Mean field limit for bosons and propagation of Wigner measures

Z. Ammari*  F. Nier †

July 2008

Abstract

We consider the $N$-body Schrödinger dynamics of bosons in the mean field limit with a bounded pair-interaction potential. According to the previous work [AmNi], the mean field limit is translated into a semiclassical problem with a small parameter $\epsilon \to 0$, after introducing an $\epsilon$-dependent bosonic quantization. The limit is expressed as a push-forward by a nonlinear flow (e.g. Hartree) of the associated Wigner measures. These object and their basic properties were introduced in [AmNi] in the infinite dimensional setting. The additional result presented here states that the transport by the nonlinear flow holds for rather general class of quantum states in their mean field limit.

2000 Mathematics subject classification: 81S30, 81S05, 81T10, 35Q55

1 Introduction

The mathematical analysis of the mean field limit of the $N$-body quantum dynamics of bosons started with the work of [Hep] and [GiVe]. Since, the problem has experienced intensive investigations using mainly the so-called BBGKY hierarchy method explained in [Spo]. Interest was focused on studying the cases of singular interaction potential (see for example [BGM], [EY], [BEGMY], [ESY]).

Recently, a new method was given in [FGS] (see also [FKP]) for a scalar bounded potential which inspires this work. The convergence of the quantum dynamics are typically tested on the above quoted articles, either on coherent states or on Hermite states. Even when such specific choices are avoided, the convergence on arbitrary states still has to be studied.

In the work [AmNi], Wigner measures were extended to the infinite dimensional setting, as Borel probability measures under general assumptions. It was also explained how previous weak formulations of the mean field limit are contained in the definition of these asymptotic Wigner measures, after a reformulation of the $N$-body problem as a semiclassical problem with the small parameter $\epsilon = \frac{1}{N} \to 0$. The basic properties of these Wigner measures were considered and they were used to check that the mean field dynamics for the coherent states and Hermite states are essentially equivalent.

In this paper, the problem of the mean field dynamics is considered under some restrictive assumptions on the initial data. The convergence of $N$-body Schrödinger dynamics of bosons in the mean field limit will be proved for a class of density operator sequences, which contains all the common examples. Remember that contrary to the finite dimensional case no natural pseudodifferential calculus can be deformed by arbitrary nonlinear flows, and the propagation of Wigner measures as dual objects cannot be straightforward in the infinite dimensional case. The limit is expressed as push-forward by a nonlinear flow (e.g. Hartree) of Wigner measures associated with the sequence of density operators. The result holds here when the pair interaction potential is bounded on $L^2(\mathbb{R}^{2d})$.

*Département de Mathématiques, Université de Cergy-Pontoise UMR-CNRS 8088, 2, avenue Adolphe Chauvin 95302 Cergy-Pontoise Cedex France. Email: zied.ammari@u-cergy.fr
†IRMAR, UMR-CNRS 6625, Université de Rennes I, campus de Beaulieu, 35042 Rennes Cedex, France. Email: francis.nier@univ-rennes1.fr
This can be considered as a regular case and subsequent work will be devoted to more singular cases like in [FKS] with a Coulombic interaction $V(x - y) = \frac{1}{x^2}$ or in the derivation of cubic nonlinear Schrödinger equations with $V(x - y) = \delta(x - y)$ like in the [ESY].

Since in the literature the non relativistic and the semi-relativistic dynamics of bosons were both studied (see [ESSc]), an abstract setting for the linear part of the flow seems relevant. Examples are reviewed in the last section.

We keep the same notations as in [AmNi]. The phase-space, a complex separable Hilbert space, is denoted by $Z$ with the scalar product $(\ldots)$. The symmetric Fock space on $Z$ is denoted by $H$ and $\bigwedge^n Z$ is the $n$-fold symmetric (Hilbert) tensor product, so that $H = \bigoplus_{n\in\mathbb{N}} \bigwedge^n Z$ as a Hilbert direct sum. Algebraic direct sums or tensor products are denoted with a $\text{alg}$ superscript. Hence $H_0 = \bigoplus_{n\in\mathbb{N}} \bigwedge^n Z$ denotes the subspace of vectors with a finite number of particles. For any $p, q \in \mathbb{N}$, the space $\mathcal{P}_{p,q}(Z)$ of complex-valued polynomials on $Z$ is defined with the following continuity condition: $b \in \mathcal{P}_{p,q}(Z)$ iff there exists a unique $\tilde{b} \in L(\bigwedge^p Z, \bigwedge^q Z)$ such that:

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

The subspace of $\mathcal{P}_{p,q}(Z)$ made of polynomials $b$ such that $\tilde{b}$ is a compact operator is denoted by $\mathcal{P}^m_{p,q}(Z)$. The Wick monomial of symbol $b \in \mathcal{P}_{p,q}(Z)$ is the linear operator $b^{\text{Wick}} : H_0 \to H_0$ defined as follows:

$$b^{\text{Wick}}|_{\bigwedge^p Z} = 1_{[p, +\infty)}(n) \sqrt{n!(n + q - p)!} (n - p)! e^{\frac{1}{2}y + \partial n \cdot \tilde{b} \otimes I_{n-p} Z},$$

where $\partial$ is the symmetrization orthogonal projection from $\bigotimes^n Z$ onto $\bigwedge^n Z$. Remark that $b^{\text{Wick}}$ depends on the scaling parameter $y$.

Consider a polynomial $Q \in \mathcal{P}_{2,2}(Z)$ such that $\tilde{Q} \in L(\bigwedge^2 Z)$ is bounded symmetric. The many-body quantum Hamiltonian of bosons is a self-adjoint operator on $H$ having the general shape:

$$H_\varepsilon = d\Gamma(A) + Q^{\text{Wick}},$$

where $A$ is a given self-adjoint operator on $Z$. The time evolution of the quantum system is given by $U_\varepsilon(t) = e^{-itH_\varepsilon}$ and $U_\varepsilon^{(0)}(t) = e^{-it\frac{d\Gamma(A)}{dt}}$ for the free motion. The commutation $[Q^{\text{Wick}}, N] = 0$ with the number operator $N = d\Gamma(1) = |z|^2$ Wick ensures the essential self-adjointness of $H_\varepsilon$ on $\mathcal{P}(d\Gamma(A)) \cap H_0$ and the fact that both dynamics preserve the number.

