TOWARDS A RIGOROUS DERIVATION OF THE CUBIC NLSE IN DIMENSION ONE

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ABSTRACT. We consider a system of N particles in dimension one, interacting through a zero-range repulsive potential whose strength is proportional to N^{-1}. We construct the finite and the infinite Schrödinger hierarchies for the reduced density matrices of subsystems with n particles. We show that the solution of the finite hierarchy converges in a suitable sense to a solution of the infinite one. Besides, the infinite hierarchy is solved by a factorized state, built as a tensor product of many identical one-particle wave functions which fulfil the cubic nonlinear Schrödinger equation. Therefore, choosing a factorized initial datum and assuming propagation of chaos, we provide a derivation for the cubic NLSE. The result, achieved with operator-analysis techniques, can be considered as a first step towards a rigorous deduction of the Gross-Pitaevskii equation in dimension one. The problem of proving propagation of chaos is left untouched.

1. Introduction

The study of the nonlinear Schrödinger equation with a cubic nonlinearity (CNLSE) has received a considerable attention in the mathematical literature due to its relevance in applications in many fields of physics (see [C], [SS], and references therein).

In particular CNLSE in dimension two and three is widely used in quantum physics as an effective one-particle equation for the analysis of the Bose-Einstein condensation phenomenon, which is a relevant quantum effect produced by bosons at low temperature ([DGPS] and references therein).

For the sake of precision, we mention that in order to describe the ground state of a Bose-Einstein condensate, CNLSE should be supplied with an external potential term, whose rôle lies in the confinement of the system to some bounded spatial region.

At least at a formal level it is generally believed that the dynamics of a system of N identical bosons interacting via a short range two-body potential V factorizes for $N \to \infty$. Moreover, in that limit, the potential felt at each point x by a particle is proportional to the probability to find the particle at the position x. The limit dynamics of each particle is then described by a nonlinear Schrödinger equation with an effective nonlinear potential of the form $\alpha|\psi(t,x)|^2$, where ψ is the wave function of the particle itself and $\alpha > 0$ is a physical parameter associated to the two-body potential V.

Still, a rigorous derivation of the nonlinear equation starting from the N-particle dynamics in the short-range scaling limit has been approached only recently.

In particular, in [LSSY] interesting and detailed results have been obtained for the stationary, i.e. for the time-independent, case.

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Here we consider the problem of the derivation of the time-dependent evolution equation and we give some partial results in a simple one dimensional case, which can be considered as a version of the model introduced in [LL] with a scaled potential.

More precisely, we analyse a system of N identical bosons in dimension one interacting via a two-body δ-function potential, i.e. a point interaction, of strength αN^{-1}, with $\alpha > 0$.

Our techniques are inspired to those employed in [BGM] (see also [S], [BEGMY] and [EY]) for the analysis of the problem of the mean field limit. In particular in [BGM] a three-dimensional system has been investigated consisting of N particles that interact via a possibly singular potential V, rescaled as $\frac{V}{N}$ (which is called the mean-field or weak-coupling scaling).

As a result, it has been found that in the limit $N \to \infty$ the dynamics is factorized and the one-particle wave function representing the state of any single particle is given by the solution of the Hartree equation, namely the Schrödinger equation with a non-local nonlinearity of the type $V * |\psi(t)|^2$.

We want to stress that in order to model physical systems like Bose-Einstein condensates, we have to consider a different kind of scaling limit, namely the short-range one. It is due to the introduction of the delta interactions, that our scaling translates to a kind of mean-field one, as one can see with the following argument.

For a generic two-body potential V in dimension one the short-range scaling is $V_N(x) = V(Nx)$; taking into account that, for large N, $NV(Nx)$ approaches $\alpha\delta(x)$, where $\alpha = \int dx V(x)$ (see e.g. [AGH-KH]), we replace $V_N(x)$ by its asymptotic limit $\alpha N^{-1}\delta(x)$, which is easier to handle.

In this perspective, the choice of the point interaction has the only meaning to simplify the analysis of the limit $N \to \infty$.

The techniques used in [BGM] refer to the "method of the hierarchy", which consists in considering the reduced density matrices $\hat{\rho}_{N,n}(t)$ associated to the subsystems of n particles ($1 \le n \le N$). Such density matrices can in principle be computed at any time from the wave function of the entire system $\Psi_N(t)$; alternatively, they can be regarded as the solutions of a system of N evolution equations, called the finite Schrödinger hierarchy.
The limit for $N \to \infty$ leads to consider an infinite hierarchy, called the infinite Schrödinger hierarchy.

It is easily seen that a solution of the infinite hierarchy considered in [BGM] is given by the sequence of density matrices $\hat{\rho}_n(t)$, $n \in \mathbb{N}^*$, where $\hat{\rho}_n(t)$ describes the evolution of n independent particles satisfying the Hartree equation. In other words, the infinite hierarchy is solved by the factorized state consisting of the product of single particle wave functions which follow a nonlinear evolution equation.
In [BGM] the convergence of the solution of the finite hierarchy to the factorized solution of the infinite one is proved in two steps:

(1) The sequence of the solutions of the finite hierarchy converges (in the sense of distributions) to a solution of the infinite hierarchy.
(2) The infinite hierarchy has a unique solution.

For the N-particles system considered here, we shall give a proof of the first step. Notice that if one assumes the validity of the second step, one obtains a limit dynamics governed by the Schrödinger equation with a nonlinearity of the type $\alpha\delta * |\psi(t)|^2$, i.e. the CNLSE

$$i\hbar\partial_t\psi(t,x) = -\frac{\hbar^2}{2m}\Delta\psi(t,x) + \alpha|\psi(t,x)|^2\psi(t,x) \tag{1.1}$$

The question of the uniqueness of the solution of the infinite hierarchy, i.e. the second step, is left untouched here. We only observe that the proof cannot be obtained by a straightforward application of the strategy used for the standard mean-field problem. We plan to come back to this question in a further work.

We preliminarily fix some notation.
We shall denote by N the number of particles in the whole system. The configuration of the system will be indicated by the vector $X_N \in \mathbb{R}^N$, $X_N = (x_1, ..., x_N)$, $x_j \in \mathbb{R}$.
It will be useful to introduce the vector of the positions of the "last $N-n$ particles": $X_N^{n+1} \in \mathbb{R}^{N-n}$, $X_N^{n+1} = (x_{n+1}, ..., x_N)$ and the "traced" vector of positions $X_N^{ij} \in \mathbb{R}^N$, $X_N^{ij} = X_N + (x_i - x_j)\mathbf{e}_{j,N}$, where $\mathbf{e}_{j,N}$ is in $\mathbb{R}^N$ and its k^{th} coordinate $[\mathbf{e}_{j,N}]^k$ equals δ_{jk}. In the sequel we shall also make use of the following $N-1$ dimensional measure of integration: $dX_N^j = dx_1...dx_{j-1}dx_{j+1}...dx_N$, for any $j > 1$. In general we shall denote an operator by a hat in order to distinguish it from its integral kernel.
We shall denote by $\tilde{f}$ the Fourier transform of f, defined as follows

$$\tilde{f}(\Xi_N) = \int_{\mathbb{R}^N} dX_N\, f(X_N)\, e^{iX_N\Xi_N} \tag{1.2}$$

The so-called trace with respect to degrees of freedom from the $k+1^{\text{th}}$ to the N^{th} will be denoted by the symbol $\mathrm{Tr}_{[k+1,N]}$. Namely, if $\hat{f}$ is the operator represented by the integral kernel $f(X_N; Y_N)$, then the operator $\mathrm{Tr}_{[k+1,N]}\hat{f}$ is represented by the integral kernel

$$g(X_k, Y_k) = \int_{\mathbb{R}^{N-k}} dZ_N^{k+1} f(X_k, Z_N^{k+1}; Y_k, Z_N^{k+1}) \tag{1.3}$$

With the symbols $\mathcal{L}_1(X)$ and $\mathcal{L}_2(X)$ we shall denote respectively the space of the trace class operators and the space of the Hilbert-Schmidt operators on the Hilbert space X.

