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Quantum mean-field asymptotics and multiscale analysis

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We study, via multiscale analysis, a defect-of-compactness phenomenon which occurs in bosonic and fermionic quantum mean-field problems. The approach relies on a combination of mean-field asymptotics and second microlocalized semiclassical measures. The phase space geometric description is illustrated by various examples.

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1. Introduction

Motivations. Over the past three decades, microlocal and semiclassical analysis has provided interesting mathematical techniques for the study of quantum field theory and quantum many-body theory; see for instance [Ammari and Nier 2008; Brunetti and Fredenhagen 2000; Fournais et al. 2015; Fröhlich et al. 2007; Gérard and Wrochna 2014; Ivrii and Sigal 1993; Lieb and Yau 1987; Amour et al. 2001]. In the present article we follow this fruitful stream of ideas and study the mathematical problem of defect of compactness for density matrices in the bosonic or fermionic Fock spaces. Previously, in a series of papers [Ammari and Nier 2008; 2009; 2011; 2015], the authors have introduced Wigner (or semiclassical) measures of density matrices in the bosonic Fock space and showed that it is a very useful

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tool to study the mean-field approximation of Bose gases. Moreover, it was noticed that a certain defect of compactness of density matrices is one of the difficulties that occurs in this context. So towards a better understanding of these concentration and defect-of-compactness phenomena we introduced here a multiscale analysis inspired by second microlocalization. We believe that this approach will be of interest to the study of the mean-field theory of Fermi and Bose gases; see, e.g., [Bach et al. 2016; Benedikter et al. 2014; Fournais et al. 2015]. We indeed provide here some simple applications to the Bose and Fermi free gases and leave more involved applications to further investigations.

Let us briefly describe the main question we consider here. As mentioned before, in the analysis of general bosonic mean-field problems the following defect-of-compactness problem arises. In fact, if ϱ_ε are density matrices in the (fermionic or bosonic) Fock space and $\gamma_\varepsilon^{(p)}$ are its p -particle reduced density matrices, one may have

$$\lim_{\varepsilon \rightarrow 0} \text{Tr}[\gamma_\varepsilon^{(p)} \tilde{b}] = \text{Tr}[\gamma_0^{(p)} \tilde{b}] \quad (1)$$

for any p -particle *compact* observable $\tilde{b}$, while it is not true for a general bounded $\tilde{b}$; e.g.,

$$\lim_{\varepsilon \rightarrow 0} \text{Tr}[\gamma_\varepsilon^{(p)}] > \text{Tr}[\gamma_0^{(p)}].$$

This reflects the difference between the weak* convergence of trace-class operators and convergence with respect to the trace norm. In the fermionic case, it is even worse, because mean-field asymptotics cannot be described in terms of finitely many quantum states and the right-hand side of (1) is usually 0, while $\lim_{\varepsilon \rightarrow 0} \text{Tr}[\gamma_\varepsilon^{(p)}] > 0$ (see Proposition 4.6). From the analysis of finite-dimensional partial differential equations, it is known that such a defect of compactness can be localized geometrically with accurate quantitative information by introducing scales and small parameters within semiclassical techniques; see, e.g., [Gérard 1991; Gérard et al. 1997; Tartar 1990]. We are thus led to introduce two small parameters $\varepsilon > 0$ for the mean-field asymptotics and $h > 0$ for the semiclassical quantization of finite-dimensional p -particle phase space. The small parameter ε stands for $\frac{1}{n}$, where $n \rightarrow \infty$ is the typical number of particles, while h is the *rescaled* Planck constant measuring the proximity of quantum mechanics to classical mechanics. Such scaling appears already in the mathematical physics literature with a specific relation between h and ε depending on the considered problem; see, e.g., [Fournais et al. 2015; Narnhofer and Sewell 1981; Lieb and Yau 1987]. The combined analysis of this article is concerned with the general situation when $\varepsilon = \varepsilon(h)$ with $\lim_{h \rightarrow 0} \varepsilon(h) = 0$. In order to keep track of the information at the quantum level, especially in the bosonic case, we also introduce finite-dimensional multi-scale observables in the spirit of [Bony 1986; Fermanian-Kammerer and Gérard 2002; Fermanian Kammerer 2005; Nier 1996].

Framework. The 1-particle space $\mathcal{H}$ is a separable complex Hilbert space endowed with the scalar product $\langle \cdot, \cdot \rangle$ (antilinear in the left-hand side). For a Hilbert space $\mathfrak{h}$ the set of bounded operators is denoted by $\mathcal{L}(\mathfrak{h})$, while the Schatten classes are denoted by $\mathcal{L}^p(\mathfrak{h})$, $1 \leq p \leq \infty$, the case $p = \infty$ corresponding to the space of compact operators. Let $\Gamma_{\pm}(\mathcal{H})$ be the bosonic (+) or fermionic (−) Fock space built on the separable Hilbert space $\mathcal{H}$:

$$\Gamma_{\pm}(\mathcal{H}) = \bigoplus_{n \in \mathbb{N}}^{\perp} \mathcal{S}_{\pm}^n \mathcal{H}^{\otimes n},$$

where tensor products and direct sums are Hilbert completed. The operator $\mathcal{S}_{\pm}^n$ is the orthogonal projection given by

$$\mathcal{S}_{\pm}^n(f_1 \otimes \cdots \otimes f_n) = \frac{1}{n!} \sum_{\sigma \in \mathfrak{S}_n} s_{\pm}(\sigma) f_{\sigma(1)} \otimes \cdots \otimes f_{\sigma(n)}, \quad (2)$$

where $s_{+}(\sigma)$ equals 1, while $s_{-}(\sigma)$ denotes the signature of the permutation σ and $\mathfrak{S}_n$ is the n -symmetric group.

The dense set of many-body state vectors with a finite number of particles is

$$\Gamma_{\pm}^{\text{fin}}(\mathcal{H}) = \bigoplus_{n \in \mathbb{N}}^{\perp, \text{alg}} \mathcal{S}_{\pm}^n \mathcal{H}^{\otimes n},$$

where the $\perp, \text{alg}$ superscript stands for the algebraic orthogonal direct sum. We shall also use the notation $[A, B]_{+} = [A, B] = \text{ad}_A B = AB - BA$ for the commutator of two operators and the notation $[A, B]_{-} = AB + BA$ for the anticommutator.

One way to investigate the mean-field asymptotics relies on parameter-dependent *canonical (anti-)commutation relations* (CCR or CAR). The small parameter $\varepsilon > 0$ has to be thought of as the inverse of the typical number of particles and the CCR (resp. CAR) relations are given by

$$[a_{\pm}(g), a_{\pm}(f)]_{\pm} = [a_{\pm}^{*}(g), a_{\pm}^{*}(f)]_{\pm} = 0, \quad [a_{\pm}(g), a_{\pm}^{*}(f)]_{\pm} = \varepsilon \langle g, f \rangle.$$

Let $(\varrho_{\varepsilon})_{\varepsilon > 0}$ be a family of normal states (i.e., nonnegative and normalized trace-class operators) on the Fock space $\Gamma_{\pm}(\mathcal{H})$, depending on $\varepsilon > 0$; we want to investigate the asymptotic behavior of reduced density matrices, defined below, as $\varepsilon \rightarrow 0$, by possibly introducing another scale $h > 0$ on the p -particle phase space, with $\varepsilon = \varepsilon(h)$ and $\lim_{h \rightarrow 0} \varepsilon(h) = 0$.

Outline. In Section 2, we recall how Wick observables are used to define the reduced density matrices $\gamma_{\varepsilon}^{(p)}$. Note that it is much more convenient here, in the general grand canonical framework, to work with nonnormalized reduced density matrices. Some symmetrization formulas are also recalled in this section. In

Section 3, we present the geometry of the classical p -particle phase space and introduce the formalism of double scale semiclassical measures, after [Fermanian Kammerer 2005; Fermanian-Kammerer and Gérard 2002]. In Section 4, we combine the mean-field asymptotics with semiclassical analysis, the two parameters ε and h being related through $\varepsilon = \varepsilon(h)$ with $\lim_{h \rightarrow 0} \varepsilon(h) = 0$. Instead of studying the collection of nonnormalized reduced density matrices $(\gamma_{\varepsilon(h)}^{(p)})_{p \in \mathbb{N}}$, it is more convenient to associate generating functions

$$z \mapsto \text{Tr}[\varrho_{\varepsilon(h)} e^{z \, d\Gamma_{\pm}(a^{\mathcal{Q},h})}],$$

and to use holomorphy arguments presented there. In Section 5, some classical examples with various asymptotics illustrate the general framework: coherent states in the bosonic setting; simple Gibbs states in the fermionic case; more involved Gibbs states in the bosonic case, which make explicit the separation of condensate and noncondensate phases for rather general noninteracting steady Bose gases. The appendices collect or revisit known things about multiscale semiclassical measures, the (PI)-condition of bosonic mean-field problems, Wick composition formulas, and traces of non-self-adjoint second quantized contractions.

2. Wick observables and reduced density matrices

2A. Wick observables.

Notation. For $n \in \mathbb{N}$, the operator $S_{\pm}^n$ given in (2) is an orthogonal projection in $\mathcal{X}^{\otimes n}$ so that $(S_{\pm}^n)^* = S_{\pm}^n$. However, we consider $S_{\pm}^n$ as a bounded operator from $\mathcal{X}^{\otimes n}$ onto $S_{\pm}^n \mathcal{X}^{\otimes n}$, and its adjoint, denoted by $S_{\pm}^{n,*} : S_{\pm}^n \mathcal{X}^{\otimes n} \rightarrow \mathcal{X}^{\otimes n}$, is nothing but the natural embedding.

Let $\tilde{b} \in \mathcal{L}(S_{\pm}^p \mathcal{X}^{\otimes p}; S_{\pm}^q \mathcal{X}^{\otimes q})$. The Wick quantization of $\tilde{b}$ is the operator on $\Gamma_{\pm}^{\text{fin}}(\mathcal{X})$ defined by

$$\tilde{b}^{\text{Wick}}|_{S_{\pm}^{n+p} \mathcal{X}^{\otimes(n+p)}} = \varepsilon^{\frac{p+q}{2}} \frac{\sqrt{(n+p)! (n+q)!}}{n!} S_{\pm}^{n+q} (\tilde{b} \otimes \text{Id}_{\mathcal{X}^{\otimes n}}) S_{\pm}^{n+p,*}.$$

In the bosonic case, an element $\tilde{b} \in \mathcal{L}(S_{+}^p \mathcal{X}^{\otimes p}; S_{+}^q \mathcal{X}^{\otimes q})$ is determined by a related “symbol” $\mathcal{X} \ni z \mapsto b(z) = \langle z^{\otimes q}, \tilde{b} z^{\otimes p} \rangle$ which is a homogeneous polynomial. So b admits Gâteaux differentials

$$\partial_z^k \partial_z^{k'} b(w)[u_1, \dots, u_k, v_1, \dots, v_{k'}] = \bar{\partial}_{u_1} \cdots \bar{\partial}_{u_k} \partial_{v_1} \cdots \partial_{v_{k'}} b(w),$$

where $\bar{\partial}_u, \partial_v$ are the complex directional derivatives relative to $u, v \in \mathcal{X}$ at the point $w \in \mathcal{X}$. In particular, we have the relation

$$\tilde{b} = \frac{1}{q! p!} \partial_z^q \partial_z^p b.$$

Observe that $b(w)$ admits higher Gâteaux derivatives with the natural identification of $\partial_z^{k'} b(w)$ as a continuous form on $\mathcal{S}_+^{k'} \mathcal{X}^{\otimes k}$ and $\partial_{\bar{z}}^k b(w)$ as a vector in $\mathcal{S}_+^k \mathcal{X}^{\otimes k}$. With the above form-vector identification we define, for any symbols b_1, b_2 ,

$$\partial_z^k b_1(w) \cdot \partial_{\bar{z}}^k b_2(w) = \partial_z^k b(w) [\partial_{\bar{z}}^k b(w)] \in \mathbb{C}.$$

We shall also use the notation $b^{\text{Wick}} = \tilde{b}^{\text{Wick}}$.

Examples.

- (a) The annihilation operator $a_{\pm}(f)$, $f \in \mathcal{X}$, is the Wick quantization of $\tilde{b} = \langle f | : \mathcal{X}^{\otimes 1} = \mathcal{X} \ni \varphi \mapsto \langle f, \varphi \rangle \in \mathcal{X}^{\otimes 0} = \mathbb{C}$.
- (b) The creation operator $a_{\pm}^*(f)$, $f \in \mathcal{X}$, is the Wick quantization of $\tilde{b} = |f \rangle : \mathcal{X}^{\otimes 0} = \mathbb{C} \ni \lambda \mapsto \lambda f \in \mathcal{X}^{\otimes 1} = \mathcal{X}$.
- (c) For $\tilde{b} \in \mathcal{L}(\mathcal{X})$ its Wick quantization $\tilde{b}^{\text{Wick}}$ is nothing but

$$d\Gamma_{\pm}(\tilde{b})|_{\mathcal{S}_{\pm}^n \mathcal{X}^{\otimes n}} = \varepsilon [\tilde{b} \otimes \text{Id}_{\mathcal{X}} \otimes \cdots \otimes \text{Id}_{\mathcal{X}} + \cdots + \text{Id}_{\mathcal{X}} \otimes \cdots \otimes \text{Id}_{\mathcal{X}} \otimes \tilde{b}].$$

A particular case is $\tilde{b} = \text{Id}_{\mathcal{X}}$ associated with the scaled number operator ($N_{\pm, \varepsilon=1}$ stands for the usual ε -independent number operator):

$$\tilde{b}^{\text{Wick}} = d\Gamma_{\pm}(\text{Id}_{\mathcal{X}}) = N_{\pm} = \varepsilon N_{\pm, \varepsilon=1}.$$

When $\tilde{b}$ is self-adjoint one has

$$d\Gamma_{\pm}(\tilde{b}) = i \partial_t e^{-it} d\Gamma_{\pm}(\tilde{b})|_{t=0} = i \partial_t \Gamma_{\pm}(e^{-i\varepsilon t \tilde{b}})|_{t=0},$$

while for a contraction $C \in \mathcal{L}(\mathcal{X}; \mathcal{X})$,

$$\Gamma_{\pm}(C)|_{\mathcal{S}_{\pm}^n \mathcal{X}^{\otimes n}} = C \otimes \cdots \otimes C.$$

From the definition of the Wick quantization one easily checks the following properties; see [Ammari 2004].

Proposition 2.1. For $\tilde{b} \in \mathcal{L}(\mathcal{S}_{\pm}^p \mathcal{X}^{\otimes p}; \mathcal{S}_{\pm}^q \mathcal{X}^{\otimes q})$:

- $[\tilde{b}^{\text{Wick}}]^* = [\tilde{b}^*]^{\text{Wick}}$.
- The operator $(1 + N_{\pm})^{-\frac{m}{2}} \tilde{b}^{\text{Wick}} (1 + N_{\pm})^{-\frac{m'}{2}}$ extends to a bounded operator on $\Gamma_{\pm}(\mathcal{X})$ if $m + m' \geq p + q$ with

$$\|(1 + N_{\pm})^{-\frac{m}{2}} \tilde{b}^{\text{Wick}} (1 + N_{\pm})^{-\frac{m'}{2}}\|_{\mathcal{L}(\Gamma_{\pm}(\mathcal{X}))} \leq C_{m, m'} \|\tilde{b}\|_{\mathcal{L}(\mathcal{S}_{\pm}^p \mathcal{X}; \mathcal{S}_{\pm}^q \mathcal{X})}, \quad (3)$$

with $C_{m, m'}$ independent of $\tilde{b}$ and of $\varepsilon \in (0, \varepsilon_0)$.

- $(\tilde{b} \geq 0) \iff (\tilde{b}^{\text{Wick}} \geq 0)$, while this makes sense only for $q = p$.

Wick quantized operators are generally unbounded operators on $\Gamma_{\pm}(\mathcal{Z})$ (e.g., $N_{\pm}$) but they are well-defined on the dense set $\Gamma_{\pm}^{\text{fin}}(\mathcal{Z})$, which is preserved by their action. Hence $\tilde{b}_1^{\text{Wick}} \circ \tilde{b}_2^{\text{Wick}}$ makes sense at least on $\Gamma_{\pm}^{\text{fin}}(\mathcal{Z})$ and the following composition law holds true.

Proposition 2.2 (composition of Wick operators). *Let $\tilde{b}_j \in \mathcal{L}(S_{\pm}^{p_j} \mathcal{Z}^{\otimes p_j}; S_{\pm}^{q_j} \mathcal{Z}^{\otimes q_j})$, $j = 1, 2$. Then*

$$\tilde{b}_1^{\text{Wick}} \circ \tilde{b}_2^{\text{Wick}} = \sum_{k=0}^{\min\{p_1, q_2\}} (\pm 1)^{(p_1-k)(p_2+q_2)} \frac{\varepsilon^k}{k!} (\tilde{b}_1 \sharp^k \tilde{b}_2)^{\text{Wick}}, \quad (4)$$

where

$$\tilde{b}_1 \sharp^k \tilde{b}_2 := \frac{p_1!}{(p_1-k)!} \frac{q_2!}{(q_2-k)!} S_{\pm}^{q_1+q_2-k} (\tilde{b}_1 \otimes \text{Id}^{\otimes q_2-k}) (\text{Id}^{\otimes p_1-k} \otimes \tilde{b}_2) S_{\pm}^{p_1+p_2-k,*}.$$

For the reader's convenience, the proof of Proposition 2.2 is provided in Appendix C.

In the bosonic case the symbols $b(z) = \langle z^{\otimes q}, \tilde{b} z^{\otimes p} \rangle$ are convenient for writing the composition of Wick quantized operators. If $b_1 \sharp^{\text{Wick}} b_2$ denotes the symbol of $\tilde{b}_1^{\text{Wick}} \circ \tilde{b}_2^{\text{Wick}}$, the composition law is summarized below; see [Ammari and Nier 2008, Proposition 2.7].

Proposition 2.3 (composition of Wick symbols in the bosonic case). *We have*

$$b_1 \sharp^{\text{Wick}} b_2(z) = e^{\varepsilon \partial_{z_1} \cdot \partial_{\bar{z}_2}} b_1(z_1) b_2(z_2)|_{z_1=z_2=z} = \sum_{k=0}^{\min\{p_1, q_2\}} \frac{\varepsilon^k}{k!} \partial_z^k b_1(z) \cdot \partial_{\bar{z}}^k b_2(z).$$

The commutator of Wick operators in the bosonic case is given by

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

where the k -th order Poisson bracket is given by

$$\{b_1, b_2\}^{(k)}(w) = \partial_z^k b_1(w) \cdot \partial_{\bar{z}}^k b_2(w) - \partial_z^k b_2(w) \cdot \partial_{\bar{z}}^k b_1(w).$$

Proposition 2.4. *Let $p, m, m' \in \mathbb{N}$ such that $m + m' \geq 2p - 2$. Then, there exist coefficients $C_{j_1, \dots, j_k} \geq 0$ such that, for any $\tilde{b} \in \mathcal{L}(\mathcal{Z}; \mathcal{Z})$,*

$$\begin{aligned} d\Gamma_{\pm}(\tilde{b})^p - (\tilde{b}^{\otimes p})^{\text{Wick}} \\ = \sum_{k=1}^{p-1} \varepsilon^{p-k} \sum_{\substack{0 \leq j_1 \leq \dots \leq j_k \\ j_1 + \dots + j_k = p}} C_{j_1, \dots, j_k} (S_{\pm}^k \tilde{b}^{j_1} \otimes \dots \otimes \tilde{b}^{j_k} S_{\pm}^{k,*})^{\text{Wick}} \end{aligned} \quad (5)$$

and the estimate

$$\| (1 + N_{\pm})^{-\frac{m}{2}} (d\Gamma_{\pm}(\tilde{b})^p - (\tilde{b}^{\otimes p})^{\text{Wick}}) (1 + N_{\pm})^{-\frac{m'}{2}} \|_{\mathcal{L}(\Gamma_{\pm}(\mathcal{Z}))} \leq \varepsilon B_p \|\tilde{b}\|_{\mathcal{L}(\mathcal{Z})}^p$$

holds in both the bosonic and fermionic cases, with B_p the p -th Bell number.

Remark 2.5. The p -th Bell number B_p can be defined as the number of partitions of a set with p elements and satisfies $B_p < (0.792p/\ln(p+1))^p$, see [Berend and Tassa 2010], and hence it grows much slower than $p!$.

Proof. We first prove formula (5) by induction on $p \in \mathbb{N}^*$.

For $p = 1$, formula (5) holds because $d\Gamma_{\pm}(\tilde{b}) = (\tilde{b})^{\text{Wick}}$.

We then set $r_p(\tilde{b}) := d\Gamma_{\pm}(\tilde{b})^p - (\tilde{b}^{\otimes p})^{\text{Wick}}$. Assuming the result holds for some $p \in \mathbb{N}^*$, one can compute

$$d\Gamma_{\pm}(\tilde{b})^{p+1} = (\tilde{b}^{\otimes p})^{\text{Wick}}(\tilde{b})^{\text{Wick}} + r_p(\tilde{b})^{\text{Wick}}(\tilde{b})^{\text{Wick}}$$

using the composition formula (4) for

$$(\tilde{b}^{\otimes p})^{\text{Wick}}(\tilde{b})^{\text{Wick}} = (\tilde{b}^{\otimes p+1})^{\text{Wick}} + p\varepsilon (S_{\pm}^p \tilde{b}^{\otimes p-1} \otimes \tilde{b}^2 S_{\pm}^{p,*})^{\text{Wick}}$$

and for

$$\begin{aligned} \varepsilon^{p-k} (S_{\pm}^k \tilde{b}^{j_1} \otimes \dots \otimes \tilde{b}^{j_k} S_{\pm}^{k,*})^{\text{Wick}}(\tilde{b})^{\text{Wick}} \\ = \varepsilon^{p+1-(k+1)} (S_{\pm}^{k+1} \tilde{b} \otimes \tilde{b}^{j_1} \otimes \dots \otimes \tilde{b}^{j_k} S_{\pm}^{k+1,*})^{\text{Wick}} \\ + k\varepsilon^{p+1-k} (S_{\pm}^k (\tilde{b}^{j_1} \otimes \dots \otimes \tilde{b}^{j_k}) S_{\pm}^{k,*} S_{\pm}^k (\tilde{b} \otimes \text{Id}_{\mathcal{Z}^{\otimes j_1} + \dots + j_k - 1}) S_{\pm}^{k,*})^{\text{Wick}}, \end{aligned}$$

which yields the expected form for $r_{p+1}(\tilde{b})$, and achieves the induction.