Now we turn to the description of the nonlinear classical dynamics analogues of (1).

Let us first recall some notations from [AmNi]. Polynomials in $\mathcal{P}_{p,q}(Z)$ admit Fréchet differentials. For $b \in \mathcal{P}_{p,q}(Z)$, set

$$\partial_b(z)[u] = \frac{\partial b(z)}{\partial z} u |_{\partial z = 0}, \quad \partial_b(z)[u] = \frac{\partial b(z)}{\partial z} u |_{\partial z = 0},$$

where $\partial$ and $\partial$ are the usual derivatives over $\mathbb{C}$. Moreover, $\partial^k b(z)$ naturally belongs to $(\bigwedge^p Z)^* \times (\bigwedge^q Z)^*$ (i.e.: $k$-linear symmetric functionals) while $\partial^k b(z)$ is identified via the scalar product with an element of $\bigwedge^k Z$, for any fixed $z \in Z$. For $b_1 \in \mathcal{P}_{p,q_1}(Z)$, $i = 1, 2$ and $k \in \mathbb{N}$, set

$$\partial_{b_1} \partial_{b_2}(z) = \langle \partial^k b_1(z), \partial^k z\partial_{b_2}(z) \rangle_{\bigwedge^k Z} \in \mathcal{P}_{p_1 + p_2 - k, q_1 + q_2 - k}(Z).$$

The multiple Poisson brackets are defined by

$$\{b_1, b_2\}^{(k)} = \partial^k b_1 \partial^k b_2 - \partial^k b_2 \partial^k b_1, \quad \{b_1, b_2\} = \{b_1, b_2\}^{(1)}.$$ 

The energy functional

$$h(z) = \langle z, Az \rangle + Q(z), \quad z \in \mathcal{P}(A),$$

has the associated vector field $X : \mathcal{P}(A) \to Z, X(z) = Az + \partial_z Q(z)$ and the nonlinear field equation

$$i\partial_t z = X(z).$$
with initial condition $z_0 = z \in \mathcal{D}(A)$. For our purpose, we only need the integral form of the later equation

$$z_t = e^{-itA}z - i \int_0^t e^{-i(t-s)A} \partial_t Q(z_s) \, ds, \quad \text{for } z \in \mathcal{Z}.$$  \tag{2}

The standard fixed point argument implies that (2) admits a unique global $C^0$-flow on $\mathcal{Z}$ which is denoted by $F : \mathbb{R} \times \mathcal{Z} \to \mathcal{Z}$ (i.e.: $F$ is a $C^0$-map satisfying $F_{t+s}(z) = F_t \circ F_s(z)$ and $F_t(z)$ solves (2) for any $z \in \mathcal{Z}$). While considering the evolution of the Wick symbols, the action of the free flow $e^{-itA}$ will be summarized by the next notation:

$$b_t = b \circ e^{-itA} : \mathcal{Z} \ni z \mapsto b_t(z) = b(e^{-itA}z), \quad b_t \in \oplus_{p,q \in \mathbb{N}} \mathcal{P}_{p,q}(\mathcal{Z}),$$  \tag{3}

for any $b \in \oplus_{p,q \in \mathbb{N}} \mathcal{P}_{p,q}(\mathcal{Z})$ and any $t \in \mathbb{R}$. Moreover, if $z_t$ solves (2), and $Q_t$ is defined according to (3), then $w_t = e^{itA}z_t$ solves the differential equation

$$\frac{d}{dt} w_t = -i \partial_t Q_t(w_t).$$

This yields for any $z \in \mathcal{Z}$ and $b \in \oplus_{p,q \in \mathbb{N}} \mathcal{P}_{p,q}(\mathcal{Z})$, the Duhamel formula

$$b \circ F_t(z) = b_t(z) + i \int_0^t \{Q_t, b_{t-t_1}\} \circ F_t(z) \, dt_1,$$  \tag{4}

by observing that $\{Q_t, b_{t-t_1}\}(z_t) = \{Q, b_{t-t_1}\}(z_t)$.

2 Results

While introducing or using Wigner measures, all the arguments are carried out with extracted sequences (or subsequences) $(\varepsilon_n)_{n \in \mathbb{N}}$ such that $\lim_{n \to \infty} \varepsilon_n = 0$, instead of considering a non countable range $(0, \mathcal{I})$, $\mathcal{I} > 0$, of values for the small parameter $\varepsilon$. Without loss of generality (see [AmNi]) one can consider a countable family $(\rho_{\varepsilon_n})_{n \in \mathbb{N}}$ of density matrices, $\rho_{\varepsilon_n} \geq 0$, $\text{Tr}[\rho_{\varepsilon_n}] = 1$, and test them with $\varepsilon_n$-quantized (Wick, Weyl or anti-Wick) observables before taking the limit $\varepsilon_n \to 0$. For the sake of conciseness, the $\varepsilon$ or $\varepsilon_n$ parameter does not appear in the notations of quantized observables.