The sequel of the paper is organized as follows.
In section 2 we shall state the problem and explictly write the finite and infinite Schrödinger hierarchies.
In section 3 we will exploit the conservation of the energy in order to prove some estimates on the derivatives of $\rho_{N,n}(t)$; we will also introduce the operator spaces in which we shall work.
In section 4 we will prove the convergence of $\rho_{N,n}(t)$ to a solution $\rho_n(t)$ of the infinite hierarchy.

2. The finite and infinite Schrödinger hierarchies

Let us recall some basic tools about the formalism of the density matrix.
For a system with N degrees of freedom being in the state represented by the normalized wave function $\Psi_N(t)$, the density matrix $\hat{\rho}_N(t)$ is the orthogonal projection on the linear space spanned by $\Psi_N(t)$, namely an integral operator whose kernel $\rho_N(t)$ reads

$$\rho_N(t; X_N; Y_N) = \Psi_N(t; X_N)\overline{\Psi_N(t; Y_N)} \tag{2.1}$$

The time evolution of the density matrix is given by the von Neumann equation

$$i\hbar\partial_t\hat{\rho}_N(t) = [H_N, \hat{\rho}_N(t)] \tag{2.2}$$

where H_N is the hamiltonian operator of the system.

For the integral kernel representing the density matrix, equation (2.2) implies the following evolution of the Schrödinger type

$$i\hbar\partial_t\rho_N(t; X_N; Y_N) = \mathcal{H}_N\rho_N(t; X_N; Y_N) \tag{2.3}$$

where we defined $\mathcal{H}_N$ as the self-adjoint operator on $L^2(\mathbb{R}^{2N})$

$$\mathcal{H}_N \equiv H_N \otimes \mathbb{I} - \mathbb{I} \otimes H_N \tag{2.4}$$

Here the factors in the tensor products are intended to act on the space of the variable X_N and on the space of the variable Y_N respectively. The symbol $\mathbb{I}$ denotes the identity operator.

In our problem, the hamiltonian for the N-particles system is given by

$$H_N \equiv -\frac{\hbar^2}{2m}\Delta_{X_N} + \frac{\alpha}{N}\sum_{1\leq i<j\leq N}\delta(x_j - x_j) \tag{2.5}$$

where $\Delta_{X_N} = \sum_{j=1}^N \partial^2_{x_j}$.
¿From the theory of point interactions (see e.g.[AGH-KH], [LL]), we know that such a hamiltonian can be defined as a self-adjoint operator on $L^2(\mathbb{R}^N)$. Therefore, owing to Stone's theorem, the Cauchy problem

$$\begin{aligned} i\hbar\partial_t\Psi_N(t, X_N) &= -\frac{\hbar^2}{2m}\Delta_{X_N}\Psi_N(t, X_N) + \frac{\alpha}{N}\sum_{1\leq i<j\leq N}\delta(x_i - x_j)\Psi_N(t, X_N) \\ \Psi_N(0, X_N) &= \Psi_N^I(X_N) \end{aligned} \tag{2.6}$$

has a unique, global, square integrable, weak solution for any $\Psi_N^I \in L^2(\mathbb{R}^N)$. Moreover, the solution is strong if Ψ_N^I belongs to the domain of H_N, whilst it is mild if Ψ_N^I lies in the form domain of H_N. In fact, this form domain coincides with $H^1(\mathbb{R}^N)$, due to the smallness of the δ potential in the sense of quadratic form ([RS2], sec. X.3).
We also know that the L^2 norm of the solution is preserved by time evolution. Besides, due to the time invariance of the system, the energy

$$E_N(\Psi(t)) = \frac{\hbar^2}{2m}\|\nabla_N\Psi(t)\|^2_{L^2(\mathbb{R}^N;\mathbb{C}^N)} + \frac{\alpha}{N}\sum_{1\leq i<j\leq N}\int_{\mathbb{R}^{N-1}} dX_N^j\,|\Psi(t, X_N^{ij})|^2 \tag{2.7}$$

is conserved.

Since we are dealing with a system of bosons, we will choose a symmetrized initial datum, namely a Ψ_N^I such that

$$\Psi_N^I(x_{\sigma(1)}, ..., x_{\sigma(N)}) = \Psi_N^I(x_1, ..., x_N) \tag{2.8}$$

for any permutation σ of the indices $1, ..., N$. In particular Ψ_N^I is symmetric under exchanges of pair of particles. This feature is also known as undistinguishability of particles and is preserved by time evolution.

Factorized states, namely wave functions of the type

$$\Psi_N^I(X_N) = \prod_{j=1}^{N} \psi^I(x_j) \tag{2.9}$$

are a particular case of symmetric states; in general, property of factorization is not preserved by time evolution, while symmetrization is.

The initial states we shall consider are normalized in $L^2(\mathbb{R}^N)$

$$\|\Psi_N^I\|_{L^2(\mathbb{R}^N)} = 1 \tag{2.10}$$

Let us formulate the problem for the integral kernel of the density matrix. Equation (2.3) gives

$$\begin{aligned} i\hbar\partial_t \rho_N(t; X_N; Y_N) = &-\frac{\hbar^2}{2m}(\Delta_{X_N} - \Delta_{Y_N})\rho_N(t; X_N; Y_N) \\ &+ \frac{\alpha}{N} \sum_{1 \le i < j \le N} [\delta(x_i - x_j) - \delta(y_i - y_j)]\rho_N(t; X_N; Y_N) \end{aligned} \tag{2.11}$$

The subsystem of the first n particles is described by the "reduced density matrix", which is also a positive trace class operator. Its integral kernel reads

$$\rho_{N,n}(t; X_n; Y_n) = \int_{\mathbb{R}^{N-n}} dZ_N^{n+1}\, \rho_N(t; X_n, Z_N^{n+1}; Y_n, Z_N^{n+1}) \tag{2.12}$$

It is easily seen that $\|\hat{\rho}_{N,n}(t)\|_{\mathcal{L}_1(L^2(\mathbb{R}^n))} = 1$ at any time t, $\|\hat{\rho}_{N,n}(t)\|_{\mathcal{L}_2(L^2(\mathbb{R}^n))} \le 1$ and equality holds if and only if $\hat{\rho}_{N,n}(t)$ is a projection on a one-dimensional space (namely if it represents a pure state).

