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ON THE RATE OF CONVERGENCE FOR THE MEAN FIELD APPROXIMATION OF BOSONIC MANY-BODY QUANTUM DYNAMICS*

ZIED AMMARI†, MARCO FALCONI‡, AND BORIS PAWILOWSKI§

Abstract. We consider the time evolution of quantum states by many-body Schrödinger dynamics and study the rate of convergence of their reduced density matrices in the bosonic mean field limit. If the prepared state at initial time is of coherent or factorized type and the number of particles n is large enough then it is known that $1/n$ is the correct rate of convergence at any time. We show in the simple case of bounded pair potentials that the previous rate of convergence holds in more general situations with possibly correlated prepared states. In particular, it turns out that the coherent structure at initial time is unessential and the important fact is rather the speed of convergence of all reduced density matrices of the prepared states. We illustrate our result with several numerical simulations and examples of multi-partite entangled quantum states borrowed from quantum information.

Key words. Mean field limit, reduced density matrices, Wigner measures, entangled quantum states.

AMS subject classifications. 81S30, 81S05, 81T10, 35Q55, 81P40.

1. Introduction

The mean field theory provides in principle a fair approximation of time evolved quantum states by many-body Schrödinger dynamics in the mean field scaling; namely when the number of particles is large and the pair interaction potential is proportionally weak. During the last decade, a strong activity around the mean-field problem has occurred within the community of mathematical physics (see for instance [9, 26, 28, 36, 52] for bosons and [8, 12, 20, 27] for fermions). This in particular have led to a rigorous justification of the bosonic mean field approximation for singular potentials including Coulomb interaction as well as the derivation of the Gross–Pitaevskii equation from many-body quantum dynamics (e.g. [2, 6, 10, 16, 21–24, 29, 35, 39, 45] and also [32, 33] for older results). More recently, emphasis has been placed on the speed of convergence of the mean-field approximation. This seems to be motivated by providing useful quantitative bounds and understanding higher order corrections (see [7, 14, 15, 25, 34, 40, 48, 50]).

The aim of our article is to give at the level of a simple model more insight on the aforementioned problem for bosonic systems. Actually, the rate of convergence is essentially understood in the case of coherent or factorized type states with a particular structure. So, we can ask the following natural questions:

- What should we expect if we start from another prepared state which is more correlated?

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†IRMAR, Université de Rennes I, UMR-CNRS 6625, Campus de Beaulieu, 35042 Rennes Cedex, France (zied.ammari@univ-rennes1.fr).
‡IRMAR, Université de Rennes I, UMR-CNRS 6625, Campus de Beaulieu, 35042 Rennes Cedex, France (marco.falconi@univ-rennes1.fr).
§Fak. Mathematik, Univ. Wien, Oskar-Morgenstern-Platz 1, 1090 Wien, Austria (boris.pawilowski@univie.ac.at).

- Is the specific coherent structure of the known examples important?
- Can we determine the optimal rate of convergence in some examples?
- Does the rate of convergence improves under the effect of the quantum dynamics?

We will show that the rate of convergence at a given time depends essentially on the rate of convergence of all reduced density matrices of the prepared state at time $t=0$. In fact, we are able to give a general condition on the prepared state that guarantees a given speed of convergence at any time. The assumption we require at time zero, which is rather easy to check in initial states, is true at any time if it holds at $t=0$. This allows in particular to consider the question of improvement of the convergence over time while the question of optimality will be addressed through numerical analysis.

Consider for instance the many-body Schrödinger Hamiltonian of an n-boson system

$$\mathbf{H}_n=\sum_{i=1}^{n}-\Delta_{x_i}+\frac{1}{n}\sum_{1\leq i<j\leq n}V(x_i-x_j), \tag{1.1}$$

where $(x_1,\dots,x_n)\in\mathbb{R}^{dn}$ and V is a real bounded potential satisfying $V(x)=V(-x)$. The self-adjoint operator $\mathbf{H}_n$ acts on the space $L^2_s(\mathbb{R}^{dn})$ of symmetric square integrable functions. A function $\Psi_n\in L^2(\mathbb{R}^{dn})$ is symmetric if $\Psi_n(x_1,\dots,x_n)=\Psi_n(x_{\sigma_1},\dots,x_{\sigma_n})$ for any permutation σ of the symmetric group $\mathfrak{S}(n)$. Suppose that the system is in a prepared quantum state ϱ_n at initial time $t=0$ (i.e. ϱ_n is a non-negative trace class operator with $\mathrm{Tr}[\varrho_n]=1$). So, under the action of the Schrödinger dynamics the system at time t evolves into the state

$$\varrho_n(t)=e^{it\mathbf{H}_n}\varrho_n e^{-it\mathbf{H}_n}.$$

The mean field approximation at the dynamical level is usually understood as the following picture: if the system is in an uncorrelated state $\varrho_n=|\varphi^{\otimes n}\rangle\langle\varphi^{\otimes n}|$, with $||\varphi||_{L^2(\mathbb{R}^d)}=1$, at initial time $t=0$ then it will evolve into a state close in some sense to an uncorrelated one $\varrho_n(t)\simeq|\varphi_t^{\otimes n}\rangle\langle\varphi_t^{\otimes n}|$ when n is large and φ_t is the solution of the nonlinear Hartree equation

$$\begin{cases} i\partial_t\varphi_t=-\Delta\varphi_t+(V*|\varphi_t|^2)\varphi_t,\\ \varphi_{t=0}=\varphi. \end{cases} \tag{1.2}$$

The above convergence is neither a strong nor a weak one but rather in the sense of reduced density matrices. More precisely, the convergence is understood as

$$\lim_{n\to\infty}\mathrm{Tr}[\varrho_n(t)A\otimes 1^{\otimes(n-p)}]=\langle\varphi_t^{\otimes p},A\varphi_t^{\otimes p}\rangle_{L^2(\mathbb{R}^{dp})},$$

for any bounded (or compact) operator A on $L^2(\mathbb{R}^{dp})$ and any $p\in\mathbb{N}^*$ (p is kept fixed while $n\to\infty$).

In some sense, the mean field approximation says essentially that the measurements

$$\mathrm{Tr}[\varrho_n(t)A\otimes 1^{\otimes(n-p)}],\quad n\geq p, \tag{1.3}$$

for any observable A on $L^2(\mathbb{R}^{dp})$ converge, when n goes to infinity while p is kept fixed, to some classical or one particle quantities to be determined. Hence, the main quantities to be analyzed are the reduced density matrices of the time evolved states $\varrho_n(t)$. Recall that for each $p\in\mathbb{N}^*$, the p-reduced density matrix of $\varrho_n(t)$ is the unique non-negative trace class operator $\varrho_n^{(p)}(t)$ on $L^2_s(\mathbb{R}^{dp})$ satisfying

$$\mathrm{Tr}\left[\varrho_n(t)\, A\otimes 1^{\otimes(n-p)}\right]=\mathrm{Tr}\left[\varrho_n^{(p)}(t)\, A\right], \tag{1.4}$$

for any bounded operator A on $L^2(\mathbb{R}^{dp})$. Therefore, the point is to determine for each $p\in\mathbb{N}^*$ the limit and the rate of convergence of these quantities (1.4) when the number of particles n goes to infinity. It turns out that the limit at $t=0$ may not exist and actually there is a difference between requiring convergence in (1.4) for all bounded operators A on $L^2(\mathbb{R}^{dp})$, or convergence for compact operators only, since the weak and weak-$*$ topologies differ on the space of trace-class operators. However, one can characterize all the limit points of $(\varrho_n^{(p)})_{n\geq p}$ with respect to the weak-$*$ topology in the space of trace-class operators (which is the dual space of compact operators) and also describe their structure. Indeed, at time $t=0$, we can show that there exists always a subsequence $(\varrho_{n_k})_{k\in\mathbb{N}}$ such that for each $p\in\mathbb{N}$, $1\leq p\leq n_k$, the reduced density matrices $(\varrho_{n_k}^{(p)})_{k\in\mathbb{N}^*}$ converge to non-negative trace-class operators $\varrho_\infty^{(p)}$ in the weak-$*$ topology. Moreover, there exists a Borel probability measure μ on $L^2(\mathbb{R}^d)$ such that

$$\varrho_\infty^{(p)}=\int_{L^2(\mathbb{R}^d)}|z^{\otimes p}\rangle\langle z^{\otimes p}|\,d\mu(z).$$

In this way we have characterized all the possible limit points via subsequences of the reduced density matrices $(\varrho_n^{(p)})_{n\geq p}$ and identified their structure. More details are given in Subsection 3.1 while here we summarize the main result in the proposition below. We will use often the notation $\mathscr{L}^k(\mathfrak{h})$, $1\leq k\leq\infty$, to refer to the Schatten classes with $||\cdot||_k$ denoting their norms; and denote by $\mathscr{L}(\mathfrak{h})$ the space of bounded operators.

PROPOSITION 1.1. *Let $(\varrho_n)_{n\in\mathbb{N}^*}$ be a sequence of density matrices with $\varrho_n\in\mathscr{L}^1(L^2_s(\mathbb{R}^{dn}))$ for each $n\in\mathbb{N}^*$. Suppose that for any $p\in\mathbb{N}^*$ and each compact operator $A\in\mathscr{L}^\infty(L^2_s(\mathbb{R}^{dp}))$ the sequence $(\mathrm{Tr}[\varrho_n^{(p)}A])_{n\geq p}$ converges. Then there exists a unique Borel probability measure μ_0 on $L^2(\mathbb{R}^d)$ invariant with respect to the unitary group $U(1)$ and such that for any $p\in\mathbb{N}^*$ and any $A\in\mathscr{L}^\infty(L^2_s(\mathbb{R}^{dp}))$,*

$$\lim_{n\to\infty}\mathrm{Tr}[\varrho_n^{(p)}A]=\mathrm{Tr}[\varrho_\infty^{(p)}A],\qquad \textit{with}\qquad \varrho_\infty^{(p)}=\int_{L^2(\mathbb{R}^d)}|z^{\otimes p}\rangle\langle z^{\otimes p}|\,d\mu_0(z).$$

Moreover, the measure μ_0 is concentrated on the unit ball $B(0,1)$ of $L^2(\mathbb{R}^d)$ centered at the origin and of radius one (i.e., $\mu_0(B(0,1))=1$).

Actually, the measure μ_0 is the unique Wigner measure of the sequence $(\varrho_n)_{n\in\mathbb{N}^*}$ (see Subsection 3.1 for definition and details). Once this is understood we can consider the problem of rate of convergence for more general correlated states.

THEOREM 1.2. *Let $(\alpha(n))_{n\in\mathbb{N}^*}$ be a sequence of positive numbers with $\lim\alpha(n)=\infty$ and such that $(\frac{\alpha(n)}{n})_{n\in\mathbb{N}^*}$ is bounded. Let $(\varrho_n)_{n\in\mathbb{N}^*}$ and $(\varrho_\infty^{(p)})_{p\in\mathbb{N}^*}$ be two sequences of density matrices with $\varrho_n\in\mathscr{L}^1(L^2_s(\mathbb{R}^{dn}))$ and $\varrho_\infty^{(p)}\in\mathscr{L}^1(L^2_s(\mathbb{R}^{dp}))$ for each $n,p\in\mathbb{N}^*$. Assume that there exist $C_0>0$, $C>2$ and $\gamma\geq 1$ such that for all $n,p\in\mathbb{N}^*$ with $n\geq\gamma p$*

$$\left\|\varrho_n^{(p)}-\varrho_\infty^{(p)}\right\|_1\leq C_0\frac{C^p}{\alpha(n)}. \tag{1.5}$$

Then for any $T>0$ *there exists* $C_T>0$ *such that for all* $t\in[-T,T]$ *and all* $n,p\in\mathbb{N}^*$ *with* $n\geq\gamma p$,

$$\left\|\varrho_n^{(p)}(t)-\varrho_\infty^{(p)}(t)\right\|_1\leq C_T\frac{C^p}{\alpha(n)},\tag{1.6}$$

where

$$\varrho_\infty^{(p)}(t)=\int_{L^2(\mathbb{R}^d)}|z^{\otimes p}\rangle\langle z^{\otimes p}|\,d\mu_t(z),$$

with $\mu_t=(\Phi_t)_\sharp\mu_0$ *the push-forward of the initial measure* μ_0 *(given in Proposition 1.1) by the well defined and continuous Hartree flow* Φ_t *on* $L^2(\mathbb{R}^d)$ *of the equation* (1.2) *(given in Subsection 2.2).*

Remarks 1.3.