The first condition which characterizes our class of $\varepsilon_n$-dependent density matrices reads:

$$\exists \lambda > 0 : \forall k \in \mathbb{N}, \quad \text{Tr}[N^k \rho_{\varepsilon_n}] \leq \lambda^k \quad \text{uniformly in } n \in \mathbb{N}, (N = N_{\varepsilon_n}).$$  \tag{H0}

Wigner measures were constructed in [AmNi] Corollary 6.14 for the sequence $(\rho_{\varepsilon_n})_{n \in \mathbb{N}}$. Possibly extracting a subsequence still denoted $(\varepsilon_n)_{n \in \mathbb{N}}$, there exists a Borel probability measure $\mu$ called Wigner measure such that:

$$\lim_{\varepsilon_n \to 0} \text{Tr}[\rho_{\varepsilon_n} b^{\text{Wick}}] = \int_{\mathcal{Z}} b(z) \, d\mu(z), \quad \text{for any } b \in \oplus_{\alpha,\beta \in \mathbb{N}} \mathcal{P}_{\alpha,\beta}(\mathcal{Z}),$$  \tag{5}

with again $b^{\text{Wick}} = b^{\text{Wick}}_{\varepsilon_n}$.

The statement (5) does not hold in general for all $b \in \oplus_{\alpha,\beta \in \mathbb{N}} \mathcal{P}_{\alpha,\beta}(\mathcal{Z})$ and counterexamples exhibiting the phenomenon of dimensional defect of compactness were given in [AmNi]. The extension of (5) to the larger class of symbols $\oplus_{\alpha,\beta \in \mathbb{N}} \mathcal{P}_{\alpha,\beta}(\mathcal{Z})$ depends on the sequence $(\rho_{\varepsilon_n})_{n \in \mathbb{N}}$ and it turns out to be an important fact when studying the mean field limit. In the following, a sequence $(\rho_{\varepsilon_n})_{n \in \mathbb{N}}$ with a single Wigner measure $\mu$ will have the property (P) when:

$$\lim_{\varepsilon_n \to 0} \text{Tr}[\rho_{\varepsilon_n} b^{\text{Wick}}] = \int_{\mathcal{Z}} b(z) \, d\mu(z), \quad \text{for any } b \in \oplus_{\alpha,\beta \in \mathbb{N}} \mathcal{P}_{\alpha,\beta}(\mathcal{Z}).$$  \tag{P}

Here is the main theorem.
Theorem 2.1 Let the sequence \((\rho_{e_n})_{n\in\mathbb{N}}\) of density matrices, \(\rho_{e_n} \geq 0, \operatorname{Tr}[\rho_{e_n}] = 1, \lim_{n \to \infty} \varepsilon_n = 0\), satisfy (H0) and (P). Then the limit
\[
\lim_{n \to \infty} \operatorname{Tr}[\rho_{e_n} e^{i \frac{1}{e_n} H_{e_n}} b_{\text{Wick}} e^{-i \frac{1}{e_n} H_{e_n}}] = \int_{\mathfrak{F}} (b \circ F_l)(z) \, d\mu,
\]
holds for any \(t \in \mathbb{R}\) and any \(b \in \bigoplus_{\alpha, \beta \in \mathbb{N}} \mathcal{D}_{\alpha, \beta}(\mathfrak{F})\) with \(b_{\text{Wick}} = b_{e_n}^{\text{Wick}}\).

Remark 2.2 Since \(F\) is a \(C^0\)-map the r.h.s. of (6) can be written as
\[
\int_{\mathfrak{F}} (b \circ F_l)(z) \, d\mu = \int_{\mathfrak{F}} b(z) \, d\mu_1,
\]
where \(\mu_1\) is a push-forward measure defined by \(\mu_1(B) = \mu(F^{-1}(B))\) for any Borel set \(B\).

We refer the reader to [AmNi] for the definition of Weyl observables and the Schwartz class of cylindrical functions \(\mathcal{S}(\mathfrak{F})\).

Corollary 2.3 Let the sequence \((\rho_{e_n})_{n\in\mathbb{N}}\) of density matrices, \(\rho_{e_n} \geq 0, \operatorname{Tr}[\rho_{e_n}] = 1, \lim_{n \to \infty} \varepsilon_n = 0\), satisfy (H0) and (P). Then the limit
\[
\lim_{e_n \to 0} \operatorname{Tr}[\rho_{e_n} e^{i \frac{1}{e_n} H_{e_n}} b_{\text{Wick}} e^{-i \frac{1}{e_n} H_{e_n}}] = \int_{\mathfrak{F}} b \circ F_l(z) \, d\mu,
\]
holds for any \(b \in \mathcal{S}(\mathfrak{F})\) and any \(t \in \mathbb{R}\).

Proof. A consequence of Thm. 2.1 and [AmNi] Prop. 6.15 is that the sequence
\[
\rho_{e_n}(t) = U_{e_n}(t) \rho_{e_n} U_{e_n}(t)^*\]
admits a single Wigner measure given by \(\mu_t\). Hence, by definition
\[
\lim_{e_n \to 0} \operatorname{Tr}[\rho_{e_n}(t) b_{\text{Wick}}] = \lim_{e_n \to 0} \int_{\mathfrak{F}} \mathcal{F}[b](\xi) \operatorname{Tr}[\rho_{e_n}(t) W(\sqrt{2} \pi \xi)] L_p(d\xi)
\]
\[
= \int_{\mathfrak{F}} \mathcal{F}[b](\xi) \int_{\mathfrak{F}} e^{2\pi i \text{Re}(z, \xi)} d\mu(z) L_p(d\xi).
\]

Another formulation states that the Wigner measure \(\mu_t\) satisfies a transport equation in an integral form.

Corollary 2.4 Let \((\rho_{e_n}(t))_{n\in\mathbb{N}}\) be as above and let \(\mu_t\) denote its Wigner measure. Then \(t \in \mathbb{R} \mapsto \mu_t\) is a solution to the transport equation:
\[
\mu_t(b) = \mu_0^0(b) + i \int_0^t \mu_s(\{Q, b_{t-s}\}) ds,
\]
for any \(b \in \bigoplus_{\alpha, \beta \in \mathbb{N}} \mathcal{D}(\mathfrak{F})\) and where \(\mu_0^0(B) = \mu(e^{-\mu A} B)\) for any borel set \(B\).

