_+, denoted by $\{J_i\}_{i\geq 1}$. Define the metric on H_- by

$$\rho(\Gamma,\widetilde{\Gamma}) := \sum_{i=1}^{\infty} 2^{-i} \Big| \sum_{k=1}^{\infty} \int \mathrm{d}\mathbf{x}_k \mathrm{d}\mathbf{x}'_k \overline{J_i^{(k)}(\mathbf{x}_k;\mathbf{x}'_k)} \big[\gamma^{(k)}(\mathbf{x}_k;\mathbf{x}'_k) - \widetilde{\gamma}^{(k)}(\mathbf{x}_k;\mathbf{x}'_k)\big] \Big| \,. \tag{2.14}$$

Then the topology induced by $\rho(.,.)$ and the weak* topology are equivalent on the unit ball B_- of H_-. We equip $C([0,T],H_-)$ with the metric

$$\widehat{\rho}(\Gamma,\widetilde{\Gamma}) := \sup_{0\leq t\leq T} \rho\left(\Gamma(t),\widetilde{\Gamma}(t)\right) . \tag{2.15}$$

We are now ready to state our main theorem.

Theorem 2.1. *Assume the potential $V(x)$ is positive, smooth, and has compact support, and set $V_a(x) = a^{-3}V(x/a)$. Suppose that $a = N^{-\varepsilon}$, for some $0 < \varepsilon < 3/5$. Choose an initial density matrix $\gamma_{N,0}$ such that*

$$Tr\, H_N^k \gamma_{N,0} \leq C^k N^k$$

for some constant C and for all $k \geq 1$. Let $\Gamma_{N,0} = \{\gamma_{N,0}^{(k)}\}_{k=1}^N$ be the family of marginal distributions corresponding to the initial density matrix $\gamma_{N,0}$. Fix now $T > 0$ and denote by $\Gamma_{N,t} = \{\gamma_{N,t}^{(k)}\}$, for $t \in [0,T]$, the solution to the BBGKY Hierarchy (1.6) corresponding to the initial data $\Gamma_{N,0}$.

i) The sequence $\Gamma_{N,t}$ is compact in $C([0,T],H_-)$ with respect to the metric $\widehat{\rho}$.

ii) Let $\Gamma_{\infty,t} = \{\gamma_{\infty,t}^{(k)}\}_{k\geq 1} \in C([0,T],H_-)$ be any limit point of $\Gamma_{N,t}$ with respect to the metric $\widehat{\rho}$. Then there is a constant C such that

$$Tr \big| S_1 \dots S_k \, \gamma_{\infty,t}^{(k)} S_k \dots S_1 \big| \leq C^k \tag{2.16}$$

for every $k \geq 1$. Here we use the notation $S_j = (1-\Delta_j)^{1/2}$.

iii) $\Gamma_{\infty,t}$ is non trivial. In particular we have

$$Tr \gamma_{\infty,t}^{(k)} = 1 \tag{2.17}$$

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

iv) Assume $h_r(x) = r^{-3}h(x/r)$ for any $h \in C_0^\infty(\Lambda)$ with $\int_\Lambda h = 1$. Then, for any $k \geq 1$ and $t \in [0,T]$, the limit

$$\begin{aligned} \lim_{r,r'\to 0} \int \mathrm{d}x'_{k+1} \mathrm{d}x_{k+1} \, h_r(x'_{k+1} - x_{k+1}) h_{r'}(x_{k+1} - x_j) \gamma_{\infty,t}^{(k)}(\mathbf{x}_k, x_{k+1}; \mathbf{x}'_k, x'_{k+1}) \\ =: \gamma_{\infty,t}^{(k)}(\mathbf{x}_k, x_j; \mathbf{x}'_k, x_j) \end{aligned} \tag{2.18}$$

exists in the weak $W^{-1,1}(\Lambda^k \times \Lambda^k)$*-sense and defines* $\gamma^{(k)}(\mathbf{x}_k, x_j; \mathbf{x}'_k, x_j)$ *as a distribution of* $2k$ *variables* [1]*.*

v) $\Gamma_{\infty,t}$ *satisfies the infinite Gross-Pitaevski Hierarchy (1.8) in the following sense: For any* $J^{(k)}(\mathbf{x}_k, \mathbf{x}'_k) \in W^{2,\infty}(\Lambda^k \times \Lambda^k)$ *we have*

$$\begin{aligned}\int \mathrm{d}\mathbf{x_k}\mathrm{d}\mathbf{x}'_k\, J^{(k)}(\mathbf{x}_k, \mathbf{x}'_k)\gamma^{(k)}_{\infty,t}(\mathbf{x}_k, \mathbf{x}'_k) &= \int \mathrm{d}\mathbf{x}_k\mathrm{d}\mathbf{x}'_k J^{(k)}(\mathbf{x}_k, \mathbf{x}'_k)\gamma^{(k)}_{\infty,0}(\mathbf{x}_k, \mathbf{x}'_k)\\ &\quad -i\sum_{j=1}^{k}\int_0^t \mathrm{d}s \int \mathrm{d}\mathbf{x}_k\mathrm{d}\mathbf{x}'_k\, J^{(k)}(\mathbf{x}_k, \mathbf{x}'_k)\,(-\Delta_j + \Delta'_j)\gamma^{(k)}_{\infty,s}(\mathbf{x}_k, \mathbf{x}'_k)\\ &\quad -ib\sum_{j=1}^{k}\int_0^t \mathrm{d}s \int \mathrm{d}\mathbf{x}_k\mathrm{d}\mathbf{x}'_k\mathrm{d}x_{k+1}\, J^{(k)}(\mathbf{x}_k, \mathbf{x}'_k)(\delta(x_j - x_{k+1}) - \delta(x'_j - x_{k+1}))\\ &\qquad \times \gamma^{(k+1)}_{\infty,s}(\mathbf{x}_k, x_{k+1}; \mathbf{x}'_k, x_{k+1})\,.\end{aligned} \tag{2.19}$$

Here the action of the δ*-functions on* $\gamma^{(k+1)}$ *is well defined (through a regularization of the* δ*-function) by part iv).*

3 Energy Estimates

The main tool in the proof of Theorem 2.1 is the following proposition, which proves bounds for the L^2-norm of the derivatives of a wave function ψ in terms of the expectation of powers of the Hamiltonian H_N (defined in (1.1)) in the state described by ψ. The proof of this proposition requires some standard Sobolev-type inequalities, which are collected, for completeness, in Appendix A.

Proposition 3.1. *Suppose* V *is smooth and positive. Put* $V_a(x) = a^{-3}V(x/a)$ *and assume* $a = N^{-\varepsilon}$*, with* $0 < \varepsilon < 3/5$*. Put*

$$\tilde{H}_N = \sum_{j=1}^{N} S_j^2 + \frac{1}{N}\sum_{\ell \neq m} V_a(x_\ell - x_m) = H_N + N.$$

Fix $k \in \mathbb{N}$ *and* $0 < C < 1$*. Then there is* $N_0 = N_0(k, C)$ *such that*

$$(\psi, \tilde{H}_N^k \psi) \geq C^k N^k\, (\psi, S_1^2 S_2^2 \dots S_k^2 \psi) \tag{3.20}$$

for all $N > N_0$ *and all* $\psi \in D(H_N^k)$ *(*ψ *is assumed to be symmetric with respect to any permutation of all its variables).*

[1]Here and in the following $W^{p,q}(\Lambda^k \times \Lambda^k)$ denotes the usual Sobolev space over $\Lambda^k \times \Lambda^k$.