By (2.3) one has that the integral kernel in (2.12) solves the following finite Schrödinger hierarchy

$$\begin{aligned} i\hbar\partial_t \rho_{N,n}(t; X_n; Y_n) = &-\frac{\hbar^2}{2m}(\Delta_{X_n} - \Delta_{Y_n})\rho_{N,n}(t; X_n; Y_n) \\ &+ \frac{\alpha}{N} \sum_{1 \le i < j \le n} [\delta(x_i - x_j) - \delta(y_i - y_j)]\rho_{N,n}(t; X_n; Y_n) \\ &+ \alpha \frac{N-n}{N} \sum_{1 \le i \le n} [\rho_{N,n+1}(t; X_n, x_i; Y_n, x_i) - \rho_{N,n+1}(t; X_n, y_i; Y_n, y_i)] \end{aligned} \tag{2.13}$$

The infinite Schrödinger hierarchy is obtained from the finite one as a formal limit for $N \to \infty$

$$\begin{aligned} i\hbar\partial_t \rho_n(t; X_n; Y_n) = &-\frac{\hbar^2}{2m}(\Delta_{X_n} - \Delta_{Y_n})\rho_n(t; X_n; Y_n) \\ &+ \alpha \sum_{1 \le i \le n} [\rho_{n+1}(t; X_n, x_i; Y_n, x_i) - \rho_{n+1}(t; X_n, y_i; Y_n, y_i)] \end{aligned} \tag{2.14}$$

It is easily verified that the family of factorized density matrices

$$\rho_n(t; X_n; Y_n) = \prod_{j=1}^{n} \psi(t, x_j)\overline{\psi(t, y_j)} \;\; n \in \mathbb{N}^* \tag{2.15}$$

solves the infinite hierarchy (2.14) if and only if ψ solves CNLSE (1.1).

It is our aim to show that the limit from the finite to the infinite hierarchy is valid in the sense that the solution of (2.13) converges to a solution of (2.14).

In the following sections we will give a rigorous meaning to this statement.

3. Some regularity estimates for the reduced density matrix

Conservation of energy (2.7) gives a basic estimate on the derivates of the wave function $\Psi_N(t)$, as shown by the following proposition.

Proposition 3.1. *If the intial datum $\Psi_N^I \in H^1(\mathbb{R}^N)$ is symmetrized like in (2.8), then the solution $\Psi_N(t)$ to problem (2.6) satisfies the inequality*

$$\sup_{1\le j\le N} \int_{\mathbb{R}^N} dX_N \, |\partial_j \Psi_N(t, X_N)|^2 \le \frac{2m}{\hbar^2 N} E_N(\Psi_N^I) \tag{3.1}$$

Proof. ¿From conservation of energy the following inequality holds

$$\|\nabla_N \Psi_N(t)\|^2_{L^2(\mathbb{R}^N;\mathbb{C}^N)} \le \frac{2m}{\hbar^2} E_N(\Psi_N(t)) = \frac{2m}{\hbar^2} E_N(\Psi_N^I) \tag{3.2}$$

Moreover, by undistinguishability of particles (2.8)

$$\|\nabla_N \Psi_N(t)\|^2_{L^2(\mathbb{R}^N;\mathbb{C}^N)} = N \|\partial_l \Psi_N(t)\|^2_{L^2(\mathbb{R}^N)} \tag{3.3}$$

¿From (3.3) and (3.2) we conclude

$$\|\partial_l \Psi_N(t)\|_{L^2(\mathbb{R}^N)} \le \frac{2m}{\hbar^2 N} E_N(\Psi_N^I) \tag{3.4}$$

for any $l \in \{1, ..., N\}$. □

Remark 3.2. Let us stress the fact that there exist sequences $(\Psi_N^I)_{N\in\mathbb{N}^*}$ of initial data in $H^1(\mathbb{R}^N)$ such that the corresponding values of the energy form a sequence which is $O(N)$ for $N \to \infty$. An example is provided by factorized states like (2.9), for which

$$E_N(\Psi_N^I) = \frac{\hbar^2 N}{2m} \|(\psi^I)'\|^2_{L^2(\mathbb{R})} + \alpha \frac{N-1}{2} \|\psi^I\|^4_{L^4(\mathbb{R})} \tag{3.5}$$

¿From (3.4) it is clear that whenever a sequence of initial data is chosen such that $E_N(\Psi_N^I) = O(N)$, then

$$C \equiv \sup\{\|\partial_l \Psi_N(t)\|^2_{L^2(\mathbb{R}^N)}, \; N \in \mathbb{N}^*, \, 1 \le l \le N, \, t \in \mathbb{R}\} \tag{3.6}$$

is a finite quantity.

Remark 3.3. Although useless in this paper, we would like to point out the role of $\hbar$. As a matter of fact, it is easy to show that

$$\sup_{1\leq j\leq N}\int_{\mathbb{R}^N} dX_N\,|\partial_j\Psi_N(t,X_N)|^2 \leq \frac{c_1}{\hbar^2}+\frac{c_2}{\hbar^2 N}+c_3 \tag{3.7}$$

where the coefficient $c_i's$ do not depend on $\hbar$. In particular they are given by $c_1 = m\alpha\int_{\mathbb{R}^{N-1}}|\Psi^I_N(t,X^{kj}_N)|^2\,dX^j_N$, $c_2 = -m\alpha\int_{\mathbb{R}^{N-1}}|\Psi^I_N(t,X^{kj}_N)|^2\,dX^j_N$ and $c_3 = \|\partial_i\Psi^I_N(t)\|^2_2$, for any i,j and k in $\{1,...,N\}$. Furthermore, for a factorized initial datum they do not depend on N.

Inequality (3.6) leads to consider the H^1 spaces as somewhat natural for the analysis of the problem. Then we proceed defining the analog of the H^1 spaces in the context of trace class operator spaces. Actually, it suffices to consider only one space derivative.

Indeed, we consider the space E_n which consists of all bounded operators $\hat{T}$ on $L^2(\mathbb{R}^n)$ such that the operator $(\mathbb{I}-\partial^2_n)^{\frac12}\hat{T}(\mathbb{I}-\partial^2_n)^{\frac12}$ is trace class.

Notice that ∂_n represents the operator of differentiation with respect to the n^{th} variable. From well-known theory of trace-class operators ([RS1], section VI.6) it is easy to show the following result.

Proposition 3.4. *The space* $E_n = \{\hat{T}\in\mathcal{L}(L^2(\mathbb{R}^n)),\,(\mathbb{I}-\partial^2_n)^{\frac12}\hat{T}(\mathbb{I}-\partial^2_n)^{\frac12}\in\mathcal{L}^1(L^2(\mathbb{R}^n))\}$ *endowed with the norm*

$$\|\hat{T}\|_{E_n}\equiv\|(\mathbb{I}-\partial^2_n)^{\frac12}\hat{T}(\mathbb{I}-\partial^2_n)^{\frac12}\|_{\mathcal{L}^1(L^2(\mathbb{R}^n))} \tag{3.8}$$

is a Banach space.