Proof. The relation (8) is given by testing (4) on \(\mu = \mu_0\).

3 Criteria for the property \((P)\)

In the following, two conditions which ensure the property \((P)\) are formulated. Recall that for any \(P \in \mathcal{L}(\mathfrak{F})\) the operator \(\Gamma(P)\) acting on \(\mathcal{H}\) is defined by
\[
\Gamma(P)|_{\mathfrak{F}} = P \otimes P \cdots \otimes P
\]
and \(\Gamma(P)\) is an orthogonal projector if \(P\) is too. The first criterion is a ‘tightness’ assumption with respect to the trace norm of the state
\[
\forall \eta > 0, \exists P \in \mathcal{L}(\mathfrak{F}) \text{ finite rank orthogonal projector}, \forall n \in \mathbb{N}: \operatorname{Tr}[(1 - \Gamma(P)) \rho_{e_n}] < \eta \quad (T).
\]
The dual version is formulated as an equicontinuity assumption with respect to the Wick symbols:

\[ \forall p, q \in \mathbb{N}, \forall \eta > 0, \exists W_0 \subset \mathcal{L}(\sqrt{p} \mathcal{Z}, \sqrt{q} \mathcal{Z}) \forall b \in W_0, \forall n \in \mathbb{N} : |\text{Tr}[\rho_{b_n} b_{\text{Wick}}]| < \eta, \quad (E) \]

where \( W_0 \) is a neighborhood of zero in \( \mathcal{L}(\sqrt{p} \mathcal{Z}, \sqrt{q} \mathcal{Z}) \) endowed with the \( \sigma \)-weak topology.

Lemma 3.1 Assume that \( (\rho_{b_n})_{n \in \mathbb{N}} \) satisfies (H0). Then

(i) \((T) \Rightarrow (P)\),

(ii) \((E) \Rightarrow (P)\).

Proof. We aim to prove \((P)\) for \( b \in \mathcal{P}_{p,q}(\mathcal{Z}) \).

(i) Start with

\[ \text{Tr}[\rho_{b_n} b_{\text{Wick}}] = \text{Tr}[\rho_{b_n} \Gamma(P)b_{\text{Wick}} \Gamma(P)] + \text{Tr}[\rho_{b_n}(1 - \Gamma(P))b_{\text{Wick}} \Gamma(P)] + \text{Tr}[\rho_{b_n} \Gamma(P)b_{\text{Wick}} (1 - \Gamma(P))] + \text{Tr}[\rho_{b_n}(1 - \Gamma(P))b_{\text{Wick}} (1 - \Gamma(P))] \]

Estimate all the terms containing \((1 - \Gamma(P))\) in a similar way. For example, we have

\[ |\text{Tr}[\rho_{b_n}(1 - \Gamma(P))b_{\text{Wick}} \Gamma(P)]| = |\text{Tr}[\langle N \rangle^{\frac{p+q}{2}} \rho_{b_n}(1 - \Gamma(P))b_{\text{Wick}} \langle N \rangle - \frac{p+q}{2} \Gamma(P)]| \]

\[ \leq C_{p,q}(b) \left\| \langle N \rangle^{\frac{p+q}{2}} \rho_{b_n}^{1/2} \rho_{b_n}^{1/2} (1 - \Gamma(P)) \right\|_1 \]

\[ \leq C_{p,q}(b) \left\| \langle N \rangle^{\frac{p+q}{2}} \rho_{b_n}^{1/2} \rho_{b_n}^{1/2} (1 - \Gamma(P)) \right\|_1 \left\| (1 - \Gamma(P))\rho_{b_n}(1 - \Gamma(P)) \right\|_1^2 \]

\[ \leq \tilde{C}_{p,q}(b) |\text{Tr}[\rho_{b_n}(1 - \Gamma(P))]|^{1/2}. \]

First \((10)\) comes from the number estimate \( \left\| b_{\text{Wick}} \langle N \rangle - \frac{p+q}{2} \right\| \leq C_{p,q}(b) \) then Cauchy-Schwarz inequality yields \((11)\). The last estimate \((12)\) is possible with \((H0)\). Remark that \( \Gamma(P)b_{\text{Wick}} \Gamma(P) = \Gamma(P)b(PZ)_{\text{Wick}} \Gamma(P) \) and that the polynomial \( b(PZ) \in \mathcal{B}_{p,q}(\mathcal{Z}) \) when \( P \) is finite rank orthogonal projector. The hypothesis \((T)\) and the above argument allow to approximate \( \text{Tr}[\rho_{b_n} b_{\text{Wick}}] \) by the quantity \( \text{Tr}[\rho_{b_n} b(PZ)_{\text{Wick}}] \) using \( \eta/3 \) argument.

Now, write

\[ |\text{Tr}[\rho_{b_n} b_{\text{Wick}}] - \int_{\mathcal{Z}} b(z) d\mu| \leq |\text{Tr}[\rho_{b_n} \left( b_{\text{Wick}} - b(PZ)_{\text{Wick}} \right)] + \text{Tr}[\rho_{b_n} b(PZ)_{\text{Wick}}] - \int_{\mathcal{Z}} b(PZ) d\mu| \]

So, the property \((T)\) implies \((P)\).

(ii) There exists a sequence \( b_k \in \mathcal{B}_{p,q}(\mathcal{Z}) \) such that \( b_k \) converges in the \( \sigma \)-weak topology to \( b \). We have

\[ |\text{Tr}[\rho_{b_n} b_{\text{Wick}}] - \int_{\mathcal{Z}} b(z) d\mu| \leq |\text{Tr}[\rho_{b_n} \left( b_{\text{Wick}} - b_k \right)] + \left( \text{Tr}[\rho_{b_n} b_k(z)_{\text{Wick}}] - \int_{\mathcal{Z}} b_k(z) d\mu \right) + \int_{\mathcal{Z}} |b_k(z) - b(z)| d\mu |. \]

So, \((P)\) holds by an \( \eta/3 \) argument and using respectively \((E)\), \((5)\) and dominated convergence for each term in the (r.h.s.) of \((13)\).