Proof. The proof of the proposition is by a two step induction over k. For $k = 0$ and $k = 1$ the claim is trivial (because of the positivity of the potential). Now we assume the proposition is true for all $k \leq n$, and we prove it for $k = n + 2$. To this end we apply the induction assumption and we find, for $N > N_0(n, C)$,

$$(\psi, \tilde{H}_N^{n+2}\psi) = (\psi, \tilde{H}_N \tilde{H}_N^n \tilde{H}_N \psi) \geq C^n N^n (\psi \tilde{H}_N S_1^2 \dots S_n^2 \tilde{H}_N \psi)\,. \tag{3.21}$$

We put

$$H^{(n)} = \sum_{j=1}^n S_j^2 + \frac{1}{N} \sum_{j<m}^N V_{jm}$$

with $V_{jm} = a^{-3} V((x_j - x_m)/a)$. Then we have

$$\begin{aligned}(\psi \tilde{H}_N S_1^2 \dots S_n^2 \tilde{H}_N \psi) = &\sum_{j_1, j_2 \geq n+1} (\psi, S_{j_1}^2 S_1^2 \dots S_n^2 S_{j_2}^2 \psi) + \sum_{j \geq n+1} \Big((\psi, S_j^2 S_1^2 \dots S_n^2 H^{(n)} \psi) + \text{c.c.} \Big) \\ &+ (\psi, H^{(n)} S_1^2 \dots S_n^2 H^{(n)} \psi)\,.\end{aligned}$$

Since $H^{(n)} S_1^2 \dots S_n^2 H^{(n)} \geq 0$, we find, using the symmetry with respect to permutations,

$$\begin{aligned}(\psi \tilde{H}_N S_1^2 \dots S_n^2 \tilde{H}_N \psi) \geq\ &(N-n)(N-n-1)(\psi, S_1^2 \dots S_{n+2}^2 \psi) + (2n+1)(N-n)(\psi, S_1^4 S_2^2 \dots S_{n+1}^2 \psi) \\ &+ \frac{n(n+1)(N-n)}{2N} \big((\psi, V_{12} S_1^2 \dots S_{n+1}^2 \psi) + \text{c.c.} \big) \\ &+ \frac{(n+1)(N-n)(N-n-1)}{N} \big((\psi, V_{1,n+2} S_1^2 \dots S_{n+1}^2 \psi) + \text{c.c.} \big)\,,\end{aligned} \tag{3.22}$$

where c.c. denotes the complex conjugate. Here we also used that $(\psi, V_{jm} S_1^2 \dots S_{n+1}^2 \psi) \geq 0$ if $j, m > n + 1$, because of the positivity of the potential. Next we consider the term on the second line of (3.22): note that this term vanishes if $n = 0$, so we can assume $n \geq 1$. Then we have

$$\begin{aligned}(\psi, V_{12} S_1^2 \dots S_{n+1}^2 \psi) + \text{c.c.} =\ &(\psi, S_{n+1} \dots S_3 V_{12} S_1^2 S_2^2 S_3 \dots S_{n+1} \psi) + \text{c.c.} \\ &= (\psi, S_{n+1} \dots S_3 V_{12} (1 + p_1^2)(1 + p_2^2) S_3 \dots S_{n+1} \psi) + \text{c.c.} \\ &\geq 2(\psi, S_{n+1} \dots S_3 V_{12} p_2^2 S_3 \dots S_{n+1} \psi) + (\psi, S_{n+1} \dots S_3 V_{12} p_1^2 p_2^2 S_3 \dots S_{n+1} \psi) + \text{c.c.} \\ &\geq 2(\psi, S_{n+1} \dots S_3 \nabla V_{12} p_2 S_3 \dots S_{n+1} \psi) + (\psi, S_{n+1} \dots S_3 p_2 \nabla V_{12} p_1 p_2 S_3 \dots S_{n+1} \psi) \\ &\quad + (\psi, S_{n+1} \dots S_3 \nabla V_{12} p_1^2 p_2 S_3 \dots S_{n+1} \psi) + \text{c.c.}\end{aligned}$$

where $\nabla V_{12} = a^{-4}(\nabla V)((x_1 - x_2)/a)$. Applying Schwarz inequality we get

$$\begin{aligned}
(\psi, &V_{12} S_1^2 \dots S_{n+1}^2 \psi) + \text{c.c.} \\
&\geq -2\{\alpha_1 (\psi, S_{n+1} \dots S_3 |\nabla V_{12}| S_3 \dots S_{n+1}\psi) + \alpha_1^{-1} (\psi, S_{n+1} \dots S_3 |p_2| |\nabla V_{12}| |p_2| S_3 \dots S_{n+1}\psi)\} \\
&\quad - \{\alpha_2 (\psi, S_{n+1} \dots S_3 |p_2| |\nabla V_{12}| |p_2| S_3 \dots S_{n+1}\psi) \\
&\qquad\qquad + \alpha_2^{-1} (\psi, S_{n+1} \dots S_3 |p_2| |p_1| |\nabla V_{12}| |p_1| |p_2| S_3 \dots S_{n+1}\psi)\} \\
&\quad - \{\alpha_3 (\psi, S_{n+1} \dots S_3 |\nabla V_{12}| S_3 \dots S_{n+1}\psi) + \alpha_3^{-1} (\psi, S_{n+1} \dots S_3 |p_2| p_1^2 |\nabla V_{12}| p_1^2 |p_2| S_3 \dots S_{n+1}\psi)\}\,.
\end{aligned}$$

Using Lemma A.1 we find

$$\begin{aligned}
(\psi, &V_{12} S_1^2 \dots S_{n+1}^2 \psi) + \text{c.c.} \\
&\geq -C\{\alpha_1 a^{-1} (\psi, S_{n+1} \dots S_3 S_1^2 S_2^2 S_3 \dots S_{n+1}\psi) + \alpha_1^{-1} a^{-2} (\psi, S_{n+1} \dots S_3 S_1^2 p_2^2 S_3 \dots S_{n+1}\psi)\} \\
&\quad - C\{\alpha_2 a^{-2} (\psi, S_{n+1} \dots S_3 S_1^2 p_2^2 S_3 \dots S_{n+1}\psi) + \alpha_2^{-1} a^{-2} (\psi, S_{n+1} \dots S_3 S_1^2 p_1^2 p_2^2 S_3 \dots S_{n+1}\psi)\} \\
&\quad - C\{\alpha_3 a^{-1} (\psi, S_{n+1} \dots S_3 S_1^2 S_2^2 S_3 \dots S_{n+1}\psi) + \alpha_3^{-1} a^{-4} (\psi, S_{n+1} \dots S_3 p_2^2 p_1^4 S_3 \dots S_{n+1}\psi)\} \\
&\geq -C N^{-3/2} a^{-5/2} \{N^2 (\psi, S_1^2 S_2^2 S_3^2 \dots S_{n+1}^2 \psi) + N (\psi, S_1^4 S_2^2 \dots S_{n+1}^2 \psi)\}
\end{aligned} \tag{3.23}$$