1) Our result holds true in a more general framework. We can replace $L^2(\mathbb{R}^d)$ by any separable Hilbert space $\mathscr{Z}$, $-\Delta$ by any self-adjoint operator h_0, and V by any two-particle bounded interaction (see Subsection 2.2). So from now on we will consider this setting, which has the advantage of covering several situations: e.g. either finite or infinite dimensional systems, as well as semi or non relativistic ones.
2) The assumption (1.5) implies that we can apply Proposition 1.1 and hence obtain the existence of the initial measure μ_0 at $t=0$.
3) The condition $C>2$ in the main assumption of Theorem 1.2 can be replaced by $C>0$ at the cost of slightly changing the conclusion, by replacing C in (1.6) by $C+2$.
4) We can apply Theorem 1.2 backward in time. So, if the estimates (1.6) hold true at a given time t, then (1.5) should also hold at time $t=0$. This answers the question of improvement of the rate of convergence under the action of the quantum evolution. Indeed, if we suppose that inequalities (1.6) hold with a faster rate of convergence $\beta(n)$, $\lim\frac{\alpha(n)}{\beta(n)}=0$, then the "initial" estimate (1.5) should also hold with $\beta(n)$ instead of $\alpha(n)$ by backward evolution.
5) The proof of Theorem 1.2 allows to start with a rate of convergence $\alpha(n)$ faster than $1/n$ at time $t=0$. However, we can't recover a better convergence at time $t\neq 0$. This is why we have restricted $\alpha(n)$ to be of order n or less. However, this feature do not seem to be an artifact of the proof: numerical simulations on product states indicate a $1/n$ order of convergence even when at time $t=0$ the reduced density matrices coincide with their limit.

The mathematical analysis of the mean field limit is quite rich and indeed there are several approaches and techniques applicable to this problem. For example coherent states analysis [32, 33, 36], BBGKY hierarchy method [52], Egorov type theorem [26, 28, 29], Wigner measures approach [3, 6, 44] or deviation estimates [40, 48]. Hence the combination of these different techniques may lead to interesting results. The proof of our main Theorem 1.2 relies on two ingredients: an Egorov type theorem proved in [26, 28] and a Wigner measures characterization of the limit points of reduced density matrices studied in [3–5]. So the first step is to use second quantization formalism and Wick observables, then the result in [26, 28] provides the asymptotics of time-evolved Wick observables as

$$e^{it\mathbf{H}_n}\,b^{\mathrm{Wick}}e^{-it\mathbf{H}_n}{}_{|L^2_s(\mathbb{R}^{dn})}=b(t)^{\mathrm{Wick}}{}_{|L^2_s(\mathbb{R}^{dn})}+R(n),\tag{1.7}$$

where $\lim_{n\to\infty} R(n) = 0$ in some specific sense and where $b(t)^{\text{Wick}}$ is an infinite sum of Wick operators with time-dependent kernels or symbols (see subsections 2.1 and 2.3). The mean field expansion (1.7) gives actually the convergence of the correlation functions (1.4). So that, if we use the idea of Wigner measures extended to this framework in [3], we can obtain the rate of convergence for the quantities (1.4). Once this is proved, one can get the announced trace norm estimates for the difference between reduced density matrices.

The article is organized as follows. The second quantization formalism and Wick symbolic calculus is recalled in Subsection 2.1. The mean field expansion is explained in Subsection 2.3 while the quantum and classical dynamics are introduced in Subsection 2.2. In Section 3, we analyse the relationship between reduced density matrices (RDM) and Wigner measures and provide the proof of Proposition 1.1. Our main result is proved in Section 4 with some preliminary lemmas. Examples and numerical simulations are discussed in the last Section 5.

2. Mean field expansion

The mean field theory is concerned with quantum dynamical systems which preserve the number of particles and can be worked out in the setting of multi-particles Schrödinger operators (1.1). Nevertheless, it is advantageous to use the more general setting of second quantization. Actually, the Hamiltonian (1.1) can be reformulated as

$$\mathbf{H}_n = \varepsilon^{-1} H_{\varepsilon_{|L^2_s(\mathbb{R}^{dn})}}, \tag{2.1}$$

with $\varepsilon = \frac{1}{n}$ and H_ε a Hamiltonian on the symmetric Fock space over $L^2(\mathbb{R}^d)$ given by

$$H_\varepsilon = \varepsilon \int_{\mathbb{R}^d} \nabla a^*(x) \nabla a(x)\, dx + \frac{\varepsilon^2}{2} \int_{\mathbb{R}^{2d}} V(x-y) a^*(x) a^*(y) a(x) a(y)\, dx dy, \tag{2.2}$$

where a, a^* are the usual creation-annihilation operator-valued distributions, i.e.,

$$[a(x), a^*(y)] = \delta(x-y),\ [a^*(x), a^*(y)] = 0 = [a(x), a(y)]. \tag{2.3}$$

Our investigation of the mean field approximation for the quantum dynamics (1.1) is made through the analysis of the Hamiltonian (2.2). The strategy relies on a specific Schwinger–Dyson expansion of the time dependent correlation functions (1.3) elaborated in [26, 28] combined to some tools (Wigner measures) from semiclassical analysis extended to infinite dimensional setting in [3]. The Schwinger–Dyson expansion, called here mean field expansion, is explained in Subsection 2.3 and leads naturally to the consideration of several multiple commutators which we need to normal order using Wick's theorem. So, for reader convenience we recall some basic results on normal ordering and Wick operators written in more systematic and in some sense more efficient way: it makes possible the use of a symbolic calculus, for an algebra of Wick operators, similar to the pseudo-differential calculus in finite dimension (for other presentations of second quantization see [11, 19]).

2.1. Wick calculus. From now on we will wok in a general setting. Let $\mathscr{Z}$ be a separable Hilbert space. The symmetric Fock space over $\mathscr{Z}$ is the Hilbert space

$$\mathscr{H} = \overset{\infty}{\underset{n=0}{\oplus}} \vee^n \mathscr{Z},$$

where $\vee^n \mathscr{Z}$ denotes the n-fold symmetric tensor product. The dense subspace of finite particle vectors is denoted by

$$\mathscr{H}_0 = \overset{\text{alg}}{\underset{n\geq 0}{\oplus}} \vee^n \mathscr{Z}.$$

For any $n\in\mathbb{N}$, we define the symmetrizer $\mathcal{S}_n$ to be the orthogonal projection of $\mathscr{Z}^{\otimes n}$ onto the closed subspace $\vee^n\mathscr{Z}$. So, the creation and annihilation operators $a^*(f)$ and $a(f)$, parameterized by $\varepsilon>0$, are then defined by the following:

$$a(f)\varphi^{\otimes n}=\sqrt{\varepsilon n}\,\langle f,\varphi\rangle\varphi^{\otimes(n-1)} \tag{2.4}$$

$$a^*(f)\varphi^{\otimes n}=\sqrt{\varepsilon(n+1)}\,\mathcal{S}_{n+1}(f\otimes\varphi^{\otimes n}),\ \forall\varphi\in\mathscr{Z}. \tag{2.5}$$

To avoid cumbersome notations, we choose not to emphasize the dependence of the creation-annihilation operators on the small parameter ε. Thus, we warn the reader that each creation or annihilation operator scales henceforth as $\sqrt{\varepsilon}$ according to (2.4)–(2.5).
It is well known that $a(f)$ and $a^*(f)$ are closable operators, adjoint of each other and satisfy the canonical commutation relations (CCR):

$$[a(f),a^*(g)]=\varepsilon\langle f,g\rangle 1,\ [a^*(f),a^*(g)]=[a(f),a(g)]=0,\quad \forall f,g\in\mathscr{Z}.$$

The ε-dependent Weyl operators are

$$W(f)=e^{\frac{i}{\sqrt{2}}[a^*(f)+a(f)]},\quad f\in\mathscr{Z},$$

and they satisfy the Weyl commutation relations

$$W(f)W(g)=e^{-\frac{i\varepsilon}{2}\mathrm{Im}\langle f,g\rangle}\,W(f+g),\quad \forall f,g\in\mathscr{Z}.$$

For any (possibly unbounded) operator $A:\mathcal{D}(A)\subset\mathscr{Z}\to\mathscr{Z}$, we define $\mathrm{d}\Gamma(A)$ as

$$\mathrm{d}\Gamma(A)_{|\vee^{n,\mathrm{alg}}\mathcal{D}(A)}=\varepsilon\sum_{k=1}^{n}1^{\otimes(k-1)}\otimes A\otimes 1^{\otimes(n-k)}, \tag{2.6}$$

where $\vee^{n,\mathrm{alg}}\mathcal{D}(A)$ denotes the n-fold algebraic symmetric tensor product of $\mathcal{D}(A)$. The ε-dependent $\mathrm{d}\Gamma(A)$ operator scales as ε since it is essentially a sum of products of one creation with one annihilation operator.

Any Wick operator preserving the number of particles could be written in the case of $\mathscr{Z}=L^2(\mathbb{R}^d)$ as a quadratic form using the integral formula

$$b^{\mathrm{Wick}}=\varepsilon^k\int_{\mathbb{R}^{2kd}}\prod_{i=1}^{k}a^*(x_i)B(x_1,\ldots,x_k;y_1,\ldots,y_k)\prod_{j=1}^{k}a(y_j)\,dx_1\cdots dx_k dy_1\cdots dy_k,$$

with $B(x_1,\ldots,x_k;y_1,\ldots,y_k)$ denotes the distribution kernel of the operator B on $L^2(\mathbb{R}^{kd})$ and $a^*(x),a(y)$ are ε-independent operator-valued distributions satisfying (2.3). For general Hilbert spaces, this formula can be generalized as follows.

DEFINITION 2.1 (Class of symbols). *For any $p,q\in\mathbb{N}$, define $\mathscr{P}_{p,q}$ to be the space of homogeneous complex-valued polynomials on $\mathscr{Z}$ such that $b\in\mathscr{P}_{p,q}$ if and only if there exists a (unique) bounded operator $\tilde{b}\in\mathscr{L}(\vee^p\mathscr{Z},\vee^q\mathscr{Z})$ such that for all $z\in\mathscr{Z}$:*

$$b(z)=\langle z^{\otimes q},\tilde{b}z^{\otimes p}\rangle. \tag{2.7}$$

We will often use the identification between homogeneous polynomials $b\in\mathscr{P}_{p,q}$ and their associated operators $\tilde{b}\in\mathscr{L}(\vee^p\mathscr{Z},\vee^q\mathscr{Z})$ according to (2.7). The algebraic sum

$$\mathscr{P}=\overset{\mathrm{alg}}{\underset{p,q\geq 0}{\oplus}}\mathscr{P}_{p,q}$$

is clearly an algebra of polynomials. These spaces $\mathscr{P}$ and $\mathscr{P}_{p,q}$ play a similar role, in some sense, to classes of symbols in pseudo-differential calculus. For this reason we sometimes call the polynomials $b\in\mathscr{P}$ symbols (see for instance [13]). The subspace of $\mathscr{P}_{p,q}$ made of polynomials b such that $\tilde{b}$ is a compact operator is denoted by $\mathscr{P}^{\infty}_{p,q}$ and

$$\mathscr{P}^{\infty}=\overset{\text{alg}}{\underset{p,q\geq 0}{\oplus}}\mathscr{P}^{\infty}_{p,q}.$$

DEFINITION 2.2 (Wick operators). *A Wick operator with symbol $b\in\mathscr{P}_{p,q}$ is a linear operator b^{Wick} with domain $\mathscr{H}_0$ defined as*

$$b^{\mathrm{Wick}}{}_{|\vee^n\mathscr{Z}}=1_{[p,+\infty)}(n)\frac{\sqrt{n!(n+q-p)!}}{(n-p)!}\,\varepsilon^{\frac{p+q}{2}}\,\mathcal{S}_{n-p+q}\Big(\tilde{b}\otimes 1^{\otimes(n-p)}\Big),\tag{2.8}$$

where $\tilde{b}$ denotes the operator associated to the symbol b according to (2.7).

Remark again that for simplicity we use the notation b^{Wick} without stressing the dependence on the scaling parameter ε. Our definition of ε-dependent Wick operators is suitable for the study of the mean-field limit and provides naturally an efficient symbolic calculus similar to the one in finite dimension. So, it makes computations more systematic and one can easily keep track of the meaningful ε-dependence when computing commutators.