Remark 3.2

1) The space of bounded operators \( \mathcal{L}(\sqrt{p} \mathcal{Z}, \sqrt{q} \mathcal{Z}) \) endowed with the \( \sigma \)-weak topology is not a Baire space when \( \mathcal{Z} \) is infinite dimensional. Otherwise, \((E)\) and hence \((P)\) would be fulfilled by any sequence \( (\rho_{b_n})_{n \in \mathbb{N}} \) satisfying \((H0)\), according to Banach-Steinhaus Theorem (Uniform Boundedness Principle).

2) The hypothesis \((H0)\) in the above lemma, can be replaced by the weaker statement (see AmNi Prop.6.15)

\[ \exists C > 0 : \forall k \in \mathbb{N}, \text{Tr}[\rho_{b_n} N^k] \leq C(k)^k \]

uniformly in \( \varepsilon_n \). This can be interpreted as an analyticity property of \( t \rightarrow \text{Tr}[e^{iN^2} \rho_{b_n} e^{iN^2}] \) in \(|t| < 1/C\), uniformly w.r.t. \( \varepsilon_n \).

5
4 Proof of Thm. 2.1

Definition 4.1 For $m \in \mathbb{N}$, $r \in \{0, \ldots, m\}$ and $t_1, \cdots, t_m, t_0 \in \mathbb{R}$, associate with any $b \in \mathcal{P}_{p,q}(\mathcal{F})$ the polynomial:

$$C_r^{(m)}(t_m, \ldots, t_1, t) = \frac{1}{2^r} \sum_{\gamma(1,2)} \{Q_{m_\gamma}, \ldots, \{Q_{m_\gamma}, b_1\}^{(\gamma_2)} \cdots \{\gamma_1\} \} \in \mathcal{P}_{p-r+m, q-r+m}(\mathcal{F}). \quad (14)$$

Note that for shortness the dependence of $C_r^{(m)}(t_m, \ldots, t_1, t)$ on $b$ is not made explicit on the notation and even sometimes we will write $C_r^{(m)}$. By convention we set $C_0^{(0)}(t) = b_1$.

We collect some statements from [AmNi]. Remember that $	ilde{b}$ denotes the operator $\tilde{b} = \frac{\partial^p g_p}{\partial^p p} b(z) \in \mathcal{L}(\mathcal{V}^{p,\mathcal{F}}, \mathcal{V}^{q,\mathcal{F}})$ associated with $b \in \mathcal{P}_{p,q}(\mathcal{F})$.

Lemma 4.2 Let $b \in \mathcal{P}_{p,q}(\mathcal{F})$.

(i) The following inequality holds true

$$\|\{Q_{\gamma}, b_1\}]_2 \mathcal{L}(\mathcal{V}^{p,\mathcal{F}}, \mathcal{V}^{q,\mathcal{F}}) \leq 2[p(p-1) + q(q-1)] \|Q\| \|\tilde{b}\|_\mathcal{L}(\mathcal{V}^{p,\mathcal{F}}, \mathcal{V}^{q,\mathcal{F}}),$$

(ii) For any $m \in \mathbb{N}$ and $r \in \{0, 1, \ldots, m\}$, we have

$$\|\tilde{C}_r^{(m)} \mathcal{L}(\mathcal{V}^{p+r,\mathcal{F}}, \mathcal{V}^{q+r,\mathcal{F}}) \leq 2^{m-r} \binom{m}{r} (p+m-r|r) \binom{p+m-r-1}{r-1} \|\tilde{Q}\|^{m-r} \|\tilde{b}\|_\mathcal{L}(\mathcal{V}^{p,\mathcal{F}}, \mathcal{V}^{q,\mathcal{F}}),$$

when $p \geq q$ with a similar expression when $q \geq p$ (replace $(p+m-r, p-1)$ with $(q+m-r, q-1)$).

Proof. See [AmNi] Lemma 5.8, 5.9. \qed

Lemma 4.3 For any $\delta > 0$ there exists $T > 0$ such that for all $0 < t < T$:

$$\sum_{m=0}^{\infty} \delta^m \int_0^t dt_1 \cdots \int_0^{t_{m-1}} dt_m \left| C_0^{(m)}(t_m, \ldots, t_1, t) \right| \mathcal{L}(\mathcal{V}^{p,\mathcal{F}}, \mathcal{V}^{q,\mathcal{F}}) < \infty \quad (15)$$

Proof. It is enough to bound (15) in the case $p \geq q$. Using Lemma 4.2(iii) with $r = 0$, we obtain

$$\sum_{m=0}^{\infty} \delta^m \int_0^t dt_1 \cdots \int_0^{t_{m-1}} dt_m \left| C_0^{(m)}(t_m, \ldots, t_1, t) \right| \leq 2^{p-1} \|\tilde{b}\| \sum_{m=0}^{\infty} (23 \delta t |\tilde{Q}|)^m.$$