where we optimized the choice of $\alpha_1, \alpha_2, \alpha_3$. As for the last term on the r.h.s. of (3.22) we have

$$\begin{aligned}
(\psi, V_{1,n+2} S_1^2 \dots S_{n+1}^2 \psi) + \text{c.c.} &= (\psi, S_{n+1} \dots S_2 V_{1,n+2} S_1^2 S_2 \dots S_{n+1}\psi) + \text{c.c.} \\
&\geq (\psi, S_{n+1} \dots S_2 V_{1,n+2} p_1^2 S_2 \dots S_{n+1}\psi) + \text{c.c.} \\
&\geq (\psi, S_{n+1} \dots S_2 \nabla V_{1,n+2} p_1 S_2 \dots S_{n+1}\psi) + \text{c.c.} \\
&\geq -\alpha (\psi, S_{n+1} \dots S_2 |\nabla V_{1,n+2}| S_2 \dots S_{n+1}\psi) \\
&\qquad\qquad - \alpha^{-1} (\psi, S_{n+1} \dots S_2 |p_1| |\nabla V_{1,n+2}| |p_1| S_2 \dots S_{n+1}\psi) \\
&\geq -C(\alpha a^{-1} + \alpha^{-1} a^{-2})\, (\psi, S_1^2 \dots S_{n+2}^2 \psi) \\
&\geq -C a^{-3/2} (\psi, S_1^2 \dots S_{n+2}^2 \psi)\,.
\end{aligned}$$

Inserting last equation and (3.23) in the r.h.s. of (3.22) we get

$$\begin{aligned}
(\psi \tilde{H}_N S_1^2 \dots S_n^2 \tilde{H}_N \psi) \geq (N-n)(N-n-1) &\left(1 - \frac{C}{N a^{3/2}} - \frac{C}{N^{3/2} a^{5/2}}\right) (\psi, S_1^2 \dots S_{n+2}^2 \psi) \\
+ (2n+1)(N-n) &\left(1 - \frac{C}{N^{3/2} a^{5/2}}\right) (\psi, S_1^4 S_2^2 \dots S_{n+1}^2 \psi)\,.
\end{aligned}$$

Since $a = N^{-\varepsilon}$ with $\varepsilon < 3/5$, we have $N^{3/2} a^{5/2} \gg 1$ and $N a^{3/2} \gg 1$. From the last equation, for any fixed $C < 1$ and $n \in \mathbb{N}$, we can find N_0 so that

$$(\psi, \tilde{H}_N S_1^2 \dots S_n^2 \tilde{H}_N \psi) \geq C^2 N^2 (\psi, S_1^2 \dots S_{n+2}^2 \psi) \tag{3.24}$$

for every $N \geq N_0$. This, together with (3.21) completes the proof of the proposition. □

Corollary 3.2. *Suppose the initial density matrix $\gamma_{N,0}$ satisfies*

$$Tr\, H_N^k \gamma_{N,0} \leq C_1^k N^k \,.$$

Let $\gamma_{N,t}$ be the solution of (1.3)*, and let $\{\gamma_{N,t}^{(k)}\}_{k=0}^N$ be the corresponding marginal distributions. Then, for any $C \geq C_1$ and any $k \in \mathbb{N}$ there is $N_0 = N_0(k, C)$ such that*

$$Tr\, S_1 \dots S_k \gamma_{N,t}^{(k)} S_k \dots S_1 \leq C^k \tag{3.25}$$

for all $t \in \mathbb{R}$ and all $N \geq N_0$.

4 Proof of the Main Theorem

In this section we prove our main result, Theorem 2.1. To this end we will make use of the following lemma. We use here the notation

$$\langle J^{(k)}, \gamma^{(k)} \rangle = \int \mathrm{d}\mathbf{x}_k \mathrm{d}\mathbf{x}'_k J^{(k)}(\mathbf{x}_k, \mathbf{x}'_k)\, \gamma^{(k)}(\mathbf{x}_k, \mathbf{x}'_k) \,. \tag{4.26}$$

Lemma 4.1. *Fix $k \geq 1$ and $J^{(k)} \in W^{1,\infty}(\Lambda^k \times \Lambda^k)$. For $\beta > 0$ set $\delta_\beta(x) = (4\pi\beta^3/3)^{-1}\chi(|x| \leq \beta)$. Then we have*

$$\begin{aligned}
\langle J^{(k)}, \gamma_{N,t}^{(k)} \rangle = {} & \langle J^{(k)}, \gamma_{N,0}^{(k)} \rangle - i \sum_{j=1}^k \int_0^t \mathrm{d}s \int \mathrm{d}\mathbf{x}_k \mathrm{d}\mathbf{x}'_k J^{(k)}(\mathbf{x}_k, \mathbf{x}'_k)(-\Delta_{x_j} + \Delta_{x'_j})\gamma_{N,s}^{(k)}(\mathbf{x}_k, \mathbf{x}'_k) \\
& - ib \sum_{j=1}^k \int_0^t \mathrm{d}s \int \mathrm{d}\mathbf{x}_k \mathrm{d}\mathbf{x}'_k \mathrm{d}x_{k+1} J^{(k)}(\mathbf{x}_k, \mathbf{x}'_k)(\delta_\beta(x_j - x_{k+1}) - \delta_\beta(x'_j - x_{k+1})) \\
& \qquad \times \gamma_{N,s}^{(k+1)}(\mathbf{x}_k, x_{k+1}, \mathbf{x}'_k, x_{k+1}) \\
& + t \left(kO(\beta^{1/2}) + kO(a^{1/2}) + k^2 O\left(\frac{1}{Na^{1/2}}\right)\right) \sup_{s \in [0,t]} Tr|S_1 S_2 \gamma_{N,s}^{(2)} S_2 S_1| \,.
\end{aligned} \tag{4.27}$$

Proof. We start from the BBGKY Hierarchy (1.7). After multiplying with $J^{(k)} \in L^2(\Lambda^k \times \Lambda^k)$ we get

$$\langle J^{(k)}, \gamma^{(k)}_{N,t}\rangle = \langle J^{(k)}, \gamma^{(k)}_{N,0}\rangle - i\sum_{j=1}^k \int_0^t \mathrm{d}s \int \mathrm{d}\mathbf{x}_k \mathrm{d}\mathbf{x}'_k J^{(k)}(\mathbf{x}_k,\mathbf{x}'_k)(-\Delta_{x_j} + \Delta_{x'_j})\gamma^{(k)}_{N,s}(\mathbf{x}_k,\mathbf{x}'_k)$$
$$- \frac{i}{N}\sum_{j\neq \ell}^k \int_0^t \mathrm{d}s \int \mathrm{d}\mathbf{x}_k \mathrm{d}\mathbf{x}'_k\, J^{(k)}(\mathbf{x}_k,\mathbf{x}'_k)(V_a(x_j-x_\ell) - V_a(x'_j - x'_\ell))\gamma^{(k)}_{N,s}(\mathbf{x}_k,\mathbf{x}'_k)$$
$$- i(1-\frac{k}{N})\sum_{j=1}^k \int_0^t \mathrm{d}s \int \mathrm{d}\mathbf{x}_k \mathrm{d}\mathbf{x}'_k \mathrm{d}x_{k+1}\, J^{(k)}(\mathbf{x}_k,\mathbf{x}'_k)\,(V_a(x_j - x_{k+1}) - V_a(x'_j - x_{k+1}))$$
$$\times\, \gamma^{(k+1)}_{N,s}(\mathbf{x}_k, x_{k+1}, \mathbf{x}'_k, x_{k+1}). \tag{4.28}$$