Moreover, E_n *is the dual of the space* E_{n*} *of the operators* $\hat{K}$ *such that* $(\mathbb{I}-\partial^2_n)^{-\frac12}\hat{K}(\mathbb{I}-\partial^2_n)^{-\frac12}$ *is a compact operator on* $L^2(\mathbb{R}^n)$, *whilst the dual* E^*_n *of* E_n *is the space of operators* $\hat{K}$ *such that* $(\mathbb{I}-\partial^2_n)^{-\frac12}\hat{K}(\mathbb{I}-\partial^2_n)^{-\frac12}$ *is a bounded operator on* $L^2(\mathbb{R}^n)$.

Here, the action of $\hat{T}$ *on* $\hat{K}$ *as a linear functional is understood as follows*

$$\hat{K}\to\mathrm{Tr}(\hat{T}\hat{K}) \tag{3.9}$$

for any $n\leq N\in\mathbb{N}^*$ *and* $t\in\mathbb{R}$.

In the following proposition we prove that the quantity $\|\hat{\rho}_{N,n}(t)\|_{E_n}$ is uniformly bounded in N, n and t.

Proposition 3.5. *Let* $(\Psi^I_N)_{N\in\mathbb{N}^*}$ *be a sequence of initial data for problems (2.6), such that the energy* $E_N(\Psi^I_N)$ *is* $O(N)$ *for* $N\to\infty$.

Then there exists $M>0$, *independent of* N, n *and* t, *such that the family of reduced density matrices* $\hat{\rho}_{N,n}(t)$ *fulfils the following estimate*

$$\|\hat{\rho}_{N,n}(t)\|_{E_n}\leq M \tag{3.10}$$

for any N, n and t, with $n\leq N$.

Proof. By definition (3.6), the quantity $\|\partial_j\Psi_N(t)\|^2_{L^2(\mathbb{R}^N)}$ is estimated uniformly in N, n and t by the quantity C.

Then we consider the operator $(\mathbb{I}-\partial^2_n)^{\frac12}\hat{\rho}_N(t)(\mathbb{I}-\partial^2_n)^{\frac12}$, which is proportional to the orthogonal projection in $L^2(\mathbb{R}^N)$ on the subspace spanned by the vector $(\mathbb{I}-\partial^2_n)^{\frac12}\Psi_N(t)$.

A computation of the trace class norm of this projector yields

$$\begin{aligned}\|(\mathbb{I}-\partial_n^2)^{\frac12}\hat\rho_N(t)(\mathbb{I}-\partial_n^2)^{\frac12}\|_{\mathcal{L}^1(L^2(\mathbb{R}^N))} =&\|(\mathbb{I}-\partial_n^2)^{\frac12}\Psi_N(t)\|^2_{L^2(\mathbb{R}^N)}\\ \le&1+\|\partial_n\Psi_N(t)\|^2_{L^2(\mathbb{R}^N)}\\ \le&1+C\end{aligned} \tag{3.11}$$

It suffices now to apply the definition of reduced density matrix (2.12) to find

$$\mathrm{Tr}_{[n+1,N]}\left[(\mathbb{I}-\partial_n^2)^{\frac12}\hat\rho_N(t)(\mathbb{I}-\partial_n^2)^{\frac12}\right]=(\mathbb{I}-\partial_n^2)^{\frac12}\hat\rho_{N,n}(t)(\mathbb{I}-\partial_n^2)^{\frac12} \tag{3.12}$$

and then to conclude

$$\begin{aligned}\|\hat\rho_{N,n}(t)\|_{E_n} =&\|(\mathbb{I}-\partial_n^2)^{\frac12}\hat\rho_{N,n}(t)(\mathbb{I}-\partial_n^2)^{\frac12}\|_{\mathcal{L}^1(L^2(\mathbb{R}^n))}\\ =&\|(\mathbb{I}-\partial_n^2)^{\frac12}\hat\rho_{N}(t)(\mathbb{I}-\partial_n^2)^{\frac12}\|_{\mathcal{L}^1(L^2(\mathbb{R}^N))}\\ \le&\ 1+C\end{aligned} \tag{3.13}$$

If we define $M=1+C$ then the proof is complete. □

Before stating the main result, we need the following lemma

Lemma 3.6. *Let Γ_N be an element of $H^1(\mathbb{R}^n)$. Then*

$$\begin{aligned}&\int_{\mathbb{R}^{N-1}}|\Gamma_N(X_{N-2},x,x)|^2\,dX_{N-2}dx\\ &\le\frac{1}{2\sqrt2}\left[\|\Gamma_N\|_{L^2(\mathbb{R}^n)}+\frac{1}{\sqrt2}\|\partial_{N-1}\Gamma_N\|_{L^2(\mathbb{R}^n)}+\frac{1}{\sqrt2}\|\partial_N\Gamma_N\|_{L^2(\mathbb{R}^n)}\right]^2\end{aligned} \tag{3.14}$$

Proof. We define the function Θ_N as follows

$$\Theta_N(X_{N-2},x'_{N-1},x'_N)\equiv\Gamma_N\left(X_{N-2},\frac{x'_{N-1}-x'_N}{\sqrt2},\frac{x'_{N-1}+x'_N}{\sqrt2}\right) \tag{3.15}$$

¿From Parseval inequality one has

$$\begin{aligned}\int_{\mathbb{R}^{N-1}}|\Gamma_N(X_{N-2},x,x)|^2\,dX_{N-2}dx &= \frac{1}{\sqrt2}\int_{\mathbb{R}^{N-1}}|\Theta_N(X_{N-2},x,0)|^2\,dX_{N-2}dx\\ &= \frac{1}{\sqrt2(2\pi)^{N+1}}\int_{\mathbb{R}^{N-1}}d\Xi_{N-1}\left|\int_{\mathbb{R}}\tilde\Theta_N(\Xi_{N-1},\xi)d\xi\right|^2\end{aligned} \tag{3.16}$$

Applying the Cauchy-Schwarz inequality to the last integral one obtains

$$\begin{aligned}\int_{\mathbb{R}^{N-1}}|\Gamma_N(X_{N-2},x,x)|^2\,dX_{N-2}dx &\le \frac{\pi}{\sqrt2(2\pi)^{N+1}}\int_{\mathbb{R}^N}d\Xi_{N-1}d\xi\left|\widetilde{(1-\partial_N^2)^{\frac12}\Theta_N}(\Xi_{N-1},\xi)\right|^2\\ &= \frac{1}{2\sqrt2}\|(1-\partial_N^2)^{\frac12}\Theta_N\|^2_{L^2(\mathbb{R}^N)}\\ &\le \frac{1}{2\sqrt2}\left[\|\Theta_N\|_{L^2(\mathbb{R}^N)}+\|\partial_N\Theta_N\|_{L^2(\mathbb{R}^N)}\right]^2\end{aligned} \tag{3.17}$$

Then, to conclude the proof it suffices to remark that

$$\|\partial_N\Theta_N\|_{L^2(\mathbb{R}^N)}\le\frac{1}{\sqrt2}\|\partial_{N-1}\Gamma_N\|_{L^2(\mathbb{R}^N)}+\frac{1}{\sqrt2}\|\partial_N\Gamma_N\|_{L^2(\mathbb{R}^N)} \tag{3.18}$$

□

Remark 3.7. Applying the result in lemma (3.6) to $\Psi_N(t;X_N^{ij})$, and exploiting undistinguishability (2.8), one has

$$\begin{aligned}\int_{\mathbb{R}^{N-1}}|\Psi_N(t;X_N^{ij})|^2dX_N^j \leq & \frac{1}{2\sqrt{2}}\left[\|\Psi_N(t)\|_{L^2(\mathbb{R}^N)}+\sqrt{2}\|\partial_N\Psi_N(t)\|_{L^2(\mathbb{R}^N)}\right]^2 \\ \leq & \frac{(1+\sqrt{2})^2}{2\sqrt{2}}\|(\mathbb{I}-\partial_N^2)^{\frac{1}{2}}\Psi_N(t)\|^2_{L^2(\mathbb{R}^N)}\end{aligned} \tag{3.19}$$

4. Convergence of the finite hierarchy to the infinite one

We first establish a convergence result for the sequence of reduced density matrices $\hat{\rho}_{N,n}(t)$ with $N \in \mathbb{N}^*$.