We then remark that the sum of coefficients of order k ,

$$S_2(p, k) = \sum_{\substack{0 \leq j_1 \leq \dots \leq j_k \\ j_1 + \dots + j_k = p}} C_{j_1, \dots, j_k},$$

satisfies the recurrence relation $S_2(p, k) = kS_2(p-1, k) + S_2(p-1, k-1)$, with $S_2(p, 1) = 1 = S_2(1, k)$ for all $p, k \in \mathbb{N}^*$, where the $S_2(p, k)$ are the Stirling numbers of the second kind. Observe that, for $\frac{M}{2} \geq k$, and for any $\tilde{c} \in \mathcal{L}(S_{\pm}^k \mathcal{Z}^{\otimes k})$,

$$\|\tilde{c}^{\text{Wick}}(1 + N_{\pm})^{-\frac{M}{2}}\|_{\mathcal{L}(\Gamma_{\pm}(\mathcal{Z}))} \leq \|\tilde{c}\|_{\mathcal{L}(S_{\pm}^k \mathcal{Z}^{\otimes k}; S_{\pm}^k \mathcal{Z}^{\otimes k})}.$$

We thus get,

$$\begin{aligned} \|(1 + N_{\pm})^{-\frac{m}{2}} (d\Gamma_{\pm}(\tilde{b})^p - (\tilde{b}^{\otimes p})^{\text{Wick}}) (1 + N_{\pm})^{-\frac{m'}{2}}\|_{\mathcal{L}(\Gamma_{\pm}(\mathcal{Z}))} \\ \leq \sum_{k=1}^{p-1} \varepsilon^{p-k} S_2(p, k) \|\tilde{b}\|_{\mathcal{L}(\mathcal{Z})}^p \end{aligned}$$

and the estimate then follows from $\sum_{k=1}^{p-1} \varepsilon^{p-k} S_2(p, k) \leq \varepsilon \sum_{k=1}^p S_2(p, k) = \varepsilon B_p$, with B_p the p -th Bell number. $\square$

2B. Reduced density matrices. Reduced density matrices emerge naturally in the study of correlation functions of quantum gases [Spohn 1980]. In particular, in quantum mean-field theory they are the main quantities to be analyzed; see, e.g.,

[Bardos et al. 2000; Knowles and Pickl 2010; Lewin et al. 2016]. However, we shall work with *nonnormalized* reduced density matrices, which are easier to handle. Going back to the more natural reduced density matrices with trace equal to 1 requires attention when normalizing and taking the limits.

Definition 2.6. Let $\varrho_\varepsilon \in \mathcal{L}^1(\Gamma_\pm(\mathcal{Z}))$ ($\varepsilon > 0$ is fixed here) be such that $\varrho_\varepsilon \geq 0$, $\text{Tr}[\varrho_\varepsilon] = 1$ and $\text{Tr}(\varrho_\varepsilon e^{cN_\pm}) < \infty$ for some $c > 0$. The nonnormalized reduced density matrix of order $p \in \mathbb{N}$, $\gamma_\varepsilon^{(p)} \in \mathcal{L}^1(\mathcal{S}_\pm^p \mathcal{Z}^{\otimes p})$, is defined by duality according to,

$$\text{for all } \tilde{b} \in \mathcal{L}(\mathcal{S}_\pm^p \mathcal{Z}^{\otimes p}; \mathcal{S}_\pm^p \mathcal{Z}^{\otimes p}), \quad \text{Tr}[\gamma_\varepsilon^{(p)} \tilde{b}] = \text{Tr}[\varrho_\varepsilon \tilde{b}^{\text{Wick}}].$$

The definition makes sense owing to the number estimate (3) and to

$$(1 + N_\pm)^k e^{-cN_\pm} \in \mathcal{L}(\Gamma_\pm(\mathcal{Z})).$$

When $\text{Tr}[\gamma_\varepsilon^{(p)}] \neq 0$, the normalized density matrix $\bar{\gamma}_\varepsilon^{(p)}$ is defined by $\bar{\gamma}_\varepsilon^{(p)} = \gamma_\varepsilon^{(p)} / \text{Tr}[\gamma_\varepsilon^{(p)}]$; that is, for all $\tilde{b} \in \mathcal{L}(\mathcal{S}_\pm^p \mathcal{Z}^{\otimes p})$,

$$\text{Tr}[\bar{\gamma}_\varepsilon^{(p)} \tilde{b}] = \frac{\text{Tr}[\varrho_\varepsilon \tilde{b}^{\text{Wick}}]}{\text{Tr}[\varrho_\varepsilon (\text{Id}_{\mathcal{S}_\pm^p \mathcal{Z}^{\otimes p}})^{\text{Wick}}]} = \frac{\text{Tr}[\varrho_\varepsilon \tilde{b}^{\text{Wick}}]}{\text{Tr}[\varrho_\varepsilon N_\pm (N_\pm - \varepsilon) \cdots (N_\pm - \varepsilon(p-1))]}.$$

These normalized reduced density matrices $\bar{\gamma}_\varepsilon^{(p)}$ are commonly used, especially when $\varrho_\varepsilon \in \mathcal{L}^1(\mathcal{S}_\pm \mathcal{Z}^{\otimes n})$, with $n\varepsilon \sim 1$, for the following reason: when $\varrho_\varepsilon \in \mathcal{L}^1(\mathcal{S}_\pm^n \mathcal{Z}^{\otimes n})$ lies in the n -particle sector in the mean-field regime $n\varepsilon \rightarrow 1$, one has

$$\text{Tr}[\bar{\gamma}_\varepsilon^{(p)} \tilde{b}] = \text{Tr}[\varrho_\varepsilon (\tilde{b} \otimes \text{Id}_{\mathcal{Z}^{\otimes (n-p)}})] \quad \text{and} \quad \lim_{\substack{n\varepsilon \sim 1 \\ \varepsilon \rightarrow 0}} \text{Tr}[\bar{\gamma}_\varepsilon^{(p)} \tilde{b}] = \lim_{\substack{n\varepsilon \sim 1 \\ \varepsilon \rightarrow 0}} \text{Tr}[\gamma_\varepsilon^{(p)} \tilde{b}], \quad (6)$$

since for $n > p$,

$$\tilde{b}^{\text{Wick}}|_{\mathcal{S}_\pm^n \mathcal{Z}^{\otimes n}} = \varepsilon^p \frac{n!}{(n-p)!} \mathcal{S}_\pm^n (\tilde{b} \otimes \text{Id}_{\mathcal{Z}^{\otimes (n-p)}}) \mathcal{S}_\pm^{n,*}$$

and $\varepsilon^p n(n-1) \cdots (n-p+1) \rightarrow 1$ when $n\varepsilon \rightarrow 1$.

Moreover, one often works with kernels of (normalized) reduced density matrices $\bar{\gamma}_\varepsilon^{(p)}$ when $\mathcal{Z} = L^2(M; dv)$ with the following relation deduced from the left-hand side of (6):

$$\bar{\gamma}_\varepsilon^{(p)}(x_1, \dots, x_p; x'_1, \dots, x'_p) = \int_{M^{n-p}} \varrho_\varepsilon(x_1, \dots, x_p, x; x'_1, \dots, x'_p, x) dv^{\otimes (n-p)}(x).$$

But, if the states ϱ_ε are not localized on the n -particles then $\gamma_\varepsilon^{(p)}$ and $\bar{\gamma}_\varepsilon^{(p)}$ do not coincide even asymptotically in the mean-field regime (i.e., the right-hand side of (6) may not hold true). As well there is no simple relation between the

nonnormalized density matrices $\gamma_\varepsilon^{(p+1)}$ and $\gamma_\varepsilon^{(p)}$. Actually, we have

$$\begin{aligned} (S_\pm^{p+1}(\tilde{b} \otimes \text{Id}_{\mathcal{Z}})S_\pm^{p+1,*})^{\text{Wick}} \Big|_{S_\pm^{n+p+1} \mathcal{Z}^{\otimes(n+p+1)}} \\ = \varepsilon^{p+1} \frac{(n+p+1)!}{n!} S_\pm^{n+p+1}(\tilde{b} \otimes \text{Id}_{\mathcal{Z}^{\otimes(n+1)}})S_\pm^{n+p+1,*} \\ = \varepsilon(n+1)\tilde{b}^{\text{Wick}} \Big|_{S_\pm^{n+p+1} \mathcal{Z}^{\otimes(n+p+1)}}, \end{aligned}$$

from which we deduce

$$\text{Tr}[\gamma_\varepsilon^{(p+1)}(\tilde{b} \otimes \text{Id}_{\mathcal{Z}})] = \text{Tr}[\varrho_\varepsilon(N_\pm - \varepsilon p)\tilde{b}^{\text{Wick}}],$$

while

$$\text{Tr}[\gamma_\varepsilon^{(p)}\tilde{b}] = \text{Tr}[\varrho_\varepsilon\tilde{b}^{\text{Wick}}],$$

where we have again identified $\gamma_\varepsilon^{(p+1)}$ as an element of $\mathcal{L}^1(\mathcal{Z}^{\otimes(p+1)})$. We thus conclude with the following important remark.

Remark 2.7. Assume $\varrho_\varepsilon = \varrho_\varepsilon 1_{[\nu-\delta(\varepsilon), \nu+\delta(\varepsilon)]}(N_\pm)$ with $\nu > 0$ and $\lim_{\varepsilon \rightarrow 0} \delta(\varepsilon) = 0$. Then the following simple asymptotic relations between $\gamma_\varepsilon^{(p)}$ and $\gamma_\varepsilon^{(p')}$ (or the normalized versions $\tilde{\gamma}_\varepsilon^{(p)}$ and $\tilde{\gamma}_\varepsilon^{(p')}$) hold true for any $p' > p$ and any $\tilde{b} \in \mathcal{L}(S_\pm^p \mathcal{Z}^{\otimes p}; S_\pm^p \mathcal{Z}^{\otimes p})$,

$$\begin{aligned} \lim_{\varepsilon \rightarrow 0} \text{Tr}[\gamma_\varepsilon^{(p')}(\tilde{b} \otimes \text{Id}_{\mathcal{Z}^{\otimes(p'-p)}})] &= \nu^{p'-p} \lim_{\varepsilon \rightarrow 0} \text{Tr}[\gamma_\varepsilon^{(p)}\tilde{b}], \\ \lim_{\varepsilon \rightarrow 0} \text{Tr}[\tilde{\gamma}_\varepsilon^{(p')}(\tilde{b} \otimes \text{Id}_{\mathcal{Z}^{\otimes(p'-p)}})] &= \lim_{\varepsilon \rightarrow 0} \text{Tr}[\tilde{\gamma}_\varepsilon^{(p)}\tilde{b}]. \end{aligned}$$

We shall use recurrently with variations the following lemma, with the notation

$$\tilde{b}_1 \odot \cdots \odot \tilde{b}_p = \frac{1}{p!} \sum_{\sigma \in \mathfrak{S}_p} \tilde{b}_{\sigma(1)} \otimes \cdots \otimes \tilde{b}_{\sigma(p)}$$

for $\tilde{b}_1, \dots, \tilde{b}_p \in \mathcal{L}(\mathcal{Z})$.

We also abbreviate $(S_\pm^p(\tilde{b}_1 \odot \cdots \odot \tilde{b}_p)S_\pm^{p,*})^{\text{Wick}}$ by $(\tilde{b}_1 \odot \cdots \odot \tilde{b}_p)^{\text{Wick}}$ and $(S_\pm^p(\tilde{b}^{\otimes p})S_\pm^{p,*})^{\text{Wick}}$ by $(\tilde{b}^{\otimes p})^{\text{Wick}}$.

Lemma 2.8 (quantum symmetrization lemma). *In the bosonic and fermionic cases for any $p \in \mathbb{N}$, the equality*

$$S_\pm^p(\tilde{b}_1 \otimes \cdots \otimes \tilde{b}_p)S_\pm^{p,*} = S_\pm^p(\tilde{b}_1 \odot \cdots \odot \tilde{b}_{\sigma(p)})S_\pm^{p,*} \quad (7)$$

holds in $\mathcal{L}(S_\pm^p \mathcal{Z}^{\otimes p}; S_\pm^p \mathcal{Z}^{\otimes p})$ for all $\tilde{b}_1, \dots, \tilde{b}_p \in \mathcal{L}(\mathcal{Z}; \mathcal{Z})$.

As a consequence, under the assumptions of Definition 2.6, the nonnormalized (resp. normalized if possible) reduced density matrix $\gamma_\varepsilon^{(p)}$ (resp. $\tilde{\gamma}_\varepsilon^{(p)}$), $p \in \mathbb{N}$, is completely determined by the set of quantities $\{\text{Tr}[\varrho_\varepsilon(\tilde{b}^{\otimes p})^{\text{Wick}}], \tilde{b} \in \mathcal{B}\}$ when $\mathcal{B}$ is any dense subset of $\mathcal{L}^\infty(\mathcal{Z}; \mathcal{Z})$.

Remark 2.9. While computing $\text{Tr}[\gamma_\varepsilon^{(p)}]$ or studying $\bar{\gamma}_\varepsilon^{(p)}$ one can simply add to $\mathcal{B}$ the element $\text{Id}_{\mathcal{Z}}$ owing to $S_\pm^p \text{Id}_{\mathcal{Z}}^{\otimes p} S_\pm^{p,*} = \text{Id}_{S_\pm^p \mathcal{Z}^{\otimes p}}$. For $\varepsilon > 0$ fixed it is not necessary because compact observables are sufficient to determine the total trace owing to

$$\text{Tr}[\gamma_\varepsilon^{(p)}] = \sup_{\substack{B \in \mathcal{L}^\infty(S_\pm^p \mathcal{Z}^{\otimes p}) \\ 0 \leq B \leq \text{Id}}} \text{Tr}[\gamma_\varepsilon^{(p)} B].$$

However, while considering weak*-limits as $\varepsilon \rightarrow 0$, adding the identity operator $\text{Id}_{S_\pm^p \mathcal{Z}^{\otimes p}}$ to the set of compact observables, or possibly replacing $\mathcal{B}$ by the Calkin algebra $\mathbb{C}\text{Id}(\mathcal{Z}) \oplus \mathcal{L}^\infty(\mathcal{Z})$, is useful in order to control the asymptotic total mass.

Proof. For $\tilde{b}_1, \dots, \tilde{b}_p \in \mathcal{L}(\mathcal{Z})$, we decompose

$$S_\pm^p(\tilde{b}_1 \otimes \dots \otimes \tilde{b}_p) S_\pm^{p,*} S_\pm^p(\psi_1 \otimes \dots \otimes \psi_p)$$

as

$$\begin{aligned} S_\pm^p & \left[\frac{1}{p!} \sum_{\sigma' \in \mathfrak{S}_p} s_\pm(\sigma') (\tilde{b}_1 \psi_{\sigma'(1)}) \otimes \dots \otimes (\tilde{b}_p \psi_{\sigma'(p)}) \right] \\ &= \frac{1}{p! p!} \left[\sum_{\sigma \in \mathfrak{S}_p} \sum_{\sigma' \in \mathfrak{S}_p} s_\pm(\sigma) s_\pm(\sigma') (\tilde{b}_{\sigma(1)} \psi_{\sigma \circ \sigma'(1)}) \otimes \dots \otimes (\tilde{b}_{\sigma(p)} \psi_{\sigma \circ \sigma'(p)}) \right]. \end{aligned}$$

Setting $\sigma'' = \sigma \circ \sigma'$, with $s_\pm(\sigma'') = s_\pm(\sigma) s_\pm(\sigma')$ yields (7), after noting that $\tilde{b}_1 \odot \dots \odot \tilde{b}_p = \frac{1}{p!} \sum_{\sigma \in \mathfrak{S}_p} \tilde{b}_{\sigma(1)} \otimes \dots \otimes \tilde{b}_{\sigma(p)}$ commutes with $S_\pm^p$ in both the bosonic and fermionic cases.

Now the nonnormalized reduced density matrix is determined by

$$\text{Tr}[\gamma_\varepsilon^{(p)} \tilde{B}] = \text{Tr}[\varrho_\varepsilon \tilde{B}^{\text{Wick}}]$$

for $\tilde{B} \in \mathcal{L}^\infty(S_\pm^p \mathcal{Z}^{\otimes p})$ as $\mathcal{L}^1(S_\pm^p \mathcal{Z}^{\otimes p})$ is the dual of $\mathcal{L}^\infty(S_\pm^p \mathcal{Z}^{\otimes p})$. But $\tilde{B} \in \mathcal{L}^\infty(S_\pm^p \mathcal{Z}^{\otimes p})$ means $\tilde{B} = S_\pm^p \tilde{B}' S_\pm^{p,*}$ with $\tilde{B}' \in \mathcal{L}^\infty(\mathcal{Z}^{\otimes p})$, while the algebraic tensor product $\mathcal{L}^\infty(\mathcal{Z})^{\otimes_{\text{alg}} p}$ is dense in $\mathcal{L}^\infty(\mathcal{Z}^{\otimes p})$.

With the estimate

$$\begin{aligned} |\text{Tr}[\varrho_\varepsilon \tilde{B}^{\text{Wick}}]| &= |\text{Tr}[e^{\frac{\varepsilon}{2} N} \varrho_\varepsilon e^{\frac{\varepsilon}{2} N} e^{-\frac{\varepsilon}{2} N} \tilde{B}^{\text{Wick}} e^{-\frac{\varepsilon}{2} N}]| \\ &\leq C \text{Tr}[\varrho_\varepsilon e^{cN}] \|\tilde{B}\|_{\mathcal{L}(S_\pm^p \mathcal{Z}^{\otimes p}; S_\pm^p \mathcal{Z}^{\otimes p})}, \end{aligned}$$

it suffices to consider $\tilde{B} = S_\pm^p \tilde{B}' S_\pm^{p,*}$ with $\tilde{B}' \in \mathcal{L}^\infty(\mathcal{Z})^{\otimes_{\text{alg}} p}$. By linearity and density, $\gamma_\varepsilon^{(p)}$ is determined by the quantities $\text{Tr}[\varrho_\varepsilon \tilde{B}^{\text{Wick}}]$ with $\tilde{B}' = \tilde{b}_1 \otimes \dots \otimes \tilde{b}_p$, $\tilde{b}_i \in \mathcal{B}$. We conclude with

$$S_\pm^p(\tilde{b}_1 \otimes \dots \otimes \tilde{b}_p) S_\pm^{p,*} = S_\pm^p(\tilde{b}_1 \odot \dots \odot \tilde{b}_p) S_\pm^{p,*},$$

and the polarization identity

$$\tilde{b}_1 \odot \cdots \odot \tilde{b}_p = \frac{1}{2^p p!} \sum_{\varepsilon_i = \pm 1} \varepsilon_1 \cdots \varepsilon_p \left(\sum_{i=1}^p \varepsilon_i \tilde{b}_i \right)^{\otimes p}. \quad \square$$

Remark 2.10. In the bosonic case, the nonnormalized reduced density matrices $\gamma_\varepsilon^{(p)}$ are also characterized by the values of $\text{Tr}[\gamma_\varepsilon^{(p)} B]$ for B in

$$\mathcal{B} = \{|\psi^{\otimes p}\rangle\langle\psi^{\otimes p}| : \psi \in \mathcal{X}\} \cup \{\text{Id}_{\mathcal{X}^{\otimes p}}\}.$$

This does not hold in the fermionic case.

The rest of the article is devoted to the asymptotic analysis of $\gamma_\varepsilon^{(p)}$ as $\varepsilon \rightarrow 0$. In particular we shall study their concentration at the quantum level while testing with fixed observable $\tilde{b}$ (with $\tilde{b}$ compact) and their semiclassical behavior after taking semiclassically quantized observables, e.g., $a(x, hD_x)$ with some relation $\varepsilon = \varepsilon(h)$ between ε and h .

3. Classical phase-space and h -quantizations

When $\mathcal{X} = L^2(M^1, dx)$, with $M^1 = M$ a smooth manifold with volume measure dx , the classical 1-particle phase space is $\mathcal{X}^1 = \mathcal{X} = T^*M^1$ and we will focus on the h -dependent quantization which associates with a symbol $a(x, \xi) = a(X)$, $X \in \mathcal{X}^1$ an operator $a^{Q,h} = a(x, hD_x)$ with the standard semiclassical quantization or when $M^1 = \mathbb{R}^d$, $a^{Q,h} = a^{W,h} = a^W(h^t x, h^{1-t} D_x)$, by using the Weyl quantization, $t \in \mathbb{R}$ being fixed.

Note that in later sections the parameters ε and h will be linked through $\varepsilon = \varepsilon(h)$ with $\lim_{h \rightarrow 0} \varepsilon(h) = 0$. In relation with the symmetrization result, Lemma 2.8, we introduce the adapted p -particle phase space which was also considered in [Dereziński 1998], and the corresponding semiclassical observables.

3A. Classical p -particle phase space. A fundamental principle of quantum mechanics is that identical particles are indistinguishable. The classical description is thus concerned with indistinguishable classical particles. If one classical particle is characterized by its position-momentum $(x, \xi) \in \mathcal{X}^1 = T^*M^1$, $x \in M$ being the position coordinate and ξ the momentum coordinates, p indistinguishable particles will be described by their position-momentum coordinates $(X_1, \dots, X_p) = (x_1, \xi_1, \dots, x_p, \xi_p) \in \mathcal{X}^p / \mathfrak{S}_p = (T^*M)^p / \mathfrak{S}_p = T^*(M^p) / \mathfrak{S}_p$, where the quotient by $\mathfrak{S}_p$ simply implements the identification,

$$\text{for all } \sigma \in \mathfrak{S}_p, \quad (X_{\sigma(1)}, \dots, X_{\sigma(p)}) \equiv (X_1, \dots, X_p).$$

The grand canonical description of a classical particles system then takes place in the disjoint union

$$\bigsqcup_{p \in \mathbb{N}} \mathcal{X}^p / \mathfrak{S}_p = \bigsqcup_{p \in \mathbb{N}} (T^*M)^p / \mathfrak{S}_p.$$

A p -particle classical observable will be a function on $\mathcal{X}^p/\mathfrak{S}_p$ and, when the number of particles is not fixed, a collection of functions $(a^{(p)})_{p \in \mathbb{N}}$, each $a^{(p)}$ being a function on $\mathcal{X}^p/\mathfrak{S}_p$. The situation is presented in this way in [Dereziński 1998]. A p -particle observable is a function $a^{(p)}$ on $\mathcal{X}^p/\mathfrak{S}_p$ and a p -particle classical state is a probability measure (and when the normalization is forgotten, a nonnegative measure) on $\mathcal{X}^p/\mathfrak{S}_p$.