The above Wick quantization maps the algebra of symbols or polynomials $\mathscr{P}$ into an algebra of operators in the Fock space. In particular, the composition of two given Wick operators b_1^{Wick} and b_2^{Wick} is again a Wick operator c^{Wick} with c belonging to $\mathscr{P}$ and given by an explicit formula involving multiple Poisson brackets like in pseudo-differential calculus of finite dimension.

Let us introduce the precise meaning of the multiple Poisson brackets. Remark that all polynomials in $\mathscr{P}_{p,q}$ admit Fréchet differentials and therefore they all have directional derivatives. Remark also that we don't need a particular conjugation on the Hilbert space $\mathscr{Z}$ in order to define the derivatives $\partial_{\bar{z}}$ and ∂_z. In fact, for $b\in\mathscr{P}_{p,q}$ we define

$$\partial_{\bar{z}}b(z)[u]=\bar{\partial}_r b(z+ru)_{|r=0},\partial_z b(z)[u]=\partial_r b(z+ru)_{|r=0},$$

where $\bar{\partial}_r,\partial_r$ are the usual derivatives over $\mathbb{C}$. Moreover, $\partial_z^k b(z)$ naturally belongs to $(\vee^k\mathscr{Z})^*$ (i.e., k-linear symmetric functionals) while $\partial_{\bar{z}}^j b(z)$ is identified via the scalar product with an element of $\vee^j\mathscr{Z}$, for any fixed $z\in\mathscr{Z}$. For $b_i\in\mathscr{P}_{p_i,q_i}$, $i=1,2$ and $k\in\mathbb{N}$, set

$$\partial_z^k b_1\cdot\partial_{\bar{z}}^k b_2(z)=\langle\partial_z^k b_1(z),\partial_{\bar{z}}^k b_2(z)\rangle_{(\vee^k\mathscr{Z})^*,\vee^k\mathscr{Z}}=\partial_z^k b_1(z)[\partial_{\bar{z}}^k b_2(z)]\in\mathscr{P}_{p_1+p_2-k,q_1+q_2-k}\,.$$

The multiple *Poisson brackets* are defined by

$$\{b_1,b_2\}^{(k)}=\partial_z^k b_1\cdot\partial_{\bar{z}}^k b_2-\partial_z^k b_2\cdot\partial_{\bar{z}}^k b_1\quad\text{ and }\quad\{b_1,b_2\}=\{b_1,b_2\}^{(1)}.\tag{2.9}$$

PROPOSITION 2.3. *Let $b_1\in\mathscr{P}_{p_1,q_1}$ et $b_2\in\mathscr{P}_{p_2,q_2}$. For all $k\in\{0,\ldots,\min(p_1,q_2)\}$, the polynomial $\partial_z^k b_1\cdot\partial_{\bar{z}}^k b_2$ belongs to $\mathscr{P}_{p_1+p_2-k,q_1+q_2-k}$ with the following formulas holding true on $\mathscr{H}_0$:*

$$b_1^{\mathrm{Wick}}\circ b_2^{\mathrm{Wick}}=\Big[\sum_{k=0}^{\min(p_1,q_2)}\frac{\varepsilon^k}{k!}\partial_z^k b_1\cdot\partial_{\bar{z}}^k b_2\Big]^{\mathrm{Wick}}.$$

$$[b_1^{\mathrm{Wick}}, b_2^{\mathrm{Wick}}] = \sum_{k=1}^{\max(\min(p_1,q_2),\min(p_2,q_1))} \frac{\varepsilon^k}{k!}\left[\{b_1,b_2\}^{(k)}\right]^{\mathrm{Wick}}.$$

2.2. Classical and Quantum dynamics. Instead of analyzing the Schrödinger Hamiltonian (1.1), we prefer to deal with an abstract general many-body operator using the ε-dependent Wick quantization of the previous subsection. Consider a polynomial $Q \in \mathscr{P}_{2,2}$ such that $\tilde{Q} \in \mathscr{L}(\vee^2 \mathscr{Z})$ is bounded and symmetric. In all the sequel we consider the many-body quantum Hamiltonian of bosons to be the operator defined by

$$H_\varepsilon = \mathrm{d}\Gamma(\tilde{h}_0) + Q^{\mathrm{Wick}}, \tag{2.10}$$

where $\tilde{h}_0$ is a given self-adjoint operator on $\mathscr{Z}$ with domain $\mathcal{D}(\tilde{h}_0)$. Both operators $\mathrm{d}\Gamma(\tilde{h}_0)$ and Q^{Wick} are ε-dependent according to (2.6) and (2.8), respectively. The mean field nature of this abstract Hamiltonian H_ε is enlightened by the relation (2.1) when $\mathscr{Z} = L^2(\mathbb{R}^d)$. By standard perturbation theory, and thanks to the conservation of the number of particles, it is easy to prove that H_ε is essentially self-adjoint on $\mathcal{D}(\mathrm{d}\Gamma(\tilde{h}_0)) \cap \mathscr{H}_0$. We denote respectively the time evolution of the perturbed and the free quantum system by

$$U(t) = e^{-i\frac{t}{\varepsilon}H_\varepsilon} \quad \text{and} \quad U_0(t) = e^{-i\frac{t}{\varepsilon}\mathrm{d}\Gamma(\tilde{h}_0)}.$$

It is known that in the mean field limit we obtain the Hartree equation (1.2), when the many-body Schrödinger Hamiltonian (1.1) is considered. In our abstract setting the limit equation has the energy functional

$$h(z) = \langle z, \tilde{h}_0 z\rangle + Q(z),\ z \in \mathcal{D}(\tilde{h}_0),$$

which is actually the Wick symbol of the quantum Hamiltonian (2.10). So, the associated nonlinear field equation reads

$$i\partial_t z_t = X(z_t) \tag{2.11}$$

with $X : \mathcal{D}(\tilde{h}_0) \to \mathscr{Z}$ is the vector field given by $X(z) = \tilde{h}_0 z + \partial_{\bar{z}} Q(z)$. In order to solve this equation we write it in the integral form

$$z_t = e^{-it\tilde{h}_0} z_0 - i\int_0^t e^{-i(t-s)\tilde{h}_0}\,\partial_{\bar{z}} Q(z_s)\,ds, \ \text{for } z_0 \in \mathscr{Z}. \tag{2.12}$$

Since $\tilde{Q}$ is a bounded operator then a standard fixed point argument implies that (2.12) admits a unique continuous local solution for each initial condition $z_0 \in \mathscr{Z}$. Thanks to the conservation of the Hilbert norm on $\mathscr{Z}$ we see that any local solution extends to a global continuous one. Therefore, we have a well defined global continuous flow on $\mathscr{Z}$ which we denote by $\Phi : \mathbb{R} \times \mathscr{Z} \to \mathscr{Z}$. In other terms Φ is a C^0-map satisfying $\Phi_{t+s}(z) = \Phi_t \circ \Phi_s(z)$ and $z_t := \Phi_t(z_0)$ solves (2.12) for any $z_0 \in \mathscr{Z}$. Moreover, if $\mathbb{R} \ni t \mapsto z_t$ is the solution of (2.12) and Q_t is the polynomial in $\mathscr{P}_{2,2}$ given as $Q_t(z) = Q(e^{-it\tilde{h}_0} z)$, then the curve $w_t = e^{it\tilde{h}_0} z_t$ solves the differential equation

$$\frac{d}{dt} w_t = -i\partial_{\bar{z}} Q_t(w_t).$$

Hence, a simple computation yields for any $b \in \mathscr{P}_{p,q}$ the identity

$$\frac{d}{dt} b(w_t) = i\partial_z Q_t(w_t)[\partial_{\bar{z}} b(w_t)] + \partial_z b(w_t)[-i\partial_{\bar{z}} Q_t(w_t)] = i\{Q_t, b\}(w_t),$$

where the brackets are defined according to (2.9). So, we obtain the following Duhamel formula for all $t\in\mathbb{R}$:

$$b(z_t)=b_t(w_0)+i\int_0^t \{Q_{t_1},b_t\}(w_{t_1})\,dt_1, \tag{2.13}$$

with $t\in\mathbb{R}\mapsto z_t$ a (mild) solution of the nonlinear field equation (2.11) and $w_t=e^{it\tilde{h}_0}z_t$.

2.3. Mean field expansion. The main point is to study the time evolution of Wick operators with respect to the small mean field parameter ε which is essentially the inverse of the number of particles. This was done in [26, 28] and in fact we can prove in some sense that

$$e^{i\frac{t}{\varepsilon}H_\varepsilon}\,A^{\mathrm{Wick}}e^{-i\frac{t}{\varepsilon}H_\varepsilon}=A(t)^{\mathrm{Wick}}+R(\varepsilon), \tag{2.14}$$

with $R(\varepsilon)\to 0$ when $\varepsilon\to 0$ (see [26, 28] and also [3, Thm. 5.5]) and where $A(t)^{\mathrm{Wick}}$ is an infinite sum of Wick operators with time-dependent symbols related to the Hartree dynamics. In order to prove (2.14), we use an iterated integral formula (the so-called Dyson–Schwinger expansion) with a specific use of Wick calculus (Proposition 2.3) in order to expand commutators of Wick operators with respect to the ε parameter. We will work in the interaction representation. Hence, the following notation is useful

$$b_t=b\circ e^{-it\tilde{h}_0}\ :\ \mathscr{Z}\ni z\mapsto b_t(z)=b(e^{-it\tilde{h}_0}z),$$

for $b\in\mathscr{P}$ and $t\in\mathbb{R}$ (remark that b_t belongs to $\mathscr{P}$). We also know that multiple commutators in the Schwinger–Dyson expansion lead to Wick operators with multiple Poisson brackets symbols. For this reason we make the following definition.

DEFINITION 2.4. *For $m\in\mathbb{N}$ and $(t_1,\dots,t_m,t)\in\mathbb{R}^{m+1}$, we associate to any $b\in\mathscr{P}_{p,p}$ the polynomial:*

$$C_0^{(0)}(t)=b_t \text{ and } C_0^{(m)}(t_m,\dots,t_1,t)=\Big\{Q_{t_m},\cdots,\Big\{Q_{t_1},b_t\Big\}\cdots\Big\}\in\mathscr{P}_{p+m,p+m}. \tag{2.15}$$

For simplicity the dependence of $C_0^{(m)}(t_m,\dots,t_1,t)$ on the symbol b is not made explicit and sometimes we will write $C_0^{(m)}$ for shortness.

The above polynomials $C_0^{(m)}$ satisfy the following iteration formula.

LEMMA 2.5. *For $m\in\mathbb{N}$ and $(t_1,\dots,t_m,t)\in\mathbb{R}^{m+1}$,*

$$\begin{aligned}\frac{1}{\varepsilon}\big[Q_{t_m}^{\mathrm{Wick}},C_0^{(m-1)}(t_{m-1},\dots,t_1,t)^{\mathrm{Wick}}\big]&=C_0^{(m)}(t_m,\dots,t_1,t)^{\mathrm{Wick}}\\&\quad+\frac{\varepsilon}{2}\left(\Big\{Q_{t_m},C_0^{(m-1)}(t_{m-1},\dots,t_1,t)\Big\}^{(2)}\right)^{\mathrm{Wick}}.\end{aligned}$$

Proof. This is a straightforward consequence of the definition of $C_0^{(m)}$ and the composition formula in Proposition 2.3. ∎

We consider a sequence $(\varrho_n)_{n\in\mathbb{N}^*}$ of density matrices such that $\varrho_n\in\mathscr{L}^1(\vee^n\mathscr{Z})$. For shortness, we denote

$$\varrho_n(t)=U(t)\,\varrho_n\,U(t)^* \quad\text{ and }\quad \tilde{\varrho}_n(t)=U_0(t)^*\,\varrho_n(t)\,U_0(t) \quad\text{ with }\quad \varepsilon=\frac{1}{n},$$

and for simplicity write A^{Wick} for the Wick operator with symbol $\langle z^{\otimes p}, A z^{\otimes p}\rangle$ with $A \in \mathscr{L}(\vee^p \mathscr{Z})$.