The r.h.s. is finite whenever $0 < t < T = (23 \delta |\tilde{Q}|)^{-1}$. \qed

Proof of Thm. 2.1

First consider the following expansion proved in [AmNi] (50)-(52) for any positive integer $M$:

$$U_{\varepsilon}(t)^* b^{\text{Wick}} U_{\varepsilon}(t) = \sum_{m=0}^{M-1} \delta^m \int_0^t dt_1 \cdots \int_0^{t_{m-1}} dt_m \left[ C_0^{(m)}(t_m, \ldots, t_1, t) \right]^{\text{Wick}}$$

$$+ \frac{\varepsilon}{2} \sum_{m=1}^{M} \delta^m \int_0^t dt_1 \cdots \int_0^{t_{m-1}} dt_m U(t_m)^* U_0(t_m) \left\{ Q_{m_\gamma}, C_0^{(m-1)}(t_{m-1}, \ldots, t_1, t) \right\} \right]^{(2)}^{\text{Wick}}$$

$$+ \varepsilon M \int_0^t dt_1 \cdots \int_0^{t_{M-1}} dt_m U(t_m)^* U_0(t_m) \left[ C_0^{(M)}(t_m, \ldots, t_1, t) \right]^{\text{Wick}} U_0(t_m)^* U(t_m) \right].$$

where the equality holds in $\mathcal{L}(\mathcal{V}^{p,\mathcal{F}}, \mathcal{V}^{p+q-p,\mathcal{F}})$ for any $s \in \mathbb{N}, s \geq q-p$. Multiplying on the left the above identity by $\rho_{\varepsilon_n}$ and then using number estimates with the help of (H0), yields an identity
on \( L(\mathcal{H}) \) on which we take the trace. This leads to

\[
\text{Tr}[\rho_{\epsilon_n} U_{\epsilon_n}(t)^* b^{\text{Wick}} U_{\epsilon_n}(t)] = \sum_{m=0}^{M-1} \int_0^t dt_1 \cdots \int_0^{t_{m-1}} dt_m \text{Tr}\left[\rho_{\epsilon_n} \left( C^{(m)}_0 (t_m, \cdots, t_1, t) \right)^{\text{Wick}} \right]
\]

(16)

\[
+ \sum_{m=1}^M \int_0^t dt_1 \cdots \int_0^{t_{m-1}} dt_m \text{Tr}\left[\rho_{\epsilon_n} U_{\epsilon_n}(t_m)^* U_{\epsilon_n}(t_m) \left( \{ \mathcal{Q}_{\epsilon_n}, C^{(m-1)}_0 (t_{m-1}, \cdots, t_1, t) \}^{(2)} \right)^{\text{Wick}} U_{\epsilon_n}(t_m)^* U_{\epsilon_n}(t_m) \right] + i M \int_0^t dt_1 \cdots \int_0^{t_{m-1}} dt_m \text{Tr}\left[\rho_{\epsilon_n} U_{\epsilon_n}(t_m)^* U_{\epsilon_n}(t_m) \left( C^{(M)}_0 (t_M, \cdots, t_1, t) \right)^{\text{Wick}} U_{\epsilon_n}(t_m)^* U_{\epsilon_n}(t_m) \right].
\]

(17)

(18)

The interchange of trace and integrals on the r.h.s. is justified by the bounds on Lemma 4.2. Lemma 4.3 implies that the term of (16) and (17) are bounded by

\[
A_m = \lambda^{m+\frac{m+2}{2}} \text{sign}(t)^m \int_0^t dt_1 \cdots \int_0^{t_{m-1}} dt_m \left| C^{(m)}_0 \right|
\]

\[
B_m = \epsilon_n \left| Q \right| (p + q + m - 1)^2 \lambda^{m-1+\frac{m+2}{2}} \text{sign}(t)^m \int_0^t dt_1 \cdots \int_0^{t_{m-1}} dt_m \left| C^{(m-1)}_0 \right|
\]

while the remainder (18) is estimated by

\[
\left| (18) \right| \leq \text{sign}(t)^M \int_0^t dt_1 \cdots \int_0^{t_{M-1}} dt_m \left| C^{(M)}_0 \right| = C_M.
\]

By Lemma 4.2, the series \( \sum_{m=0}^\infty A_m \) and \( \sum_{m=0}^\infty B_m \) converge as soon as \( |t| < T_0 = (2^3 \lambda |Q|)^{-1} \) while \( \lim_{m \to \infty} C_M = 0 \). Hence the relation (16)(17)(18) holds with \( M = \infty \) with a vanishing third term and a second term bounded by \( \sum_{m=0}^\infty B_m = \mathcal{O}(\epsilon_n) \). Therefore, we obtain

\[
\lim_{\epsilon_n \to 0} \sum_{m=0}^\infty \int_0^t dt_1 \cdots \int_0^{t_{m-1}} dt_m \text{Tr}\left[\rho_{\epsilon_n} \left( C^{(m)}_0 (t_m, \cdots, t_1, t) \right)^{\text{Wick}} \right] = 0.
\]

Owing to the condition \( (P) \) which provides the pointwise convergence and the uniform bound of \( \sum_{m=0}^\infty A_m \), the Lebesgue’s convergence theorem implies

\[
\lim_{\epsilon_n \to 0} \sum_{m=0}^\infty \int_0^t dt_1 \cdots \int_0^{t_{m-1}} dt_m \text{Tr}\left[\rho_{\epsilon_n} \left( C^{(m)}_0 (t_m, \cdots, t_1, t) \right)^{\text{Wick}} \right] = \sum_{m=0}^\infty \int_0^t dt_1 \cdots \int_0^{t_{m-1}} dt_m \int_\mathcal{X} C^{(m)}_0 (t_m, \cdots, t_1, t ; z) d\mu.
\]

(19)

Now, we interchange the sum over \( m \) and the integrals on \( (t_1, \cdots, t_m, t) \) with the integral over \( \mathcal{X} \) on (19) simply with a Fubini argument based on the absolute convergence (written here for \( t > 0 \)):

\[
\sum_{m=0}^\infty \int_0^t dt_1 \cdots \int_0^{t_{m-1}} dt_m \int_\mathcal{X} \left| C^{(m)}_0 (t_m, \cdots, t_1, t ; z) \right| d\mu \leq \sum_{m=0}^\infty \left( \int_\mathcal{X} |z|^{p+q+2m} d\mu \right) \int_0^t dt_1 \cdots \int_0^{t_{m-1}} dt_m \left| C^{(m)}_0 (t_m, \cdots, t_1, t) \right|.
\]