However while quantizing a classical observable, it is better to work in $\mathcal{X}^p$, which equals $T^*(M^p)$, a function $a^{(p)}$ on $\mathcal{X}^p/\mathfrak{S}_p$ being nothing but a function on $\mathcal{X}^p$ which satisfies,

$$\text{for all } \sigma \in \mathfrak{S}_p, \quad \sigma^* a^{(p)} = a^{(p)},$$

where,

$$\text{for all } (X_1, \dots, X_p) \in \mathcal{X}^p, \quad \sigma^* a^{(p)}(X_1, \dots, X_p) = a^{(p)}(X_{\sigma(1)}, \dots, X_{\sigma(p)}),$$

and

$$a^{(p)} = \frac{1}{p!} \sum_{\sigma \in \mathfrak{S}_p} \sigma^* a^{(p)}.$$

In the same way, we define for a Borel measure ν on $\mathcal{X}^p$ and $\sigma \in \mathfrak{S}_p$, the measure $\sigma_* \nu$ by $\int_{\mathcal{X}^p} \sigma^* a^{(p)} d\nu = \int_{\mathcal{X}^p} a^{(p)} d(\sigma_* \nu)$ for all $a^{(p)} \in \mathcal{C}_c^0(\mathcal{X}^p)$, or alternatively $\sigma_* \nu(E) = \nu(\sigma^{-1}(E))$ for all Borel subsets E of $\mathcal{X}^p$. A nonnegative measure on $\mathcal{X}^p/\mathfrak{S}_p$ is identified with a nonnegative measure ν on $\mathcal{X}^p$ such that,

$$\text{for all } \sigma \in \mathfrak{S}_p, \quad \sigma_* \nu = \nu = \frac{1}{p!} \sum_{\tilde{\sigma} \in \mathfrak{S}_p} \tilde{\sigma}_* \nu. \quad (8)$$

Lemma 3.1 (classical symmetrization lemma). *Any Borel measure $\mu^{(p)}$ on $\mathcal{X}^p/\mathfrak{S}_p$ is characterized by the quantities $\{\int_{\mathcal{X}^p} a^{\otimes p} d\mu^{(p)} : a \in \mathcal{C}\}$ where the tensor power $a^{\otimes p}$ means $a^{\otimes p}(X_1, \dots, X_p) = \prod_{i=1}^p a(X_i)$ and $\mathcal{C}$ is any dense set in $\mathcal{C}_\infty^0(\mathcal{X}^1) = \{f \in \mathcal{C}^0(\mathcal{X}^1) : \lim_{X \rightarrow \infty} f(X) = 0\}$.*

Proof. By the Stone–Weierstrass theorem the subalgebra generated by the algebraic tensor product $\mathcal{C}^{\otimes_{\text{alg}} p}$ is dense in $\mathcal{C}_\infty^0(\mathcal{X}^p)$. Hence it suffices to consider

$$a_1 \odot \dots \odot a_p = \frac{1}{p!} \sum_{\sigma \in \mathfrak{S}_p} a_{\sigma(1)} \otimes \dots \otimes a_{\sigma(p)}, \quad a_i \in \mathcal{C}.$$

We conclude again with the polarization identity

$$a_1 \odot \dots \odot a_p = \frac{1}{2^p p!} \sum_{\varepsilon_i = \pm 1} \varepsilon_1 \dots \varepsilon_p \left(\sum_{i=1}^p \varepsilon_i a_i \right)^{\otimes p}. \quad \square$$

We will work essentially with $M = \mathbb{R}^d$ and $\mathcal{X} = T^*\mathbb{R}^d$ and therefore on $\mathcal{X}^p = T^*\mathbb{R}^{dp} \sim \mathbb{R}^{2dp}$ and recall the invariance properties, if possible, by a change of variable in order to extend it to the general case. Remember that on $\mathbb{R}^{dp}$,

the standard and Weyl semiclassical quantization are asymptotically equivalent: $a(x, hD_x) - a^W(x, hD_x) = O(h)$ when $a \in S(1, dX^2)$ ($\sup_{X \in T^*\mathbb{R}^{dp}} |\partial_X^\alpha a(X)| < \infty$ for all $\alpha \in \mathbb{N}^{2d}$). Moreover on $\mathbb{R}^{dp}$, $a^W(x, hD_x)$ is unitary equivalent to $a^W(h^t x, h^{1-t} D_x)$ for any fixed $t \in \mathbb{R}$ so that result can be adapted to different scalings.

3B. Semiclassical and multiscale measures. We recall the notions of semiclassical (or Wigner) measures and multiscale measures in the finite-dimensional case. We start with the results on $M = \mathbb{R}^D$ (think of $D = dp$) and review the invariance properties for applications to some more general manifolds M .

3B1. In the Euclidean space. On $\mathbb{R}^D$ the semiclassical Weyl quantization of a symbol $a \in \mathcal{S}'(\mathbb{R}^{2D})$ will be written $a^{W,h} = a^W(h^t x, h^{1-t} D_x)$, with $t > 0$ fixed, while $c^W(x, D_x)$ is given by its kernel:

$$[c^W(x, D_x)](x, y) = \int_{\mathbb{R}^d} e^{i\xi \cdot (x-y)} c\left(\frac{x+y}{2}, \xi\right) \frac{d\xi}{(2\pi)^d}.$$

Definition 3.2. Let $(\gamma_h)_{h \in \mathcal{E}}$ with $0 \in \bar{\mathcal{E}}$, $\mathcal{E} \subset (0, +\infty)$, be a family of trace-class nonnegative operators on $L^2(\mathbb{R}^D)$ such that $\lim_{h \rightarrow 0} \text{Tr}[\gamma_h] < +\infty$. The semiclassical quantization $a \mapsto a^{W,h} = a^W(h^t x, h^{1-t} D_x)$ is said to be *adapted* to the family $(\gamma_h)_{h \in \mathcal{E}}$ if

$$\lim_{\delta \rightarrow 0^+} \limsup_{\substack{h \in \mathcal{E} \\ h \rightarrow 0}} \text{Re Tr}[(1 - \chi(\delta \cdot)^{W,h})\gamma_h] = 0$$

for some $\chi \in \mathcal{C}_0^\infty(T^*\mathbb{R}^D)$ such that $\chi \equiv 1$ in a neighborhood of 0.

The set of *Wigner measures* $\mathcal{M}(\gamma_h, h \in \mathcal{E})$ is the set of nonnegative measures ν on $T^*\mathbb{R}^D$ such that there exists $\mathcal{E}' \subset \mathcal{E}$, $0 \in \bar{\mathcal{E}'}$, such that,

$$\text{for all } a \in \mathcal{C}_0^\infty(T^*\mathbb{R}^D), \quad \lim_{\substack{h \in \mathcal{E}' \\ h \rightarrow 0}} \text{Tr}[\gamma_h a^{W,h}] = \int_{T^*\mathbb{R}^D} a(X) d\nu(X).$$

The following well-known statement, see [Colin de Verdière 1985; Helffer et al. 1987; Gérard 1991; Gérard et al. 1997; Lions and Paul 1993; Shnirel'man 1974], results from the asymptotic positivity of the semiclassical quantization and it is actually the finite-dimensional version of bosonic mean-field Wigner measures (with the change of parameter $\varepsilon = 2h$); see [Ammari and Nier 2008, Section 3.1].

Proposition 3.3. *Let $(\gamma_h)_{h \in \mathcal{E}}$ with $0 \in \bar{\mathcal{E}}$, $\mathcal{E} \subset (0, +\infty)$, such that $\gamma_h \geq 0$ and $\lim_{h \rightarrow 0} \text{Tr}[\gamma_h] < +\infty$. The set of semiclassical measures $\mathcal{M}(\gamma_h, h \in \mathcal{E})$ is nonempty. The semiclassical quantization $a^{W,h}$ is adapted to the family $(\gamma_h)_{h \in \mathcal{E}}$ if and only if any $\nu \in \mathcal{M}(\gamma_h, h \in \mathcal{E})$ satisfies $\nu(\mathbb{R}^{2D}) = \lim_{h \rightarrow 0} \text{Tr}[\gamma_h]$.*

Remark 3.4. (1) The manifold version, with $a^{\mathcal{Q},h} = a(x, hD_x)$ instead of $a^{W,h}$ results from the semiclassical Egorov theorem.

- (2) By reducing $\mathcal{E}$ to some subset $\mathcal{E}'$ (think of subsequence extraction), one can always assume that there is a unique semiclassical measure.
- (3) While considering a time evolution problem, or adding another uncountable parameter, $(\gamma_{t,h})_{h \in \mathcal{E}, t \in \mathbb{R}}$, finding simultaneously the subset $\mathcal{E}'$ for all $t \in \mathbb{R}$ requires some compactness argument with respect to the parameter $t \in \mathbb{R}$, usually obtained by equicontinuity properties.

We now review the multiscale measures introduced in [Fermanian-Kammerer and Gérard 2002; Fermanian Kammerer 2005]. For the reader's convenience, details are given in Appendix A, concerning the relationship between Proposition 3.5 below and the more general statement of [Fermanian Kammerer 2005].

The class of symbols $S^{(2)}$ is defined as the set of $a \in C^\infty(\mathbb{R}^{2D} \times \mathbb{R}^{2D})$ such that

- there exists $C > 0$ such that for all $Y \in \mathbb{R}^{2D}$, $a(\cdot, Y) \in C_0^\infty(B(0, C))$;
- there exists a function $a_\infty \in C_0^\infty(\mathbb{R}^{2D} \times \mathbb{S}^{2D-1})$ such that $a(X, R\omega) \rightarrow a_\infty(X, \omega)$, as $R \rightarrow \infty$, in $C^\infty(\mathbb{R}^{2D} \times \mathbb{S}^{2D-1})$.

Those symbols are quantized according to

$$a^{(2),h} = a_h^{W,h}, \quad a_h(X) = a\left(X, \frac{X}{h^{\frac{1}{2}}}\right).$$

A geometrical interpretation of those double scale symbols can be given by matching the compactified quantum phase space with the blow-up at $r = 0$ of the macroscopic phase space; see Figure 1.

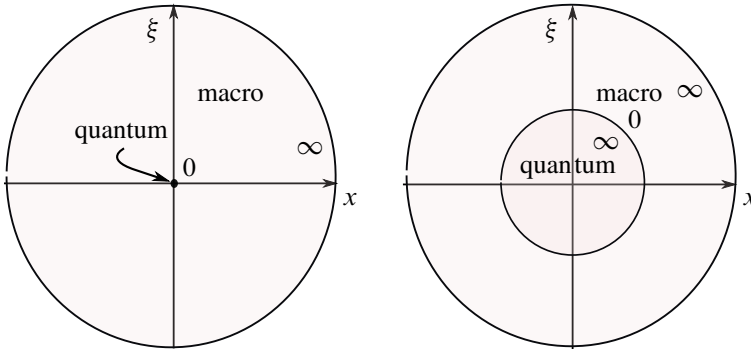


Figure 1. On the left-hand side, the macroscopic phase space with its sphere at infinity. On the right-hand side, the matched quantum and macroscopic phase spaces for which the quantum sphere at infinity and the $r = 0$ macroscopic sphere coincide.

Proposition 3.5. *Let $(\gamma_h)_{h \in \mathcal{E}}$ be a bounded family of nonnegative trace-class operators on $L^2(\mathbb{R}^D)$ with $\lim_{h \rightarrow 0} \text{Tr}[\gamma_h] < +\infty$. There exist $\mathcal{E}' \subset \mathcal{E}$, $0 \in \bar{\mathcal{E}}'$, nonnegative measures ν and $\nu_{(I)}$ on $\mathbb{R}^{2D}$ and $\mathbb{S}^{2D-1}$, and a $\gamma_0 \in \mathcal{L}^1(L^2(\mathbb{R}^D))$ such that $\mathcal{M}(\gamma_h, h \in \mathcal{E}') = \{\nu\}$ and, for all $a \in S^{(2)}$,*

$$\lim_{\substack{h \in \mathcal{E}' \\ h \rightarrow 0}} \text{Tr}[\gamma_h a^{(2),h}] = \int_{\mathbb{R}^{2D} \setminus \{0\}} a_\infty\left(X, \frac{X}{|X|}\right) d\nu(X) \\ + \int_{\mathbb{S}^{2D-1}} a_\infty(0, \omega) d\nu_{(I)}(\omega) + \text{Tr}[a(0, x, D_x)\gamma_0].$$

Definition 3.6. $\mathcal{M}^{(2)}(\gamma_h, h \in \mathcal{E})$ denotes the set of all triples $(\nu, \nu_{(I)}, \gamma_0)$ which can be obtained in Proposition 3.5 for suitable choices of $\mathcal{E}' \subset \mathcal{E}$, $0 \in \bar{\mathcal{E}}'$.

Remark 3.7. Actually when $a^{W,h} = a^W(\sqrt{h}x, \sqrt{h}D_x)$, this trace class operator γ_0 is nothing but the weak*-limit of γ_h . Take simply $\tilde{a}(X, Y) = \chi(X)\alpha(Y)$ with $\chi, \alpha \in C_0^\infty(\mathbb{R}^{2D})$, $\chi \equiv 1$ in a neighborhood of 0 for which

$$\lim_{h \rightarrow 0} \|\tilde{a}^{(2),h} - \alpha^W(x, D_x)\|_{\mathcal{L}(L^2)} = 0.$$

The above results says $\lim_{h \rightarrow 0} \text{Tr}[\gamma_h \alpha^W(x, D_x)] = \text{Tr}[\gamma_0 \alpha^W(x, D_x)]$ for all $\alpha \in C_0^\infty(\mathbb{R}^{2D}) \subset L^2(\mathbb{R}^{2D}, dX)$, and by the density of the embeddings $C_0^\infty(\mathbb{R}^{2D}) \subset L^2(\mathbb{R}^{2D}, dx) \sim \mathcal{L}^2(L^2(\mathbb{R}^D)) \subset \mathcal{L}^\infty(L^2(\mathbb{R}^D))$, the test observable $\alpha^W(x, D_x)$ can be replaced by any compact operator $K \in \mathcal{L}^\infty(L^2(\mathbb{R}^D, dx))$. Moreover the relationship between ν and the triple $(1_{(0,+\infty)}(|X|)\nu, \nu_{(I)}, \gamma_0)$ can be completed in this case by

$$\nu(\{0\}) = \int_{\mathbb{S}^{2D-1}} d\nu_{(I)}(\omega) + \text{Tr}[\gamma_0], \quad (9)$$

and $\nu_{(I)} \equiv 0$ is equivalent to $\nu(\{0\}) = \text{Tr}[\gamma_0]$.

Because products of spheres are not spheres, handling the part $\nu_{(I)}$ in the p -particle space, $D = dp$, is not straightforward within a tensorization procedure; see Figure 2.

Actually we expect in the applications that a well chosen quantization will lead to $\nu_{(I)} = 0$. This leads to the following definition.

Definition 3.8. Assume that the quantization $a^{W,h} = a^W(\sqrt{h}x, \sqrt{h}D_x)$ is adapted to the family $(\gamma_h)_{h \in \mathcal{E}}$, $\gamma_h \geq 0$, $\text{Tr}[\gamma_h] = 1$. We say that the quantization $a^{W,h} = a^W(\sqrt{h}x, \sqrt{h}D_x)$ is *separating* for the family $(\gamma_h)_{h \in \mathcal{E}}$ if one of the three following (equivalent) conditions is satisfied:

- (1) For any triple $(\nu, \nu_{(I)}, \gamma_0) \in \mathcal{M}^{(2)}(\gamma_h, h \in \mathcal{E})$, we have $\nu_{(I)} = 0$.
- (2)
$$\left. \begin{aligned} &\mathcal{M}(\gamma_h, h \in \mathcal{E}') = \{\nu\}, \\ &\text{w}^*\text{-}\lim_{h \in \mathcal{E}', h \rightarrow 0} \gamma_h = \gamma_0 \quad \text{in } \mathcal{L}^1(L^2(\mathbb{R}^D)) \end{aligned} \right\} \implies \nu(\{0\}) = \text{Tr}[\gamma_0].$$
- (3) For any triple $(\nu, \nu_{(I)}, \gamma_0) \in \mathcal{M}^{(2)}(\gamma_h, h \in \mathcal{E})$, we have $\nu(\{0\}) = \text{Tr}[\gamma_0]$.

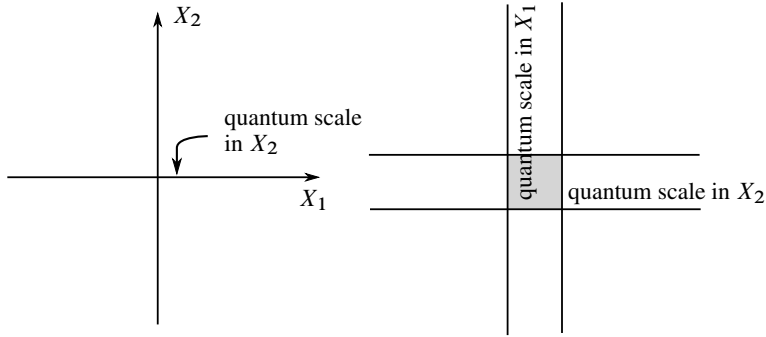


Figure 2. Tensor product of two blow-ups. The product of the two matching spheres is not a sphere: the corners of the gray square correspond to the case when the quantum variables $|X_1|$ and $|X_2|$ go to infinity without any proportionality rule.

Remark 3.9. This terminology expresses the fact that the mass localized at any intermediate scale vanishes asymptotically when $\nu_I \equiv 0$. Accordingly, the microscopic quantum scale and the macroscopic scale are well-identified and separated.

Hence we can get all the information by computing the weak*-limit of γ_h and the semiclassical measure ν and then by checking a posteriori the equality $\nu(\{0\}) = \text{Tr}[\gamma_0]$.

This will suffice when the quantum part corresponds, within a macroscopic scale, to a point in the phase space. When $M = \mathbb{R}^d$, we have enough flexibility by choosing the small parameter $h > 0$ and using some dilation in $\mathbb{R}^D$ in order to reduce many problems to such a case. On a manifold M if we can first localize the analysis around a point $x_0 \in M$, the problem can be transferred to $\mathbb{R}^D$ and then analyzed with the suitable scaling.

3B2. On a compact manifold. We now consider another interesting case of a smooth compact manifold M with the semiclassical calculus $a^{\mathcal{Q},h} = a(x, hD_x)$. This case is not completely treated in [Fermanian Kammerer 2005] because the geometric invariance properties do not follow only from the microlocal equivariance of semiclassical calculus. We assume $\mathcal{X} = L^2(M, dx)$ to be defined globally on the compact manifold M (e.g., by introducing a metric, dx being the associated volume measure).

Remark 3.10. When M is a general manifold, replace $a^{W,h}$ in Definition 3.2 by $a^{\mathcal{Q},h} = a(x, hD_x)$, and $\chi(\delta \cdot)$ with $\delta \rightarrow 0$ by some increasing sequence of compactly supported cut-off functions $(\chi_n)_{n \in \mathbb{N}}$ such that $\bigcup_{n \in \mathbb{N}} \chi_n^{-1}(\{1\}) = T^*M$.

To adapt Proposition 3.5 to the case of a compact manifold, we consider another notion instead of the symbols $S^{(2)}$. For the observables we shall consider the pair

(K, a) , where $K \in \mathcal{L}^\infty(L^2(M, dx))$ and $a \in \mathcal{C}_0^\infty(S^*M \sqcup (T^*M \setminus M))$, with $S^*M \sqcup (T^*M \setminus M)$ being described in local coordinates through the identification

$$M \times [0, \infty) \times \mathbb{S}^{D-1} \ni (x, r, \omega) \mapsto \begin{cases} (x, \omega) \in S^*M & \text{if } r = 0, \\ (x, \xi = r\omega) \in T^*M \setminus M & \text{otherwise.} \end{cases}$$

We have identified the 0-section of the cotangent bundle T^*M with M . After introducing an additional parameter $\delta > 0$, $\delta \geq h$, and a $\mathcal{C}^\infty$ partition of unity $(1 - \chi) + \chi \equiv 1$ on T^*M with $1 - \chi \in \mathcal{C}_0^\infty(T^*M)$, $1 - \chi \equiv 1$ in a neighborhood of M , we can quantize a as

$$a^{(2) \mathcal{Q}, \delta, h} = [\chi(x, \xi) a(x, h\delta^{-1}\xi)]^{\mathcal{Q}, \delta}.$$

Note that K and the quantization of a are geometrically defined modulo $\mathcal{O}(\delta)$ when $h \leq \delta$ in $\mathcal{L}(L^2(M, dx))$: use local charts for the semiclassical calculus with parameter δ , while $\mathcal{L}^\infty(L^2(M, dx))$ is globally defined like all natural spaces associated with $L^2(M, dx)$. Actually in local coordinates the seminorms of the symbol $\chi(x, \xi) a(x, h\delta^{-1}\xi)$ in $S(1, dx^2 + d\xi^2)$ are uniformly bounded with respect to $h \in (0, \delta]$ by seminorms of a in $\mathcal{C}_0^\infty((T^*M \setminus M) \sqcup S^*M)$. Moreover, when the symbol a is nonnegative one has

$$\|(\chi a(\cdot, h\delta^{-1}\cdot))^{\mathcal{Q}, \delta} - \text{Re}[(\chi a(\cdot, h\delta^{-1}\cdot))^{\mathcal{Q}, \delta}]\| \leq C_a \delta, \quad (10)$$

$$\|a\|_{L^\infty} + C_a \delta \geq \text{Re}[(\chi a(\cdot, h\delta^{-1}\cdot))^{\mathcal{Q}, \delta}] \geq -C_a \delta, \quad (11)$$

uniformly with respect to $h \in (0, \delta]$.

Proposition 3.11. *Let $(\gamma_h)_{h \in \mathcal{E}}$ be a family of nonnegative trace class operators on $L^2(M, dx)$ such that $\lim_{h \rightarrow 0} \text{Tr}[\gamma_h] < +\infty$. Then there exist $\mathcal{E}' \subset \mathcal{E}$, $0 \in \bar{\mathcal{E}}'$, with $\mathcal{M}(\gamma_h, h \in \mathcal{E}') = \{\nu\}$, a nonnegative measure $\nu_{(I)}$ on S^*M and a nonnegative $\gamma_0 \in \mathcal{L}^1(L^2(M, dx))$ such that, for any $K \in \mathcal{L}^\infty(L^2(M, dx))$,*

$$\lim_{\substack{h \in \mathcal{E}' \\ h \rightarrow 0}} \text{Tr}[\gamma_h K] = \text{Tr}[\gamma_0 K],$$

and, for any $a \in \mathcal{C}_0^\infty(S^*M \sqcup (T^*M \setminus M))$, and any partition of unity $(1 - \chi) + \chi \equiv 1$ with $1 - \chi \in \mathcal{C}_0^\infty(T^*M)$, $1 - \chi \equiv 1$ in a neighborhood of M ,

$$\lim_{\delta \rightarrow 0} \lim_{\substack{h \in \mathcal{E}' \\ h \rightarrow 0}} \text{Tr}[\gamma_h a^{(2) \mathcal{Q}, \delta, h}] = \int_{T^*M \setminus M} a(X) d\nu(X) + \int_{S^*M} a(X) d\nu_{(I)}(X).$$

Additionally $(\nu_{(I)}, \gamma_0)$ is related to ν by

$$\nu(E) = \nu_{(I)}(\pi^{-1}(E)) + \nu_0(E)$$

for any Borel set $E \subset M$ identified with $E \times \{0\}$, when $\pi : S^*M \rightarrow M$ is the natural projection and ν_0 is defined by $\int_M \varphi(x) d\nu_0(x) = \text{Tr}[\gamma_0 \varphi]$, where $\varphi \in \mathcal{C}^\infty(M)$ is identified with the multiplication operator by the function φ .

Proof. When γ_h is bounded in $\mathcal{L}^1(L^2(M, dx))$, after extraction of a sequence $h_n \rightarrow 0$ from $\mathcal{E}$, we have $\mathcal{M}((\gamma_{h_n})_{n \in \mathbb{N}}) = \{\nu\}$, and the weak*-limit γ_0 of (γ_{h_n}) , and the associated measure ν_0 are well-defined objects on the manifold M .