Proposition 2.6. *Let $(\varrho_n)_{n\in\mathbb{N}^*}$ be a sequence of density matrices such that $\varrho_n \in \mathscr{L}^1(\vee^n \mathscr{Z})$ for each $n \in \mathbb{N}^*$. Then for any $n,p \in \mathbb{N}^*$ such that $p \leq n$, $A \in \mathscr{L}(\vee^p \mathscr{Z})$, $M \in \mathbb{N}^*$, and $t \in \mathbb{R}$*

$$\begin{aligned}\mathrm{Tr}[\varrho_n(t)\, A^{\mathrm{Wick}}] = &\sum_{k=0}^{M-1} i^k \int_0^t dt_1 \cdots \int_0^{t_{k-1}} dt_k \,\mathrm{Tr}\left[\varrho_n\, C_0^{(k)}(t_k,\ldots,t_1,t)^{\mathrm{Wick}}\right] \\ &+ \frac{\varepsilon}{2}\sum_{k=1}^{M} i^k \int_0^t dt_1 \cdots \int_0^{t_{k-1}} dt_k \,\mathrm{Tr}\left[\tilde{\varrho}_n(t_k)\left(\left\{Q_{t_k}, C_0^{(k-1)}(t_{k-1},\ldots,t_1,t)\right\}^{(2)}\right)^{\mathrm{Wick}}\right] \\ &+ i^M \int_0^t dt_1 \cdots \int_0^{t_{M-1}} dt_M \,\mathrm{Tr}\left[\tilde{\varrho}_n(t_M)\, C_0^{(M)}(t_M,\ldots,t_1,t)^{\mathrm{Wick}}\right], \qquad (2.16)\end{aligned}$$

with $C_0^{(k)}$ given by (2.15)*, replacing b_t by $A_t = U_0^*(t) A U_0(t)$, and the multiple Poisson bracket defined in* (2.9).

Proof. The expansion is obtained by iteration. Let $b \in \mathscr{P}_{p,p}$ then

$$\frac{d}{dt} U(t)^* U_0(t) b^{\mathrm{Wick}} U_0(t)^* U(t)_{|\vee^n \mathscr{Z}} = \frac{i}{\varepsilon} U(t)^* U_0(t) [Q_t^{\mathrm{Wick}}, b^{\mathrm{Wick}}] U_0(t)^* U(t)_{|\vee^n \mathscr{Z}}.$$

A simple integration yields

$$\begin{aligned}U(t)^* U_0(t) b^{\mathrm{Wick}} U_0(t)^* U(t)_{|\vee^n \mathscr{Z}} = b^{\mathrm{Wick}}{}_{|\vee^n \mathscr{Z}} + \frac{i}{\varepsilon}\int_0^t dt_1 U(t_1)^* U_0(t_1) \\ [Q_{t_1}^{\mathrm{Wick}}, b^{\mathrm{Wick}}] U_0(t_1)^* U(t_1)_{|\vee^n \mathscr{Z}}. \qquad (2.17)\end{aligned}$$

Taking $b^{\mathrm{Wick}} = U_0(t)^* A^{\mathrm{Wick}} U_0(t) = A_t^{\mathrm{Wick}}$ in the above formula, gives

$$\begin{aligned}U(t)^* A^{\mathrm{Wick}} U(t)_{|\vee^n \mathscr{Z}} = &U_0(t)^* A^{\mathrm{Wick}} U_0(t)_{|\vee^n \mathscr{Z}} \\ &+ \frac{i}{\varepsilon}\int_0^t dt_1 U(t_1)^* U_0(t_1) \left[Q_{t_1}, A_t^{\mathrm{Wick}}\right] U_0(t_1)^* U(t_1)_{|\vee^n \mathscr{Z}}.\end{aligned}$$

Hence using Lemma 2.5, we get

$$\begin{aligned}U(t)^* A^{\mathrm{Wick}} U(t)_{|\vee^n \mathscr{Z}} = &U_0(t)^* A^{\mathrm{Wick}} U_0(t)_{|\vee^n \mathscr{Z}} \\ &+ i\int_0^t dt_1 \underbrace{U(t_1)^* U_0(t_1)\, C_0^1(t_1,t)^{\mathrm{Wick}} U_0(t_1)^* U(t_1)}_{(\mathrm{T})}{}_{|\vee^n \mathscr{Z}} \\ &+ i\frac{\varepsilon}{2}\int_0^t dt_1 U(t_1)^* U_0(t_1) \left(\left\{Q_{t_1}, A_t\right\}^{(2)}\right)^{\mathrm{Wick}} U_0(t_1)^* U(t_1)_{|\vee^n \mathscr{Z}}.\end{aligned}$$

Remark that the first two terms in the right-hand side are of order $O(1)$ while the last one is of order $O(\varepsilon)$. By using again (2.17) to expand the term (T) above with $b = C_0^1(t_1,t)$ we obtain, after taking the trace with ϱ_n, the formula (2.16) for $M = 2$. So, iterating this process $M-1$ times and following the same scheme of splitting commutators into two parts one of order $O(1)$ and the second of order $O(\varepsilon)$, we get

$$U(t)^* A^{\mathrm{Wick}} U(t)_{|\vee^n \mathscr{Z}}$$

$$
\begin{aligned}
&= \sum_{k=0}^{M-1} i^k \int_0^t dt_1 \cdots \int_0^{t_{k-1}} dt_k \, C_0^{(k)}(t_k,\ldots,t_1,t)^{\mathrm{Wick}} \\
&\quad + i^M \int_0^t dt_1 \cdots \int_0^{t_{M-1}} dt_M \, U(t_M)^* U_0(t_M) \left[C_0^{(M)}(t_M,\ldots,t_1,t)\right]^{\mathrm{Wick}} U_0(t_M)^* U(t_M) \\
&\quad + \frac{\varepsilon}{2} \sum_{k=1}^{M-1} i^k \int_0^t dt_1 \cdots \int_0^{t_{k-1}} dt_k \, U(t_k)^* U_0(t_k) \left(\left\{ Q_{t_k} ; C_0^{(k-1)}(t_{k-1},\ldots,t_1,t) \right\}^{(2)} \right)^{\mathrm{Wick}} U_0(t_k)^* U(t_k).
\end{aligned}
$$

Hence, by taking the trace with ϱ_n we prove the proposition. ◻

The next step is to let $M \to \infty$ in the formula (2.16). But to do this we need to prove some estimates which guarantee the absolute convergence of these series.

Lemma 2.7. *For any $b \in \mathscr{P}_{p,p}$ the symbols $\{Q_s, b_t\}^{(2)} \in \mathscr{P}_{p,p}$ and $C_0^{(m)} \in \mathscr{P}_{p+m,p+m}$ with the following inequalities holding true:*
(i)

$$
\left\| \widetilde{\{Q_s, b_t\}^{(2)}} \right\|_{\mathscr{L}(\vee^p \mathscr{Z})} \le 4p(p-1) \, \|\tilde{Q}\| \, \|\tilde{b}\|_{\mathscr{L}(\vee^p \mathscr{Z})}.
$$

(ii) For any $m \in \mathbb{N}$,

$$
\left\| \widetilde{C_0^{(m)}}(t_m,\ldots,t_1,t) \right\|_{\mathscr{L}(\vee^{p+m} \mathscr{Z})} \le 4^m \, \frac{(p+m-1)!}{(p-1)!} \, \|\tilde{Q}\|^m \, \|\tilde{b}\|_{\mathscr{L}(\vee^p \mathscr{Z})}.
$$

Here $\widetilde{\{Q_s, b_t\}^{(2)}}$ and $\widetilde{C_0^{(m)}}$ are respectively the operators associated to the polynomials $\{Q_s, b_t\}^{(2)}$ and $C_0^{(m)}$ according to Definition 2.1.

Proof. See [3, Lemma 5.8, 5.9]. ◻

Proposition 2.8. *Let $(\varrho_n)_{n \in \mathbb{N}^*}$ be a sequence of density matrices such that $\varrho_n \in \mathscr{L}^1(\vee^n \mathscr{Z})$ for each $n \in \mathbb{N}^*$. Then for any $n, p \in \mathbb{N}^*$ such that $p \le n$, $A \in \mathscr{L}(\vee^p \mathscr{Z})$ and $|t| < \frac{1}{8\|\tilde{Q}\|}$ and $\varepsilon = \frac{1}{n}$*

$$
\begin{aligned}
\mathrm{Tr}[\varrho_n(t) \, A^{\mathrm{Wick}}] &= \sum_{k=0}^{\infty} i^k \int_0^t dt_1 \cdots \int_0^{t_{k-1}} dt_k \, \mathrm{Tr}\left[\varrho_n \, C_0^{(k)}(t_k,\ldots,t_1,t)^{\mathrm{Wick}}\right] \\
&\quad + \frac{\varepsilon}{2} \sum_{k=1}^{\infty} i^k \int_0^t dt_1 \cdots \int_0^{t_{k-1}} dt_k \, \mathrm{Tr}\left[\tilde{\varrho}_n(t_k) \left(\left\{ Q_{t_k}, C_0^{(k-1)}(t_{k-1},\ldots,t_1,t) \right\}^{(2)} \right)^{\mathrm{Wick}} \right],
\end{aligned}
$$

with $C_0^{(k)}$ are given in (2.15), the multiple Poisson bracket defined in (2.9).

Proof. Proposition 2.6 says that

$$
\mathrm{Tr}[\varrho_n(t) \, A^{\mathrm{Wick}}] = \sum_{k=0}^{M-1} C_k + \frac{\varepsilon}{2} \sum_{k=1}^{M} B_k + R_M,
$$

where A_k, B_k, and R_M are short notations for the terms appearing in (2.16). Applying Lemma 2.7 and using the fact that we integrate k-times, we get for $n \ge p+k$

$$
\left| C_k \right| \le 4^k \frac{(p+k-1)!}{(p-1)! k!} (|t| \, \|\tilde{Q}\|)^k \, \|A\|,
$$

$$\begin{aligned}\left|B_k\right| &\leq 4^k(p+k-1)(p+k-2)\frac{(p+k-1)!}{(p-1)!k!}(|t|\,||\tilde{Q}||)^k\,||A||, \qquad (2.18)\\ \left|R_M\right| &\leq 4^M\frac{(p+M-1)!}{(p-1)!M!}(|t|\,||\tilde{Q}||)^M\,||A||.\end{aligned}$$

Therefore, using the bound $C_{p+k-1}^k \leq 2^{p+k-1}$, we see that for times $|t| < \frac{1}{8||\tilde{Q}||}$ the two series $\sum_{k=0}^{M-1} C_k$ and $\sum_{k=1}^{M} B_k$ are absolutely convergent and $R_M \to 0$ when $M \to \infty$. □

PROPOSITION 2.9. *Let $(\varrho_n)_{n\in\mathbb{N}^*}$ be a sequence of density matrices such that $\varrho_n \in \mathscr{L}^1(\vee^n \mathscr{Z})$ for each $n \in \mathbb{N}^*$. Then for any $C > 2$ there exists $C_0 > 0$ such that for any $n,p \in \mathbb{N}^*$, $p \leq n$, $A \in \mathscr{L}(\vee^p \mathscr{Z})$, $|t| < \frac{1}{16||\tilde{Q}||}$ and $\varepsilon = \frac{1}{n}$:*

$$\begin{aligned}&\left|\mathrm{Tr}[\varrho_n(t)\,A^{\mathrm{Wick}}] - \sum_{k=0}^{\infty} i^k \int_0^t dt_1 \cdots \int_0^{t_{k-1}} dt_k\, \mathrm{Tr}\left[\varrho_n\, C_0^{(k)}(t_k,\ldots,t_1,t)^{\mathrm{Wick}}\right]\right|\\ &\leq C_0\,\frac{C^p}{n}||A||. \qquad (2.19)\end{aligned}$$

Proof. This follows by Proposition 2.8 and estimate (2.18). In fact, we see that the left-hand side of (2.19) is bounded by

$$\frac{2^{p-1}}{2n}\sum_{k=1}^{\infty}(k+p)^2\big(8|t|\,||\tilde{Q}||\big)^k\,||A|| \leq \frac{2^p}{2n}\sum_{k=1}^{\infty}(k^2+p^2)\big(8|t|\,||\tilde{Q}||\big)^k\,||A|| \leq \frac{2^p}{n}(3+p^2)\,||A||.$$

Taking $C_0 = \max_{p\geq 1}\frac{2^p(3+p^2)}{C^p}$ for $C > 2$, we obtain the inequality (2.19). □

3. Reduced density matrices

In this section, we explain the notion of Wigner measures and its relationship with reduced density matrices. Most of the results we need are proved in [3,5], but for reader convenience we briefly recall them since they play an essential role in the proof of our main result. The main observation is that reduced density matrices of a given sequence of normal states have limit points with respect to the weak-$*$ topology when $n \to \infty$ and these limit points have a very particular structure. Actually, a noncommutative de Finetti theorem [53] due to Størmer (motivated by classification of C^*-algebras and type factors) provides in some sense the structure of these limiting states. This is more apparent in the work of Hudson and Moody [37,38] where the authors focus on normal states which are also used in our setting. Actually, it turns out that with Wigner measures we can characterize the structure of the limit points more easily, without appealing to C^*-algebras formalism, and using probability measures in more natural sets. Moreover, some compactness defect phenomena can be easily understood with the latter tool (see [3, 5]). More recently, the authors Lewin, Nam, and Rougerie in [43] gave an alternative proof of the noncommutative de Finetti theorem (see also [17, 42] for application of this type of result).