We shall consider $\hat{\rho}_{N,n}$ as a function of the time variable in the space E_n and we will prove that there exists a subsequence of $\{\hat{\rho}_{N,n}\}_{N\in\mathbb{N}^*}$ which converges in a suitable topology for any value of n.

Proposition 4.1. *There exists an increasing function $\phi : \mathbb{N}^* \to \mathbb{N}^*$ such that for any $n \in \mathbb{N}^*$, the sequence $\{\hat{\rho}_{\phi(N),n}\}_{N\in\mathbb{N}^*}$ converges in the space $L^\infty(\mathbb{R}, E_n)$ in the sense of the weak-$*$ topology.*

Proof. ¿From proposition 3.5 we know that $\hat{\rho}_{N,n}$ is an element of $L^\infty(\mathbb{R}; E_n)$ which is the dual of the space $L^1(\mathbb{R}; E_{n*})$ (see proposition 3.4); besides, the norm of $\hat{\rho}_{N,n}$ in $L^\infty(\mathbb{R}; E_n)$ is uniformly bounded in N and n.
Therefore, by Alaoglu theorem we know that there is an increasing function $\phi_1 : \mathbb{N}^* \to \mathbb{N}^*$ such that the sequence $\{\hat{\rho}_{\phi_1(N),1}\}_{N\in\mathbb{N}^*}$ converges in the space $L^\infty(\mathbb{R}, E_1)$ in the sense of the weak-$*$ topology.
We define by induction the increasing function $\phi_{n+1} : \mathbb{N}^* \to \phi_n(\mathbb{N}^*)$: let us consider the sequence $\{\hat{\rho}_{(\phi_n\circ\phi_{n-1}\circ\ldots\circ\phi_1)(N),n+1}\}_{N\in\mathbb{N}^*}$. As before, there exists an increasing function ϕ_{n+1} : $\mathbb{N}^* \to \phi_n(\mathbb{N}^*)$ such that the sequence $\{\hat{\rho}_{(\phi_{n+1}\circ\phi_n\circ\ldots\circ\phi_1)(N),n+1}\}_{N\in\mathbb{N}^*}$ converges in the space $L^\infty(\mathbb{R}, E_{n+1})$ in the sense of the weak-$*$ topology.
Mimicing the “diagonal trick”, we find that $\phi(n) = (\phi_n \circ \phi_{n-1} \circ \ldots \circ \phi_1)(n)$ is the increasing function we looked for. □

Now we come to the main result, which establishes the convergence of the finite hierarchy to the infinite one.

Theorem 4.2. *Let $\Psi_N \in C^0(\mathbb{R}; H^1(\mathbb{R}^N))$ be a mild solution of problem (2.6), with initial datum $\Psi_I \in H^1(\mathbb{R}^N)$ satisfying the assumption of indistinguishable particles (2.8), the normalization condition (2.10) and the condition of finite energy density, namely $E_N(\Psi_N^I) = O(N)$ for $N \to \infty$, with E_N given by (2.7).*
Furthermore we assume that, for all $n \leq N$, the integral operator $\hat{\rho}^I_{N,n}$, acting on $L^2(\mathbb{R}^n)$ and defined by the kernel

$$\rho^I_{N,n}(X_n, Y_n) = \int_{\mathbb{R}^{N-n}} \Psi^I_N(X_n, Z_N^{n+1})\overline{\Psi^I_N(Y_n, Z_N^{n+1})}\, dZ_N^{n+1} \tag{4.1}$$

converges to the operator $\hat{\rho}^I_n$, represented by the kernel $\rho^I_n(X_n, Y_n)$, weak-$*$ in E_n as $N \to \infty$, with E_n defined in proposition 3.4.

Let the density matrix $\hat\rho_N$ be defined by (2.1) and (2.2) with its marginal distributions $\hat\rho_{N,n}$ defined by (2.12).
Then, any limit point as $N\to\infty$ of the family of integral kernels $\rho_{N,n}$ of partial traces $\hat\rho_{N,n}$ solves the infinite Schrödinger hierarchy (2.14) in the sense of distributions $\mathcal{D}'(\mathbb{R}^{2n+1})$.
Here, limit points are understood in the sense of the product topology on $\prod_{n\geq 1} L^\infty(\mathbb{R};E_n)$, each factor being equipped with the weak-$*$ topology.

In order to avoid a cluttered proof we first prove the following technical lemma.

Lemma 4.3. *Under the hypotheses of theorem 4.2 the following inequality holds*
(4.2)
$$\int_{\mathbb{R}} dz \left[\int_{\mathbb{R}^{2n-1}} dX_n^i dY_n \left|\rho_{N,n+1}(t;X_{i-1},z,X_n^{i+1},z;Y_n,z)\right|^2\right]^{\frac12} \leq \frac{1+\sqrt2}{2^{\frac34}}\|\hat\rho_{N,n+1}(t)\|_{E_{n+1}}$$

Proof. First, let us choose i, n and N in $\mathbb{N}^*$, $i\leq n\leq N$ and a function $\chi\in C_c^\infty(\mathbb{R})$. Then we construct the function $\pi_N^{i,n}$ as follows

$$\pi_N^{i,n}(t;X_N,Y_N)\equiv\Psi_N(t;X_{i-1},x_n,X_N^{i+1})\chi(x_i)\overline{\Psi_N(t;Y_N)} \tag{4.3}$$

The operator $\hat\pi_N^{i,n}(t)$ having the function $\pi_N^{i,n}(t)$ as an integral kernel has a one-dimensional range, therefore it is a trace class operator on $L^2(\mathbb{R}^N)$.

Notice that in general $\hat\pi_N^{i,n}(t)$ is neither positive nor self-adjoint, nonetheless its trace class norm can be easily computed observing that

$$\hat\pi_N^{i,n}(t)=\|\Phi_N^{i,n}(t)\|_{L^2(\mathbb{R}^N)}\left(\Psi_N(t),\cdot\right)_N\frac{\Phi_N^{i,n}(t)}{\|\Phi_N^{i,n}(t)\|_{L^2(\mathbb{R}^N)}} \tag{4.4}$$

where we intoduced the function $\Phi_N^{i,n}(t,X_N)\equiv\Psi_N(t;X_{i-1},x_n,X_N^{i+1})\chi(x_i)$ and $(\cdot,\cdot)_N$ denotes the ordinary scalar product in $L^2(\mathbb{R}^N)$.