Let us construct a measure $\tilde{\nu}$ on

$$(T^*M \setminus M) \sqcup S^*M = \{(x, r\omega) : x \in M, \omega \in S^{d-1}, r \in [0, \infty)\}$$

and a subset $\mathcal{E}' \subset \mathcal{E}$, $0 \in \bar{\mathcal{E}}'$, such that

$$\lim_{\delta \rightarrow 0} \lim_{\substack{h \in \mathcal{E}' \\ h \rightarrow 0}} \text{Tr}[\gamma_h(\chi a(\cdot, h\delta^{-1} \cdot)) \mathcal{Q}^{\delta}] = \int_{(T^*M \setminus M) \sqcup S^*M} a d\tilde{\nu} \quad (12)$$

holds for all $a \in \mathcal{C}_0^\infty((T^*M \setminus M) \sqcup S^*M)$.

Fix first the partition of unity $(1 - \chi) + \chi \equiv 1$, $1 - \chi \in \mathcal{C}_0^\infty(T^*M)$, $1 - \chi \equiv 1$ in a neighborhood of M , and $\delta = \delta_0 > 0$. For a given $a \in \mathcal{C}_0^\infty((T^*M \setminus M) \sqcup S^*M)$, the inequalities (10) and (11) imply that one can find a subsequence $(h_{k, \chi, \delta_0, a})_{k \in \mathbb{N}}$ of $(h_n)_{n \in \mathbb{N}}$ such that

$$\lim_{k \rightarrow \infty} \text{Tr}[\gamma_{h_{k, \chi, \delta_0, a}}(\chi a(\cdot, h_{k, \chi, \delta_0, a} \delta_0^{-1} \cdot)) \mathcal{Q}^{\delta_0}] = \ell_{\chi, \delta_0, a} \in \mathbb{C}. \quad (13)$$

For a different partition of unity $(1 - \tilde{\chi}) + \tilde{\chi} \equiv 1$ the symbol $[\chi - \tilde{\chi}]a(x, h\delta_0^{-1}\xi)$ is supported in $C_{\chi, \tilde{\chi}, \delta_0}^{-1} \leq |\xi| \leq C_{\chi, \tilde{\chi}, \delta_0}$ and equals

$$[\chi - \tilde{\chi}]a(x, h\delta_0^{-1}\xi) = [\chi - \tilde{\chi}]a_0\left(x, \frac{\xi}{|\xi|}\right) + hr_{\chi, \tilde{\chi}, \delta_0, h}(x, \xi),$$

where $a_0 = a|_{S^*M}$ and with $r_{\chi, \tilde{\chi}, \delta_0, h}$ uniformly bounded in $S(1, dx^2 + d\xi^2)$. For $\delta_0 > 0$ fixed, the operator $[(\chi - \tilde{\chi})a_0] \mathcal{Q}^{\delta_0}$ is a compact operator and we obtain

$$\lim_{h \rightarrow 0} \text{Tr}[\gamma_h(\chi a(\cdot, h\delta_0^{-1} \cdot)) \mathcal{Q}^{\delta_0}] - \text{Tr}[\gamma_h(\tilde{\chi} a(\cdot, h\delta_0^{-1} \cdot)) \mathcal{Q}^{\delta_0}] = \text{Tr}[\gamma_0((\chi - \tilde{\chi})a_0) \mathcal{Q}^{\delta_0}].$$

Therefore the subsequence extraction, which ensures the convergence (13), can be done independently of the choice of $\tilde{\chi}$ and by taking $\tilde{\chi}(x, \xi) = \chi(x, \delta\delta_0^{-1}\xi)$ independently of $\delta > 0$. For $\mathcal{E}_a = (h_{k, a})_{k \in \mathbb{N}}$ such a sequence of parameters, the limits can be compared by

$$\begin{aligned} \ell_{\tilde{\chi}, \delta, a} - \ell_{\chi, \delta_0, a} &= \lim_{\substack{h \in \mathcal{E}_a \\ h \rightarrow 0}} \text{Tr}[\gamma_h(\tilde{\chi} a(\cdot, h\delta^{-1} \cdot)) \mathcal{Q}^{\delta}] - \text{Tr}[\gamma_h(\chi a(\cdot, h\delta_0^{-1} \cdot)) \mathcal{Q}^{\delta_0}] \\ &= \text{Tr}[(\tilde{\chi}(\delta\delta_0^{-1}) - \chi)a_0] \mathcal{Q}^{\delta_0} \gamma_0. \end{aligned} \quad (14)$$

By choosing $\tilde{\chi} = \chi$ above, the inequality $0 \leq (\chi - \chi(\delta\delta_0^{-1}))a_0 \leq \chi a_0$ for $a_0 \geq 0$ and $\delta \leq \delta_0$, and the δ_0 -Gårding inequality implies

$$|\text{Tr}[(\tilde{\chi}(\delta\delta_0^{-1}) - \chi)a_0] \mathcal{Q}^{\delta_0} \gamma_0| \leq \text{Tr}[(\chi a_0) \mathcal{Q}^{\delta_0} \gamma_0] + \mathcal{O}(\delta_0)$$

uniformly with respect to $\delta \leq \delta_0$. Thus the quantity $\ell_{\chi,\delta,a}$ satisfies the Cauchy criterion as $\delta \rightarrow 0$ because $\text{s-lim}_{\delta \rightarrow 0} (\chi a_0)^{\mathcal{Q},\delta_0} = 0$ and γ_0 is fixed in $\mathcal{L}^1(L^2(M, dx))$. Hence the limit

$$\ell_{\chi,a} = \lim_{\delta \rightarrow 0} \ell_{\chi,\delta,a} = \lim_{\delta \rightarrow 0} \lim_{\substack{h \in \mathcal{E}'_a \\ h \rightarrow 0}} \text{Tr}[\gamma_h(\chi a(\cdot, h\delta^{-1}\cdot))^{\mathcal{Q},\delta}]$$

exists for any fixed $a \in \mathcal{C}_0^\infty((T^*M \setminus M) \sqcup S^*M)$. Using (14) with $\delta = \delta_0$, but a general pair $(\chi, \tilde{\chi})$, and taking the limit as $\delta \rightarrow 0$ shows $\ell_{\tilde{\chi},a} = \ell_{\chi,a} = \ell_a$. The inequalities (10) and (11) give $0 \leq \ell_a \leq \|a\|_{L^\infty}$. By the usual diagonal extraction process according to a countable set $\mathcal{N} \subset \mathcal{C}_0^\infty((T^*M \setminus M) \sqcup S^*M)$ dense in the set of continuous functions with limit 0 at infinity, we have found a subset $\mathcal{E}' \subset \mathcal{E}$, $0 \in \bar{\mathcal{E}}'$, and a nonnegative measure $\tilde{\nu}$ such that (12) holds. Note that we have also proved

$$\begin{aligned} \int_{(T^*M \setminus M) \sqcup S^*M} a \, d\tilde{\nu} &= \lim_{\delta \rightarrow 0} \lim_{\substack{h \in \mathcal{E}' \\ h \rightarrow 0}} \text{Tr}[\gamma_h(\chi a(\cdot, h\delta^{-1}\cdot))^{\mathcal{Q},\delta}] \\ &= \lim_{\delta \rightarrow 0} \lim_{\substack{h \in \mathcal{E}' \\ h \rightarrow 0}} \text{Tr}[(\gamma_h - \gamma_0)(\chi a(\cdot, h\delta^{-1}\cdot))^{\mathcal{Q},\delta}], \end{aligned}$$

where neither limit depends on the partition of unity $(1 - \chi) + \chi \equiv 1$ with $1 - \chi \in \mathcal{C}_0^\infty(T^*M)$ equal to 1 in a neighborhood of M .

We still have to compare $\tilde{\nu}$ and ν . For this take $a \in \mathcal{C}_0^\infty(T^*M)$ and set $a_0(x, \omega) = \varphi(x) = a(x, 0)$. The symbol identity

$$\begin{aligned} a(x, h\delta^{-1}\xi) &= a(x, h\delta^{-1}\xi)(1 - \chi) + a(x, h\delta^{-1}\xi)\chi \\ &= \varphi(x)(1 - \chi) + a(x, h\delta^{-1}\xi)\chi + hr_{a,\chi,\delta,h}, \end{aligned}$$

with $r_{a,\delta,\chi,h}$ uniformly bounded in $S(1, dx^2 + d\xi^2)$ with respect to h , leads after δ -quantization to

$$\begin{aligned} \int_{T^*M} a \, d\nu &= \lim_{\substack{h \in \mathcal{E}' \\ h \rightarrow 0}} \text{Tr}[\gamma_h a^{\mathcal{Q},h}] \\ &= \lim_{\substack{h \in \mathcal{E}' \\ h \rightarrow 0}} \text{Tr}[\gamma_h(\varphi(x)(1 - \chi))^{\mathcal{Q},\delta}] + \lim_{\substack{h \in \mathcal{E}' \\ h \rightarrow 0}} \text{Tr}[\gamma_h(\chi a(\cdot, h\delta^{-1}\cdot))^{\mathcal{Q},\delta}]. \end{aligned}$$

For $\delta > 0$ fixed, $(\varphi(x)(1 - \chi))^{\mathcal{Q},\delta}$ is a fixed compact operator so that the first limit is

$$\lim_{\substack{h \in \mathcal{E}' \\ h \rightarrow 0}} \text{Tr}[\gamma_h(\varphi(x)(1 - \chi))^{\mathcal{Q},\delta}] = \text{Tr}[\gamma_0(\varphi(x)(1 - \chi))^{\mathcal{Q},\delta}],$$

while the second one is exactly the quantity occurring in the definition of $\tilde{\nu}$. Taking the limit as $\delta \rightarrow 0$ with $\text{s-lim}_{\delta \rightarrow 0} (\varphi(x)(1 - \chi))^{\mathcal{Q},\delta} = \varphi(x)$, yields $\nu|_{T^*M \setminus M} =$

$\tilde{v}|_{T^*M \setminus M}$. Finally setting $\nu_{(I)} = \tilde{v}|_{S^*M}$ yields, for any $a \in \mathcal{C}_0^\infty(T^*M)$,

$$\int_{T^*M} a \, d\nu = \int_{T^*M \setminus M} a \, d\nu + \int_{S^*M} a_0 \, d\nu_{(I)} + \int_M \varphi \, d\nu_0,$$

which implies the relation for the measures. $\square$

Definition 3.12. $\mathcal{M}^{(2)}(\gamma_h, h \in \mathcal{E})$ denotes the set of all triples $(\nu, \nu_{(I)}, \gamma_0)$ which can be obtained in Proposition 3.11 for suitable choices of $\mathcal{E}' \subset \mathcal{E}$, $0 \in \bar{\mathcal{E}}'$.

We note that the equality $\nu(M) = \text{Tr}[\gamma_0]$ implies $\nu_{(I)} \equiv 0$ and this leads, as in the previous case, to the following definition.

Definition 3.13. On a compact manifold M , assume that the quantization $a^{\mathcal{Q},h} = a(x, hD_x)$ is adapted to the family $(\gamma_h)_{h \in \mathcal{E}}$, with $\gamma_h \in \mathcal{L}^1(L^2(M))$, $\gamma_h \geq 0$ and $\lim_{h \rightarrow 0} \text{Tr}[\gamma_h] < \infty$. We say that the quantization is *separating* if for any $\mathcal{E}' \subset \mathcal{E}$, $0 \in \bar{\mathcal{E}}'$,

$$\left. \begin{array}{l} \mathcal{M}(\gamma_h, h \in \mathcal{E}') = \{\nu\}, \\ \text{w}^*\text{-}\lim_{h \in \mathcal{E}', h \rightarrow 0} \gamma_h = \gamma_0 \text{ in } \mathcal{L}^1(L^2(M)) \end{array} \right\} \implies \nu(\{\xi = 0\}) = \text{Tr}[\gamma_0].$$

While doing the double scale analysis of the nonnormalized reduced density matrices $\bar{\gamma}_h^{(p)}$, especially with the help of tensorization arguments, we will simply study their weak*-limit in $\mathcal{L}^1$ and their semiclassical measures. The equality of Definition 3.8 or 3.13 will be checked a posteriori in order to ensure $\nu_{(I)} \equiv 0$.

4. Mean-field asymptotics with h -dependent observables

We now combine the mean-field asymptotics with semiclassically quantized observables. This means that the parameter ε appearing in CCR (resp. CAR) relations in Section 2 is bound to the semiclassical parameter h of Section 3 parametrizing observables $a^{W,h}$ (or $a^{\mathcal{Q},h}$):

$$\varepsilon = \varepsilon(h) > 0 \quad \text{with} \quad \lim_{h \rightarrow 0} \varepsilon(h) = 0.$$

So, from now on we consider families of density matrices on the fermionic or bosonic Fock space $\Gamma_\pm(\mathcal{H})$ labeled as $(Q_\varepsilon(h))_{h \in \mathcal{E}}$ with their reduced density matrices denoted by $(\gamma_{\varepsilon(h)}^{(p)})_{h \in \mathcal{E}}$. Firstly, we give a sufficient condition in terms of semiclassical 1-particle observables and of the family $(Q_\varepsilon(h))_{h \in \mathcal{E}}$ so that a quantization $a^{W,h}$ defined on the p -particle phase space $\mathcal{X}^p$ is adapted to the nonnormalized reduced density matrix $\gamma_{\varepsilon(h)}^{(p)}$ for all $p \in \mathbb{N}$. After this, the quantum and classical symmetrization results, Lemmas 2.8 and 3.1, then provide simple ways to identify the weak*-limits $\gamma_0^{(p)}$ or the semiclassical measures associated with the family $(\gamma_{\varepsilon(h)}^{(p)})_{h \in \mathcal{E}}$ for all $p \in \mathbb{N}$. According to the discussion in Section 2 about Definitions 3.8 and 3.13, a simple mass argument allows one to check that all the

multiscale information has been classified. Recall that if

$$\lim_{h \rightarrow 0} \text{Tr}[\gamma_{\varepsilon(h)}^{(p)}] = \lim_{h \rightarrow 0} \text{Tr}[\varrho_{\varepsilon(h)} N_{\pm}^p] = T^{(p)}$$

then the semiclassical measures $\nu^{(p)} \in \mathcal{M}(\gamma_{\varepsilon(h)}^{(p)}, h \in \mathcal{E})$ (or multiscale asymptotic triples $(\nu^{(p)}, \nu_{(I)}^{(p)}, \gamma_0^{(p)})$) have a total mass equal to $T^{(p)}$.

Remember that the nonnormalized reduced density matrices $\gamma_{\varepsilon(h)}^{(p)}$ are defined for $h > 0$ by,

$$\text{for all } \tilde{b} \in \mathcal{L}(S_{\pm}^p \mathcal{X}^{\otimes p}), \quad \text{Tr}[\gamma_{\varepsilon(h)}^{(p)} \tilde{b}] = \text{Tr}[\varrho_{\varepsilon(h)} \tilde{b}^{\text{Wick}}].$$

They are well-defined and uniformly bounded trace-class operators with respect to $h \in \mathcal{E}$, as soon as $\text{Tr}[\varrho_{\varepsilon(h)} N_{\pm}^p]$ is bounded uniformly with respect to $h \in \mathcal{E}$ for every $p \in \mathbb{N}$. Actually, it is more convenient in many cases, and not so restrictive, to work with exponential weights in terms of the number operator $N_{\pm}$.

Hypothesis 4.1. *The family $(\varrho_{\varepsilon(h)})_{h \in \mathcal{E}}$ in $\mathcal{L}^1(\Gamma_{\pm}(\mathcal{X}))$ satisfies:*

- (i) *For all $h \in \mathcal{E}$, we have $\varrho_{\varepsilon(h)} \geq 0$ and $\text{Tr}[\varrho_{\varepsilon(h)}] = 1$.*
- (ii) *There exist $c, C > 0$ such that $\text{Tr}[\varrho_{\varepsilon(h)} e^{cN_{\pm}}] \leq C$ for all $h \in \mathcal{E}$.*

When the 1-particle phase space is $\mathcal{X}^1 = T^*\mathbb{R}^d$ we use the Weyl quantization on $\mathcal{X}^p = T^*\mathbb{R}^{dp}$, $a^{\mathcal{Q},h} = a^{W,h} = a^W(h^t x, h^{1-t} D_x)$, $x \in \mathbb{R}^{dp}$, and when M^1 is a compact manifold, $\mathcal{X}^p = T^*M^p$, we use $a^{\mathcal{Q},h} = a(x, hD_x)$, $x \in M^p$.

Proposition 4.2. *Assume Hypothesis 4.1. Let $\chi \in \mathcal{C}_0^\infty(T^*M^1)$ satisfy $0 \leq \chi \leq 1$ and $\chi \equiv 1$ in a neighborhood of 0 (resp. in a neighborhood of the null section $\{(x, \xi) \in T^*M : \xi = 0\} = M$) when $M = \mathbb{R}^d$ (resp. M is a compact manifold) and let $\chi_\delta(X) = \chi(\delta X)$ (resp. $\chi_\delta(x, \xi) = \chi(x, \delta\xi)$). For $c' < c$, where c is given by Hypothesis 4.1(ii), if*

$$s_{c',\chi}(\delta) = \limsup_{h \rightarrow 0} \text{Re} \text{Tr}[\varrho_{\varepsilon(h)}(e^{c'N_{\pm}} - e^{c'd\Gamma_{\pm}(\chi_\delta^{\mathcal{Q},h})})] \rightarrow 0 \quad \text{as } \delta \rightarrow 0, \quad (15)$$

then for all $p \in \mathbb{N}$, the quantization $a^{\mathcal{Q},h}$ is adapted to the family $\gamma_{\varepsilon(h)}^{(p)}$.

Lemma 4.3. *Let $A \in \mathcal{L}(\mathcal{X})$ and $\alpha \geq \|A\|$. For z in the open disc $D(0, \alpha/\|A\|) \subset \mathbb{C}$, the operator $e^{zd\Gamma_{\pm}(A)} e^{-\alpha N_{\pm}} = e^{d\Gamma_{\pm}(zA - \alpha \text{Id}_{\mathcal{X}})}$ is a contraction in $\Gamma_{\pm}(\mathcal{X})$ and the function $z \mapsto e^{d\Gamma_{\pm}(zA - \alpha \text{Id}_{\mathcal{X}})}$ is holomorphic in $D(0, \alpha/\|A\|)$ with*

$$\begin{aligned} \frac{1}{p!} d\Gamma_{\pm}(A)^p e^{-\alpha N_{\pm}} &= e^{-\alpha N_{\pm}} \frac{1}{p!} d\Gamma_{\pm}(A)^p \\ &= \frac{1}{2i\pi} \int_{|z|=r} e^{d\Gamma_{\pm}(zA - \alpha \text{Id}_{\mathcal{X}})} \frac{dz}{z^{p+1}}, \end{aligned} \quad (16)$$

which holds true in $\mathcal{L}(\Gamma_{\pm}(\mathcal{X}))$ for all $p \in \mathbb{N}$ and all $r \in (0, \alpha/\|A\|)$.

Assume moreover that $A, B \in \mathcal{L}(\mathcal{Z})$, and $\alpha > \alpha_0 = \max\{\|A\|, \|B\|\}$. Then:

(1) For all $z \in D(0, \alpha/\alpha_0)$,

$$\|(e^{zd\Gamma_{\pm}(B)} - e^{zd\Gamma_{\pm}(A)})e^{-\alpha N_{\pm}}\|_{\mathcal{L}(\Gamma_{\pm}(\mathcal{Z}))} \leq \frac{\alpha\|B - A\|_{\mathcal{L}(\mathcal{Z})}}{\alpha_0(\alpha - \alpha_0)e}.$$

(2) For all $p \in \mathbb{N}$ and $r \in (0, \alpha/\alpha_0)$,

$$\|(d\Gamma_{\pm}(B)^p - d\Gamma_{\pm}(A)^p)e^{-\alpha N_{\pm}}\|_{\mathcal{L}(\Gamma_{\pm}(\mathcal{Z}))} \leq \frac{\alpha p! \|B - A\|_{\mathcal{L}(\mathcal{Z})}}{\alpha_0(\alpha - \alpha_0)e r^p}.$$

Proof of Lemma 4.3. After setting $A' = zA$ with $|z| < \alpha/\|A\|$ so that $\|A'\| < \alpha$, notice that $\|e^{\varepsilon(A' - \alpha)}\| \leq e^{\varepsilon\|A'\|}e^{-\varepsilon\alpha} < 1$. Hence, the operators $\Gamma_{\pm}(e^{-\varepsilon(A' - \alpha)}) = e^{-\alpha N_{\pm}}e^{d\Gamma_{\pm}(A')} = e^{d\Gamma_{\pm}(A')}e^{-\alpha N_{\pm}}$ are contractions on $\Gamma_{\pm}(\mathcal{Z})$. The holomorphy and the Cauchy formula are then standard.

For the second statement, set $B' = zB$ and $A' = zA$, $|z| < \alpha/\alpha_0$, and use Duhamel's formula:

$$\begin{aligned} e^{-d\Gamma_{\pm}(\alpha - B')} - e^{-d\Gamma_{\pm}(\alpha - A')} \\ = \int_0^1 e^{-(1-t)d\Gamma_{\pm}(\alpha_0 - A')} d\Gamma_{\pm}(B' - A') e^{-(\alpha - \alpha_0)N_{\pm}} e^{-td\Gamma_{\pm}(\alpha_0 - B')} dt. \end{aligned}$$

Since $e^{-(1-t)d\Gamma_{\pm}(\alpha_0 - A')}$ and $e^{-td\Gamma_{\pm}(\alpha_0 - B')}$ are contractions, the inequality

$$\|d\Gamma_{\pm}(B' - A')e^{-(\alpha - \alpha_0)N_{\pm}}\| \leq \frac{\alpha}{\alpha_0}\|B - A\| \sup_{n \in \mathbb{N}} \varepsilon n e^{-(\alpha - \alpha_0)\varepsilon n} \leq \frac{\alpha\|B - A\|}{\alpha_0(\alpha - \alpha_0)e}$$

yields part (1).