Next we estimate

$$\begin{aligned}\Big|\int \mathrm{d}\mathbf{x}_k \mathrm{d}\mathbf{x}'_k\, J^{(k)}(\mathbf{x}_k,\mathbf{x}'_k) V_a(x_j - x_\ell)\gamma^{(k)}_{N,s}(\mathbf{x}_k,\mathbf{x}'_k)\Big| &= \Big|\mathrm{Tr} J^{(k)} V_a(x_j-x_\ell)\gamma^{(k)}_{N,s}\Big| \\ &\leq \|S_j^{-1} J^{(k)} S_j\|\, \|S_j^{-1} V_a(x_j - x_\ell) S_j^{-1} S_\ell^{-1}\|\, \|S_\ell^{-1}\|\, \mathrm{Tr} S_j S_\ell \gamma^{(k)}_{N,s} S_j S_\ell \\ &\leq C_k a^{-1/2}\, \mathrm{Tr}\, S_1 S_2 \gamma^{(2)}_{N,s} S_2 S_1\end{aligned} \tag{4.29}$$

where we used that, by Lemma A.1, $\|(V_a)^{1/2}(x_j-x_\ell)S_j^{-1}\| \leq C a^{-1/2}$, and $\|(V_a)^{1/2}(x_j - x_\ell)S_j^{-1}S_\ell^{-1}\| \leq C$. Moreover we used that $\|S_j^{-1}J^{(k)}S_j\| \leq \|J^{(k)}S_j\|$ and that

$$\|J^{(k)}S_j\|^2 \leq \|J^{(k)}S_j^2 (J^{(k)})^*\| \leq \mathrm{Tr}\, J^{(k)} S_j^2 (J^{(k)})^* = \int \mathrm{d}\mathbf{x}_k \mathrm{d}\mathbf{x}'_k\, \left(|J^{(k)}(\mathbf{x}_k,\mathbf{x}'_k)|^2 + |\nabla_j J^{(k)}(\mathbf{x}_k,\mathbf{x}'_k)|^2\right) \tag{4.30}$$

which is bounded, because of the finiteness of the volume, and because, by assumption $J^{(k)} \in W^{1,\infty}(\Lambda^k \times \Lambda^k)$.

In the same way we can bound the contribution arising from the term $V_a(x'_j - x'_\ell)$, and so we find

$$\Big|\frac{1}{N}\sum_{j\neq\ell}^k \int_0^t \mathrm{d}s \int \mathrm{d}\mathbf{x}_k \mathrm{d}\mathbf{x}'_k\, J^{(k)}(\mathbf{x}_k,\mathbf{x}'_k)(V_a(x_j - x_\ell) - V_a(x'_j - x'_\ell))\gamma^{(k)}_{N,s}(\mathbf{x}_k,\mathbf{x}'_k)\Big|$$
$$\leq \frac{C_k t}{N a^{1/2}} \sup_{s\in[0,t]} \mathrm{Tr}\, S_1 S_2 \gamma^{(2)}_{N,s} S_2 S_1\,. \tag{4.31}$$

Analogously we also get

$$
\begin{aligned}
&\Big|\frac{k}{N}\sum_{j=1}^{k}\int_0^t \mathrm{d}s \int \mathrm{d}\mathbf{x}_k \mathrm{d}\mathbf{x}_k' \mathrm{d}x_{k+1}\, J^{(k)}(\mathbf{x}_k,\mathbf{x}_k')\,(V_a(x_j-x_{k+1})-V_a(x_j'-x_{k+1}))\\
&\qquad\qquad \times \gamma_{N,s}^{(k+1)}(\mathbf{x}_k,x_{k+1},\mathbf{x}_k',x_{k+1})\Big|\\
&\qquad \le \frac{C_k t}{N}\|J^{(k)}\|\|S_{k+1}^{-1}V_a(x_j-x_{k+1})S_{k+1}^{-1}S_j^{-1}\|\|S_j^{-1}\| \sup_{s\in[0,t]} \operatorname{Tr} S_1S_2\gamma_{N,s}^{(2)}S_2S_1\\
&\qquad \le \frac{C_k t}{Na^{1/2}} \sup_{s\in[0,t]} \operatorname{Tr} S_1S_2\gamma_{N,s}^{(2)}S_2S_1\,.
\end{aligned}
\tag{4.32}
$$

Applying Lemma 4.2 twice (once with $\beta_2=a$ and once with $\beta_2=\beta$; in both cases with $\beta_1=0$), we have

$$
\begin{aligned}
\Big|\int \mathrm{d}\mathbf{x}_k \mathrm{d}\mathbf{x}_k'\, J^{(k)}(\mathbf{x}_k,\mathbf{x}_k')\,(V_a(x_j-x_{k+1})-b\delta_\beta(x_j-x_{k+1}))\,\gamma_{N,s}^{(k+1)}(\mathbf{x}_k,x_{k+1},\mathbf{x}_k',x_{k+1})\Big|&\\
\le C(a^{1/2}+\beta^{1/2})\operatorname{Tr} S_1S_2\gamma_{N,s}^{(2)}S_2S_1&
\end{aligned}
$$

for some constant C which only depends on $J^{(k)}$, but is independent of N, of β, and of $s\in[0,t]$. □

The following lemma is used to regularize the action of the δ-function. It was already used in the proof of Lemma 4.1. It will be used again to prove the convergence to the infinite BBGKY hierarchy. Its proof can be found in [4] (see Proposition 8.1).

Lemma 4.2. *Suppose $\delta_\beta(x)$ is a radially symmetric function, with $0\le\delta_\beta(x)\le C\beta^{-3}\chi(|x|\le\beta)$ and $\int\delta_\beta(x)\mathrm{d}x=1$ (for example $\delta_\beta(x)=\beta^{-3}h(x/\beta)$, for a radially symmetric probability density $h(x)$ supported in $\{x:|x|\le 1\}$). Then, for any $J^{(k)}\in W^{1,\infty}(\Lambda^k\times\Lambda^k)$ and for any smooth function $\gamma^{(k+1)}(\mathbf{x}_{k+1};\mathbf{x}_{k+1}')$ corresponding to a $(k+1)$-particle density matrix, we have, for any fixed $j\le k$,*

$$
\begin{aligned}
\Big|\int &\mathrm{d}\mathbf{x}_k\mathrm{d}\mathbf{x}_k'\mathrm{d}x_{k+1}\mathrm{d}x_{k+1}'\, J^{(k)}(\mathbf{x}_k;\mathbf{x}_k')\,\big(\delta_{\beta_1}(x_{k+1}'-x_{k+1})\delta_{\beta_2}(x_j-x_{k+1})-\delta(x_{k+1}'-x_{k+1})\delta(x_j-x_{k+1})\big)\\
&\times\gamma^{(k+1)}(\mathbf{x}_k,x_{k+1};\mathbf{x}_k',x_{k+1}')\Big|\\
&\qquad\le C[\,\|J\|_\infty+\|\nabla_j J\|_\infty\,]\,(\beta_1+\sqrt{\beta_2})\ \mathit{Tr}\,|S_jS_{k+1}\gamma^{(k+1)}S_jS_{k+1}|\,.
\end{aligned}
\tag{4.33}
$$

4.1 Compactness of the sequence $\Gamma_N(t)$

The aim of this section is to prove part i) of Theorem 2.1.