3.1. Wigner measures. In finite dimension, Wigner (or semi-classical) measures are well-known tools in the analysis of PDEs with particular scaling (see for instance [30, 31, 46, 47, 49, 54]). This idea was extended to the infinite dimensional case in [3] and adapted to the framework of the mean field problem. Actually, the Borel probability measures μ_0 appearing in Proposition 1.1 is what we call Wigner measures of the sequence of density matrices $(\varrho_n)_{n\in\mathbb{N}^*}$. This concept is more general and one can deal with arbitrary families of normal states (or even trace class operators) on the Fock space. The main advantage is that we can identify these measures μ_0 by means of simpler quantities involving the Weyl operators (see Theorem 3.1) according to the following formula:

$$\lim_{n\to\infty} \mathrm{Tr}[\varrho_n W(\xi)] = \int_{\mathscr{Z}} e^{i\sqrt{2}\mathrm{Re}\langle \xi, z\rangle}\, d\mu_0(z), \quad \forall \xi \in \mathscr{Z},$$

where $W(\xi)$ refers to the Weyl operator on the Fock space $\mathscr{H}$ with $\varepsilon = \frac{1}{n}$. Therefore the mean field problem becomes a propagation problem of Wigner measures along the nonlinear flow of the (Hartree) equation (2.11). To enlighten the discussion let us consider a concrete example. Let $\Psi_n = \varphi^{\otimes n}$ with $\varphi \in \mathscr{Z}$ and $||\varphi||_{\mathscr{Z}} = 1$. It is easy to see that the p-reduced density matrices of $\varrho_n = |\Psi_n\rangle\langle\Psi_n|$ are $\varrho_n^{(p)} = |\varphi^{\otimes p}\rangle\langle\varphi^{\otimes p}|$ and one can compute explicitly the Wigner measure of the sequence $(\varrho_n)_{n\in\mathbb{N}}$ according to Proposition 1.1:

$$\lim_{n\to\infty} \mathrm{Tr}[\varrho_n^{(p)} B] = \langle \varphi^{\otimes p}, B\varphi^{\otimes p}\rangle = \int_{\mathscr{Z}} \langle z^{\otimes p}, B z^{\otimes p}\rangle\, d\mu_0(z), \quad \text{with } \mu_0 = \frac{1}{2\pi}\int_0^{2\pi} \delta_{e^{i\theta}\varphi}\, d\theta,$$

where $\delta_{e^{i\theta}\varphi}$ denotes the Dirac measure on $\mathscr{Z}$ at the point $e^{i\theta}\varphi$. So Theorem 1.2 gives in particular the convergence of the evolved reduced density matrices and in our example it yields

$$\lim_{n\to\infty} \mathrm{Tr}[\varrho_n^{(p)}(t) B] = \int_{\mathscr{Z}} \langle z^{\otimes p}, B z^{\otimes p}\rangle\, d\mu_t(z), \quad \text{with} \quad \mu_t = (\Phi_t)_\sharp \mu_0 = \frac{1}{2\pi}\int_0^{2\pi} \delta_{e^{i\theta}\varphi_t}\, d\theta,$$

where φ_t is the solution of the nonlinear field (Hartree) equation (2.11) with initial condition φ. So, working with Wigner measures allows to understand the superposition of states that may interact in the mean field limit (see [3]); and hence it provides a general and flexible point of view. We recall below the result that gives the construction of Wigner measures. It is a slight adaptation of [3, Theorem 6.2] including [5, Lemma 2.14].

THEOREM 3.1. *Let $(\varrho_n)_{n\in\mathbb{N}^*}$ be a sequence of density matrices such that $\varrho_n \in \mathscr{L}^1(\vee^n \mathscr{Z})$ for each $n \in \mathbb{N}^*$. Then there exists a subsequence $(n_k)_{k\in\mathbb{N}^*}$ and a Borel probability measure μ on $\mathscr{Z}$, called a Wigner measure, such that for any $\xi \in \mathscr{Z}$,*

$$\lim_{k\to\infty} \mathrm{Tr}[\varrho_{n_k} W(\xi)] = \int_{\mathscr{Z}} e^{i\sqrt{2}\mathrm{Re}\langle \xi, z\rangle}\, d\mu(z), \tag{3.1}$$

with $W(\xi)$ referring to the Weyl operator on the Fock space $\mathscr{H}$ with the scaling $\varepsilon = \frac{1}{n}$. Moreover, the probability measure μ is $U(1)$ invariant and it is concentrated on the unit ball $B(0,1)$ of the Hilbert space $\mathscr{Z}$ (i.e., $\mu_0(B(0,1)) = 1$).

The $U(1)$-invariance of the measure μ is a straightforward consequence of the fact that $\varrho_n \in \mathscr{L}^1(\vee^n \mathscr{Z})$ for each $n \in \mathbb{N}^*$. So, the above theorem says that the set of Wigner measures of a sequence $(\varrho_n)_{n\in\mathbb{N}^*}$ is never empty and we denote it by

$$\mathscr{M}(\varrho_n, n \in \mathbb{N}^*).$$

In practice and without loss of generality, one can assume in the analysis of the mean field problem that the set $\mathscr{M}(\varrho_n, n \in \mathbb{N}^*)$ only contains a single measure.

3.2. De Finetti Theorem. In this subsection we give the proof of Proposition 1.1 which can be considered as a noncommutative de Finetti theorem. Moreover, the convergence (3.1) extends to Wick quantized symbols with compact kernels belonging to $\mathscr{P}^\infty$ and hence this proves the weak-$*$ convergence of reduced density matrices. This result is proved in [3, Corollary 6.14] and a slight adaptation of it is recalled below.

PROPOSITION 3.2. *Let $(\varrho_n)_{n\in\mathbb{N}^*}$ be a sequence of density matrices such that $\varrho_n\in\mathscr{L}^1(\vee^n\mathscr{Z})$ for each $n\in\mathbb{N}^*$ and assume that $\mathscr{M}(\varrho_n,n\in\mathbb{N}^*)=\{\mu_0\}$. Then the convergence*

$$\lim_{n\to\infty}\mathrm{Tr}[\varrho_n^{(p)}A]=\mathrm{Tr}[\varrho_\infty^{(p)}A],\qquad \textit{with}\qquad \varrho_\infty^{(p)}=\int_{\mathscr{Z}}|z^{\otimes p}\rangle\langle z^{\otimes p}|\,d\mu_0(z),\tag{3.2}$$

holds for any $p\in\mathbb{N}^*$ and any $A\in\mathscr{L}^\infty(\vee^p\mathscr{Z})$.

Proof. (Proof of Proposition 1.1.) Suppose that for each $p\in\mathbb{N}^*$ and each compact operator $A\in\mathscr{L}^\infty(\vee^p\mathscr{Z})$ the sequence $(\mathrm{Tr}[\varrho_n^{(p)}A])_{n\in\mathbb{N}^*}$ converges. Then there exist trace-class operators $0\leq\varrho_\infty^{(p)}\leq 1$, $p\in\mathbb{N}^*$, such that

$$\lim_{n\to\infty}\mathrm{Tr}[\varrho_n^{(p)}A]=\mathrm{Tr}[\varrho_\infty^{(p)}A],\quad \forall A\in\mathscr{L}^\infty(\mathscr{Z}).$$

Let μ be any Wigner measure in $\mathscr{M}(\varrho_n,n\in\mathbb{N}^*)\neq\varnothing$. Then by Proposition 3.2, up to extraction of subsequences, we see that

$$\varrho_\infty^{(p)}=\int_{\mathscr{Z}}|z^{\otimes p}\rangle\langle z^{\otimes p}|\,d\mu(z).$$

So, this provides the existence of a Borel probability measure μ on $\mathscr{Z}$ with the appropriate properties. The uniqueness follows by [3, Proposition 6.15]. □

3.3. Defect of compactness. The convergence in Proposition 3.2 is with respect to the weak-$*$ topology on $\mathscr{L}^1(\vee^p\mathscr{Z})$ which is the topological dual of $\mathscr{L}^\infty(\vee^p\mathscr{Z})$ and the statement (3.2) does not hold in general for all $A\in\mathscr{L}(\vee^p\mathscr{Z})$, $p\in\mathbb{N}^*$. Counterexamples exhibiting this phenomenon of dimensional defect of compactness are given in [3] (we call it in this way because of the similarity with finite dimension, although the source of defect here is the fact the phase-space is of infinite dimension and so bounded sets are not relatively compact in the norm topology). Actually, the extension of (3.2) to all bounded operators $A\in\mathscr{L}(\vee^p\mathscr{Z})$ and $p\in\mathbb{N}^*$ depends on the sequence $(\varrho_n)_{n\in\mathbb{N}^*}$ and it turns out to be an important point in the mean field problem: we need this information when we take the limit $n\to\infty$ in the mean field expansion. Let $(\varrho_n)_{n\in\mathbb{N}^*}$ be a sequence of density matrices such that $\varrho_n\in\mathscr{L}^1(\vee^n\mathscr{Z})$ for each $n\in\mathbb{N}^*$. The reduced density matrices $(\varrho_n^{(p)})_{n\in\mathbb{N}^*}$ weakly converges to $\varrho_\infty^{(p)}\in\mathscr{L}^1(\vee^p\mathscr{Z})$ if

$$\lim_{n\to\infty}\mathrm{Tr}[\varrho_n^{(p)}A]=\mathrm{Tr}[\varrho_\infty^{(p)}A],\quad \forall A\in\mathscr{L}(\vee^p\mathscr{Z}).\tag{3.3}$$

The following proposition provides a strong relationship between the Wigner measures of a sequence of density matrices and the convergence of their reduced density matrices in the $\mathscr{L}^1$-norm topology.

PROPOSITION 3.3. *Let $(\varrho_n)_{n\in\mathbb{N}^*}$ be a sequence of density matrices with $\varrho_n\in\mathscr{L}^1(\vee^n\mathscr{Z})$ for each $n\in\mathbb{N}^*$. Suppose that the reduced density matrices $(\varrho_n^{(p)})_{n\in\mathbb{N}^*}$ weakly converge* *to* $\varrho_\infty^{(p)} \in \mathscr{L}^1(\vee^p \mathscr{Z})$ *for each* $p \in \mathbb{N}^*$ *according to* (3.3)*. Then there exists a unique* $U(1)$*-invariant Borel probability measure* μ_0 *on* $\mathscr{Z}$ *such that for any* $p \in \mathbb{N}^*$*,*

$$\lim_{n\to\infty} ||\varrho_n^{(p)} - \varrho_\infty^{(p)}||_1 = 0, \quad \text{with} \quad \varrho_\infty^{(p)} = \int_{\mathscr{Z}} |z^{\otimes p}\rangle\langle z^{\otimes p}| \, d\mu_0(z).$$

Moreover, μ_0 *is the unique Wigner measure of* $(\varrho_n)_{n\in\mathbb{N}^*}$ *and it is concentrated on the unit sphere* $S(0,1)$ *of* $\mathscr{Z}$ *centred at the origin and of radius one (i.e.,* $\mu_0(S(0,1)) = 1$*).*