Therefore

$$\hat\pi_N^{i,n}(t)^*\hat\pi_N^{i,n}(t)=\|\Phi_N^{i,n}(t)\|^2_{L^2(\mathbb{R}^N)}\left(\Psi_N(t),\cdot\right)_N\Psi_N(t) \tag{4.5}$$

Then

$$\left|\hat\pi_N^{i,n}(t)\right|=\left[\hat\pi_N^{i,n}(t)^*\hat\pi_N^{i,n}(t)\right]^{\frac12}=\|\Phi_N^{i,n}(t)\|_{L^2(\mathbb{R}^N)}\left(\Psi_N(t),\cdot\right)_N\Psi_N(t) \tag{4.6}$$

By definition of trace class norm

$$\|\hat\pi_N^{i,n}(t)\|_{\mathcal{L}^1(L^2(\mathbb{R}^N))}=\mathrm{Tr}\left[\left|\hat\pi_N^{i,n}(t)\right|\right]=\|\Phi_N^{i,n}(t)\|_{L^2(\mathbb{R}^N)} \tag{4.7}$$

Now we can consider the operator $\hat\pi_{N,m}^{i,n}(t)$ defined by the following integral kernel

$$\pi_{N,m}^{i,n}(t;X_m;Y_m)\equiv\int_{\mathbb{R}^{N-m}}\pi_N^{i,n}(t;X_m,Z_N^{m+1};Y_m,Z_N^{m+1}) \tag{4.8}$$

¿From lemma 2.1 in [BGM], $\hat\pi_{N,m}^{i,n}(t)$ is a trace class operator and

$$\|\hat\pi_{N,m}^{i,n}(t)\|_{\mathcal{L}^1(L^2(\mathbb{R}^N))}\leq\|\hat\pi_N^{i,n}(t)\|_{\mathcal{L}^1(L^2(\mathbb{R}^N))}=\|\Phi_N^{i,n}(t)\|_{L^2(\mathbb{R}^N)} \tag{4.9}$$

Let us consider the operator $\hat{\pi}^{i,n+1}_{N,n+1}(t)$. Following (4.3) and (4.8), we know that its integral kernel is given by

(4.10)

$$\begin{aligned}\pi^{i,n+1}_{N,n+1}(t;X_{n+1};Y_{n+1}) &= \int_{\mathbb{R}^{N-n-1}} dZ_N^{n+2}\,\Phi_N^{i,n+1}(t;X_{n+1},Z_N^{n+2})\overline{\Psi_N(t;Y_{n+1},Z_N^{n+2})}\\ &= \chi(x_i)\int_{\mathbb{R}^{N-n-1}} dZ_N^{n+2}\Psi_N(t;X_{i-1},x_{n+1},X^{i+1}_{n+1},Z_N^{n+2})\overline{\Psi_N(t,Y_{n+1},Z_N^{n+2})}\\ &= \chi(x_i)\rho_{N,n+1}(t;X_{i-1},x_{n+1},X^{i+1}_{n+1};Y_{n+1})\end{aligned}$$

¿From inequality (2.28) in [BGM], the operator $\hat{\pi}^{i,n+1}_{N,n+1}(t;z)$ acting on $L^2(\mathbb{R}^n)$ and defined for fixed z by the integral kernel $\pi^{i,n+1}_{N,n+1}(t;X_n,z;Y_n,z)$, belongs to $L^1(\mathbb{R};\mathcal{L}^1(L^2(\mathbb{R}^n)))$ as a function of the variable z. Moreover, the following inequality holds

$$\int_{\mathbb{R}} dz\,\|\hat{\pi}^{i,n+1}_{N,n+1}(t;z)\|_{\mathcal{L}^1(L^2(\mathbb{R}^n))} \le \|\hat{\pi}^{i,n+1}_{N,n+1}(t)\|_{\mathcal{L}^1(L^2(\mathbb{R}^{n+1}))} \tag{4.11}$$

Now, recalling that the space of trace class operators is embedded in the space of the Hilbert-Schmidt operators, which is isomorphic to the space of integral kernels endowed with the L^2-norm, we get

$$\|\chi\|_{L^2(\mathbb{R})}\int_{\mathbb{R}} dz\,\left[\int_{\mathbb{R}^{2n-1}} dX_n^i dY_n\,\left|\rho_{N,n+1}(t;X_{i-1},z,X_n^{i+1},z;Y_n,z)\right|^2\right]^{\frac{1}{2}}$$

$$\le \|\hat{\pi}^{i,n+1}_{N,n+1}(t)\|_{\mathcal{L}^1(L^2(\mathbb{R}^{n+1}))} \le \|\hat{\pi}^{i,n+1}_{N}(t)\|_{\mathcal{L}^1(L^2(\mathbb{R}^N))} \tag{4.12}$$

$$= \|\Phi^{i,n+1}_N(t)\|_{L^2(\mathbb{R}^N)} = \|\chi\|_{L^2(\mathbb{R})}\left[\int_{\mathbb{R}^{N-1}} dX_N^i\left|\Psi_N(t;X_{i-1},x_{n+1},X_N^{i+1})\right|^2\right]^{\frac{1}{2}} \tag{4.13}$$

$$\le \frac{1+\sqrt{2}}{2^{\frac{3}{4}}}\|\chi\|_{L^2(\mathbb{R})}\|(1+\partial^2_{n+1})^{\frac{1}{2}}\Psi_N(t)\|_{L^2(\mathbb{R}^N)} \le \frac{1+\sqrt{2}}{2^{\frac{3}{4}}}\|\chi\|_{L^2(\mathbb{R})}\|\hat{\rho}_N(t)\|_{E_{n+1}} \tag{4.14}$$

Let us explain the chain of inequalities written above. In (4.12) we exploited formula (2.28) in [BGM]. In (4.13) we used equation (4.7) and the definition of $\pi^{i,n}_N(t)$. Then in (4.14) we made use of remark 3.7, of the definition of the spaces E_n and of the fact that $\|\hat{\rho}_N(t)\|_{E_{n+1}}$ is greater than one.

Finally, by the intermediate step in equality (3.13), which states that the E_n-norm of $\hat{\rho}_N$ equals the E_n-norm of $\hat{\rho}_{N,n}$, and getting rid of the factor $\|\chi\|_{L^2(\mathbb{R})}$, we obtain inequality (4.2) □

Now we prove theorem 4.2.

Proof. In this proof we will always omit the indication of the converging subsequence $\hat{\rho}_{\phi(N),n}$, constructed like in proposition 4.1, so the symbol $\hat{\rho}_{N,n}$ must be interpreted as a converging sequence, for $N\to\infty$, in the weak-$*$ topology of $L^\infty(\mathbb{R};E_n)$.

Let $\hat{\rho}_n$ be the limit of $\hat{\rho}_{N,n}$. We show that it satisfies the infinite Schrödinger hierarchy (2.14) in the sense of distributions.