Part (2) follows from (16) and part (1). $\square$

Proof of Proposition 4.2. Fix $p \in \mathbb{N}$. We want to find $\tilde{\chi} \in \mathcal{C}_0^{\infty}(T^*M^p)$, $0 \leq \tilde{\chi} \leq 1$, and $\tilde{\chi} \equiv 1$ in a neighborhood of $\{X \in \mathbb{R}^{2dp} : X = 0\}$ (resp. $\{(x, \xi) \in T^*M^p : \xi = 0\} = M^p$) when $M^p = \mathbb{R}^{dp}$ (resp. when M is a compact manifold), such that

$$\lim_{\delta \rightarrow 0} \limsup_{h \rightarrow 0} \mathcal{T}(\delta, h) = 0,$$

with

$$\begin{aligned} \mathcal{T}(\delta, h) &:= \operatorname{Re} \operatorname{Tr}[\gamma_{\varepsilon(h)}^{(p)} (\operatorname{Id}_{S_{\pm}^p \mathcal{Z}^{\otimes p}} - \tilde{\chi}_{\delta}^{Q, h})] \\ &= \operatorname{Re} \operatorname{Tr}[\varrho_{\varepsilon(h)} (\operatorname{Id}_{S_{\pm}^p \mathcal{Z}^{\otimes p}} - \tilde{\chi}_{\delta}^{Q, h})^{\operatorname{Wick}}]. \end{aligned}$$

We know that $\chi^{\otimes p} \in \mathcal{C}_0^{\infty}(T^*M^p)$, with $0 \leq \chi^{\otimes p} \leq 1$. Take $\tilde{\chi}$ such that $\chi^{\otimes p} \leq \tilde{\chi} \leq 1$. For a constant $\kappa_{\delta} > 0$ to be fixed, the inequalities of symbols

$$\begin{aligned} 0 &\leq \chi_{\delta}^{\otimes p} \leq \tilde{\chi}_{\delta} \leq 1, \\ 0 &\leq \chi_{\delta} + \kappa_{\delta} h \leq 1 + \kappa_{\delta} h \end{aligned}$$

and the semiclassical calculus imply

$$\|(1 - \tilde{\chi}_\delta)^{\mathcal{Q},h} - \operatorname{Re}[(1 - \tilde{\chi}_\delta)^{\mathcal{Q},h}]\|_{\mathcal{L}(\mathcal{X}^{\otimes p})} \leq C_\delta h,$$

$$\|\chi_\delta^{\mathcal{Q},h} - \operatorname{Re}[\chi_\delta^{\mathcal{Q},h}]\| \leq C_\delta h,$$

$$\begin{aligned} 0 &\leq \operatorname{Re}[(1 - \chi_\delta^{\otimes p})^{\mathcal{Q},h}] + C'_\delta h = 1 - (\operatorname{Re}[\chi_\delta^{\mathcal{Q},h}])^{\otimes p} + C'_\delta h \\ &\leq (1 + 2\kappa_\delta h)^p - (\operatorname{Re}[(\chi_\delta + \kappa_\delta h)^{\mathcal{Q},h}])^{\otimes p} + C''_\delta h \quad \text{in } \mathcal{L}(\mathcal{X}^{\otimes p}) \end{aligned}$$

for some constants $C_\delta, C'_\delta, C''_\delta > 0$, chosen according to $p \in \mathbb{N}$, $\delta > 0$ and $\kappa_\delta > 0$. Moreover for $\delta > 0$ fixed, the constant κ_δ can be chosen so that

$$0 \leq \operatorname{Re}[(\chi_\delta + \kappa_\delta h)^{\mathcal{Q},h}] \leq 1 + 2\kappa_\delta h.$$

With

$$\|(1 + N_\pm)^p e^{-\frac{\epsilon}{2} N_\pm}\|_{\mathcal{L}(\Gamma_\pm(\mathcal{X}))} \leq C_{p,c'},$$

the number estimate (3) and the positivity property ($\tilde{b} \geq 0$) $\Rightarrow$ ($\tilde{b}^{\operatorname{Wick}} \geq 0$), writing

$$\mathcal{Q}_\varepsilon(h) = e^{-\frac{\epsilon}{2} N_\pm} e^{\frac{\epsilon}{2} N_\pm} \mathcal{Q}_\varepsilon(h) e^{\frac{\epsilon}{2} N_\pm} e^{-\frac{\epsilon}{2} N_\pm},$$

leads to

$$\begin{aligned} \mathcal{T}(\delta, h) &:= \operatorname{Re} \operatorname{Tr}[\mathcal{Q}_\varepsilon(h)(\operatorname{Id}_{S_\pm^p \mathcal{X}^{\otimes p}} - \tilde{\chi}_\delta^{\mathcal{Q},h})^{\operatorname{Wick}}] \\ &= \operatorname{Tr}[\mathcal{Q}_\varepsilon(h)(\operatorname{Id}_{S_\pm^p \mathcal{X}^{\otimes p}} - \operatorname{Re}[\tilde{\chi}_\delta^{\mathcal{Q},h}])^{\operatorname{Wick}}] + \mathcal{O}_\delta(h) \\ &\leq \operatorname{Tr}[\mathcal{Q}_\varepsilon(h)((1 + 2\kappa_\delta h)^p - (\operatorname{Re}[(\chi_\delta + \kappa_\delta h)^{\mathcal{Q},h}])^{\otimes p})^{\operatorname{Wick}}] + \mathcal{O}_\delta(h). \end{aligned}$$

We now use Proposition 2.4 for

$$\mathcal{T}(\delta, h) \leq \operatorname{Tr}[\mathcal{Q}_\varepsilon(h)(d\Gamma_\pm(1 + 2\kappa_\delta h)^p - d\Gamma_\pm(\operatorname{Re}[(\chi_\delta + \kappa_\delta h)^{\mathcal{Q},h}])^p)] + \mathcal{O}_\delta(h + \varepsilon(h)).$$

The two operators $\mathcal{A} = d\Gamma_\pm(1 + 2\kappa_\delta h)$ and $\mathcal{B} = d\Gamma_\pm(\operatorname{Re}[(\chi_\delta + \kappa_\delta h)^{\mathcal{Q},h}])$ are commuting self-adjoint operators such that $0 \leq \mathcal{B} \leq \mathcal{A}$, so that $0 \leq \mathcal{A}^p - \mathcal{B}^p \leq C_{p,c'}[e^{c'\mathcal{A}} - e^{c'\mathcal{B}}]$. We deduce

$$\begin{aligned} \mathcal{T}(\delta, h) &\leq C_{p,c'} \operatorname{Tr}[\mathcal{Q}_\varepsilon(h) e^{cN_\pm} e^{-cN_\pm} (e^{d\Gamma_\pm(c'(1+2\kappa_\delta h))} - e^{d\Gamma_\pm(c' \operatorname{Re}[(\chi_\delta + \kappa_\delta h)^{\mathcal{Q},h}]})] \\ &\quad + \mathcal{O}_\delta(h + \varepsilon(h)). \end{aligned}$$

We apply Lemma 4.3 with $z = 1$, $A = c'(1 + 2\kappa_\delta h)$ and $B = c'$, or $A = c' \operatorname{Re}[(\chi_\delta + \kappa_\delta h)^{\mathcal{Q},h}]$ and $B = c' \chi_\delta^{\mathcal{Q},h}$, and finally

$$\alpha = c > \alpha_0 = \frac{c + c'}{2} \geq c' \max\{1 + 2\kappa_\delta h, \|(\chi_\delta + \kappa_\delta h)^{\mathcal{Q},h}\|, \|\chi_\delta^{\mathcal{Q},h}\|\} \quad \text{for } h \leq h_{\delta,c'}$$

and we get

$$\mathcal{T}(\delta, h) \leq \operatorname{Re} \operatorname{Tr}[\mathcal{Q}_\varepsilon(h)(e^{c'N_\pm} - e^{c'd\Gamma_\pm(\chi_\delta^{\mathcal{Q},h})})] + \mathcal{O}_\delta(h + \varepsilon(h)).$$

We thus obtain

$$\limsup_{h \rightarrow 0} \mathcal{T}(\delta, h) \leq s_{c', \chi}(\delta)$$

and our assumption $\lim_{\delta \rightarrow 0} s_{c', \chi}(\delta) = 0$ gives the desired conclusion. $\square$

Notation. For any open set $\Omega \subseteq \mathbb{C}$ the Hardy space $H^\infty(\Omega)$ is the space of bounded holomorphic functions on Ω .

Proposition 4.4. *Assume Hypothesis 4.1. Then:*

- (i) *The set $\mathcal{E}$ can be reduced to $\mathcal{E}'$ so that $\mathcal{M}(\gamma_{\varepsilon(h)}^{(p)}, h \in \mathcal{E}') = \{v^{(p)}\}$ for all $p \in \mathbb{N}$, where $v^{(p)}$ is a nonnegative measure on $T^*M^p/\mathfrak{S}_p$, i.e., a measure on $(T^*M)^p$ with the invariance (8).*
- (ii) *When (15) is satisfied, this implies*

$$\lim_{\substack{h \in \mathcal{E}' \\ h \rightarrow 0}} \text{Tr}[\gamma_{\varepsilon(h)}^{(p)}] = \int_{T^*M^p} dv^{(p)}(X) \quad \text{for all } p \in \mathbb{N}.$$

- (iii) *For any $a \in C_0^\infty(\mathbb{R}^{2d})$ there exists $r_a > 0$ such that the function $\Phi_{a,h} : s \mapsto \text{Tr}[\varrho_{\varepsilon(h)} e^{sd\Gamma_\pm(a^{W,h})}]$ is uniformly bounded in $H^\infty(D(0, r_a))$ and, locally uniformly in s ,*

$$\lim_{\substack{h \in \mathcal{E}' \\ h \rightarrow 0}} \Phi_{a,h}(s) = \Phi_{a,0}(s) := \sum_{p=0}^{\infty} \frac{s^p}{p!} \int_{T^*M^p} a^{\otimes p}(X) dv^{(p)}(X). \quad (17)$$

Conversely, if we know that $\Phi_{a,h}$ converges, pointwise on the interval $(-r_a, r_a)$ or in $\mathcal{D}'((-r_a, r_a))$, to some function $\Phi_{a,0}$ as $h \rightarrow 0$, $h \in \mathcal{E}$, then $\mathcal{M}(\gamma_{\varepsilon(h)}^{(p)}, h \in \mathcal{E}) = \{v^{(p)}\}$ for all $p \in \mathbb{N}$ and $\Phi_{a,0}$ is equal to (17) with $\mathcal{E}' = \mathcal{E}$.

Proof. The uniform bound

$$\text{Tr}[\gamma_{\varepsilon(h)}^{(p)}] \leq \text{Tr}[\varrho_{\varepsilon(h)} \langle N_\pm \rangle^p] \leq C_{p,c} \text{Tr}[\varrho_{\varepsilon(h)} e^{cN_\pm}]$$

and Hypothesis 4.1 ensure for each $p \in \mathbb{N}$ the existence of $\mathcal{E}^{(p)} \subseteq \mathcal{E}^{(p-1)} \subseteq \mathcal{E}$, $0 \in \bar{\mathcal{E}}^{(p)}$, such that $\mathcal{M}(\gamma_{\varepsilon(h)}^{(p)}, h \in \mathcal{E}^{(p)}) = \{v^{(p)}\}$ (see Proposition 3.3 and Remark 3.4). A diagonal extraction with respect to p determines $\mathcal{E}' \subset \mathcal{E}$, $0 \in \bar{\mathcal{E}}'$, such that $\mathcal{M}(\gamma_{\varepsilon(h)}^{(p)}, h \in \mathcal{E}') = \{v^{(p)}\}$ for all $p \in \mathbb{N}$.

The second statement (ii) is a straightforward application of Proposition 4.2 and Proposition 3.3.

In the statement (iii), the holomorphy of the function $\Phi_{a,h}$ on the domain $D(0, c/\|a^{W,h}\|)$ follows by Lemma 4.3. Hypothesis 4.1 now combined with

$$\|e^{-cN_\pm} e^{zd\Gamma_\pm(a^{W,h})}\| = \|\Gamma(e^{\varepsilon(z\alpha^{W,h}-c)})\| \leq 1 \quad \text{and} \quad \|a^{W,h}\| \leq C_a$$

provides the uniform boundedness with respect to $h \in \mathcal{E}$ of $\Phi_{a,h}$ in $H^\infty(D(0, r_a))$ with $r_a = c/C_a$. Moreover, Lemma 4.3(2) shows that $\Phi_{a,h}$ is given by the entire function

$$\Phi_{a,h}(s) = \sum_{p=0}^{\infty} \frac{s^p}{p!} \operatorname{Tr}[\varrho_{\varepsilon(h)} d\Gamma_{\pm}(a^{W,h})^p],$$

which is absolutely convergent on $s \in D(0, r_a)$ uniformly in $h \in \mathcal{E}$ since the estimate

$$\|d\Gamma_{\pm}(a^{W,h})^p e^{-cN_{\pm}}\|_{\mathcal{L}(\Gamma_{\pm}(\mathcal{X}))} \lesssim \frac{p!}{r_a^p} \quad (18)$$

holds true uniformly for all $p \in \mathbb{N}$ and $h \in \mathcal{E}$. According to (i) and Proposition 2.4,

$$\begin{aligned} \lim_{\substack{h \in \mathcal{E}' \\ h \rightarrow 0}} \operatorname{Tr}[\varrho_{\varepsilon(h)} d\Gamma_{\pm}(a^{W,h})^p] &= \lim_{\substack{h \in \mathcal{E}' \\ h \rightarrow 0}} \operatorname{Tr}[\varrho_{\varepsilon(h)} ((a^{W,h})^{\otimes p})^{\operatorname{Wick}}] \\ &= \lim_{\substack{h \in \mathcal{E}' \\ h \rightarrow 0}} \operatorname{Tr}[\gamma_{\varepsilon(h)}^{(p)} (a^{W,h})^{\otimes p}] = \int_{T^*M^p} a^{\otimes p} dv^{(p)}. \end{aligned}$$

Hence, by dominated convergence, $\Phi_{a,h}$ converges locally uniformly in $D(0, r_a)$ to $\Phi_{a,0}$ given by (17) and consequently $\Phi_{a,0}$ belongs to $H^\infty(D(0, r_a))$ as well.

Moreover, assume for any $a \in \mathcal{C}_0^\infty(\mathbb{R}^{2d})$ the convergence of $\Phi_{a,h}$ to $\Phi_{a,0}$ in a weak topology on the interval $(-r_a, r_a)$ as $h \in \mathcal{E}$, $h \rightarrow 0$. Let $\nu_1^{(p)}, \nu_2^{(p)} \in \mathcal{M}(\gamma_h^{(p)}, h \in \mathcal{E})$, for $p \in \mathbb{N}$. Then according to (i) and the first part of (iii), one has, for any $s \in (-r_a, r_a)$,

$$\Phi_{a,0}(s) = \sum_{p=0}^{\infty} \frac{s^p}{p!} \int_{T^*M^p} a^{\otimes p}(X) dv_1^{(p)}(X) = \sum_{p=0}^{\infty} \frac{s^p}{p!} \int_{T^*M^p} a^{\otimes p}(X) dv_2^{(p)}(X).$$

The uniform estimate (18) shows that $\Phi_{a,0}$ admits a holomorphic extension on $D(0, r_a)$ and consequently

$$\int_{T^*M^p} a^{\otimes p}(X) dv_1^{(p)}(X) = \int_{T^*M^p} a^{\otimes p}(X) dv_2^{(p)}(X)$$

for all $p \in \mathbb{N}$. Thanks to Lemma 3.1, the measures $\nu_1^{(p)}$ and $\nu_2^{(p)}$ are determined by integrating with all the test functions $a^{\otimes p}$, $a \in \mathcal{C}_0^\infty(T^*M)$. So $\nu_1^{(p)} = \nu_2^{(p)}$, which ends the proof. $\square$

Replacing the semiclassical symmetrization Lemma 3.1 by the quantum ones, Lemma 2.8 in the above proof leads to the following similar result for the quantum part.

Proposition 4.5. *Assume Hypothesis 4.1. For all $K \in \mathcal{L}^\infty(\mathcal{X})$ there exists $r_K > 0$ such that the set $\{\Psi_{K,h}, h \in \mathcal{E}\}$ of functions $\Psi_{K,h}(s) := \operatorname{Tr}[\varrho_{\varepsilon(h)} e^{sd\Gamma_{\pm}(K)}]$ is bounded in $H^\infty(D(0, r_K))$.*

The pointwise or $\mathcal{D}'((-r_K, r_K))$ -convergence $\lim_{h \in \mathcal{E}, h \rightarrow 0} \Psi_{K,h} = \Psi_{K,0}$ is equivalent to w^* - $\lim_{h \in \mathcal{E}, h \rightarrow 0} \gamma_h^{(p)} = \gamma_0^{(p)}$ (remember $\mathcal{L}^1 = (\mathcal{L}^\infty)^*$) with

$$\Psi_{K,0}(s) = \sum_{p=0}^{\infty} \text{Tr}[\gamma_0^{(p)} K^{\otimes p}] \frac{s^p}{p!}.$$

Let us consider a specific feature of the fermionic case:

Proposition 4.6. *Let $(\varrho_\varepsilon)_{\varepsilon \in \mathcal{E}}$ be a family of nonnegative, trace-1 operators in $\mathcal{L}^1(\Gamma_-(\mathcal{Z}))$. Let $\gamma_\varepsilon^{(p)}$ denote the corresponding nonnormalized reduced density matrices of order p . If $\gamma_0^{(p)} \in \mathcal{L}^1(\mathcal{S}_-^p \mathcal{Z}^{\otimes p})$ is such that,*

$$\text{for all } K \in \mathcal{L}^\infty(\mathcal{S}_-^p \mathcal{Z}^{\otimes p}), \quad \lim_{\substack{\varepsilon \in \mathcal{E} \\ \varepsilon \rightarrow 0}} \text{Tr}[\gamma_\varepsilon^{(p)} K] = \text{Tr}[\gamma_0^{(p)} K],$$

then $\gamma_0^{(p)} = 0$.

As a consequence, the weak*-limits $\gamma_0^{(p)}$ always vanish in the fermionic case.

Proof. First consider K a nonnegative finite-rank operator. Then

$$\lim_{\substack{\varepsilon \in \mathcal{E} \\ \varepsilon \rightarrow 0}} \text{Tr}[\varrho_\varepsilon K^{\text{Wick}}] = \text{Tr}[\gamma_0^{(p)} K].$$

For fermions, $K^{\text{Wick}} \leq \varepsilon^p \text{Tr}[K]$, and hence $\text{Tr}[\varrho_\varepsilon K^{\text{Wick}}] \leq \varepsilon(h)^p \rightarrow 0$ as $\varepsilon \rightarrow 0$. Since any finite-rank operator is of the form $K = K_1 - K_2 + i(K_3 - K_4)$ for some nonnegative finite-rank operators K_j , $j \in \{1, 2, 3, 4\}$, the limit $\text{Tr}[\varrho_\varepsilon K^{\text{Wick}}] \rightarrow 0 = \text{Tr}[\gamma_0^{(p)} K]$ holds for any finite-rank operator K . Hence, by density of the finite-rank operators in the compact operators for the operator norm, $\text{Tr}[\gamma_0^{(p)} K] = 0$ for any $K \in \mathcal{L}^\infty(\mathcal{S}_-^p \mathcal{Z}^{\otimes p})$, i.e., $\gamma_0^{(p)} = 0$. $\square$

5. Examples

5A. h -dependent coherent states in the bosonic case. We first recall our normalization for a coherent state. If we use the identification $\mathcal{S}_\pm^0 \mathcal{Z} \equiv \mathbb{C}$, then the vacuum-state vector is defined as $\Omega = (1, 0, 0, \dots) \in \Gamma_\pm(\mathcal{Z})$. We then introduce the usual field operators $\Phi(f) = (1/\sqrt{2})(a^*(f) + a(f))$, with $f \in \mathcal{Z}$, and the Weyl operators are $W(f) = \exp((i/\sqrt{2})\Phi(f))$. A coherent state is a pure state $E_z = W(\sqrt{2}z/(i\varepsilon))\Omega$, with $z \in \mathcal{Z}$. One then can also speak of a coherent state for the corresponding density matrix $|E_z\rangle\langle E_z|$. One of the useful properties of coherent states is that

$$b(z) = \langle E(z), b^{\text{Wick}} E(z) \rangle. \quad (19)$$

See, e.g., [Ammari and Nier 2008, Proposition 2.10]. The case of coherent states is simple:

Proposition 5.1. *Let $(z_\varepsilon)_{\varepsilon \in (0,1]}$ be a bounded family of $\mathcal{Z}$, choose the semiclassical quantization $a \mapsto a^{W,h} = a^W(\sqrt{h}x, \sqrt{h}D_x)$, and fix a function $\varepsilon = \varepsilon(h) \rightarrow 0$ as $h \rightarrow 0$. Up to an extraction, $z_{\varepsilon(h)} \rightharpoonup z_0 \in \mathcal{Z}$ weakly, and $\mathcal{M}(|z_{\varepsilon(h)}\rangle\langle z_{\varepsilon(h)}|, h \in \mathcal{E}) = \{v\}$. Assume that the semiclassical quantization $a^{W,h} = a^W(\sqrt{h}x, \sqrt{h}D_x)$ is adapted to $(|z_{\varepsilon(h)}\rangle\langle z_{\varepsilon(h)}|)_h$ and separating for $(|z_{\varepsilon(h)}\rangle\langle z_{\varepsilon(h)}|)_h$. Then the family $(\varrho_\varepsilon(h) = |E_{z_{\varepsilon(h)}}\rangle\langle E_{z_{\varepsilon(h)}}|)_{h \in \mathcal{E}}$ has*

$$\gamma_{\varepsilon(h)}^{(p)} = |z_{\varepsilon(h)}^{\otimes p}\rangle\langle z_{\varepsilon(h)}^{\otimes p}|$$

as (nonnormalized) reduced density matrices of order p , for which the quantization is adapted and separating, and

$$\mathcal{M}^{(2)}(\gamma_{\varepsilon(h)}^{(p)}, h \in \mathcal{E}) = \{(v^{\otimes p}, 0, |z_0^{\otimes p}\rangle\langle z_0^{\otimes p}|)\}.$$

Proof. Formula (19) yields, for $B \in \mathcal{L}(S_+^p \mathcal{Z}^{\otimes p})$,

$$\langle z_{\varepsilon(h)}^{\otimes p}, B z_{\varepsilon(h)}^{\otimes p} \rangle = \langle E_{z_{\varepsilon(h)}} | B^{\text{Wick}} | E_{z_{\varepsilon(h)}} \rangle = \text{Tr}[\varrho_{\varepsilon(h)} B^{\text{Wick}}] = \text{Tr}[\gamma_{\varepsilon(h)}^{(p)} B],$$

which implies the result. $\square$

The case of coherent states, although simple, can already exhibit interesting behaviors for some families $(z_\varepsilon)_{\varepsilon \in (0,1]}$. Indeed,

Remark 5.2. Let $(z_{j,\varepsilon(h)})_{h \in (0,1]}$, $j \in \{1, 2\}$, be families of $\mathcal{Z}$ such that

- $z_{1,\varepsilon(h)} \rightarrow z_{1,0} \in \mathcal{Z}$ as $h \rightarrow 0$, and
- $(z_{2,\varepsilon(h)})_{h \in (0,1]}$ converges weakly to 0,

$$\lim_{R \rightarrow \infty} \limsup_{h \rightarrow 0} \|(1 - \chi(R^{-1} \cdot))^{W,h} z_{2,\varepsilon(h)}\| = 0$$

for some $\chi \in C_0^\infty(\mathbb{R}^{2d})$, $\chi \equiv 1$ around 0 (no mass escaping at infinity in the phase space), and $\mathcal{M}(|z_{2,\varepsilon(h)}\rangle\langle z_{2,\varepsilon(h)}|, h \in \mathcal{E}) = \{v_2\}$, with $v_2(\{0\}) = 0$.

Then $(|z_{1,\varepsilon(h)} + z_{2,\varepsilon(h)}\rangle\langle z_{1,\varepsilon(h)} + z_{2,\varepsilon(h)}|)_{h \in (0,1]}$ satisfies the assumptions of Proposition 5.1, and $z_0 = z_{1,0}$, $v = \|z_{1,0}\|^2 \delta_0 + v_2$.