Proof of Theorem 2.1, part i). First of all we note that the sequence $\Gamma_{N,t} = \{\gamma^{(k)}_{N,t}\}_{k=1}^N$ is uniformly bounded in H_-. In fact, from $\gamma^{(k)}_{N,t} \geq 0$ and $\operatorname{Tr}\gamma^{(k)}_{N,t} = 1$ it follows immediately that

$$\|\Gamma_{N,t}\|_{H_-} = \sum_{k\geq 1} 2^{-k} \int \mathrm{d}\mathbf{x}_k \mathrm{d}\mathbf{x}'_k \, |\gamma^{(k)}_{N,t}(\mathbf{x}_k;\mathbf{x}'_k)|^2 \leq 1\,. \tag{4.34}$$

Next we prove that the sequence $\Gamma_{N,t}$ is equicontinuous in time with respect to the metric ρ (see (2.14)) defined on H_-. To check equicontinuity we use the following lemma, whose proof can be found in [4] (see Lemma 9.2).

Lemma 4.3. *The sequence $\Gamma_{N,t} = \{\gamma^{(k)}_{N,t}\}_{k=1}^N$, $N = 1, 2, \ldots$ satisfying (4.34) is equicontinuous on H_- with respect to the metric ρ if and only if for every fixed $k \geq 1$, for arbitrary $J^{(k)} \in W^{1,\infty}(\Lambda^k \times \Lambda^k)$ and for every $\varepsilon > 0$ there exists a $\delta > 0$ such that*

$$\left|\langle J^{(k)}, \gamma^{(k)}_{N,t} - \gamma^{(k)}_{N,s}\rangle\right| \leq \varepsilon \tag{4.35}$$

whenever $|t - s| \leq \delta$.

So, in order to prove that $\Gamma_{N,t}$ is equicontinuous, we choose $k \geq 1$, $J^{(k)} \in W^{1,\infty}(\Lambda^k \times \Lambda^k)$ and $\varepsilon > 0$. Then by Lemma 4.1, we have

$$\begin{aligned}
\left|\langle J^{(k)}, \gamma^{(k)}_{N,t} - \gamma^{(k)}_{N,s}\rangle\right| &\leq \sum_{j=1}^k \int_s^t \mathrm{d}\tau \left|\langle J^{(k)}, (-\Delta_{x_j} + \Delta_{x'_j})\gamma^{(k)}_{N,\tau}\rangle\right| \\
&+ b\sum_{j=1}^k \Big| \int_s^t \mathrm{d}\tau \int \mathrm{d}\mathbf{x}_k \mathrm{d}\mathbf{x}'_k \mathrm{d}x_{k+1} J^{(k)}(\mathbf{x}_k, \mathbf{x}'_k)(\delta_\beta(x_j - x_{k+1}) - \delta_\beta(x'_j - x_{k+1})) \\
&\qquad\qquad \times \gamma^{(k+1)}_{N,\tau}(\mathbf{x}_k, x_{k+1}, \mathbf{x}'_k, x_{k+1})\Big| \\
&+ |t-s| \left(kO(\beta^{1/2}) + kO(a^{1/2}) + k^2 O\left(\frac{1}{Na^{1/2}}\right)\right) \sup_{\tau\in[0,t]} \operatorname{Tr}|S_1 S_2 \gamma^{(2)}_{N,\tau} S_2 S_1|\,.
\end{aligned} \tag{4.36}$$

Next we note that

$$|\langle J^{(k)}, (-\Delta_{x_j} + \Delta_{x'_j})\gamma^{(k)}_{N,\tau}\rangle\Big| \leq 2\|S_j^{-1} J^{(k)} S_j\| \operatorname{Tr} S_j \gamma_{N,\tau} S_j \tag{4.37}$$

is uniformly bounded in N and in $\tau \in [s,t]$, because of Corollary 3.2 and of (4.30).

As for the term on the second line of (4.36) we note that, for fixed $\beta > 0$, it is bounded by

$$\begin{aligned}
b\sum_{j=1}^k \Big| \int_s^t \mathrm{d}\tau \int \mathrm{d}\mathbf{x}_k \mathrm{d}\mathbf{x}'_k \mathrm{d}x_{k+1} J^{(k)}(\mathbf{x}_k, \mathbf{x}'_k)(\delta_\beta(x_j - x_{k+1}) - \delta_\beta(x'_j - x_{k+1}))\gamma^{(k+1)}_{N,\tau}(\mathbf{x}_k, x_{k+1}, \mathbf{x}'_k, x_{k+1})\Big| \\
\leq C\beta^{-3} \sum_{j=1}^k \int_s^t \mathrm{d}\tau \, \|J^{(k)}\| \operatorname{Tr}\gamma^{(k+1)}_{N,\tau} \leq C_{\beta,k,J^{(k)}}|t-s|
\end{aligned} \tag{4.38}$$

where we used that $J^{(k)}$ is a bounded operator (this follows easily from the condition that its kernel lies in $W^{1,\infty}(\Lambda^k \times \Lambda^k)$, and from the finiteness of the volume), that the norm of δ_β is of order β^{-3}, and that the trace of $\gamma^{(k+1)}_{N,\tau}$ is one, for every τ and N. From the last three equations we find

$$\left|\langle J^{(k)}, \gamma^{(k)}_{N,t} - \gamma^{(k)}_{N,s}\rangle\right| \leq C\,|t-s| \tag{4.39}$$

for a constant C, depending on $\beta, k, J^{(k)}$, but independent of N, t, s. This implies, by Lemma 4.3 equicontinuity of $\Gamma_{N,t}$. The equicontinuity of $\Gamma_{N,t}$ then implies that $\Gamma_{N,t}$ is compact in $C([0,T], H_-)$ by the Arzela-Ascoli Theorem. □

4.2 A-priori bounds on $\Gamma_{\infty,t}$

The aim of this section is to prove part ii) of Theorem 2.1. To this end we define a new topology in the space of density matrices.