Proof. The assumption on $(\varrho_n)_{n\in\mathbb{N}^*}$ implies that $\varrho_\infty^{(p)}$ are non-negative trace class operators with $\mathrm{Tr}[\varrho_\infty^{(p)}] = 1$ and $\varrho_n^{(p)}$ converges to $\varrho_\infty^{(p)}$ with respect to the weak topology in $\mathscr{L}^1(\vee^p \mathscr{Z})$. But since $\varrho_n^{(p)}$ and $\varrho_\infty^{(p)}$ are non-negative trace-class operators with $\mathrm{Tr}[\varrho_n^{(p)}] = 1 = \mathrm{Tr}\left[\varrho_\infty^{(p)}\right]$, the $\mathscr{L}^1$-norm convergence follows according to [1, 18, 51]. In a more general framework, it is said that $\mathscr{L}^1(\vee^p \mathscr{Z})$ has the Kadec–Klee property (KK*) in the weak-$*$ topology (see [41] and references therein). The (KK*) property on a dual Banach space means that the weak-$*$ and norm convergence coincide on the unit sphere.
Thanks to the proof of Proposition 1.1, we know that μ_0 is the unique Wigner measure of the sequence $(\varrho_n)_{n\in\mathbb{N}^*}$. So, the measure μ_0 is $U(1)$-invariant and it is concentrated on the unit ball of $\mathscr{Z}$ according to Theorem 3.1. Now, using the fact that $\mathrm{Tr}[\varrho_\infty^{(p)}] = 1$, we get

$$\int_{\mathscr{Z}} ||z||^{2p} \, d\mu_0(z) = 1, \quad \forall p \in \mathbb{N}^*.$$

This easily yields that the measure is actually concentrated on the unit sphere. ∎

Corollary 3.4. *Let* $(\varrho_n)_{n\in\mathbb{N}^*}$ *be a sequence of density matrices with* $\varrho_n \in \mathscr{L}^1(\vee^n \mathscr{Z})$ *for each* $n \in \mathbb{N}^*$ *and such that* $\mathscr{M}(\varrho_n, n \in \mathbb{N}^*) = \{\mu_0\}$*. The two following conditions are equivalent:*

$$(\mu_0(S(1,0)) = 1) \Leftrightarrow \left(\forall p \in \mathbb{N}^*, \mathscr{L}^1 - \lim_{n\to\infty} \varrho_n^{(p)} = \int_{\mathscr{Z}} |z^{\otimes p}\rangle\langle z^{\otimes p}| \, d\mu_0(z)\right).$$

Proof. Suppose that the Wigner measure μ_0 is concentrated on the unit sphere, then by Proposition 3.2 we see that $(\varrho_n^{(p)})_{n\in\mathbb{N}^*}$ weak-$*$ converges to $\varrho_\infty^{(p)}$ which is a non-negative trace-class operator with $\mathrm{Tr}[\varrho_\infty^{(p)}] = 1$. So, again by the Kadec–Klee property (KK*) of $\mathscr{L}^1(\vee^p \mathscr{Z})$ we obtain the $\mathscr{L}^1$-norm convergence for each $p \in \mathbb{N}^*$. ∎

4. Rate of convergence

In this section we give the proof of our main result (Theorem 1.2). We start by proving an elementary estimate in Subsection 4.1 and then prove the result in Subsection 4.2.

4.1. Preliminary estimate. Instead of estimating the quantities $||\varrho_n^{(p)} - \varrho_\infty^{(p)}||_1$ in the trace norm, we will work essentially with

$$\left| \mathrm{Tr}[\varrho_n A^{\mathrm{Wick}}] - \int_{\mathscr{Z}} \langle z^{\otimes p}, A z^{\otimes p}\rangle \, d\mu_0 \right|.$$

In that way, we can use the mean field expansion based on Wick calculus. The two quantities are comparable and this is given by the lemma below.

LEMMA 4.1. *Let $(\varrho_n)_{n\in\mathbb{N}^*}$ be a sequence of density matrices such that $\varrho_n\in\mathscr{L}^1(\vee^p\mathscr{Z})$ for each $n\in\mathbb{N}^*$ and satisfying the assumptions of Theorem 1.2. Then for any $n,p\in\mathbb{N}^*, n\geq p$:*

$$\left| ||\varrho_n^{(p)}-\varrho_\infty^{(p)}||_1-\sup_{A\neq 0}\frac{|\mathrm{Tr}[\varrho_n A^{\mathrm{Wick}}]-\int_{\mathscr{Z}}\langle z^{\otimes p},Az^{\otimes p}\rangle\, d\mu_0|}{||A||}\right|\leq\frac{(p-1)^2}{n},$$

with μ_0 being the Wigner measure of $(\varrho_n)_{n\in\mathbb{N}^*}$ and

$$\varrho_\infty^{(p)}=\int_{\mathscr{Z}}|z^{\otimes p}\rangle\langle z^{\otimes p}|\, d\mu_0(z).$$

Proof. For any $A\in\mathscr{L}(\vee^p\mathscr{Z})$ and $\varepsilon=\frac{1}{n}$:

$$\mathrm{Tr}[\varrho_n A^{\mathrm{Wick}}]=\frac{n\cdots(n-p+1)}{n^p}\mathrm{Tr}[\varrho_n^{(p)}A]\quad\text{and}\quad \mathrm{Tr}[\varrho_\infty^{(p)}A]=\int_{\mathscr{Z}}\langle z^{\otimes p},Az^{\otimes p}\rangle\, d\mu_0(z).$$

Hence, we get

$$\begin{aligned}\left|\mathrm{Tr}[\varrho_n A^{\mathrm{Wick}}]-\int_{\mathscr{Z}}\langle z^{\otimes p},Az^{\otimes p}\rangle\, d\mu_0\right| &\leq\left|1-\frac{n\cdots(n-p+1)}{n^p}\right| ||A||+|\mathrm{Tr}[\varrho_n^{(p)}A]-\mathrm{Tr}[\varrho_\infty^{(p)}A]|\\ &\leq\left[\left|1-\frac{n\cdots(n-p+1)}{n^p}\right|+||\varrho_n^{(p)}-\varrho_\infty^{(p)}||_1\right]||A||,\end{aligned}$$

and also

$$|\mathrm{Tr}[(\varrho_n^{(p)}-\varrho_\infty^{(p)})A]|\leq\left|1-\frac{n\cdots(n-p+1)}{n^p}\right| ||A||+\left|\mathrm{Tr}[\varrho_n A^{\mathrm{Wick}}]-\int_{\mathscr{Z}}\langle z^{\otimes p},Az^{\otimes p}\rangle\, d\mu_0\right|.$$

The inequality

$$1-\frac{n\cdots(n-p+1)}{n^p}=1-\prod_{j=1}^{p-1}(1-\frac{j}{n})\leq 1-\left(1-\frac{p-1}{n}\right)^{p-1}\leq\frac{(p-1)^2}{n},$$

gives the sought estimate. ∎

4.2. Proof of the main theorem. Recall that $\mu_t=(\Phi_t)_\sharp\mu_0$ in Theorem 1.2, where μ_0 is the unique Wigner measure of the sequence $(\varrho_n)_{n\in\mathbb{N}^*}$ as provided by Proposition 1.1.

LEMMA 4.2. *For any $t\in\mathbb{R}$ such that $|t|<\frac{1}{8||\tilde{Q}||}$:*

$$\mu_t\big(\langle z^{\otimes p},Az^{\otimes p}\rangle\big)=\sum_{k=0}^{\infty}i^k\int_0^t dt_1\cdots\int_0^{t_{k-1}}dt_k\;\mu_0\left(C_0^{(k)}(t_k,\ldots,t_1,t)\right).\tag{4.1}$$

Proof. We know already that the measure μ_0 is concentrated in the ball of radius 1 centred at the origin according to Proposition 1.1. Hence, we deduce the inequality

$$\left|\mu_0\left(C_0^{(k)}(t_k,\ldots,t_1,t)\right)\right|\leq\left\|\widetilde{C_0^{(k)}}(t_k,\ldots,t_1,t)\right\|_{\mathscr{L}(\vee^{p+k}\mathscr{Z})}.$$

The right-hand side of (4.1) is absolutely convergent whenever $|t| < \frac{1}{8||\tilde{Q}||}$ thanks to the estimate (ii) of Lemma 2.7

$$\sum_{k=0}^{\infty} \int_0^t dt_1 \cdots \int_0^{t_{k-1}} dt_k \left|\mu_0\left(C_0^{(k)}(t_k,\ldots,t_1,t)\right)\right| \leq 2^{p-1}||A|| \sum_{k=0}^{\infty} \left(8\,|t|\,||\tilde{Q}||\right)^k.$$

Recall that according to (2.13) the classical solution $t \mapsto z_t$ verifies for any $b \in \mathscr{P}_{p,p}$,

$$b(z_t) = b_t(w_0) + i \int_0^t \{Q_{t_1}, b_t\}(w_{t_1})\, dt_1, \quad \text{with} \quad w_t = e^{it\tilde{h}_0} z_t.$$

Iterating this formula, with $b(z) = \langle z^{\otimes p}, A z^{\otimes p}\rangle$, and using the absolute convergence checked above gives for all $||z|| \leq 1$,

$$\langle z_t^{\otimes p}, A z_t^{\otimes p}\rangle = \sum_{k=0}^{\infty} i^k \int_0^t d_{t_1} \cdots \int_0^{t_{k-1}} dt_k\, C_0^{(k)}(t_k,\ldots,t_1,t;z).$$

Integrating with respect to μ_0 and using the fact that $\mu_t = (\Phi_t)_\sharp \mu_0$ yields (4.1). ∎

Proof. (Proof of Theorem 1.2.) We recall the assumptions of Theorem 1.2. Let $(\alpha(n))_{n\in\mathbb{N}^*}$ be a sequence of positive numbers with $\lim_{n\to\infty} \alpha(n) = \infty$ and such that $(\frac{\alpha(n)}{n})_{n\in\mathbb{N}^*}$ is bounded. Consider $(\varrho_n)_{n\in\mathbb{N}^*}$ and $(\varrho_\infty^{(p)})_{p\in\mathbb{N}^*}$ to be two sequences of density matrices with $\varrho_n \in \mathscr{L}^1(L_s^2(\mathbb{R}^{dn}))$ and $\varrho_\infty^{(p)} \in \mathscr{L}^1(L_s^2(\mathbb{R}^{dp}))$ for each $n,p \in \mathbb{N}^*$. Assume that there exist $C_0 > 0$, $C > 2$, $\gamma \geq 1$ such that for all $n,p \in \mathbb{N}^*$ with $n \geq \gamma p$,

$$\left\|\varrho_n^{(p)} - \varrho_\infty^{(p)}\right\|_1 \leq C_0 \frac{C^p}{\alpha(n)}. \tag{4.2}$$

We first prove the estimate for short times and than extend it to arbitrary times. So, suppose that $|t| < \frac{1}{8C||\tilde{Q}||}$ with $C > 2$ the constant provided by the main assumption. Thanks to Lemma 4.1 it is enough to estimate the quantity $|\mathrm{Tr}[\varrho_n(t)\, A^{\mathrm{Wick}}] - \mu_t(\langle z^{\otimes p}, A z^{\otimes p}\rangle)|$ for any bounded operator $A \in \mathscr{L}(\vee^p \mathscr{Z})$. So, the estimate in Proposition 2.9 yields

$$\left|\mathrm{Tr}[\varrho_n(t)\, A^{\mathrm{Wick}}] - \mu_t\big(\langle z^{\otimes p}, A z^{\otimes p}\rangle\big)\right| \leq C_0 \frac{C^p}{n} ||A|| + \mathfrak{R}(t), \tag{4.3}$$

for some $C_0 > 0$ and

$$\begin{aligned}\mathfrak{R}(t) &= \left|\sum_{k=0}^{\infty} i^k \int_0^t dt_1 \cdots \int_0^{t_{k-1}} dt_k\, \mathrm{Tr}\left[\varrho_n C_0^{(k)}(t_k,\ldots,t_1,t)^{\mathrm{Wick}}\right] - \mu_t\big(\langle z^{\otimes p}, A z^{\otimes p}\rangle\big)\right| \\ &= \left|\sum_{k=0}^{\infty} i^k \int_0^t dt_1 \cdots \int_0^{t_{k-1}} dt_k\, \mathrm{Tr}\left[\varrho_n C_0^{(k)}(t_k,\ldots,t_1,t)^{\mathrm{Wick}}\right] - \mu_0\big(C_0^{(k)}(t_k,\ldots,t_1,t)\big)\right|.\end{aligned}$$