5B. Gibbs states. For a given nonnegative self-adjoint hamiltonian H defined in $\mathcal{Z}$ with domain $D(H)$, the Gibbs state at positive temperature $\frac{1}{\beta}$ and with the chemical potential $\mu < 0$ is given by

$$\omega_\varepsilon(A) = \frac{\text{Tr}[\Gamma_\pm(e^{-\beta(H-\mu)})A]}{\text{Tr}[\Gamma_\pm(e^{-\beta(H-\mu)})]} = \text{Tr}[\varrho_\varepsilon A].$$

In general $\varrho_\varepsilon \in \mathcal{L}^1(\Gamma_\pm(\mathcal{Z}))$ as soon as $e^{-\beta(H-\mu)} \in \mathcal{L}^1(\mathcal{Z})$ (in the bosonic case $H \geq 0$ and $\mu < 0$ imply $\|e^{-\beta(H-\mu)}\|_{\mathcal{L}(\mathcal{Z})} < 1$, see Lemma D.1). Moreover the quasi-free state formula, see [Bratteli and Robinson 1981], with ε -dependent quantization

gives

$$\mathrm{Tr}[\varrho_\varepsilon \mathbf{N}_\pm] = \varepsilon \mathrm{Tr}[e^{-\beta(H-\mu)}(1 \mp e^{-\beta(H-\mu)})^{-1}]$$

and additionally, in the case of bosons,

$$\mathrm{Tr}[\varrho_\varepsilon W(f)] = \exp\left[-\frac{1}{4}\varepsilon \langle f, (1 + e^{-\beta(H-\mu)})(1 - e^{-\beta(H-\mu)})^{-1} f \rangle\right].$$

5B1. The fermionic case. This case is simpler than the bosonic case for two reasons: first because the quantum part vanishes (see Proposition 4.6), and second because there is no singularity to handle. To fix the ideas we consider the simple case when H is the harmonic oscillator. Actually one can treat more general pseudodifferential operators, and we do that below in the more interesting case of bosons and Bose–Einstein condensation.

Proposition 5.3. *Let $\beta > 0$, $H = \frac{1}{2}|X|^2 W, h$, $\mu(\varepsilon)$ be such that $\mu(\varepsilon) \geq C\varepsilon$ for some constant $C > 0$, and assume that $\varepsilon = \varepsilon(h) = h^d$. Let*

$$\varrho_{\varepsilon(h)} = \frac{\Gamma_-(e^{-\beta(H-\mu(\varepsilon))})}{\mathrm{Tr}[\Gamma_-(e^{-\beta(H-\mu(\varepsilon))})]}$$

and $\gamma_{\varepsilon(h)}^{(p)}$ be its nonnormalized reduced density matrix of order $p \geq 1$. Then

$$\mathcal{M}^{(2)}(\gamma_{\varepsilon(h)}^{(p)}, h \in (0, 1]) = \{(v^{(p)}, 0, 0)\},$$

where

$$dv^{(p)} = \left(\frac{e^{-\frac{\beta}{2}|X|^2}}{1 + e^{-\frac{\beta}{2}|X|^2}} \frac{dX}{(2\pi)^d} \right)^{\otimes p}.$$

Proof. From Remark 3.7 and Proposition 4.6, any

$$(v^{(p)}, v_I^{(p)}, \gamma_0^{(p)}) \in \mathcal{M}^{(2)}(\gamma_{\varepsilon(h)}^{(p)}, h \in (0, 1])$$

satisfies $\gamma_0^{(p)} = 0$.

Since we are considering a Gibbs state, the Wick formula yields

$$\gamma_{\varepsilon(h)}^{(p)} = p! \mathcal{S}_\pm^p \gamma_{\varepsilon(h)}^{(1) \otimes p} \mathcal{S}_\pm^{p,*}.$$

Moreover, in the fermionic case,

$$\gamma_{\varepsilon(h)}^{(1)} = \varepsilon(h) \frac{C}{1 + C} \quad \text{for } \varrho_{\varepsilon(h)} = \frac{\Gamma_-(C)}{\mathrm{Tr}[\Gamma_-(C)]};$$

that is to say, with $\varepsilon(h) = h^d$,

$$\gamma_{\varepsilon(h)}^{(1)} = h^d \frac{e^{-\beta(H-\mu)}}{1 + e^{-\beta(H-\mu)}}$$

in our case. The semiclassical calculus combined with the Helffer–Sjöstrand functional calculus formula yields

$$\frac{e^{-\beta(\frac{1}{2}|X|^{2W,h}-\mu)}}{1+e^{-\beta(\frac{1}{2}|X|^{2W,h}-\mu)}} = \left(\frac{e^{-\frac{\beta}{2}|X|^2}}{1+e^{-\frac{\beta}{2}|X|^2}} \right)^{W,h} + \mathcal{O}(h) \quad \text{in } \mathcal{L}(\mathcal{Z}).$$

For details we refer the reader to, e.g., [Dimassi and Sjöstrand 1999; Helffer and Nier 2005] or to the proof of Proposition 5.6. Again by the semiclassical calculus we know $h^d a^{W,h}$ is uniformly bounded in $\mathcal{L}^1(L^2(\mathbb{R}^d))$ for $a \in \mathcal{C}_0^\infty(\mathbb{R}^{2d})$. This leads to

$$\begin{aligned} \text{Tr}[(a^{W,h})^{\otimes p} \gamma_{\varepsilon(h)}^{(p)}] &= \text{Tr}[a^{W,h} \gamma_{\varepsilon(h)}^{(1)}]^p + \mathcal{O}(h) \\ &= \text{Tr} \left[\left(\frac{e^{-\frac{\beta}{2}|X|^2}}{1+e^{-\frac{\beta}{2}|X|^2}} \right)^{W,h} h^d a^{W,h} \right]^p + \mathcal{O}(h). \end{aligned}$$

We finally use

$$h^d \text{Tr}[a^{W,h} b^{W,h}] = \int_{\mathbb{R}^{2d}} a(X) b(X) \frac{dX}{(2\pi)^d},$$

which implies

$$\lim_{h \rightarrow 0} \text{Tr}[(a^{W,h})^{\otimes p} \gamma_{\varepsilon(h)}^{(p)}] = \left(\int_{\mathbb{R}^{2d}} \frac{e^{-\frac{\beta}{2}|X|^2}}{1+e^{-\frac{\beta}{2}|X|^2}} a(X) \frac{dX}{(2\pi)^d} \right)^p.$$

Hence

$$d\nu^{(p)}(X) = \left(\frac{e^{-\frac{\beta}{2}|X|^2}}{1+e^{-\frac{\beta}{2}|X|^2}} \frac{dX}{(2\pi)^d} \right)^{\otimes p}. \quad \square$$

5B2. Parameter-dependent Gibbs states and Bose–Einstein condensation in the bosonic case. The Bose–Einstein condensation phenomenon occurs when H has a ground state $\ker H = \mathbb{C}\psi_0$ and the chemical potential is scaled according to

$$-\beta\mu = \frac{\varepsilon}{\nu_C} \quad \text{for some fixed } \nu_C > 0.$$

An especially interesting case is when H is a semiclassically quantized symbol with semiclassical parameter h related to ε , or $\varepsilon = \varepsilon(h)$ according to our previous notations. The quantum and semiclassical parts arise simultaneously when $\varepsilon = h^d$. Two cases will be considered: the first one concerns $\mathcal{X} = L^2(\mathbb{R}^d)$ with a nondegenerate bottom-well hamiltonian; the second one $\mathcal{X} = L^2(M)$ with the semiclassical Laplace–Beltrami operator on the compact Riemannian manifold M .

In the first case, let $S(\langle X \rangle^m, dX^2/\langle X \rangle^2)$ denote the Hörmander class of symbols satisfying $|\partial_X^\beta a(X)| \leq C_\beta \langle X \rangle^{m-\beta}$, and let $\alpha \in S(\langle X \rangle^2, dX^2/\langle X \rangle^2)$ be elliptic in this class with a unique nondegenerate minimum at $X = 0$ (e.g., the symbol of

the harmonic oscillator hamiltonian). We can even consider small perturbations of this situation after setting

$$H = \alpha^{W,h} + B^h - \lambda_0(\alpha^{W,h} + B^h), \quad \alpha^{W,h} = \alpha(\sqrt{h}x, \sqrt{h}D_x), \quad \varepsilon = h^d,$$

where

$$B^h = B^{h*} \in \mathcal{L}(L^2(\mathbb{R}^d)), \quad \|B^h\| = o(h), \quad \lambda_0(\alpha^{W,h} + B^h) = \inf \sigma(\alpha^{W,h} + B^h).$$

It is convenient in this case to introduce the linear symplectic transformation $T \in \text{Sp}_{2d}(\mathbb{R})$ such that ${}^t X^t T^{-1} \text{Hess } \alpha(0) T^{-1} X = \sum_{j=1}^d \beta_j X_j^2$ and to introduce some unitary quantization U_T of T , i.e., a unitary operator on $L^2(\mathbb{R}^d)$ such that $U_T^* b^W U_T = b(T^{-1} \cdot)^W$.

Proposition 5.4. *Under the above assumptions with dimension $d \geq 2$, for any $p \in \mathbb{N}$, we have $\mathcal{M}^{(2)}(\gamma_{\varepsilon(h)}^{(p)}, h \in \mathcal{E}) = \{(v^{(p)}, 0, \gamma_0^{(p)})\}$ (see Definition 3.12), where*

$$\gamma_0^{(p)} = p! v_C^p |\psi_0^{\otimes p}\rangle \langle \psi_0^{\otimes p}| \quad \text{with } \psi_0(x) = U_T \frac{e^{-\frac{1}{2}x^2}}{\pi^{\frac{d}{4}}}$$

and

$$v^{(p)} = \sum_{\sigma \in \mathfrak{S}_p} \sigma_* \left[\sum_{k=0}^p \frac{1}{(p-k)!} v_C^k \delta_0^{\otimes k} \otimes v(\beta, \cdot)^{\otimes p-k} \right],$$

with

$$dv(\beta, X) = \frac{e^{-\beta\alpha(X)}}{1 - e^{-\beta\alpha(X)}} \frac{dX}{(2\pi)^d}.$$

The proof is given in Section 5B4 and needs some preliminaries, which are given in Proposition 5.6 and Lemma 5.7.

Another even simpler case, related to the example $M = \mathbb{T}^d$ presented in [Ammari and Nier 2008], is $\mathcal{Z} = L^2(M, dv_g(x))$ when (M, g) is a compact Riemannian manifold with volume $dv_g(x)$ and

$$H = -h^2 \Delta_g + B_h - \lambda_0(-h^2 \Delta_g + B_h),$$

where Δ_g is the Laplace Beltrami operator on (M, g) and $B_h = B_h^* \in \mathcal{L}(L^2(M))$, $\|B_h\| = o(h^2)$.

Proposition 5.5. *Under the above assumptions with $d \geq 3$, for any $p \in \mathbb{N}$, we have $\mathcal{M}^{(2)}(\gamma_{\varepsilon(h)}^{(p)}, h \in \mathcal{E}) = \{(v^{(p)}, 0, \gamma_0^{(p)})\}$, where*

$$\gamma_0^{(p)} = p! v_C^p |\psi_0^{\otimes p}\rangle \langle \psi_0^{\otimes p}|, \quad \psi_0 = \frac{1}{v_g(M)^{\frac{1}{2}}},$$

$$v^{(p)} = \sum_{\sigma \in \mathfrak{S}_p} \sigma_* \left[\sum_{k=0}^p \frac{1}{(p-k)!} v_C^k \left(\frac{1}{v_g(M)} dv_g(x) \otimes \delta_0(\xi) \right)^{\otimes k} \otimes v(\beta)^{\otimes (p-k)} \right],$$

with

$$dv(\beta, X) = \frac{e^{-\beta|\xi|_{g(x)}^2}}{1 - e^{-\beta|\xi|_{g(x)}^2}} \frac{dx d\xi}{(2\pi)^d},$$

and

$$|\xi|_{g(x)}^2 = \sum_{i,j \leq d} g^{ij}(x) \xi_i \xi_j \quad \text{when } g = \sum_{i,j \leq d} g_{ij}(x) dx^i dx^j, \quad (g_{ij})^{-1} = (g^{ij}).$$

We shall focus on the first case, which requires a more careful analysis, while $\sigma(-h^2 \Delta_g) = h^2 \sigma(-\Delta_g)$ reduces the problem even more easily to the integrability of $e^{-\beta|\xi|_{g(x)}^2} / (1 - e^{-\beta|\xi|_{g(x)}^2})$, valid when $d \geq 3$. The proof of Proposition 5.5 is left as an exercise, which requires the adaptation of the following arguments in the case of Proposition 3.11 with the associated Definitions 3.13 and 3.12.

5B3. Semiclassical asymptotics with a singularity at $X = 0$. We give here a general semiclassical result in $T^*\mathbb{R}^d$, which involves traces and symbols with a singularity at $X = 0$.

Proposition 5.6. *Consider the hamiltonian $H = \alpha^{W,h} + B_h - \lambda_0(\alpha^{W,h} + B_h)$, with $\alpha^{W,h} = \alpha(\sqrt{h}x, \sqrt{h}D_x)$, $\alpha \in S(\langle X \rangle^2, dX^2/\langle X \rangle^2)$ elliptic and real such that $\alpha(0) = 0$ is the unique nondegenerate minimum, $B_h = B_h^* \in \mathcal{L}(L^2(\mathbb{R}^d))$, $\|B_h\| = o(h)$, and $\lambda_0(\alpha^{W,h} + B_h) = \inf \sigma(\alpha^{W,h} + B_h)$. Assume that $f \in C^\infty((0, +\infty); \mathbb{R})$ is decreasing and satisfies*

$$0 \leq f(u) \leq Cu^{-\kappa_\infty}, \quad \lim_{u \rightarrow 0^+} u^{\kappa_0} f(u) = f_0 \in \mathbb{R}, \quad 0 < \kappa_0 < d < \kappa_\infty.$$

For $c > 0$, the operator $f(H + ch^{\frac{d}{\kappa_0}})$ is trace class with

$$\limsup_{h \rightarrow 0^+} h^d \|f(H + ch^{\frac{d}{\kappa_0}})\|_{\mathcal{L}^1(L^2(\mathbb{R}^d))} < +\infty.$$

Moreover the convergence

$$\lim_{h \rightarrow 0} h^d \operatorname{Tr}[f(H + ch^{\frac{d}{\kappa_0}})a^{W,h}] = \frac{f_0}{c^{\kappa_0}} a(0) + \int_{\mathbb{R}^{2d}} f(\alpha(X))a(X) \frac{dX}{(2\pi)^d}$$

holds for all $a \in S(1, dX^2)$. Finally, all the above estimates and convergences hold uniformly with respect to $c \in (1/A, A)$ for any fixed $A > 1$.

The following lemma gives, in a simple way, useful inequalities for our purpose, which are deduced with elementary arguments, and in a robust way with respect to the perturbation B_h , from more accurate and sophisticated results on the spectrum of $\alpha^{W,h}$; see [Charles and Vũ Ngọc 2008; Dimassi and Sjöstrand 1999].

Lemma 5.7. *Let $\alpha \in S(\langle X \rangle^2, dX^2/\langle X \rangle^2)$ be real-valued, elliptic, which means $1 + \alpha(X) \geq C^{-1}\langle X \rangle^2$, with a unique nondegenerate minimum at $X = 0$ and set*

$\alpha_0(X) = \frac{1}{2}|X|^2$. Let $B_h = B_h^* \in \mathcal{L}(L^2(\mathbb{R}^d))$ be such that $\|B_h\| = o(h)$. The ordered eigenvalues are denoted by $\lambda_j(\alpha^{W,h} + B_h)$ and $\lambda_j(\alpha_0^{W,h})$ for $j \in \mathbb{N}$:

- For $j = 0$, we have $\lambda_0(\alpha^{W,h} + B_h) = \text{Tr}[\text{Hess } \alpha(0)]h + o(h)$ and the associated spectral projection satisfies

$$\lim_{h \rightarrow 0} 1_{\{\lambda_0(\alpha^{W,h} + B_h)\}}(\alpha^{W,h} + B_h) = (\pi^{-d} e^{-|TX|^2})^W(x, D_x) \quad \text{in } \mathcal{L}^1(L^2(\mathbb{R}^d)),$$

where $T \in \text{Sp}_{2d}(\mathbb{R})$ is such that ${}^t X^t T^{-1} \text{Hess } \alpha(0) T^{-1} X = \sum_{j=1}^d \beta_j X_j^2$.

- There exist $h_0 > 0$ and $C' \geq 1$ such that, for all $j > 0$ and $h \in (0, h_0)$,

$$\begin{aligned} \frac{1}{2} C'^{-1} h d &\leq C'^{-1} \lambda_j(\alpha_0^{W,h}) \\ &\leq \lambda_j(\alpha^{W,h} + B_h) - \lambda_0(\alpha^{W,h} + B_h) \leq C' \lambda_j(\alpha_0^{W,h}). \end{aligned} \quad (20)$$

Remark 5.8. Of course $\sigma(\alpha_0^{W,h}) = \{h(\frac{d}{2} + |n|) : n \in \mathbb{N}^d\}$ and the bounds (20) are actually written in order to use this later. But for an easy use of the min-max principle it is better to write the eigenvalues $\lambda_j(\alpha_0^{W,h})$ in increasing order, with repetition according to their multiplicity.

Proof of Lemma 5.7. We start by noting that $1 + \alpha \in S(\langle X \rangle^2, dX^2 / \langle X \rangle^2)$ is fully elliptic in the sense that $(1 + \alpha)^{-1} \in S(\langle X \rangle^{-2}, dX^2 / \langle X \rangle^2)$. Therefore

$$(1 + \alpha) \sharp^{W,h} \frac{1}{1 + \alpha} = 1 + h^2 R_+(h), \quad \frac{1}{1 + \alpha} \sharp^{W,h} (1 + \alpha) = 1 + h^2 R_-(h)$$

with $R_{\pm}(h)$ uniformly bounded in $S(\langle X \rangle^{-2}, dX^2 / \langle X \rangle^2)$. The semiclassical calculus with the metric $dX^2 / \langle X \rangle^2$ then says

$$(1 + \alpha^{W,h})^{-1} = [(1 + \alpha)^{-1}]^{W,h} + \mathcal{O}(h^2) \quad \text{in } S\left(\langle X \rangle^{-2}, \frac{dX^2}{\langle X \rangle^2}\right). \quad (21)$$

The same of course also holds for $\tau \alpha_0(X) = \frac{1}{2} \tau |X|^2$ with $\tau \in (0, +\infty)$ fixed. Therefore $\alpha^{W,h} + B_h$ and $\alpha_0^{W,h}$ are self-adjoint with the same domain $D(\alpha^{W,h}) = D(\alpha_0^{W,h}) = D(\alpha_0^{W,1})$, and they have a compact resolvent. We shall collect all the necessary information by comparing the eigenvalues of $\alpha^{W,h} + B_h$ and $\alpha_0^{W,h}$ in the intervals $(-\infty, 2|\beta|h]$, $[0, 2]$ and $[1, +\infty[$, with $|\beta| = \sum_{j=1}^d \beta_j$. For the first part, we refer to the ready-made simple statement of [Charles and Vũ Ngọc 2008, Theorem 4.5] and complete the other parts with simple pseudodifferential calculus and the min-max principle.

Interval $(-\infty, 2|\beta|h]$: By Theorem 4.5 of [Charles and Vũ Ngọc 2008], there exist a family of real numbers $(\omega_n^h)_{h>0, n \in \mathbb{N}^d}$ and, for any $t > 0$, a constant $C_t > 0$ such that

$$\sigma(\alpha^{W,h}) \cap (-\infty, th] = \{\omega_n^h, n \in \mathbb{N}^d\} \cap \left[\frac{1}{2}|\beta|h, th\right]$$

and

$$\left| \omega_n^h - \sum_{j=1}^d h \beta_j \left(\frac{1}{2} + n_j \right) \right| \leq C_t h^{\frac{3}{2}}.$$

As $\|B_h\| = o(h)$, the min-max principle with $\alpha^{W,h}$ and $\alpha^{W,h} + B_h$ then gives,

$$\sigma(\alpha^{W,h} + B_h) \cap (-\infty, th] = \{\omega_n^h + o(h), n \in \mathbb{N}\} \cap [0, th].$$

By choosing $t = 2|\beta|$, the operator $\alpha^{W,h} + B_h$ is nonnegative with $\lambda_0(\alpha^{W,h} + B_h) = \frac{1}{2}|\beta|h + o(h)$ and the spectral gap is bounded from below by, for all $j \in \mathbb{N} \setminus \{0\}$,

$$\begin{aligned} \lambda_j(\alpha^{W,h} + B_h) - \lambda_0(\alpha^{W,h} + B_h) &\geq \lambda_1(\alpha^{W,h} + B_h) - \lambda_0(\alpha^{W,h} + B_h) \\ &\geq \beta_m h + o(h) \geq \frac{1}{2} \beta_m h, \end{aligned} \quad (22)$$

with $\beta_m = \min\{\beta_1, \dots, \beta_d\}$.

Let $T \in \text{Sp}_{2d}(\mathbb{R}^d)$ be such that ${}^t X^t T^{-1} \text{Hess } \alpha(0) T^{-1} X = \sum_{j=1}^d \beta_j X_j^2$, let U_T be a unitary operator such that $U_T^* b^W U_T = b(T^{-1} \cdot)^W$ and set $\varphi_T(x) = (\pi)^{-\frac{d}{4}} U_T e^{-\frac{1}{2}x^2}$. We compute

$$\begin{aligned} \langle \varphi_T, (\alpha^{W,h} + B_h) \varphi_T \rangle &= \text{Tr}[U_T^* \alpha^{W,h} U_T |\varphi_{\text{Id}}\rangle \langle \varphi_{\text{Id}}|] + o(h) \\ &= \int_{\mathbb{R}^{2d}} \alpha(\sqrt{h} T^{-1} X) e^{-|X|^2} \frac{dX}{\pi^d} + o(h). \end{aligned}$$

But since $\alpha(T^{-1} X) = \sum_{j=1}^d \frac{1}{2} \beta_j |X_j|^2 + P_3(X) + \mathcal{O}(|X|^4)$, with P_3 a homogeneous polynomial of degree 3, we obtain

$$\langle \varphi_T, (\alpha^{W,h} + B_h) \varphi_T \rangle = \frac{1}{2} h |\beta| + o(h) = \lambda_0(\alpha^{W,h} + B_h) + o(h).$$

With the spectral gap (22) this implies that the ground state ψ_0^h of $\alpha^{W,h} + B_h$ satisfies $\lim_{h \rightarrow 0} \|\psi_0^h - \varphi_T\|_{L^2} = 0$ and

$$\lim_{h \rightarrow 0} \|1_{\{\lambda_0(\alpha^{W,h} + B_h)\}} (\alpha^{W,h} + B_h) - \pi^{-d} (e^{-|TX|^2})^{W,1}\|_{\mathcal{L}^1} = 0.$$

Interval $[0, 2]$: Our assumptions on α provide a constant $C_2 \geq 1$ such that $C_2^{-1} \alpha_0 \leq \alpha \leq C_2 \alpha_0$ and therefore

$$\frac{C_2^{-1} \alpha_0}{1 + C_2^{-1} \alpha_0} \leq \frac{\alpha}{1 + \alpha} \leq \frac{C_2 \alpha_0}{1 + C_2 \alpha_0},$$

as $x \mapsto \frac{x}{1+x}$ is increasing on $\mathbb{R}^*$. Since all those symbols belong to $S(1, dX^2)$, the semiclassical Fefferman–Phong inequality for the constant metric dX^2 , see [Hörmander 1985, Lemma 18.6.1], says

$$\frac{C_2^{-1} \alpha_0^{W,h}}{1 + C_2^{-1} \alpha_0^{W,h}} - \mathcal{O}(h^2) \leq \frac{\alpha^{W,h}}{1 + \alpha^{W,h}} \leq \frac{C_2 \alpha_0^{W,h}}{1 + C_2 \alpha_0^{W,h}} + \mathcal{O}(h^2),$$

after using

$$\left(\frac{\alpha}{1+\alpha} \right)^{W,h} = \frac{\alpha^{W,h}}{1+\alpha^{W,h}} + \mathcal{O}(h^2).$$

With $\|(1+\alpha^{W,h})^{-1} - (1+\alpha^{W,h} + B_h)^{-1}\| = \mathcal{O}(\|B_h\|) = o(h)$ and $\frac{x}{1+x} = 1 - \frac{1}{1+x}$, we deduce

$$\frac{C_2^{-1}\alpha_0^{W,h}}{1+C_2^{-1}\alpha_0^{W,h}} - o(h) \leq \frac{\alpha^{W,h} + B_h}{1+\alpha^{W,h} + B_h} \leq \frac{C_2\alpha_0^{W,h}}{1+C_2\alpha_0^{W,h}} + o(h).$$

For $r = 2(1+C_2)$ and $h_0 > 0$ small enough, the above operators have a discrete spectrum in $[0, \frac{r}{1+r}]$ with eigenvalues in this interval, while the function $x \mapsto \frac{x}{1+x}$ increases on $[0, +\infty)$. Hence the min-max principle implies that there exists $C'_2 \geq 1$ such that

$$\begin{aligned} & [\lambda_j(\alpha^{W,h} + B_h) \leq 2] \\ \Rightarrow & [C_2'^{-1}\lambda_j(\alpha_0^{W,h}) - o(h) \leq \lambda_j(\alpha^{W,h} + B_h) \leq C_2'\lambda_j(\alpha_0^{W,h}) + o(h)] \end{aligned} \quad (23)$$

holds for all $j \in \mathbb{N}$. With the spectral gap (22) and $\lambda_0(\alpha^{W,h} + B_h) = \frac{1}{2}|\beta|h + o(h)$ we conclude that (20) holds when $\lambda_j(\alpha^{W,h} + B_h) \leq 2$.