Denote by $\mathcal{L}^1(\mathcal{H})$ and by $\mathcal{K}(\mathcal{H})$ the space of trace class operators and, respectively, the space of compact operators on a Hilbert space $\mathcal{H}$. Moreover let $H_k = L^2(\Lambda^k)$. For a density matrix $\gamma^{(k)} \in \mathcal{L}^1(H_k)$, we define the norm

$$\|\gamma^{(k)}\|_{\mathcal{W}_k} = \mathrm{Tr}|S_1 \dots S_k\, \gamma^{(k)}\, S_1 \dots S_k| \tag{4.40}$$

where $S_j = (1-\Delta_j)^{1/2}$. We put

$$\mathcal{W}_k = \{\gamma^{(k)} \in \mathcal{L}^1(H_k) : \|\gamma^{(k)}\|_{\mathcal{W}_k} < \infty\}\,. \tag{4.41}$$

We consider moreover the space

$$\mathcal{A}^{(k)} = \{T^{(k)} = S_1 \dots S_k\, K^{(k)}\, S_1 \dots S_k : K^{(k)} \in \mathcal{K}(H_k)\} \tag{4.42}$$

equipped with the norm

$$\|T^{(k)}\|_{\mathcal{A}^{(k)}} = \|S_1^{-1} \dots S_k^{-1} T^{(k)} S_1^{-1} \dots S_k^{-1}\| \tag{4.43}$$

where $\|.\|$ denotes the operator norm. We have

$$(\mathcal{A}^{(k)}, \|.\|_{\mathcal{A}^{(k)}})^* = (\mathcal{W}_k, \|.\|_{\mathcal{W}_k}).$$

The identification of $\mathcal{W}_k$ as the dual space to $\mathcal{A}^{(k)}$ implies the existence of a weak star topology on $\mathcal{W}_k$.

Proof of part ii) of Theorem 2.1. Let $\Gamma_{\infty,t} = \{\gamma^{(k)}_{\infty,t}\}_{k\geq 1}$ be any limit point of $\Gamma_{N,t} = \{\gamma^{(k)}_{N,t}\}_{k=1}^N$ in the space $C([0,T], H_-)$ with respect to the metric $\widehat{\rho}$. By passing to a subsequence we can assume that $\Gamma_{N,t} \to \Gamma_{\infty,t}$, for $N \to \infty$, w.r.t. the metric $\widehat{\rho}$. This implies that, for every fixed $t \in [0,T]$ and for every $k \geq 1$, we have

$$\gamma^{(k)}_{N,t} \to \gamma^{(k)}_{\infty,t} \tag{4.44}$$

with respect to the weak topology of $L^2(\Lambda^k \times \Lambda^k)$. This follows because $\|\Gamma_{N,t}\|_{H_-} \leq 1$ and because in the unit ball, the metric ρ is equivalent to the weak$*$ topology of H_-. Convergence with respect to the weak$*$ topology of H_- implies then weak convergence in every k-particle sector $L^2(\Lambda^k \times \Lambda^k)$.

By Corollary 3.2, there exists a constant C such that

$$\|\gamma_{N,t}^{(k)}\|_{\mathcal{W}_k} = \mathrm{Tr} \left| S_1 \dots S_k \gamma_{N,t}^{(k)} S_k \dots S_1 \right| \leq C^k \tag{4.45}$$

for every $t \in [0,T]$ and $k \geq 1$. By the Banach-Alaoglu Theorem, the sequence $\gamma_{N,t}^{(k)}$ is compact in $\mathcal{W}_k$ with respect to the weak$*$ topology. In particular there exists a subsequence $N_j \to \infty$, and $\widetilde{\gamma}_{\infty,t}^{(k)} \in \mathcal{W}_k$ such that $\gamma_{N_j,t}^{(k)} \to \widetilde{\gamma}_{\infty,t}^{(k)}$ and

$$\|\widetilde{\gamma}_{\infty,t}^{(k)}\|_{\mathcal{W}_k} = \mathrm{Tr} \left| S_1 \dots S_k \widetilde{\gamma}_{\infty,t}^{(k)} S_k \dots S_1 \right| \leq C^k. \tag{4.46}$$

So, the sequence $\gamma_{N_j,t}^{(k)}$ satisfies, for $j \to \infty$,

$$\begin{aligned} &\gamma_{N_j,t}^{(k)} \to \gamma_{\infty,t}^{(k)} \quad \text{w.r.t. the weak topology of } L^2(\Lambda^k \times \Lambda^k) \quad \text{and} \\ &\gamma_{N_j,t}^{(k)} \to \widetilde{\gamma}_{\infty,t}^{(k)} \quad \text{w.r.t. the weak$*$ topology of } \mathcal{W}_k\,. \end{aligned} \tag{4.47}$$

If $J^{(k)} \in L^2(\Lambda^k \times \Lambda^k)$ then the operator with kernel given by $J^{(k)}$ (which will be still denoted by $J^{(k)}$) is Hilbert-Schmidt and thus compact: in particular $J^{(k)} \in \mathcal{A}_k$. Thus, using (4.47), it is easy to verify that

$$\int \mathrm{d}\mathbf{x}_k \mathrm{d}\mathbf{x}'_k\, J^{(k)}(\mathbf{x}_k, \mathbf{x}'_k) \gamma_{\infty,t}^{(k)}(\mathbf{x}_k, \mathbf{x}'_k) = \int \mathrm{d}\mathbf{x}_k \mathrm{d}\mathbf{x}'_k\, J^{(k)}(\mathbf{x}_k, \mathbf{x}'_k) \widetilde{\gamma}_{\infty,t}^{(k)}(\mathbf{x}_k, \mathbf{x}'_k) \tag{4.48}$$

for every $J^{(k)} \in L^2(\Lambda^k \times \Lambda^k)$. This implies that $\gamma_{\infty,t}^{(k)} = \widetilde{\gamma}_{\infty,t}^{(k)}$ as elements of $L^2(\Lambda^k \times \Lambda^k)$. Thus, from (4.46), we have

$$\mathrm{Tr} \left| S_1 \dots S_k \gamma_{\infty,t}^{(k)} S_k \dots S_1 \right| \leq C^k \tag{4.49}$$

for every $t \in [0,T]$ and $k \geq 1$. More precisely one should say that there is a version of $\gamma_{\infty,t}^{(k)} \in L^2(\Lambda^k \times \Lambda^k)$ which satisfies this bound (the version we are using here is exactly the density matrix $\widetilde{\gamma}_{\infty,t}^{(k)}$). $\square$

4.3 Non-triviality of the limit points

Proof of part iii) of Theorem 2.1. Suppose $\Gamma_{\infty,t} = \{\gamma_{\infty,t}^{(k)}\}_{k\geq 1}$ is a limit point of $\Gamma_{N,t}$ in the space $C([0,T], H_-)$ with respect to the metric $\widehat{\rho}$. From Section 4.2, we know that, for every fixed $t \in [0,T]$ and $k \geq 1$, $\gamma_{\infty,t}^{(k)} \in \mathcal{W}_k$ (more precisely there is a version of $\gamma_{\infty,t}^{(k)}$ lying in the space $\mathcal{W}_k$), and that there is a subsequence $N_j \to \infty$ with $\gamma^{(k)}_{N_j,t} \to \gamma^{(k)}_{\infty,t}$ w.r.t. the weak$*$ topology of $\mathcal{W}_k$. This means that

$$\mathrm{Tr}\, J^{(k)} \left(\gamma^{(k)}_{N_j,t} - \gamma^{(k)}_{\infty,t} \right) \to 0 \tag{4.50}$$

for $j \to \infty$, and for every $J^{(k)} \in \mathcal{A}_k$ (recall that $J^{(k)} \in \mathcal{A}_k$ if and only if $S_1^{-1} \dots S_k^{-1} J^{(k)} S_k^{-1} \dots S_1^{-1}$ is compact as operator on $L^2(\Lambda^k)$). Next we note that, because of the finiteness of the volume of Λ, the identity operator is an element of $\mathcal{A}_k$ (since $S_1^{-2} \dots S_k^{-2}$ is a compact operator on $L^2(\Lambda^k)$), and thus

$$\mathrm{Tr}\, \gamma^{(k)}_{\infty,t} = \lim_{j\to\infty} \mathrm{Tr}\, \gamma^{(k)}_{N_j,t} = 1 \tag{4.51}$$

because $\mathrm{Tr}\gamma^{(k)}_{N,t} = 1$ for every N, t, k. □

4.4 Convergence to the infinite BBGKY Hierarchy

In this section we prove the last two parts of Theorem 2.1.