The last equality is a consequence of Lemma 4.2. Using now the main assumption and the fact that $C_0^{(k)}(t_k,\ldots,t_1,t)$ are polynomials in $\mathscr{P}_{p+k,p+k}$, we get the following inequality (we can assume that $t > 0$ without loss of generality)

$$\mathfrak{R}(t) \leq \sum_{k=0}^{\lfloor \frac{n}{\gamma} \rfloor - p} \int_0^t dt_1 \cdots \int_0^{t_{k-1}} dt_k \left|\mathrm{Tr}\left[\varrho_n C_0^{(k)}(t_k,\ldots,t_1,t)^{\mathrm{Wick}}\right] - \mu_0\big(C_0^{(k)}(t_k,\ldots,t_1,t)\big)\right| \tag{4.4}$$

$$+\sum_{k=\lfloor\frac{n}{\gamma}\rfloor-p+1}^{n-p}\int_0^t dt_1\cdots\int_0^{t_{k-1}}dt_k\left|\mathrm{Tr}\left[\varrho_n C_0^{(k)}(t_k,\ldots,t_1,t)^{\mathrm{Wick}}\right]-\mu_0\big(C_0^{(k)}(t_k,\ldots,t_1,t)\big)\right| \tag{4.5}$$

$$+\sum_{k=n-p+1}^{\infty}\int_0^t dt_1\cdots\int_0^{t_{k-1}}dt_k\left|\mu_0\big(C_0^{(k)}(t_k,\ldots,t_1,t)\big)\right|. \tag{4.6}$$

Thanks to the estimate (ii) of Lemma 2.7, the right-hand side of (4.4)–(4.6) is bounded by

$$(4.4)\le\frac{C^p}{\alpha(n)}\sum_{k=0}^{\lfloor\frac{n}{\gamma}\rfloor-p}(8tC||\tilde{Q}||)^k\,||A||\le\frac{C^p}{\alpha(n)}\frac{1}{1-8tC||\tilde{Q}||}\,||A||$$

$$(4.5)\le 2\sum_{k=\lfloor\frac{n}{\gamma}\rfloor-p+1}^{n-p}(8t||\tilde{Q}||)^k\,||A||\le 2\frac{(8t||\tilde{Q}||)^{\lfloor\frac{n}{\gamma}\rfloor-p+1}}{1-8t||\tilde{Q}||}\,||A||$$

$$(4.6)\le\sum_{k=n-p+1}^{\infty}(8t||\tilde{Q}||)^k\,||A||=\frac{(8t||\tilde{Q}||)^{n-p+1}}{1-8t||\tilde{Q}||}\,||A||.$$

Since $|t|<\frac{1}{8C||\tilde{Q}||}$, we easily get the bounds

$$(4.5)\le\frac{C^p}{C^{\lfloor\frac{n}{\gamma}\rfloor}}\frac{2||A||}{1-8t||\tilde{Q}||}\le\lambda\frac{C^p}{\alpha(n)}\frac{2||A||}{1-8t||\tilde{Q}||},$$

$$(4.6)\le\frac{C^p}{C^n}\frac{||A||}{1-8t||\tilde{Q}||}\le\lambda\frac{C^p}{\alpha(n)}\frac{||A||}{1-8t||\tilde{Q}||},$$

with $\lambda=\sup_{n\in\mathbb{N}^*}\frac{\alpha(n)}{C^{\lfloor\frac{n}{\gamma}\rfloor}}$ which depends only on C and the sequence $(\alpha(n))_{n\in\mathbb{N}^*}$. Collecting theses estimates, we conclude that

$$\mathfrak{R}(t)\le\frac{(1+3\lambda)}{1-8tC||\tilde{Q}||}\frac{C^p}{\alpha(n)}\,||A||.$$

So, by Lemma 4.1 there exists $C_1>0$ such that

$$\left\|\varrho_n^{(p)}(t)-\varrho_\infty^{(p)}(t)\right\|_1\le C_1\frac{C^p}{\alpha(n)},$$

uniformly in time whenever $|t|\in[0,\frac{1}{16C||\tilde{Q}||}]$. Now, iterate the same reasoning as much as needed to cover a time interval $[-T,T]$ with $T>0$ arbitrary. Then one gets the existence of $C_T>0$ such that for all $t\in[-T,T]$,

$$\left\|\varrho_n^{(p)}(t)-\varrho_\infty^{(p)}(t)\right\|_1\le C_T\frac{C^p}{\alpha(n)}.$$

∎

5. Examples and numerical simulations

In order to illustrate the main result of this article, it is useful to consider some examples and numerical simulations of states with an increasing degree of correlation. The notion of correlation is quite important in quantum information theory and it is related to the so-called quantum entanglement. So, there are several interesting examples of states in the latter field which are also useful for our purpose (Bell state, cat state, W state, GHZ state, etc.).

Numerical simulations:

In subsections 5.1 and 5.4 we will use some numerical simulations to corroborate the results of the previous sections. Here we outline briefly the dynamical system utilized in these simulations. A detailed presentation of the related numerical methods and results will be given by the third author in a separate article.

The phase space for numerical simulations is $\mathscr{Z}=\ell^2(\mathbb{Z}/K\mathbb{Z})$. It is isomorphic to the finite-dimensional space $\mathbb{C}^K$. That means each particle lies on one of the K sites represented by the set $\mathbb{Z}/K\mathbb{Z}$. The Hilbert space for n boson particles will then be isomorphic to $\vee^n\mathbb{C}^K$. The dynamics is described by the n-particle Hamiltonian

$$\mathbf{H}_n=-\sum_{\nu=1}^{n}\Delta_{disc}^{(\nu)}+\frac{1}{2n}\sum_{\nu,\mu=1}^{n}V(x_\nu-x_\mu), \tag{5.1}$$

where $-\Delta_{disc}^{(\nu)}$ is the discrete Laplacian operator of $\ell^2(\mathbb{Z}/K\mathbb{Z})$ acting on the νth variable and V is a function on $\mathbb{Z}/K\mathbb{Z}\sim\{0,1,\ldots,K-1\}$ defined by $V(x)=\frac{1}{x}$ for any $\{0,1,\ldots,K-1\}\ni x\neq 0$ and $V(0)=0$.

To estimate numerically the rate of convergence, we discretize the time interval $[0,1]$, then we compute the quantity $\max_{t\in\{t_1,\ldots,t_m\}\subset[0,1]}\left\|\varrho_n^{(p)}(t)-\varrho_\infty^{(p)}(t)\right\|_1$. For a better evaluation of the dependence in n of this object, we draw its Logarithm as a function of $\operatorname{Log} n$: an order of convergence $O(n^{-a})$ will be given by a straight line with slope $-a$ in the graph.

5.1. Product states. This is the most known example in mean field theory. It appears in the literature under the name of chaos, factorized, product or also Hermite states. It emphasizes the fact that, in the mean field limit, states $\varphi^{\otimes n}$ that are prepared uncorrelated will evolve into states which are close to be uncorrelated, namely $\varphi_t^{\otimes n}$ where φ_t is a solution of the Hartree equation (1.2) with initial condition φ. It is easy to see that the factorized states

$$\varrho_n=|\varphi^{\otimes n}\rangle\langle\varphi^{\otimes n}|, \quad \text{with } ||\varphi||=1,$$

satisfy the assumption of Theorem 1.2. In fact, the p-reduced density matrices of ϱ_n coincide with the limit

$$\varrho_n^{(p)}=|\varphi^{\otimes p}\rangle\langle\varphi^{\otimes p}|=\varrho_\infty^{(p)}. \tag{5.2}$$

This means that in this example the rate of convergence at initial time $t=0$ is arbitrarily fast. Remember that according to Theorem 1.2 the p-particle reduced density matrix $\varrho_\infty^{(p)}(t)$ is

$$\varrho_\infty^{(p)}(t)=\int_{\mathscr{Z}}|z^{\otimes p}\rangle\langle z^{\otimes p}|\,d\mu_t(z)=|\varphi_t^{\otimes p}\rangle\langle\varphi_t^{\otimes p}| \quad \text{with} \quad \mu_t=\frac{1}{2\pi}\int_0^{2\pi}\delta_{e^{i\theta}\varphi_t}\,d\theta,$$

where φ_t is a solution of the nonlinear field equation (2.11). Using the numerical simulation described in Subsection 5, we see that for the first marginal

$$\max_{t\in\{t_1,\ldots,t_m\}\subset[0,1]}\operatorname{Log}\left\|\varrho_n^{(1)}(t)-\varrho_\infty^{(1)}(t)\right\|_1=-(1+\varepsilon)\operatorname{Log}(n)+O(1);$$

with a deviation $\varepsilon\simeq-0.06$ well within the expected computational inaccuracy (see Figure 5.1). This is in very good agreement with our mathematical prevision, and indicates that the estimate in Theorem 1.2 is not far from being optimal, in some sense.

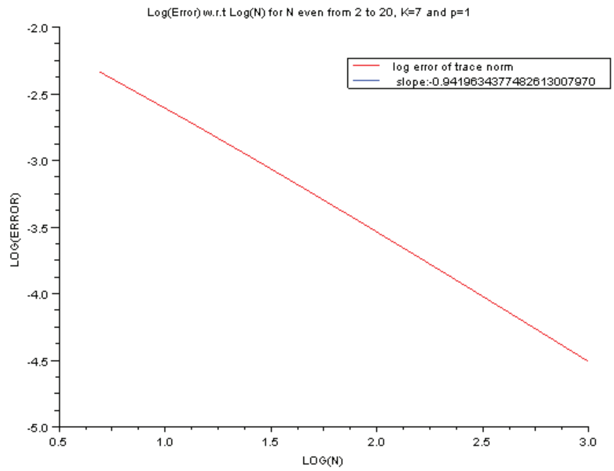

Fig. 5.1. *Log-Log plot for factorized states.*

5.2. W states. The W state is a multi-partite n-qubit entangled quantum state

$$|W\rangle = \frac{1}{\sqrt{n}}(|100...0\rangle + |010...0\rangle + \ldots + |00...01\rangle),$$

where $|1\rangle$ denotes a one particle excited state and $|0\rangle$ denotes the one particle ground state of two mode system. More generally, if $\mathscr{Z}$ is a Hilbert space and φ, ψ are two normalized orthogonal vectors in $\mathscr{Z}$ then

$$|W\rangle = \frac{1}{\sqrt{n}}(|\psi \otimes \varphi^{\otimes n-1}\rangle + |\varphi \otimes \psi \otimes \varphi^{\otimes n-2}\rangle + \cdots + |\varphi^{\otimes n-1} \otimes \psi\rangle). \tag{5.3}$$

Lemma 5.1. *Let $(\varrho_n)_{n\in\mathbb{N}^*}$ denotes a sequence of W states as in (5.3). Then for all $n, p \in \mathbb{N}^*$ such that $n \geq p$:*

$$||\varrho_n^{(p)} - \varrho_\infty^{(p)}||_1 \leq 2\,\frac{p}{n} \qquad \textit{with} \qquad \varrho_\infty^{(p)} = |\varphi^{\otimes p}\rangle\langle\varphi^{\otimes p}|.$$

Proof. A simple computation yields for any $A \in \mathscr{L}(\vee^p \mathscr{Z})$:

$$\langle W, A \otimes 1^{\otimes(n-p)} W\rangle = \frac{n-p}{n}\langle \varphi^{\otimes p}, A\varphi^{\otimes p}\rangle + \frac{p}{n}\langle W_p, AW_p\rangle,$$

where $|W_p\rangle = \frac{1}{\sqrt{p}}\big(\psi \otimes \varphi^{\otimes(p-1)} + \cdots + \varphi^{\otimes(p-1)} \otimes \psi\big)$. So that the p-reduced density matrices of ϱ_n is

$$\begin{aligned}\varrho_n^{(p)} &= \frac{n-p}{n}\,|\varphi^{\otimes p}\rangle\langle\varphi^{\otimes p}| + \frac{p}{n}\,|W_p\rangle\langle W_p| \\ &= \frac{n-p}{n}\,\varrho_\infty^{(p)} + \frac{p}{n}\,|W_p\rangle\langle W_p|,\end{aligned}$$

Hence the estimate follows since W_p is a normalized vector. $\square$

5.3. GHZ states. The GHZ (Greenberger–Horne–Zeilinger) state is a multipartite entangled quantum state. In a two-mode system it is given by the formula

$$|\mathrm{GHZ}\rangle = \frac{|0\rangle^{\otimes n} + |1\rangle^{\otimes n}}{\sqrt{2}},$$

So, it can be generalized as follows

$$|\mathrm{GHZ}\rangle = \frac{|\varphi\rangle^{\otimes n} + |\psi\rangle^{\otimes n}}{\sqrt{2}}, \tag{5.4}$$

where φ and ψ are two normalized (orthogonal) vectors in a given Hilbert space $\mathscr{Z}$. So, the n-partite GHZ states are superposition of uncorrelated states and it is again easy to check that their p-reduced density matrices coincide with their limit as in (5.2). Hence, Theorem 1.2 provides a rate of convergence for this example too with $\alpha(n) = n$ rate.