Interval $[1, +\infty)$: Our assumptions on α provide a constant $C_1 \geq 1$ such that

$$C_1^{-2} \leq \left(\frac{1+\alpha_0}{1+\alpha} \right)^2 \leq C_1^2.$$

With (21), the semiclassical Gårding inequality then gives for h_0 small enough

$$\max\{\|(1+\alpha_0^{W,h})(1+\alpha^{W,h})^{-1}\|, \|(1+\alpha^{W,h})(1+\alpha_0^{W,h})^{-1}\|\} \leq 2C_1.$$

Owing to $\|B_h\| = o(h)$, this is also true when $\alpha^{W,h}$ is replaced by $\alpha^{W,h} + B_h$. We obtain for all $\psi \in D(\alpha_0^{W,1})$,

$$(2C_1)^{-2} \langle \psi, (1+\alpha_0^{W,h})^2 \psi \rangle \leq \langle \psi, (1+\alpha^{W,h} + B_h)^2 \psi \rangle \leq (2C_1)^2 \langle \psi, (1+\alpha_0^{W,h})^2 \psi \rangle,$$

and the min-max principle gives, for all $j \in \mathbb{N}$,

$$(2C_1)^{-2} \lambda_j((1+\alpha_0^{W,h})^2) \leq \lambda_j((1+\alpha^{W,h} + B_h)^2) \leq (2C_1)^2 \lambda_j((1+\alpha_0^{W,h})^2).$$

By taking the square roots, for all $j \in \mathbb{N}$,

$$(2C_1)^{-1} (1 + \lambda_j(\alpha_0^{W,h})) \leq 1 + \lambda_j(\alpha^{W,h} + B_h) \leq 2C_1 (1 + \lambda_j(\alpha_0^{W,h})),$$

which yields (20) for $\lambda_j(\alpha^{W,h} + B_h) \geq 1$. □

Proof of Proposition 5.6. With $H = \alpha^{W,h} + B_h - \lambda_0(\alpha^{W,h} + B_h)$, Lemma 5.7 provides a constant $C' > 0$ such that,

$$\text{for all } j \in \mathbb{N} \setminus \{0\}, \quad C'^{-1} \lambda_j(\alpha_0^{W,h}) \leq \lambda_j(H) \leq C' \lambda_j(\alpha_0^{W,h}),$$

while $\lambda_0(H) = 0$ and the ground state of H is the same as the one of $\alpha^{W,h} + B_h$.

When the function f is nonnegative and decaying, we deduce

$$\begin{aligned} \text{Tr}[f(H + ch^{\frac{d}{\kappa_0}})] &= f(ch^{\frac{d}{\kappa_0}}) + \sum_{j=1}^{\infty} f(\lambda_j(H) + ch^{\frac{d}{\kappa_0}}) \\ &\leq f(ch^{\frac{d}{\kappa_0}}) + \sum_{j=1}^{\infty} f(\lambda_j(H)) \\ &\leq f(ch^{\frac{d}{\kappa_0}}) + \sum_{\substack{n \in \mathbb{N}^d \\ n \neq 0}} f(C_4^{-1}h|n|), \end{aligned} \quad (24)$$

with $C_4 = C_3(1 + 4|\beta|/\beta_m)$, and for $R > 0$,

$$\begin{aligned} \text{Tr}[f(H + ch^{\frac{d}{\kappa_0}})1_{[R,+\infty)}(H)] &= \sum_{\lambda_j(H) \geq R} f(\lambda_j(H) + ch^{\frac{d}{\kappa_0}}) \\ &\leq \sum_{\substack{n \in \mathbb{N}^d \\ h|n| \geq \frac{R}{2C_3}}} f(C_4^{-1}h|n|). \end{aligned}$$

Apply (24) first, with $f = s^{-\kappa_0} \langle s \rangle^{-\kappa_\infty + \kappa_0}$:

$$h^d \text{Tr}[f(H + ch^{\frac{d}{\kappa_0}})] \leq c^{-\kappa_0} + Ch^d \sum_{\substack{n \in \mathbb{N}^d \\ n \neq 0}} (h|n|)^{-\kappa_0} \langle h|n| \rangle^{-\kappa_\infty + \kappa_0}.$$

After splitting the sum into $\sum_{h|n| \leq 1}$ and $\sum_{h|n| \geq 1}$ and with $\#\{n \in \mathbb{N}^d : |n| = m\} = C_{m+d-1}^{d-1} = \mathcal{O}(m^{d-1})$, it becomes

$$\begin{aligned} h^d \text{Tr}[f(H + ch^{\frac{d}{\kappa_0}})] &\leq c^{-\kappa_0} + C'h^d \sum_{m=1}^{\lceil h^{-1} \rceil} h^{-\kappa_0} m^{d-1-\kappa_0} + C'h^d \sum_{m=\lfloor h^{-1} \rfloor}^{\infty} h^{-\kappa_\infty} m^{d-1-\kappa_\infty} \\ &\leq c^{-\kappa_0} + C''h^{d-\kappa_0} \lceil h^{-1} \rceil^{d-\kappa_0} + C''h^{d-\kappa_\infty} \lfloor h^{-1} \rfloor^{d-\kappa_\infty} \leq c^{-\kappa_0} + C''', \end{aligned}$$

owing to $\kappa_\infty > d$ and $\kappa_0 \in (0, d)$. With a function $f(s) = s^{-\kappa_0} \chi(s/\delta)$ with $0 \leq \chi \leq 1$ compactly supported and decaying on $[0, +\infty)$ we get similarly

$$\lim_{\delta \rightarrow 0^+} \limsup_{h \rightarrow 0} h^d \text{Tr}[f(H + ch^{\frac{d}{\kappa_0}})] - c^{-\kappa_0} = 0,$$

while with $f(s) = \langle s \rangle^{-\kappa_\infty}$, the truncated trace $\text{Tr}[f(H + ch^{\frac{d}{\kappa_0}})1_{[\delta^{-1}, +\infty)}(H)]$ satisfies

$$\lim_{\delta \rightarrow 0^+} \limsup_{h \rightarrow 0} h^d \text{Tr}[f(H + ch^{\frac{d}{\kappa_0}})1_{[\delta^{-1}, +\infty)}(H)] = 0.$$

The comparison of $\lambda_j(H)$ with $\lambda_j(\alpha_0^{W,h})$, $j \in \mathbb{N}$, stated in Lemma 5.7 does not depend on the parameter c . Neither do the constants C_3, C_4, C, C', C'' and C''' (f is nonnegative and decaying) depend on c . Therefore the previous asymptotic trace estimates are uniform with respect to $c \in (\frac{1}{A}, A)$ for any fixed $A > 1$.

Thus if $\chi \in \mathcal{C}_0^\infty(\mathbb{R})$ is a cut-off function such that $0 \leq \chi \leq 1$, $\chi \equiv 1$ in $(-1, 1)$ and if a general $f \in \mathcal{C}^\infty((0, +\infty))$ fulfills all the assumptions of Proposition 5.6, then

$$\lim_{\delta \rightarrow 0^+} \limsup_{h \rightarrow 0^+} h^d \left\| [f(H + ch^{\frac{d}{\kappa_0}}) 1_{(0, +\infty)}(H) [\chi(\delta^{-1}H) + (1 - \chi(\delta H))] \right\|_{\mathcal{L}^1} = 0. \quad (25)$$

For $g \in \mathcal{C}_0^\infty(\mathbb{R})$, with an almost analytic extension $\tilde{g} \in \mathcal{C}_0^\infty(\mathbb{C})$, the Helffer–Sjöstrand formula

$$g(\alpha^{W,h}) = \frac{1}{2i\pi} \int_{\mathbb{C}} \partial_{\bar{z}} \tilde{g}(z) (z - \alpha^{W,h}) dz \wedge d\bar{z},$$

combined with the semiclassical Beals criterion [Dimassi and Sjöstrand 1999; Helffer and Nier 2005; Nataf and Nier 1998] with the constant metric dX^2 implies

$$g(\alpha^{W,h}) - g(\alpha)^{W,h} = h r(h)^{W,h},$$

with $r(h)$ uniformly bounded (with respect to h) in $S(1, dX^2)$. Since $(1 + \alpha) \in S(\langle X \rangle^2, dX^2 / \langle X \rangle^2)$ is an invertible elliptic symbol,

$$(1 + \alpha^{W,h})^{-N} - [(1 + \alpha)^{-N}]^{W,h} = h^2 r'(h)^{W,h},$$

with $r'(h)$ uniformly bounded in $S(\langle X \rangle^{-2N-2}, dX^2 / \langle X \rangle^2) \subset S(\langle X \rangle^{-2N}, dX^2)$. For a function $f_\delta \in \mathcal{C}_0^\infty((0, +\infty))$, we take $g(s) = (1 + s)^N f_\delta(s)$ and write

$$f_\delta(\alpha^{W,h}) = g(\alpha^{W,h})(1 + \alpha^{W,h})^{-N},$$

so that

$$\begin{aligned} f_\delta(\alpha^{W,h}) - f_\delta(\alpha)^{W,h} &= [g(\alpha^{W,h}) - g(\alpha)^{W,h}](1 + \alpha^{W,h})^{-N} + g(\alpha)^{W,h}(1 + \alpha^{W,h})^{-N} - f_\delta(\alpha)^{W,h} \\ &= h r''(h)^{W,h}, \end{aligned}$$

with $r''(h)$ uniformly bounded in $S(\langle X \rangle^{-2N}, dX^2)$. In particular, $h^d r''(h)^{W,h}$ is uniformly bounded in $\mathcal{L}^1(L^2(\mathbb{R}^d))$ if we choose $N > d$.

Similarly, the Helffer–Sjöstrand formula can be used to prove $g(H + ch^{\frac{d}{\kappa_0}}) - g(\alpha^{W,h}) = o(h)$ in $\mathcal{L}(L^2(\mathbb{R}^d))$. With $h^d [(1 + H + ch^{\frac{d}{\kappa_0}})^{-N} - (1 + \alpha^{W,h})^{-N}] = o(h)$ in $\mathcal{L}^1(L^2(\mathbb{R}^d))$ due to

$$(1 + H + ch^{\frac{d}{\kappa_0}})^{-1} = [1 + (1 + \alpha^{W,h})^{-1}(B_h + ch^{\frac{d}{\kappa_0}})]^{-1}(1 + \alpha^{W,h})^{-1},$$

the same trick as above transforms the $\mathcal{L}(L^2(\mathbb{R}^d))$ estimate into

$$h^d [f_\delta(H + ch^{\frac{d}{\kappa_0}}) - f_\delta(\alpha^{W,h})] = o(h) \quad \text{in } \mathcal{L}^1(L^2(\mathbb{R}^d)) \quad (26)$$

Note again that this holds uniformly with respect to $c \in (\frac{1}{A}, A)$ for any fixed $A > 1$.

Now take $f_\delta(s) = (1 - \chi(\delta^{-2}s))\chi(\delta^2s)f(s)$ for which we note that the inequality,

$$\text{for all } s \geq 0, \quad 1 - (1 - \chi(\delta^{-2}s))\chi(\delta^2s) \leq \chi(\delta^{-1}s) + (1 - \chi(\delta s))$$

as soon as $\delta < \delta_\chi$ implies,

$$\text{for all } s \geq 0, \quad 0 \leq f(s) - f_\delta(s) \leq f(s)[\chi(\delta^{-1}s) + (1 - \chi(\delta s))]. \quad (27)$$

In the expression $h^d \text{Tr}[f(H + ch^{\frac{d}{\kappa_0}}a^{W,h})]$, we decompose $f(H + ch^{\frac{d}{\kappa_0}})$ into $(I) + (II) + (III)$, where

$$\begin{aligned} (I) &= f_\delta(H + ch^{\frac{d}{\kappa_0}}), \\ (II) &= (f(H + ch^{\frac{d}{\kappa_0}}) - f_\delta(H + ch^{\frac{d}{\kappa_0}}))1_{(0,+\infty)}(H), \\ (III) &= 1_{\{0\}}(H)f(ch^{\frac{d}{\kappa_0}}). \end{aligned}$$

We now conclude with the following steps:

- The estimate (26) yields

$$\begin{aligned} \lim_{h \rightarrow 0} h^d \text{Tr}[f_\delta(H + ch^{\frac{d}{\kappa_0}})a^{W,h}] &= \lim_{h \rightarrow 0} h^d \text{Tr}[f_\delta(\alpha)^{W,h}a^{W,h}] \\ &= \int_{\mathbb{R}^{2d}} f_\delta(\alpha(X))a(X) \frac{dX}{(2\pi)^d}, \end{aligned}$$

which provides the contribution of (I) .

- The upper bound (27) combined with (25) leads to

$$\lim_{\delta \rightarrow 0^+} \limsup_{h \rightarrow 0} |h^d \text{Tr}[(f(H + ch^{\frac{d}{\kappa_0}}) - f_\delta(H + ch^{\frac{d}{\kappa_0}}))1_{(0,+\infty)}(H)a^{W,h}]| = 0,$$

which says that (II) has a null contribution in the limit $\delta \rightarrow 0$.

- The contribution of (III) is simply computed as

$$h^d \text{Tr}[f(H + ch^{\frac{d}{\kappa_0}})1_{\{0\}}(H)a^{W,h}] = \frac{f_0}{c^{\kappa_0}} \langle \psi_0^h, a^{W,h} \psi_0^h \rangle,$$

where ψ_0^h is the ground state of $H + ch^{\frac{d}{\kappa_0}}$ with $\|\psi^h - \pi^{-\frac{d}{4}} e^{-\frac{1}{2}x^2}\| \rightarrow 0$ as $h \rightarrow 0$. This implies $\lim_{h \rightarrow 0} \langle \psi^h, a^{W,h} \psi^h \rangle = a(0)$.

- Finally, the assumptions on f ensure $f(\alpha) \in L^1(\mathbb{R}^{2d})$ and

$$\lim_{\delta \rightarrow 0} \int_{\mathbb{R}^{2d}} f_\delta(\alpha(X))a(X) dX = \int_{\mathbb{R}^{2d}} f(\alpha(X))a(X) dX. \quad \square$$

5B4. *Semiclassical analysis of the reduced density matrices in the bosonic case.*

Proof of Proposition 5.4. This will be made in two parts: we first compute the semiclassical measures $\nu^{(p)}$ and then identify the weak*-limit $\gamma_0^{(p)}$.

For the first part Proposition 4.4 says that it suffices to find the limit $\Phi_{a,0}(s)$ of $\Phi_{a,h}(s)$ for $a \in C_0^\infty(T^*\mathbb{R}^d)$, real-valued, and $s \in (-r_a, r_a)$. Actually Proposition 5.6 allows to consider more generally $a \in S(1, dX^2)$. For $a \in S(1, dX^2)$, real-valued, take $s \in \mathbb{R}$, $|s| < r_a = 1/(\nu_C C_a)$, $4\|a^{W,h}\| \leq C_a$ and set

$$DT_{a,h}(s) = \log \operatorname{Tr}[\varrho_\varepsilon \Gamma(e^{\varepsilon s a})] = -\operatorname{Tr}[\log(1 - CB_s)] + \operatorname{Tr}[\log(1 - C)],$$

$$\Phi_{a,h}(s) = \operatorname{Tr}[\varrho_\varepsilon \Gamma(e^{\varepsilon s a^{W,h}})] = \exp DT_{a,h}(s), \quad \varepsilon = h^d,$$

with $C = e^{-\beta(H + \frac{\varepsilon}{\beta \nu_C})}$ and $B_s = e^{\varepsilon s a^{W,h}}$.

Assume $s \in (-r_a, r_a)$ and compute

$$\begin{aligned} DT_{a,h}(s) &= \int_0^1 \operatorname{Tr} \left[\frac{C_{ts} \tilde{B}_{ts}}{1 - C_{ts} \tilde{B}_{ts}} \varepsilon s a^{W,h} \right] dt \\ &= \int_0^1 \operatorname{Tr} \left[\varepsilon s f \left(H + \frac{\varepsilon}{\beta} (\nu_C^{-1} - t s a(0)) \right) a^{W,h} \right] dt \\ &\quad + \int_0^1 \operatorname{Tr} [\varepsilon s [-(1 - C_{ts})^{-1} + (1 - C_{ts} \tilde{B}_{ts})^{-1}] a^{W,h}] dt, \end{aligned}$$

with

$$C_{ts} = e^{-\beta(H + \frac{\varepsilon}{\beta} (\nu_C^{-1} - t s a(0)))}, \quad \tilde{B}_{ts} = e^{\varepsilon t s (a - a(0))^{W,h}}, \quad f(u) = \frac{e^{-\beta u}}{1 - e^{-\beta u}}.$$

Note that for $t \in [0, 1]$ the parameter $\frac{1}{\beta} (\nu_C^{-1} - t s a(0))$ remains in a compact subset of $(0, +\infty)$. Proposition 5.6 implies for all $t \in [0, 1]$

$$\begin{aligned} \lim_{h \rightarrow 0} \operatorname{Tr} \left[\varepsilon s f \left(H + \frac{\varepsilon}{\beta} (\nu_C^{-1} - t s a(0)) \right) a^{W,h} \right] \\ = \frac{\nu_C s a(0)}{1 - t \nu_C s a(0)} + s \int_{\mathbb{R}^{2d}} \frac{e^{-\beta \alpha(X)}}{1 - e^{-\beta \alpha(X)}} a(X) \frac{dX}{(2\pi)^d}. \end{aligned}$$

With the uniform control with respect to $\frac{1}{\beta} (\nu_C^{-1} - t s a(0)) = c \in [\frac{1}{A}, A]$ in Proposition 5.6, we obtain for the first term

$$\begin{aligned} \lim_{h \rightarrow 0} \int_0^1 \operatorname{Tr} \left[\varepsilon s f \left(H + \frac{\varepsilon}{\beta} (\nu_C^{-1} - t s a(0)) \right) a^{W,h} \right] dt \\ = -\log(1 - s \nu_C a(0)) + s \int_{\mathbb{R}^{2d}} \frac{e^{-\beta \alpha(X)}}{1 - e^{-\beta \alpha(X)}} a(X) \frac{dX}{(2\pi)^d}. \end{aligned}$$

For the remainder term, define $\Pi_0^h = |\psi_0^h\rangle\langle\psi_0^h|$, where $\psi_0^h = U_T(\pi^{-\frac{d}{4}}e^{-\frac{x^2}{2}}) + o(h^0)$ is the ground state of H , and write

$$\begin{aligned} (1 - C_{ts}\tilde{B}_{ts}) &= 1 - C_{ts} - C_{ts}(\tilde{B}_{ts} - 1) = (1 - C_{ts}) \left[1 + \frac{C_{ts}}{1 - C_{ts}}(1 - \tilde{B}_{ts}) \right] \\ &= (1 - C_{ts}) \left[1 + \frac{C_{ts}}{1 - C_{ts}}\Pi_0^h(1 - \tilde{B}_{ts}) + \frac{C_{ts}}{1 - C_{ts}}(1 - \Pi_0^h)(1 - \tilde{B}_{ts}) \right] \\ &= (1 - C_{ts}) \left[\underbrace{1 + f\left(\frac{\varepsilon}{\beta}(\nu_C^{-1} - tsa(0))\right)\Pi_0^h(1 - \tilde{B}_{ts})}_I + \underbrace{\frac{C_{ts}}{1 - C_{ts}}(1 - \Pi_0^h)(1 - \tilde{B}_{ts})}_{II} \right]. \end{aligned}$$

We know

$$\varepsilon \times f\left(\frac{\varepsilon}{\beta}(\nu_C^{-1} - tsa(0))\right) = \frac{1}{\nu_C^{-1} - tsa(0)} + O(\varepsilon) = \frac{1}{\nu_C^{-1} - tsa(0)} + o(h).$$

We write

$$\varepsilon^{-1}(1 - \tilde{B}_{ts})\psi_0^h = - \int_0^1 e^{\varepsilon u t s(a - a(0))^{W,h}} t s(a - a(0))^{W,h} \psi_0^h du,$$

where $\psi_0^h = \pi^{-\frac{d}{4}}U_T e^{-\frac{x^2}{2}} + o(h^0)$, and $a(X) - a(0) \leq C \min\{1, |X|\}$ for some $C > 0$ implies $\lim_{h \rightarrow 0} \|(a - a(0))^{W,h} \psi_0^h\|_{L^2(\mathbb{R}^d)} = 0$. Therefore the term I in the above brackets satisfies

$$I = f\left(\frac{\varepsilon}{\beta}(\nu_C^{-1} - tsa(0))\right)\Pi_0^h(1 - \tilde{B}_{ts}) = o(h^0) \quad \text{in } \mathcal{L}^1(L^2(\mathbb{R}^d)).$$

Note that we have also proved

$$(1 - \tilde{B}_{ts})\Pi_0^h - \Pi_0^h(1 - \tilde{B}_{ts}) = o(\varepsilon) \quad \text{in } \mathcal{L}(L^2(\mathbb{R}^d)).$$

By using

$$\|1 - \tilde{B}_{ts}\| = \mathcal{O}(\varepsilon), \quad \left\| \frac{C_{ts}}{1 - C_{ts}}(1 - \Pi_0^h) \right\| = \mathcal{O}\left(\frac{1}{h}\right),$$

and

$$\begin{aligned} \lim_{h \rightarrow 0} \left\| \varepsilon \frac{C_{ts}}{1 - C_{ts}} \right\|_{\mathcal{L}^1} &= \lim_{h \rightarrow 0} \text{Tr} \left[\varepsilon f\left(H + \frac{\varepsilon}{\beta}(\nu_C^{-1} - tsa(0))\right) \right] \\ &= \frac{\nu_C}{1 - t\nu_C sa(0)} + s \int_{\mathbb{R}^{2d}} \frac{e^{-\beta\alpha(X)}}{1 - e^{-\beta\alpha(X)}} \frac{dX}{(2\pi)^d}, \end{aligned}$$

the term II in the above brackets satisfies

$$\begin{aligned} \|II\|_{\mathcal{L}^1} &= \mathcal{O}(1), \quad \|II\| = \mathcal{O}(\varepsilon h^{-1}) = o(h^0), \\ \left\| II - \frac{C_{ts}}{1 - C_{ts}}(1 - \Pi_0^h)(1 - \tilde{B}_{ts})(1 - \Pi_0^h) \right\|_{\mathcal{L}^1} &= o(h^0). \end{aligned}$$

Again all these estimates are uniform with respect to $t \in [0, 1]$, owing to the uniformity of the estimates in Proposition 5.6 with respect to $c = \frac{1}{\beta}(\nu_C^{-1} - tsa(0))$. By expanding the Neumann series $(1 + I + II)^{-1} = \sum_{k=0}^{\infty} (-1)^k (I + II)^k$ we deduce

$$\left[1 + \frac{C_{ts}}{1 - C_{ts}} (1 - \tilde{B}_{ts}) \right]^{-1} = 1 - \frac{C_{ts}}{1 - C_{ts}} (1 - \Pi_0^h) (1 - \tilde{B}_{ts}) (1 - \Pi_0^h) + R_h,$$

with $\|R_h\|_{\mathcal{L}^1} = o(h^0)$. With $\|\varepsilon(1 - C_{ts})^{-1}\| = \mathcal{O}(1)$ we finally obtain

$$\begin{aligned} & \varepsilon s [(1 - C_{ts})^{-1} - (1 - C_{ts} \tilde{B}_{ts})^{-1}] \\ &= \frac{s\varepsilon C_{ts}}{1 - C_{ts}} (1 - \Pi_0^h) (1 - \tilde{B}_{ts}) (1 - \Pi_0^h) (1 - C_{ts})^{-1} + R'_h, \quad \|R'_h\|_{\mathcal{L}^1} = o(h^0), \end{aligned}$$

while $\|\varepsilon C_{ts} (1 - C_{ts})^{-1}\|_{\mathcal{L}^1} = \mathcal{O}(1)$, $\|1 - \tilde{B}\| = \mathcal{O}(\varepsilon)$ and $\|(1 - \Pi_0^h) (1 - C_{ts})^{-1}\| = \mathcal{O}(h^{-1})$.