Again \( (H0) \) and \( (P) \) imply that for all \( k \in \mathbb{N} \) there exists \( \lambda > 0 \) such that

\[
\int_\mathcal{X} |z|^{2k} d\mu = \lim_{\epsilon_n \to 0} \text{Tr}[\rho_{\epsilon_n} (|z|^{2k})^{\text{Wick}}] = \lim_{\epsilon_n \to 0} \text{Tr}[\rho_{\epsilon_n} N^k] \leq \lambda^k.
\]

Hence, Lemma 4.3 yields for \( |t| < T_0 \):

\[
\lim_{\epsilon_n \to 0} \text{Tr}[\rho_{\epsilon_n} U_{\epsilon_n}(t)^* b^{\text{Wick}} U_{\epsilon_n}(t)] = \sum_{m=0}^\infty \int_0^t dt_1 \cdots \int_0^{t_{m-1}} dt_m \int_\mathcal{X} C^{(m)}_0 (t_m, \cdots, t_1, t ; z) d\mu
\]

\[
= \sum_{m=0}^\infty \int_0^t dt_1 \cdots \int_0^{t_{m-1}} dt_m C^{(m)}_0 (t_m, \cdots, t_1, t ; z) d\mu.
\]
where the integrand $\sum_{m=0}^{\infty} r^m \int_{0}^{t} dt_1 \cdots \int_{0}^{t_{m-1}} dt_m C_0^{(m)}(z)$ is a convergent series in $L^1(\mu)$.

The last step is the identification of the limit with the r.h.s. of (6). Indeed, an iteration of (4) reads

$$b(z) = b_t(z) + i \int_{0}^{t} \{ Q_t, b_t \}(z) dt + \sum_{m=1}^{M-1} r^m \int_{0}^{t} dt_1 \cdots \int_{0}^{t_{m-1}} dt_m C_0^{(m)}(t_m, \cdots, t_1; t; z),$$

after setting $z_t = F_t(z)$ and defining the Wick symbols $b_t$ and $Q_t$ according to (3). By induction we obtain for any $M > 1$:

$$b \circ F_t(z) = b_t(z) + \sum_{m=1}^{M-1} r^m \int_{0}^{t} dt_1 \cdots \int_{0}^{t_{m-1}} dt_m C_0^{(m)}(t_m, \cdots, t_1; t; z)$$

$$+ r^M \int_{0}^{t} dt_1 \cdots \int_{0}^{t_{M-1}} dt_m C_0^{(M)}(t_1, \cdots, t_1; t; e^{dt A} z_m).$$

An integration with respect to the measure $\mu$ leads to

$$\int_{\mathcal{Z}} b \circ F_t(z) d\mu = \sum_{m=1}^{M-1} r^m \int_{0}^{t} dt_1 \cdots \int_{0}^{t_{m-1}} dt_m \int_{\mathcal{Z}} C_0^{(m)}(t_m, \cdots, t_1; t; z) d\mu$$

$$+ r^M \int_{0}^{t} dt_1 \cdots \int_{0}^{t_{M-1}} dt_m \int_{\mathcal{Z}} C_0^{(M)}(t_1, \cdots, t_1; t; e^{dt A} z_m) d\mu.$$

Again the uniform estimate $\sum_{m=0}^{\infty} A_m$ when $|t| < T_0$ and $\lim_{M \to \infty} C_M = 0$, allow to take the limit as $M \to \infty$. This implies for $|t| < T_0$

$$\int_{\mathcal{Z}} b \circ F_t(z) d\mu = \sum_{m=1}^{\infty} r^m \int_{0}^{t} dt_1 \cdots \int_{0}^{t_{m-1}} dt_m \int_{\mathcal{Z}} C_0^{(m)}(t_m, \cdots, t_1; t; z) d\mu.$$

This proves the result for $|t| < T_0$ and it is extended to any time by the next iteration argument. Indeed, it is clear that $\rho_{e_k}(t) = U_{e_k}(t) \rho_{e_k} U_{e_k}(t)^*$ satisfies (H0) since $U_{e_k}(t)$ commute with $N$. The property (P) holds for $\rho_{e_{k_0}}(t)$ when $|t| < T_0$ by Remark 2.2 and Corollary 2.3. For $t, s$ such that $|t|, |s| < T_0$, the sequence $(\rho_{e_k}(t))_{k \in \mathbb{N}}$ satisfies (H0) and (P). Therefore, the result for short times yields

$$\lim_{k \to 0} \text{Tr}(\rho_{e_k}(t) U_{e_k}(s) \rho_{e_k}(s)^* b^{\text{Wick}} U_{e_k}(s)) = \int_{\mathcal{Z}} b \circ F_t(z) d\mu = \int_{\mathcal{Z}} b \circ F_{t+s}(z) d\mu.$$

Remark 4.4 As by product we have for any $b \in \mathcal{P}_{\alpha, \beta} \cap \mathcal{P}_{\alpha, \beta}(\mathcal{Z})$

$$b \circ F_t(z) = L^1(\mu) - \sum_{m=1}^{\infty} r^m \int_{0}^{t} dt_1 \cdots \int_{0}^{t_{m-1}} dt_m C_0^{(m)}(t_m, \cdots, t_1; t; z).$$

Moreover, the arguments used in the proof of Thm. 2.7 can not ensure the pointwise absolute convergence of the r.h.s. (20) for all $z \in \mathcal{Z}$.

5 Examples:

Models:

M1) Let $\mathcal{Z} = L^2(\mathbb{R}^d, dx)$, $A = D_x^2 + U(x)$ self-adjoint and $Q$ is a multiplication operator by $\frac{1}{2} V(x - y)$ with $V \in L^\infty(\mathbb{R}^d)$.

M2) Let $\mathcal{Z} = L^2(\mathbb{R}^d, dx)$, $A = \sqrt{D_x^2 + m^2} + U(x)$ self-adjoint and $Q$ as above.