We recall that the weak-$*$ convergence in $L^\infty(\mathbb{R};E_n)$ implies the weak-$*$ convergence in $L^\infty(\mathbb{R};L^2(\mathbb{R}^{2n}))$ and then the convergence in $\mathcal{D}'(\mathbb{R}^{2n+1})$. Therefore, the l.h.s. of (2.13) converges to the l.h.s. of (2.14), as well as the first term in the r.h.s. of (2.13) converges to the first term in the r.h.s. of (2.14).

The next term in the r.h.s. of (2.14) refers to the interactions between the first n particles and consists of $n(n-1)/2$ terms. We will prove that the generic term, evaluated on a test function, can be estimated independently of N.

Let us consider a function φ in the space $\mathcal{D}(\mathbb{R}^{2n+1})$. Then

(4.15)
$$\begin{aligned}
&\left|\int_{\mathbb{R}^{2n+1}} dt\, dX_n\, dY_n\, \delta(x_i - x_j)\rho_{N,n}(t;X_n;Y_n)\varphi(t;X_n;Y_n)\right| \\
\leq &\left|\int_{\mathbb{R}^{2n}} dt\, dX_n^j\, dY_n\, \rho_{N,n}(t;X_n^{ij};Y_n)\varphi(t;X_n^{ij};Y_n)\right| \\
\leq &\frac{1+\sqrt{2}}{2^{\frac{3}{2}}}\int_{\mathbb{R}} dt\, \left[\|\varphi(t)\|_{L^2(\mathbb{R}^{2n})} + \|\partial_i\varphi(t)\|_{L^2(\mathbb{R}^{2n})} + \|\partial_{i+1}\varphi(t)\|_{L^2(\mathbb{R}^{2n})}\right] \|(\mathbb{I}-\partial_n)^{\frac{1}{2}}\rho_{N,n}(t)\|_{L^2(\mathbb{R}^{2n})} \\
\leq &\frac{1+\sqrt{2}}{2^{\frac{3}{2}}}\int_{\mathbb{R}} dt\, \left[\|\varphi(t)\|_{L^2(\mathbb{R}^{2n})} + \|\partial_i\varphi(t)\|_{L^2(\mathbb{R}^{2n})} + \|\partial_{i+1}\varphi(t)\|_{L^2(\mathbb{R}^{2n})}\right] \|\hat{\rho}_{N,n}(t)\|_{E_n}
\end{aligned}$$

where we used the Cauchy-Schwarz inequality, lemma 3.6 (to estimate the function φ), remark 3.7 (to estimate the function $\rho_{N,n}(t)$) and the definition of the space E_n (proposition 3.4).

Recalling the uniform boundedness of the quantity $\|\hat{\rho}_{N,n}(t)\|_{E_n}$, proven in (3.5), we finally obtain

(4.16)
$$\begin{aligned}
&\left|\int_{\mathbb{R}^{2n+1}} dt\, dX_n\, dY_n\, \delta(x_i - x_j)\rho_{N,n}(t;X_n;Y_n)\varphi(t;X_n;Y_n)\right| \\
\leq &\frac{1+\sqrt{2}}{2^{\frac{3}{2}}}\mu(\mathrm{Supp_t}[\varphi])\,\left(\|\varphi\|_{L^\infty(\mathbb{R};L^2(\mathbb{R}^{2n}))} + \|\partial_i\varphi\|_{L^\infty(\mathbb{R};L^2(\mathbb{R}^{2n}))} + \|\partial_{i+1}\varphi\|_{L^\infty(\mathbb{R};L^2(\mathbb{R}^{2n}))}\right) \\
&\|\hat{\rho}_{N,n}\|_{L^\infty(\mathbb{R};E_n)}
\end{aligned}$$

where $\mu(\mathrm{Supp_t}[\varphi])$ is the Lebesgue measure of the support in t of the test function φ.

So we have proven that in the limit $N \to \infty$ the second term in the r.h.s. of (2.14) vanishes as an element of $\mathcal{D}'(\mathbb{R}^{2n+1})$.

We discuss the convergence of the last sum in the r.h.s. of (2.13) to the last sum in the r.h.s. of (2.14)

We aim to prove that, given $\varphi \in \mathcal{D}(\mathbb{R}^{2n+1})$, for $N \to \infty$ one has

$$\begin{aligned}
&\int_{\mathbb{R}^{2n+1}} \varphi(t;X_n;Y_n)\rho_{N,n+1}(t;X_n,x_i;Y_n,x_i)\, dtdX_ndY_n \\
\to &\int_{\mathbb{R}^{2n+1}} \varphi(t;X_n;Y_n)\rho_{n+1}(t;X_n,x_i;Y_n,x_i)\, dtdX_ndY_n
\end{aligned} \tag{4.17}$$

¿From lemma 4.3 the l.h.s. of (4.17) can be estimated as follows

$$\begin{aligned}
&\int_{\mathbb{R}^{2n+1}} \varphi(t;X_n;Y_n)\rho_{N,n+1}(t;X_n,x_i;Y_n,x_i)dtdX_ndY_n \\
\leq\;\; &\frac{1+\sqrt{2}}{2^{\frac{3}{4}}}\int_{\mathbb{R}} dt\, \|\varphi(t)\|_{L^\infty(\mathbb{R};L^2(\mathbb{R}^{2n-1}))}\|\hat{\rho}_{N,n+1}(t)\|_{E_{n+1}}
\end{aligned} \tag{4.18}$$

where the function $\varphi(t)$ is considered as an element of L^∞ with respect to the variable x_i and as a square integrable function with respect to other variables.

Relation (4.18) proves that at any time the l.h.s. of (4.17) can be understood as the action of a linear bounded functional on $\hat{\rho}_{N,n+1}(t)$ viewed as an element of E_{n+1}.

We would like to prove the following two statements

(1) For almost any t there exists an operator $\hat{B}(t) \in E_{n+1*}$ such that

$$\int_{\mathbb{R}^{2n}} \varphi(t; X_n; Y_n)\rho_{N,n+1}(t; X_n, x_i; Y_n, x_i)dX_n dX_n \quad = \quad \mathrm{Tr}\left[\hat{B}(t)\hat{\rho}_{N,n+1}(t)\right] \tag{4.19}$$

(2) $\hat{B}$ is integrable as a function of t in E_{n+1*}, namely

$$\int_{\mathbb{R}} dt\, \|\hat{B}(t)\|_{E_{n+1*}} = \int_{\mathbb{R}} dt\, \|(\mathbb{I} - \partial^2_{n+1})^{-\frac{1}{2}}\hat{B}(t)(\mathbb{I} - \partial^2_{n+1})^{-\frac{1}{2}}\|_{\mathcal{L}(L^2(\mathbb{R}^{n+1}))} < \infty \tag{4.20}$$

Once proven points 1. and 2. we may interpret the l.h.s. of (4.17) as a duality product in $L^\infty(\mathbb{R}; E_{n+1*})$, then the weak-$*$ convergence of $\hat{\rho}_{N,n}$ to $\hat{\rho}_N$ would suffice in order to prove (4.17).