Proof of part iv) of Theorem 2.1. Eq. (2.18) follows from part ii) of Theorem 2.1 and from Lemma 4.2, by the following simple argument. From Lemma 4.2 we find

$$\begin{aligned} \Big| \int & \mathrm{d}\mathbf{x}_k \mathrm{d}\mathbf{x}'_k \mathrm{d}x_{k+1} \mathrm{d}x'_{k+1}\, J^{(k)}(\mathbf{x}_k;\mathbf{x}'_k)\, \gamma^{(k+1)}_{\infty,t}(\mathbf{x}_k, x_{k+1}; \mathbf{x}'_k, x'_{k+1}) \\ & \times \big(\delta_{r_1}(x'_{k+1} - x_{k+1}) \delta_{r'_1}(x_j - x_{k+1}) - \delta_{r_2}(x'_{k+1} - x_{k+1}) \delta_{r'_2}(x_j - x_{k+1}) \big) \Big| \\ & \leq C \big[\|J\|_\infty + \|\nabla_j J\|_\infty \big] \left(r_1 + r_2 + \sqrt{r'_1} + \sqrt{r'_2} \right) \mathrm{Tr}\, |S_j S_{k+1} \gamma^{(k+1)}_{\infty,t} S_j S_{k+1}| \,. \end{aligned} \tag{4.52}$$

This implies, by (2.16), that the sequence

$$\begin{aligned} \int \mathrm{d}\mathbf{x}_k \mathrm{d}\mathbf{x}'_k \mathrm{d}x_{k+1} \mathrm{d}x'_{k+1}\, J^{(k)}(\mathbf{x}_k;\mathbf{x}'_k)\, \delta_r(x'_{k+1} - x_{k+1}) \delta_{r'}(x_j - x_{k+1}) \\ \times\, \gamma^{(k+1)}_{\infty,t}(\mathbf{x}_k, x_{k+1}; \mathbf{x}'_k, x'_{k+1}) \end{aligned} \tag{4.53}$$

has the Cauchy property for $r, r' \to 0$ and thus converges, if $J^{(k)} \in W^{1,\infty}(\Lambda^k \times \Lambda^k)$. □

Proof of part v) of Theorem 2.1. From Lemma 4.1 we find, for an arbitrary $J^{(k)} \in W^{1,\infty}(\Lambda^k \times \Lambda^k)$, and for N large enough,

$$\begin{aligned} \langle J^{(k)}, \gamma^{(k)}_{N,t} \rangle = \langle J^{(k)}, \gamma^{(k)}_{N,0} \rangle - i \sum_{j=1}^k \int_0^t \mathrm{d}s \int \mathrm{d}\mathbf{x}_k \mathrm{d}\mathbf{x}'_k J^{(k)}(\mathbf{x}_k, \mathbf{x}'_k)(-\Delta_{x_j} + \Delta_{x'_j}) \gamma^{(k)}_{N,s}(\mathbf{x}_k, \mathbf{x}'_k) \\ - ib \sum_{j=1}^k \int_0^t \mathrm{d}s \int \mathrm{d}\mathbf{x}_k \mathrm{d}\mathbf{x}'_k \mathrm{d}x_{k+1} J^{(k)}(\mathbf{x}_k, \mathbf{x}'_k)(\delta_\beta(x_j - x_{k+1}) - \delta_\beta(x'_j - x_{k+1})) \\ \times \gamma^{(k+1)}_{N,s}(\mathbf{x}_k, x_{k+1}, \mathbf{x}'_k, x_{k+1}) \\ + tO(\beta^{1/2}) + to(1) \end{aligned} \tag{4.54}$$

where $o(1) \to 0$ for $N \to \infty$. By passing to a subsequence we can assume that $\Gamma_{N,t} \to \Gamma_{\infty,t} = \{\gamma^{(k)}_{\infty,t}\}_{k \geq 1} \in C([0,T], H_-)$ w.r.t. the metric $\widehat{\rho}$. Since $\|\Gamma_{N,t}\|_{H_-} \leq 1$, and since the metric ρ on the unit ball of H_- is equivalent to the weak$*$ topology, it follows that $\gamma^{(k)}_{N,t} \to \gamma^{(k)}_{\infty,t}$ w.r.t. the weak topology of $L^2(\Lambda^k \times \Lambda^k)$, for every fixed $k \geq 1$ and $t \in [0,T]$. For $J^{(k)} \in W^{2,\infty}(\Lambda^k \times \Lambda^k)$, we also have $J^{(k)} \in L^2(\Lambda^k \times \Lambda^k)$ (because of the finiteness of the volume). Hence

$$\langle J^{(k)}, \gamma^{(k)}_{N,t} - \gamma^{(k)}_{\infty,t} \rangle \to 0 \quad \text{and} \quad \langle J^{(k)}, \gamma^{(k)}_{N,0} - \gamma^{(k)}_{\infty,0} \rangle \to 0 \tag{4.55}$$

for $N \to \infty$.

As for the second term on the r.h.s. of (4.54) we note that, from $J^{(k)} \in W^{2,\infty}(\Lambda^k \times \Lambda^k)$, it also follows that $\Delta_{x_j} J^{(k)}(\mathbf{x}_k; \mathbf{x}'_k)$ and $\Delta_{x'_j} J^{(k)}(\mathbf{x}_k; \mathbf{x}'_k)$ are elements of $L^2(\Lambda^k \times \Lambda^k)$. This implies that

$$\sum_{j=1}^k \int \mathrm{d}\mathbf{x}_k \mathrm{d}\mathbf{x}'_k \, \Delta_j J^{(k)}(\mathbf{x}_k; \mathbf{x}'_k) \left(\gamma^{(k)}_{N,s}(\mathbf{x}_k; \mathbf{x}'_k) - \gamma^{(k)}_{\infty,s}(\mathbf{x}_k; \mathbf{x}'_k) \right) \to 0 \tag{4.56}$$

for $N \to \infty$, and for every $s \in [0,t]$. By Lebesgue Theorem on the dominated convergence, we find

$$\sum_{j=1}^k \int_0^t \mathrm{d}s \int \mathrm{d}\mathbf{x}_k \mathrm{d}\mathbf{x}'_k J^{(k)}(\mathbf{x}_k; \mathbf{x}'_k)(-\Delta_{x_j} + \Delta_{x'_j}) \left(\gamma^{(k)}_{N,s}(\mathbf{x}_k; \mathbf{x}'_k) - \gamma^{(k)}_{\infty,s}(\mathbf{x}_k; \mathbf{x}'_k) \right) \to 0 \tag{4.57}$$

for $N \to \infty$ and for every fixed $t \in [0,T]$.