5.4. Twin states. Let $\varphi_1, \varphi_2 \in \mathscr{Z}$ be two normalized orthogonal vectors. The *twin states* are rank one projectors $\varrho_n = |\Psi_n\rangle\langle\Psi_n|$ given by

$$\Psi_n = \sqrt{\frac{n!}{n_1! n_2!}}\, \mathcal{S}_n \varphi_1^{\otimes n_1} \otimes \varphi_2^{\otimes n_2}, \tag{5.5}$$

with $n = n_1 + n_2$ and $n_1 = n_2 \in \mathbb{N}^*$. This sequence of states have a unique Wigner measure μ computed in [5]. So, after identification of the Hilbert space $\mathscr{Z}$ as $\mathbb{C}\varphi_1 \times \mathbb{C}\varphi_2 \times \mathscr{Z}_1^{\perp}$, with $\mathscr{Z}_1^{\perp}$ the orthogonal subspace to $\mathbb{C}\varphi_1 \oplus \mathbb{C}\varphi_2$, the measure μ reads

$$\mu = \delta^{S^1}_{\frac{\varphi_1}{\sqrt{2}}} \otimes \delta^{S^1}_{\frac{\varphi_2}{\sqrt{2}}} \otimes \delta_0^{\perp} \quad \text{with} \quad \delta^{S^1}_{\frac{\varphi_j}{\sqrt{2}}} = \frac{1}{2\pi}\int_0^{2\pi} \delta_{e^{i\theta}\frac{\varphi_j}{\sqrt{2}}}\, d\theta,\ j = 1,2. \tag{5.6}$$

Remark that in this example the measure $\mu_t = (\Phi_t)_\sharp \mu$ is quite correlated because of the nonlinear effect of the flow and the situation differs significantly from the simple picture of uncorrelated states (here Φ_t is the flow of the nonlinear field equation (2.11)).

LEMMA 5.2. *Let $(\varrho_n)_{n\in\mathbb{N}^*}$ be a sequence of twin states with μ its Wigner measure given in* (5.6). *Then for any $n, p \in \mathbb{N}^*$ such that $n \geq 2p$:*

$$\left\| \varrho_n^{(p)} - \varrho_\infty^{(p)} \right\|_1 \leq 2^p \frac{p^2}{n-p} \qquad \textit{with} \qquad \varrho_\infty^{(p)} = \int_{\mathscr{Z}} |z^{\otimes p}\rangle\langle z^{\otimes p}|\, d\mu.$$

Proof. Let Ψ_n be the vector given by (5.5). A simple computation yields

$$\langle \Psi_n, A \otimes 1^{\otimes(n-p)}\Psi_n\rangle = \frac{n!}{n_1! n_2!}\frac{1}{(n!)^2} \sum_{\sigma,\pi\in\mathfrak{S}(n)} \langle T_\sigma \varphi_1^{\otimes n_1} \otimes \varphi_2^{\otimes n_2}, A \otimes 1^{\otimes(n-p)} T_\pi \varphi_1^{\otimes n_1} \otimes \varphi_2^{\otimes n_2}\rangle,$$

where T_σ denotes the operator on $\otimes^n \mathscr{Z}$ defined for any $\sigma \in \mathfrak{S}(n)$ by

$$T_\sigma f_1 \otimes \cdots \otimes f_n = f_{\sigma_1} \otimes \cdots \otimes f_{\sigma_n}.$$

For $m, n \in \mathbb{N}$, $k \leq m$, we denote

$$\mathcal{I}_m^{(k)} = \left\{ i : \{1, \ldots, m\} \to \{1, 2\}, \sharp i^{-1}(\{1\}) = k \right\}.$$

So, there is a correspondence between permutations $\sigma \in \Sigma_n$ and maps $i \in \mathcal{I}_n^{(n_1)}$ according to

$$T_\sigma \varphi_1^{\otimes n_1} \otimes \varphi_2^{\otimes n_2} = \varphi_{i(1)} \otimes \cdots \otimes \varphi_{i(n)} =: \varphi(i). \tag{5.7}$$

Since the cardinality of the set of $\sigma\in\Sigma(n)$ such that (5.7) holds for the same $i\in\mathcal{I}_n^{(n_1)}$ is equal to $n_1!n_2!$, we see that

$$\langle\Psi_n, A\otimes 1^{\otimes(n-p)}\,\Psi_n\rangle = \frac{n!}{n_1!n_2!}\left(\frac{n_1!n_2!}{n!}\right)^2 \sum_{i,j\in\mathcal{I}_n^{(n_1)}} \langle\varphi(i), A\otimes 1^{\otimes(n-p)}\,\varphi(j)\rangle.$$

In the above sum if $i\neq j$ on the set $\{p+1,\dots,n\}$ then the scalar product is null because of the orthogonality condition on the vectors φ_1,φ_2. So this simplifies the sum and actually we can decompose it according to the number of occurrence of φ_1 in the first p vectors constituting $\varphi(i)$, i.e.,

$$\mathcal{I}_n^{(n_1)} = \cup_{k=0}^p \left\{ i\in\mathcal{I}_n^{(n_1)}, \sharp i^{-1}(\{1\})\cap\{1,\dots,p\}=k\right\} =: \cup_{k=0}^p \mathcal{I}_{n,k}^{(n_1)}.$$

Hence,

$$\langle\Psi_n, A\otimes 1^{\otimes(n-p)}\,\Psi_n\rangle = \frac{n_1!n_2!}{n!}\sum_{k=0}^p \sum_{i\in\mathcal{I}_{n,k}^{(n_1)}} \sum_{j\in\mathcal{I}_n^{(n_1)}, j=i_{|p+1,\dots,n}} \langle\varphi(i), A\otimes 1^{\otimes(n-p)}\,\varphi(j)\rangle.$$

If we fix the first p values of i and j and vary the $(n-p)$ others then the scalar product $\langle\varphi(i), A\otimes 1^{\otimes(n-p)}\varphi(j)\rangle$ will not change as long as $j=i_{|\{p+1,\dots,n\}}$. Actually, there are $C_{n-p}^{n_1-k}$ configurations for each choice of $i(1),\dots,i(p),j(1),\dots,j(p)$ such that $\sharp i^{-1}(\{1\})\cap\{1,\dots,p\}=\sharp j^{-1}(\{1\})\cap\{1,\dots,p\}=k$. Hence, we get

$$\langle\Psi_n, A\otimes 1^{\otimes(n-p)}\,\Psi_n\rangle = \frac{n_1!n_2!}{n!}\sum_{k=0}^p C_{n-p}^{n_1-k} \sum_{i\in\mathcal{I}_p^{(k)}} \sum_{j\in\mathcal{I}_p^{(k)}} \langle\varphi(i), A\varphi(j)\rangle.$$

Observe that for all $0\leq k\leq p$ and $2p\leq n$:

$$\lim_{n\to\infty}\frac{C_{n-p}^{n_1-k}}{C_n^{n_1}} = \frac{1}{2^p}.$$

So, we see that the limit of the p-reduced density matrices is

$$\varrho_\infty^{(p)} = \frac{1}{2^p}\sum_{k=0}^p |\psi_k\rangle\langle\psi_k| = \int_{\mathscr{Z}} |z^{\otimes p}\rangle\langle z^{\otimes p}|\,d\mu, \quad \text{with} \quad \psi_k = \sum_{i\in\mathcal{I}_p^{(k)}} \varphi(i),$$

where μ is the Wigner measure of the sequence $(\varrho_n)_{n\in\mathbb{N}^*}$ given in (5.6). In particular, the orthogonality of the family $(\psi_k)_{1,\dots,p}$ gives

$$1 = ||\varrho_\infty^{(p)}||_1 = \frac{1}{2^p}\sum_{k=0}^p \left\|\psi_k\right\|^2$$

Therefore a simple estimate yields

$$\begin{aligned}\left\|\varrho_n^{(p)} - \varrho_\infty^{(p)}\right\|_1 &\leq \max_{k=1,\dots,p}\left|1-2^p\frac{C_{n-p}^{n_1-k}}{C_n^{n_1}}\right| \sum_{k=0}^p \frac{1}{2^p}||\psi_k||^2 \\ &\leq \max_{k=1,\dots,p}\left|1-2^p\frac{C_{n-p}^{n_1-k}}{C_n^{n_1}}\right|.\end{aligned}$$

So, the result follows once we prove

$$\max_{k=1,\ldots,p}\left|1-2^p\frac{C_{n-p}^{n_1-k}}{C_n^{n_1}}\right|\leq 2^p\frac{p^2}{n-p}.$$

In fact, for any $(a_i)_{1,\ldots,r}$ such that $0\leq a_i\leq 1$ the following simple estimates hold true

$$0\leq 1-\prod_{i=1}^{r}(1-a_i)\leq r\max_{1,\ldots,r}a_i \tag{5.8}$$

$$0\leq\prod_{i=1}^{r}(1+a_i)-1\leq 2^{r-1}r\max_{1,\ldots,r}a_i. \tag{5.9}$$

By writing

$$2^p\frac{C_{n-p}^{n_1-k}}{C_n^{n_1}}=\underbrace{\prod_{i=1}^{k-1}\left(1-\frac{i}{n-i}\right)\times\prod_{j=k+1}^{p-k-1}\left(1-\frac{j-k}{n-k-j}\right)}_{T_1}\times\overbrace{\prod_{s=0}^{\min(p-k-1,k-1)}\left(1+\frac{k-s}{n-k-s}\right)}^{T_2}$$

we can see that the product $T_1=\prod_{i=1}^{p}(1-\beta_i)$ while the last one is $T_2=\prod_{j=1}^{p}(1+\gamma_j)$ with $0\leq\beta_i,\gamma_j\leq 1$ (some of the β_i,γ_j are null). Hence, applying (5.8)–(5.9), we obtain

$$\begin{aligned}|1-T_1T_2|&\leq|T_1|\,(T_2-1)+(1-T_1)\\&\leq 2^{p-1}p\max_{1,\ldots,p}\gamma_j+p\max_{1,\ldots,p}\beta_i\\&\leq 2^{p-1}p\frac{p}{n-p}+p\frac{p}{n-p}.\end{aligned}$$

∎

Again, the numerical simulation for the first marginal indicates a $1/n$ order of convergence (Figure 5.2).

Finally, we bring to reader's attention the fact that any rate of convergence is actually possible. In fact take the following example

$$\varrho_n=\left(1-\frac{1}{\alpha(n)}\right)|e_1^{\otimes n}\rangle\langle e_1^{\otimes n}|+\frac{1}{\alpha(n)}|e_2^{\otimes n}\rangle\langle e_2^{\otimes n}|,$$

with $(\alpha(n))_{n\in\mathbb{N}^*}$ such that $\alpha(n)\geq 1$, $\alpha(n)\to\infty$, and e_1,e_2 are two normalized orthogonal vectors. So, it is easy to see that

$$\varrho_n^{(p)}=\left(1-\frac{1}{\alpha(n)}\right)|e_1^{\otimes p}\rangle\langle e_1^{\otimes p}|+\frac{1}{\alpha(n)}|e_2^{\otimes p}\rangle\langle e_2^{\otimes p}|\quad\text{and}\quad\varrho_\infty^{(p)}=|e_1^{\otimes p}\rangle\langle e_1^{\otimes p}|.$$

Therefore, for each $p\in\mathbb{N}^*$, the following equality is satisfied:

$$\left\|\varrho_n^{(p)}-\varrho_\infty^{(p)}\right\|_1=\frac{2}{\alpha(n)}.$$

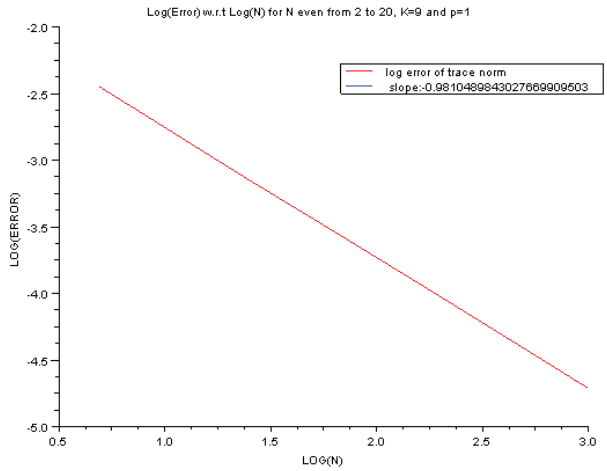

FIG. 5.2. *Log-Log plot for twin states.*

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