Let us start proving point 1. We consider the operator $\hat{\kappa}(t)$ which acts on $L^2(\mathbb{R}^{n+1})$ and whose integral kernel in Fourier space reads

$$\tilde{\kappa}(t; \Xi_{n+1}; \Lambda_{n+1}) \equiv \frac{\tilde{\varphi}(t; \Lambda_{i-1}, \lambda_i + \lambda_{n+1} + \xi_{n+1}, \Lambda^{i+1}_n; \Xi_n)}{(1+\lambda^2_{n+1})^{\frac{1}{2}}(1+\xi^2_{n+1})^{\frac{1}{2}}} \tag{4.21}$$

It is immediately seen that $\kappa(t)$ is a square integrable function, so the operator $\hat{\kappa}(t)$ is a Hilbert-Schmidt operator in $L^2(\mathbb{R}^{n+1})$. In particular it is compact and by basic embedding theorems in operator spaces one has

$$\begin{aligned} &\|\hat{\kappa}(t)\|_{\mathcal{L}(L^2(\mathbb{R}^{n+1}))} \leq \|\hat{\kappa}(t)\|_{\mathcal{L}^2(L^2(\mathbb{R}^{n+1}))} = \|\kappa(t)\|_{L^2(\mathbb{R}^{2n+2})} \\ =&(2\pi)^{-n-1}\|\tilde{\kappa}(t)\|_{L^2(\mathbb{R}^{2n+2})} = 2^{-n-1}\pi^{-n}\|\tilde{\varphi}(t)\|_{L^2(\mathbb{R}^{2n})} = \frac{1}{2}\|\varphi(t)\|_{L^2(\mathbb{R}^{2n})} \end{aligned} \tag{4.22}$$

We prove that

$$\hat{\kappa}(t) = (\mathbb{I} - \partial^2_{n+1})^{-\frac{1}{2}}\hat{B}(t)(\mathbb{I} - \partial^2_{n+1})^{-\frac{1}{2}} \tag{4.23}$$

To this purpose let us recall the canonical decomposition of $\hat{\rho}_{N,n+1}(t)$ as a compact operator,

$$\hat{\rho}_{N,n+1}(t) = \sum_k a_k \hat{P}_{\eta_k} \tag{4.24}$$

where the η_k's are normalized and mutually orthogonal elements of $L^2(\mathbb{R}^{n+1})$ and $\hat{P}_{\eta_k}$ is the orthogonal projection on the linear span of η_k. Since $\hat{\rho}_{N,n+1}(t)$ is a positive operator whose trace equals one, then all a_k's are positive and $\sum_k a_k = 1$. Both a_k's and η_k's depend on N, n and t, but we will ignore this dependence in notation. If the set of the η_k's is not complete in $L^2(\mathbb{R}^{n+1})$, then we extend it to a complete one and in correspondence to any joint η_j we set $a_j = 0$.

Let us compute the quantity

$$\begin{aligned}&\mathrm{Tr}\left[(\mathbb{I}-\partial^2_{n+1})^{\frac12}\hat\kappa(t)(\mathbb{I}-\partial^2_{n+1})^{\frac12}\hat\rho_{N,n+1}(t)\right]\\ =&\frac{1}{(2\pi)^{2n+2}}\sum_k a_k\int_{\mathbb{R}^{2n+2}}d\Xi_{n+1}d\Lambda_{n+1}\,\tilde\varphi(t;-\Lambda_{i-1},-\lambda_i-\lambda_{n+1}+\xi_{n+1},-\Lambda_n^{i+1};\Xi_n)\tilde\eta_k(\Lambda_{n+1})\overline{\tilde\eta_k(\Xi_{n+1})}\end{aligned}\tag{4.25}$$

Notice that we computed the trace on the complete orthogonal and normalized set given by the vectors η_k. We recall that the result is independent of such a choice (see e.g. [RS1], section VI.6). With the change of variables $\lambda_i'=\lambda_i+\lambda_{n+1}$ we get the following identity

$$\begin{aligned}&\mathrm{Tr}\left[(\mathbb{I}-\partial^2_{n+1})^{\frac12}\hat\kappa(t)(\mathbb{I}-\partial^2_{n+1})^{\frac12}\hat\rho_{N,n+1}(t)\right]\\ =&\frac{1}{(2\pi)^{2n+2}}\sum_k a_k\int_{\mathbb{R}^n}d\Lambda_n^i d\lambda_i'\int_{\mathbb{R}}d\lambda_{n+1}\,\tilde\eta_k(\Lambda_{i-1},\lambda_i'-\lambda_{n+1},\Lambda_{n+1}^{i+1})\\ &\int_{\mathbb{R}^{n+1}}d\Xi_{n+1}\,\tilde\varphi(t;-\Lambda_{i-1},-\lambda_i'+\xi_{n+1},-\Lambda_n^{i+1};\Xi_n)\overline{\tilde\eta_k(\Xi_{n+1})}\end{aligned}\tag{4.26}$$

Interpreting the r.h.s. of (4.26) as a scalar product in $\mathbb{R}^n$ with the measure $d\Lambda_n^i d\lambda_i'$ and coming back from Fourier to coordinates space, with the variable λ_j conjugated with x_j for $i\neq j$, and the variable λ_i' conjugated with x_i, one obtains

$$\begin{aligned}&\mathrm{Tr}\left[(\mathbb{I}-\partial^2_{n+1})^{\frac12}\hat\kappa(t)(\mathbb{I}-\partial^2_{n+1})^{\frac12}\hat\rho_{N,n+1}(t)\right]\\ =&\sum_k a_k\int_{\mathbb{R}^n}dX_n\,\eta_k(X_{n+1}^{i,n+1})\int_{\mathbb{R}^n}dY_n\,\varphi(t;X_n;Y_n)\overline{\eta_k(Y_n,x_i)}\\ =&\int_{\mathbb{R}^{2n}}dX_ndY_n\,\varphi(t;X_n;Y_n)\rho_{N,n+1}(t;X_{n+1}^{i,n+1};Y_n,x_i)\end{aligned}\tag{4.27}$$

So we managed to prove relation (4.19) with an operator $\hat B(t)$ given by (4.23). Then $\hat B(t)$ belongs to E_{n+1*} for any t and point 1. is proven.

To show point 2. it suffices to consider equality (4.22) and notice that

$$\begin{aligned}\int_{\mathbb{R}}dt\,\|\hat B(t)\|_{E_{n+1*}}&\le\frac12\int_{\mathbb{R}}dt\,\|\varphi(t)\|_{L^2(\mathbb{R}^{2n})}=\frac12\int_{\mathrm{Supp}_t[\varphi]}dt\,\|\varphi(t)\|_{L^2(\mathbb{R}^{2n})}\\ &\le\frac12\mu\left(\mathrm{Supp}_t[\varphi]\right)\sup_{t\in\mathbb{R}}\left\{\|\varphi(t)\|_{L^2(\mathbb{R}^{2n})}\right\}<\infty\end{aligned}\tag{4.28}$$

Therefore $\hat B$ is an element of $L^1(\mathbb{R};E_{n+1*})$ and the weak-$*$ convergence of $\hat\rho_{N,n+1}$ as an element of $L^1(\mathbb{R};E_{n+1})$ implies the convergence in (4.17).

This observation concludes the proof. □

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