M3) When $\mathcal{Z} = C^d \sim \mathbb{R}^d$, one recovers the standard semiclassical limit problem and the condition (P) is always satisfied if (H0) is satisfied. We refer for example the reader to [CRR] [Ger] [GMMP] [HMR] [LiPa] [Mar] [Rob] for various results about this topic.

Density operator Sequences:
1) Every sequence $(\rho_{\varepsilon_n})_{n \in \mathbb{N}}$ valued in a compact set of the Banach space of trace class operators has the Wigner measure $\delta_0$. If in addition $(\rho_{\varepsilon_n})_{n \in \mathbb{N}}$ satisfies $(H0)$ then $(P)$ holds true.

2) Let $(\rho_{\varepsilon_n})_{n \in \mathbb{N}}$ as in 1) and satisfying $(H0)$ and let $(z_n)_{n \in \mathbb{N}}$ be a sequence of $\mathcal{Z}$ such that $\lim_{n \to \infty} |z_n - z| = 0$. Then $\tilde{\rho}_{\varepsilon_n} = W(\sqrt{\frac{2}{i \varepsilon}}z_n)\rho_{\varepsilon_n}W(-\sqrt{\frac{2}{i \varepsilon}}z_n)$ admits the unique Wigner measure $\mu = \delta_z$ where $z$ and $(P)$ holds true. The push-forward measure is $\mu_t = \delta_{z_t}$.

3) Let $(z_n)_{n \in \mathbb{N}}$ be a sequence valued in a compact set of $\mathcal{Z}$. So $\rho_{\varepsilon_n} = |z_n \otimes [\varepsilon_n^{-1}]z_n \rangle \langle z_n \otimes [\varepsilon_n^{-1}]z_n |$ satisfies $(H0)$ and admits the Wigner measures $\frac{1}{2\pi} \int_0^{2\pi} \delta_{z_n} d\theta$ where $z$ is any cluster point of $(z_n)_{n \in \mathbb{N}}$. Several other examples can be obtained by superposition, see [AmNi].

4) Let $(z_n)_{n \in \mathbb{N}}$ be a sequence such that $|z_n| = 1$ in $\mathcal{Z}$ converging weakly to 0. Then $(P)$ fails for $\rho_{\varepsilon_n} = |E(z_n)\rangle \langle E(z_n)|$ with $E(z_n) = W(\sqrt{\frac{2}{i \varepsilon}}z_n |\Omega)$, although $(H0)$ holds.

References

[AmNi] Z. Ammari, F. Nier. Mean field limit for bosons and infinite dimensional phase-space analysis. [http://arxiv.org/abs/0711.4128]

[BGM] C. Bardos, F. Golse, N. Mauser Weak coupling limit of the n-particle Schrödinger equation. Methods Appl. Anal. 2, 275–293 (2000)

[BEGMY] C. Bardos, L. Erdős, F. Golse, N. Mauser, H-T. Yau Derivation of the Schrödinger-Poisson equation from the quantum N-body problem. C.R. Acad. Sci. Paris 334, 515–520 (2002)

[CRR] M. Combescure, J. Ralston, D. Robert. A proof of the Gutzwiller semiclassical trace formula using coherent states decomposition. Comm. Math. Phys. 202 (1999), no. 2, 463–480.

[ElSc] A. Elgart, B. Schlein. Mean field dynamics of boson stars Comm. Pure and Appl. Math. Vol. 60, (2005) 500–545

[EY] L. Erdös, H.T. Yau. Derivation of the nonlinear Schrödinger equation from a many body coulomb system. Adv. Theor. Math. Phys. 5, 1169–2005 (2001)

[ESY] L. Erdös, B. Schlein, H.T. Yau. Derivation of the cubic non-linear Schrödinger equation from quantum dynamics of many-body systems. Invent. Math. 167 (2007), no. 3, 515–614.

[FGS] J. Fröhlich, S. Graffi, S. Schwarz. Mean-field- and classical limit of many-body Schrödinger dynamics for bosons. Comm. Math. Phys. 271, No. 3 (2007), 681–697.

[FKP] J. Fröhlich, A. Knowles, A. Pizzo. Atomism and quantization. J. Phys. A: Math. Theor. 40 (2007) 3033–3045.

[FKS] J. Fröhlich, A. Knowles, S. Schwarz. On the Mean-field limit of bosons with Coulomb two-body interaction [http://arxiv.org/abs/0805.4299]

[Ger] P. Gérard. Mesures semi-classiques et ondes de Bloch. Séminaire sur les Équations aux Dérivées Partielles, 1990–1991, Exp. No. XVI, 19 pp., École Polytech., Palaiseau, 1991.

[GMMP] P. Gérard, P.A. Markowich, N.J. Mauser, F. Poupaud. Homogenization limits and Wigner transforms. Comm. Pure Appl. Math. 50 (1997), no. 4, 323–379.

[GiVe] J. Ginibre, G. Velo. The classical field limit of scattering theory for nonrelativistic many-boson systems. I. Comm. Math. Phys. 66, No. 1 (1979), 37–76

[HMR] B. Helffer, A. Martinez, D. Robert. Ergodicité et limite semi-classique. Comm. Math. Phys. 109 (1987), no. 2, 313–326.

[Hep] K. Hepp. The classical limit for quantum mechanical correlation functions. Comm. Math. Phys. 35 (1974), 265–277
[LiPa] P.L. Lions, T. Paul. Sur les mesures de Wigner. Rev. Mat. Iberoamericana 9 (1993), no. 3, 553–618.

[Mar] A. Martinez. An introduction to semiclassical analysis and microlocal analysis. Universitext, Springer-Verlag, (2002).

[Rob] D. Robert. Autour de l’approximation semi-classique. Progress in Mathematics, 68. Birkhäuser Boston, 1987.

[Spo] H. Spohn. Kinetic equations from Hamiltonian dynamics. Rev. Mod. Phys. 52, No. 3 (1980), 569–615