Finally we consider the limit $N \to \infty$ of the last term on the r.h.s. of (4.54). From Lemma 4.2, we have

$$\begin{aligned} \int \mathrm{d}\mathbf{x}_k \mathrm{d}\mathbf{x}'_k \mathrm{d}x_{k+1} \, J^{(k)}(\mathbf{x}_k; \mathbf{x}'_k) \left(\delta_\beta(x_j - x_{k+1}) - \delta_\beta(x'_j - x_{k+1}) \right) \gamma^{(k+1)}_{N,s}(\mathbf{x}_k, x_{k+1}; \mathbf{x}'_k, x_{k+1}) \\ = \int \mathrm{d}\mathbf{x}_k \mathrm{d}\mathbf{x}'_k \mathrm{d}x_{k+1} \mathrm{d}x'_{k+1} \, J^{(k)}(\mathbf{x}_k; \mathbf{x}'_k) \left(\delta_\beta(x_j - x_{k+1}) - \delta_\beta(x'_j - x_{k+1}) \right) \\ \times \delta_\eta(x_{k+1} - x'_{k+1}) \gamma^{(k+1)}_{N,s}(\mathbf{x}_k, x_{k+1}; \mathbf{x}'_k, x'_{k+1}) + O(\eta) \end{aligned} \tag{4.58}$$

where $O(\eta)$ is independent of β, N and s. At this point we can take the limit $N \to \infty$ with fixed β and η. Since $J^{(k)} \in W^{2,\infty}(\Lambda^k \times \Lambda^k)$, it is easy to check that, for fixed $\beta, \eta > 0$, $J^{(k)}(\mathbf{x}_k; \mathbf{x}'_k)\delta_\beta(x_j - x_{k+1})\delta_\eta(x_{k+1} - x'_{k+1})$ is an element of $L^2(\Lambda^{k+1} \times \Lambda^{k+1})$. Hence

$$\begin{aligned} \int \mathrm{d}\mathbf{x}_k \mathrm{d}\mathbf{x}'_k \mathrm{d}x_{k+1} \mathrm{d}x'_{k+1} \, J^{(k)}(\mathbf{x}_k; \mathbf{x}'_k) \left(\delta_\beta(x_j - x_{k+1}) - \delta_\beta(x'_j - x_{k+1}) \right) \delta_\eta(x_{k+1} - x'_{k+1}) \\ \times \left(\gamma^{(k+1)}_{N,s}(\mathbf{x}_k, x_{k+1}; \mathbf{x}'_k, x'_{k+1}) - \gamma^{(k+1)}_{\infty,s}(\mathbf{x}_k, x_{k+1}; \mathbf{x}'_k, x'_{k+1}) \right) \to 0 \end{aligned} \tag{4.59}$$

for $N \to \infty$, uniformly in s. Using (4.55), (4.57), and (4.59), it follows from (4.54), that

$$\begin{aligned} \langle J^{(k)}, \gamma^{(k)}_{\infty,t} \rangle = \langle J^{(k)}, \gamma^{(k)}_{\infty,0} \rangle - i \sum_{j=1}^k \int_0^t \mathrm{d}s \int \mathrm{d}\mathbf{x}_k \mathrm{d}\mathbf{x}'_k \, J^{(k)}(\mathbf{x}_k; \mathbf{x}'_k) \, (-\Delta_j + \Delta'_j) \gamma^{(k)}_{\infty,s}(\mathbf{x}_k; \mathbf{x}'_k) \\ - ib \sum_{j=1}^k \int_0^t \mathrm{d}s \int \mathrm{d}\mathbf{x}_k \mathrm{d}\mathbf{x}'_k \mathrm{d}x_{k+1} \mathrm{d}x'_{k+1} \, J^{(k)}(\mathbf{x}_k; \mathbf{x}'_k) (\delta_\beta(x_j - x_{k+1}) - \delta_\beta(x'_j - x_{k+1})) \\ \times \delta_\eta(x_{k+1} - x'_{k+1}) \gamma^{(k+1)}_{\infty,s}(\mathbf{x}_k, x_{k+1}; \mathbf{x}'_k, x'_{k+1}) + O(\beta^{1/2}) + O(\eta) \end{aligned} \tag{4.60}$$

for any fixed t and k. Finally, we apply Lemma 4.2 to replace $\delta_\eta(x_{k+1} - x'_{k+1})$ by $\delta(x_{k+1} - x'_{k+1})$ and $\delta_\beta(x_j - x_{k+1})$ (respectively, $\delta_\beta(x'_j - x_{k+1})$) by $\delta(x_j - x_{k+1})$ (respectively, by $\delta(x'_j - x_{k+1})$). The error here is of order $\beta^{1/2} + \eta$. Hence, letting $\eta \to 0$ and $\beta \to 0$ we find

$$\begin{aligned} \langle J^{(k)}, \gamma^{(k)}_{\infty,t} \rangle = \langle J^{(k)}, \gamma^{(k)}_{\infty,0} \rangle - i \sum_{j=1}^k \int_0^t \mathrm{d}s \int \mathrm{d}\mathbf{x}_k \mathrm{d}\mathbf{x}'_k \, J^{(k)}(\mathbf{x}_k; \mathbf{x}'_k) \, (-\Delta_j + \Delta'_j) \gamma^{(k)}_{\infty,s}(\mathbf{x}_k; \mathbf{x}'_k) \\ - ib \sum_{j=1}^k \int_0^t \mathrm{d}s \int \mathrm{d}\mathbf{x}_k \mathrm{d}\mathbf{x}'_k \mathrm{d}x_{k+1} \, J^{(k)}(\mathbf{x}_k; \mathbf{x}'_k) (\delta(x_j - x_{k+1}) - \delta(x'_j - x_{k+1})) \\ \times \gamma^{(k+1)}_{\infty,s}(x_1, \dots, x_{k+1}; x'_1, \dots, x'_k, x_{k+1}) \, . \end{aligned} \tag{4.61}$$

□

A Sobolev Type Inequalities

Lemma A.1. *i) Suppose $V \in L^{3/2}(\Lambda)$, and $\psi \in W^{1,2}(\Lambda)$. Then*

$$\int \mathrm{d}x |\psi(x)|^2 \frac{1}{a^2} V(x/a) \le C \|V\|_{L^{3/2}(\Lambda)} \left(\|\nabla \psi\|^2 + \|\psi\|^2 \right)^{1/2} \, . \tag{A.62}$$

ii) Suppose $V \in L^1(\Lambda)$. Then, considering $V(x-y)$ as an operator on $L^2(\Lambda, \mathrm{d}y) \otimes L^2(\Lambda, \mathrm{d}x)$ we have the operator inequality

$$\frac{1}{a^3} V\left(\frac{x-y}{a}\right) \leq C\|V\|_{L^1} (1-\Delta_x)(1-\Delta_y)\,. \tag{A.63}$$

Proof. The proof of i) can be found in [4]. The proof of ii) is in [3]. □

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