With $4\|a^{W,h}\| \leq C_a$, the remainder term tends to 0 as $h \rightarrow 0$ and we have proved, for all $s \in (-r_a, r_a)$,

$$\lim_{h \rightarrow 0} \Phi_{a,h}(s) = \Phi_{a,0}(s) = \frac{1}{1 - s\nu_C a(0)} \exp \left[s \int_{\mathbb{R}^{2d}} \frac{e^{-\beta\alpha(X)}}{1 - e^{-\beta\alpha(X)}} a(X) \frac{dX}{(2\pi)^d} \right].$$

By expanding the generating function according to Proposition 4.4, we obtain

$$\lim_{h \rightarrow 0} \text{Tr}[\varrho_\varepsilon((a^{W,h})^{\otimes p})^{\text{Wick}}] = \sum_{k=0}^p \frac{1}{(p-k)!} \nu_C^k a(0)^k \int_{\mathbb{R}^{2d(p-k)}} a^{\otimes(p-k)} dv(\beta)^{\otimes p-k}.$$

with

$$dv(\beta) = \frac{e^{-\beta\alpha(X)}}{1 - e^{-\beta\alpha(X)}} \frac{dX}{(2\pi)^d}.$$

The possibility to take $a \in S(1, dX^2)$ means that our quantization is adapted to all the $\gamma_h^{(p)}$.

Now in order to identify the weak*-limits of the $\gamma_h^{(p)}$ we compute the Wigner measure associated with $\varrho_\varepsilon(h)$. Remember, see (28) and (29),

$$\text{Tr}[\varrho_\varepsilon W(\sqrt{2\pi}f)] = \exp \left[-\frac{\varepsilon\pi^2}{2} \left\langle f, \frac{1 + e^{-\beta(H + \frac{\varepsilon}{\beta\nu_C})}}{1 - e^{-\beta(H + \frac{\varepsilon}{\beta\nu_C})}} f \right\rangle \right].$$

By using the orthonormal basis of eigenvectors $(\psi_j^h)_{j \in \mathbb{N}}$ of H with associated eigenvalues $\lambda_j^h, \lambda_0^h = 0, \lambda_j^h \geq ch$ for $j > 0$, we obtain

$$\log(\text{Tr}[\varrho_\varepsilon(h) W(\sqrt{2\pi}f)]) = -\pi^2 \nu_C |\langle f, \psi_0^h \rangle|^2 + \mathcal{O}(\varepsilon h^{-1}).$$

With $\|\psi_0^h - \psi_0\|_{L^2} = o(h)$, $\psi_0(x) = \pi^{-\frac{d}{4}} U_T e^{-\frac{x^2}{2}}$, we obtain, after decomposing $f = f_0 \psi_0 \oplus^\perp f'$,

$$\int_{L^2} e^{2i\pi \operatorname{Re}\langle f, z \rangle} d\mu(z) = \lim_{h \rightarrow 0} \operatorname{Tr}[\varrho_\varepsilon(h) W(\sqrt{2}\pi f)] = e^{-\pi^2 \nu_C |f_0|^2}.$$

We deduce, as in [Ammari and Nier 2008, Section 7.5; 2011, Section 4.4],

$$\mathcal{M}(\varrho_\varepsilon(h), h \in \mathcal{E}) = \left\{ \left(\frac{e^{-\frac{|z_0|^2}{\nu_C}}}{\pi \nu_C} L(dz_0) \right) \otimes \delta_0(z') \right\} \quad (z = z_0 \psi_0 \oplus^\perp z'),$$

and

$$\gamma_0^{(p)} = p! \nu_C^p |\psi_0^{\otimes p}\rangle \langle \psi_0^{\otimes p}| \quad \text{for all } p \in \mathbb{N}.$$

The fact that $\nu_{(I)}^{(p)} \equiv 0$ for all $p \in \mathbb{N}$, now comes from

$$\operatorname{Tr}[\gamma_0^{(p)}] = p! \nu_C^p = \nu^{(p)}(\{0\}). \quad \square$$

Appendix A. Multiscale measures

We now recall facts about multiscale measures, introduced in [Fermanian-Kammerer and Gérard 2002; Fermanian Kammerer 2005]. For this we need a new class of symbols. Let $D', D'', D''' \in \mathbb{N}$ be such that $D' + D'' + D''' = D$ and set

$$F = \{X = (x', x'', x''', \xi', \xi'', \xi''') \in \mathbb{R}^{2D} : x' = 0, x'' = \xi'' = 0\}.$$

The class of symbols $S_F^{(2)}$ is defined as the set of

$$(X, Y) \rightarrow a(X, Y) \in C^\infty(\mathbb{R}^{2D} \times \mathbb{R}^{D'+2D''})$$

(note that $\mathbb{R}^{D'+2D''} \cong F^\perp$, hence the notation $S_F^{(2)}$) such that

- there exists $C > 0$ such that for all $Y \in \mathbb{R}^{D'+2D''}$, we have $a(\cdot, Y) \in C_0^\infty(B(0, C))$;
- there exists a function $a_\infty \in C_0^\infty(\mathbb{R}^{2D} \times \mathbb{S}^{D'+2D''-1})$ such that $a(X, R\omega) \rightarrow a_\infty(X, \omega)$ as $R \rightarrow \infty$ in $C^\infty(\mathbb{R}^{2D} \times \mathbb{S}^{D'+2D''-1})$.

Those symbols are quantized according to

$$a^{(2),h} = a_h^{W,h}, \quad a_h(X) = a\left(X, \frac{x'}{h^{\frac{1}{2}}}, \frac{X''}{h^{\frac{1}{2}}}\right) \quad X = (x', x'', x''', \xi', \xi'', \xi''').$$

Theorem 0.1 in [Fermanian Kammerer 2005], which also considers the case when $(x'/h^{\frac{1}{2}}, X''/h^{\frac{1}{2}})$ is replaced by $(x'/h^s, X''/h^s)$, $s < \frac{1}{2}$, says the following.

Proposition A.1. *Let $(\gamma_h)_{h \in \mathcal{E}}$ be a bounded family of nonnegative trace-class operators on $L^2(\mathbb{R}^{2D})$ with $\lim_{h \rightarrow 0} \operatorname{Tr}[\gamma_h] < +\infty$. There exist $\mathcal{E}' \subset \mathcal{E}$, $0 \in \bar{\mathcal{E}}'$, with*

$\mathcal{M}(\gamma_h, h \in \mathcal{E}') = \{v\}$, a nonnegative measure $v_{(I)}$ on $F \times \mathbb{S}^{D'+2D''-1}$ and a $\mathcal{L}^1(L^2(\mathbb{R}^{2D''}))$ -measure m on $F \times \mathbb{R}^{D'}$ such that the convergence

$$\begin{aligned} \lim_{\substack{h \in \mathcal{E}' \\ h \rightarrow 0}} \text{Tr}[\gamma_h a^{(2),h}] &= \int_{\mathbb{R}^{2D} \setminus F} a_\infty(X, \frac{(x', X'')}{|(x', X'')|}) dv(X) \\ &\quad + \int_{F \times \mathbb{S}^{D'+2D''-1}} a_\infty(X, \omega) dv_{(I)}(X, \omega) \\ &\quad + \text{Tr} \left[\int_{F \times \mathbb{R}^{D'}} a(X, x', z, D_z) dm(X, x') \right] \end{aligned}$$

holds for all $a \in S_F^{(2)}$.

Remark A.2. With this scaling and when $a^{W,h} = a^W(x, hD_x) = a(x, hD_x) + O(h)$, $t = 0$, Fermanian Kammerer [2005] checked the equivariance by the semiclassical Egorov theorem. Hence, this construction is naturally extended to the case when $T^*\mathbb{R}^D$ is replaced by T^*M and F is replaced by a submanifold of $T^*\mathbb{R}^D$ on which the symplectic form has constant rank.

In Proposition 3.5 we use the simple case of the above result when $D' = D''' = 0$ and $D'' = D$. Note that in this case $F \times \mathbb{R}^{D'} = \{0\}$ and the trace-class-valued measure is nothing but a trace-class operator γ_0 .

Appendix B. Wigner measures in the bosonic case and condition (PI)

Bosonic mean-field analysis is like semiclassical analysis in infinite dimension. Let $\mathcal{H}$ be a separable complex Hilbert space and $\Gamma_+(\mathcal{H})$ be the associated bosonic Fock space. With the scaled CCR relations

$$[a_+(g), a_+^*(f)] = \varepsilon \langle g, f \rangle, \quad [a_+(g), a_+(f)] = [a_+^*(g), a_+^*(f)] = 0$$

and after setting

$$\Phi(f) = \frac{a_+(f) + a_+^*(f)}{\sqrt{2}}, \quad W(f) = e^{i\Phi(f)}, \quad (28)$$

mean-field Wigner measures were introduced in [Ammari and Nier 2008]. Actually the parameter ε^{-1} represents the typical number of particles. Let $(\varrho_\varepsilon)_{\varepsilon \in \mathcal{E}}$, $0 \in \bar{\mathcal{E}}$, be a family of normal states (normalized nonnegative trace-class operators) in $\Gamma_+(\mathcal{H})$. Under the sole uniform estimate $\text{Tr}[\varrho_\varepsilon(1 + N)^\delta] \leq C_\delta$ for some $\delta > 0$, Wigner measures are defined as Borel probability measures on $\mathcal{H}$ and characterized by their characteristic function as follows: $\mu \in \mathcal{M}(\varrho_\varepsilon, \varepsilon \in \mathcal{E})$ if and only if there exists $\mathcal{E}' \subset \mathcal{E}$, $0 \in \bar{\mathcal{E}}'$, such that,

$$\text{for all } f \in \mathcal{H}, \quad \lim_{\substack{\varepsilon \in \mathcal{E}' \\ \varepsilon \rightarrow 0}} \text{Tr}[\varrho_\varepsilon W(\sqrt{2}\pi f)] = \int_{\mathcal{H}} e^{2i\pi \text{Re}\langle f, z \rangle} d\mu(z). \quad (29)$$

Assuming $\text{Tr}[\varrho_\varepsilon N_+^k] \leq C^k$ for all $k \in \mathbb{N}$ (or as in Hypothesis 4.1, $\text{Tr}[\varrho_\varepsilon e^{cN_+}] \leq C$), $\mathcal{M}(\varrho_\varepsilon, \varepsilon \in \mathcal{E}) = \{\mu\}$ implies

$$\lim_{\varepsilon \rightarrow 0} \text{Tr}[\varrho_\varepsilon \tilde{b}^{\text{Wick}}] = \int_{\mathcal{Z}} \langle z^{\otimes p}, \tilde{b} z^{\otimes p} \rangle d\mu(z) \quad (30)$$

holds for all compact $\tilde{b} \in \mathcal{L}^\infty(S_+^p \mathcal{Z}^{\otimes p})$. In particular with the definition of non-normalized reduced density matrices we obtain,

$$\text{for all } p \in \mathbb{N}, \quad w^*\text{-}\lim_{\varepsilon \rightarrow 0} \gamma_\varepsilon^{(p)} = \gamma_0^{(p)} = \int_{\mathcal{Z}} |z^{\otimes p}\rangle \langle z^{\otimes p}| d\mu(z).$$

This w^* -limit can be transformed to a $\|\cdot\|_{\mathcal{L}^1}$ if and only if the restriction to compact $\tilde{b}$ in (30) can be removed. It actually suffices to check that (30) holds for $\tilde{b} \in \mathcal{L}^\infty(S_+^p \mathcal{Z}^{\otimes p})$ and $\tilde{b} = \text{Id}_{S_+^p \mathcal{Z}^{\otimes p}}$, as shows the following result.

Proposition B.1. *For a family $(\varrho_\varepsilon)_{\varepsilon \in \mathcal{E}}$ in $\mathcal{L}^1(\mathcal{H})$, $0 \in \bar{\mathcal{E}}$, such that $\varrho_\varepsilon \geq 0$, $\text{Tr}[\varrho_\varepsilon] = 1$, $\mathcal{M}(\varrho_\varepsilon, \varepsilon \in \mathcal{E}) = \{\mu\}$, the conditions (PI) and (P) are equivalent:*

$$\begin{aligned} \left[\text{(PI)} : \text{ for all } \alpha \in \mathbb{N}, \quad \lim_{\varepsilon \rightarrow 0} \text{Tr}[\varrho_\varepsilon N^\alpha] = \int_{\mathcal{Z}} |z|^{2\alpha} d\mu(z) < \infty \right] \\ \iff \left[\text{(P)} : \text{ for all } b \in \mathcal{P}_{\text{alg}}(\mathcal{Z}), \quad \lim_{\varepsilon \rightarrow 0} \text{Tr}[\varrho_\varepsilon b^{\text{Wick}}] = \int_{\mathcal{Z}} b d\mu \right], \end{aligned}$$

where

$$\mathcal{P}_{p,q}(\mathcal{Z}) = \{b : \mathcal{Z} \ni z \mapsto b(z) = \langle z^{\otimes q}, \tilde{b} z^{\otimes p} \rangle \in \mathbb{C} : \tilde{b} \in \mathcal{L}(S_+^p \mathcal{Z}^{\otimes p}; S_+^q \mathcal{Z}^{\otimes q})\},$$

$$\text{and } \mathcal{P}_{\text{alg}}(\mathcal{Z}) = \bigoplus_{p,q \in \mathbb{N}}^{\text{alg}} \mathcal{P}_{p,q}(\mathcal{Z}).$$

We give below the proof, which rectifies a minor mistake in [Ammari and Nier 2011].

Proof. For $\alpha \in \mathbb{N}^*$, we have $(|z|^{2\alpha})^{\text{Wick}} = N(N-\varepsilon) \cdots (N-(\alpha-1)\varepsilon)$. Hence the condition (PI) is equivalent to

$$(\text{PI})' : \text{ for all } \alpha \in \mathbb{N}, \quad \lim_{\varepsilon \rightarrow 0} \text{Tr}[\varrho_\varepsilon (|z|^{2\alpha})^{\text{Wick}}] = \int_{\mathcal{Z}} |z|^{2\alpha} d\mu(z) < \infty.$$

Hence the condition (PI) is a particular case of (P) and it is sufficient to prove $(\text{PI})' \Rightarrow (\text{P})$. From now, assume $(\text{PI})'$.

We want to prove (P) for a general $b \in \mathcal{P}_{\text{alg}}(\mathcal{Z}) = \bigoplus_{p,q \in \mathbb{N}}^{\text{alg}} \mathcal{P}_{p,q}(\mathcal{Z})$. Let us first consider the “diagonal” case $b \in \mathcal{P}_{p,p}(\mathcal{Z})$, $p \in \mathbb{N}^*$. Using the decomposition $\tilde{b} = \tilde{b}_{R,+} - \tilde{b}_{R,-} + i\tilde{b}_{I,+} - i\tilde{b}_{I,-}$ with all the $\tilde{b}_\bullet \geq 0$ we can assume $\tilde{b} \geq 0$. For such a $\tilde{b}$, there exists a nondecreasing sequence $(\tilde{b}_n)_{n \geq 0}$ of nonnegative compact operators in $\mathcal{L}^\infty(S_+^p \mathcal{Z})^{\otimes p}$ such that $\lim_{n \rightarrow \infty} \tilde{b}_n = \tilde{b}$ in the weak operator topology. Recall

from [Ammari and Nier 2011, Proposition 2.9] that the convergence in the (P) condition always holds when the kernel $\tilde{b}$ is compact; thus,

$$\text{for all } n \in \mathbb{N}, \quad \int_{\mathcal{X}} b_n d\mu = \lim_{\varepsilon \rightarrow 0} \text{Tr}[\varrho_\varepsilon b_n^{\text{Wick}}] \leq \liminf_{\varepsilon \rightarrow 0} \text{Tr}[\varrho_\varepsilon b^{\text{Wick}}].$$

Using $b_n(z) = \langle z^{\otimes p}, \tilde{b}_n z^{\otimes p} \rangle \rightarrow \langle z^{\otimes p}, \tilde{b} z^{\otimes p} \rangle = b(z)$ as $n \rightarrow \infty$ and Fatou's lemma yield

$$\int_{\mathcal{X}} b d\mu \leq \liminf_{\varepsilon \rightarrow 0} \text{Tr}[\varrho_\varepsilon b^{\text{Wick}}]. \quad (31)$$

The same arguments with $\tilde{b}$ replaced by $|b|_{\mathcal{P}_{p,p}} \text{Id}_{S_+^p \mathcal{X}^{\otimes p}} - \tilde{b} \geq 0$ provide

$$\liminf_{\varepsilon \rightarrow 0} \text{Tr}[\varrho_\varepsilon (|\tilde{b}|_{S_+^p \mathcal{X}^{\otimes p}} |z|^{2p} - b(z))^{\text{Wick}}] \geq \int (|\tilde{b}|_{S_+^p \mathcal{X}^{\otimes p}} |z|^{2p} - b(z)) d\mu(z).$$

With (PI)' condition, the $|z|^{2p}$ terms can be removed on both sides and thus

$$\limsup_{\varepsilon \rightarrow 0} \text{Tr}[\varrho_\varepsilon b^{\text{Wick}}] \leq \int_{\mathcal{X}} b d\mu. \quad (32)$$

The inequalities (31) and (32) show that the convergence in the (P) condition holds for all $b \in \mathcal{P}_{p,p}(\mathcal{X})$ such that $\tilde{b} \geq 0$, and hence for all $b \in \mathcal{P}_{p,p}(\mathcal{X})$.

We now consider the general case $b \in \mathcal{P}_{p,q}(\mathcal{X})$. There exists a sequence of compact operators $\tilde{b}_n \in \mathcal{L}^\infty(S_+^p \mathcal{X}^{\otimes p}, S_+^q \mathcal{X}^{\otimes q})$ such that,

$$\text{for all } n \in \mathbb{N}, \quad |b_n|_{\mathcal{P}_{p,q}} = |\tilde{b}_n|_{\mathcal{L}(S_+^p \mathcal{X}^{\otimes p}, S_+^q \mathcal{X}^{\otimes q})} \leq |\tilde{b}|_{\mathcal{L}(S_+^p \mathcal{X}^{\otimes p}, S_+^q \mathcal{X}^{\otimes q})} = |b|_{\mathcal{P}_{p,q}}$$

and,

$$\text{for all } z \in \mathcal{X}, \quad \lim_{n \rightarrow \infty} b_n(z) = \lim_{n \rightarrow \infty} \langle z^{\otimes q}, \tilde{b}_n z^{\otimes p} \rangle = \langle z^{\otimes q}, \tilde{b} z^{\otimes p} \rangle = b(z).$$

For any fixed $n \in \mathbb{N}$,

$$\begin{aligned} \limsup_{\varepsilon \rightarrow 0} \left| \text{Tr}[\varrho_\varepsilon b^{\text{Wick}}] - \int_{\mathcal{X}} b(z) d\mu(z) \right| \\ \leq \limsup_{\varepsilon \rightarrow 0} \left| \text{Tr}[\varrho_\varepsilon (b^{\text{Wick}} - b_n^{\text{Wick}})] \right| \\ + \limsup_{\varepsilon \rightarrow 0} \left| \text{Tr}[\varrho_\varepsilon b_n^{\text{Wick}}] - \int_{\mathcal{X}} b_n d\mu \right| + \int_{\mathcal{X}} |b_n - b| d\mu, \quad (33) \end{aligned}$$

where the second term of the right-hand side vanishes because $\tilde{b}_n$ is a fixed compact operator. Using the Cauchy–Schwarz inequality with $\text{Tr}[\varrho_\varepsilon] = 1$ gives

$$\left| \text{Tr}[\varrho_\varepsilon (b^{\text{Wick}} - b_n^{\text{Wick}})] \right| \leq \text{Tr}[\varrho_\varepsilon (b^{\text{Wick}} - b_n^{\text{Wick}})(b^{\text{Wick},*} - b_n^{\text{Wick},*})]^{\frac{1}{2}}.$$

From the proved result when $p = q$, we deduce

$$\limsup_{\varepsilon \rightarrow 0} \left| \text{Tr}[\varrho_\varepsilon (b^{\text{Wick}} - b_n^{\text{Wick}})] \right| \leq \left[\int_{\mathcal{X}} |b - b_n|^2 d\mu(z) \right]^{\frac{1}{2}}. \quad (34)$$

With $\int_{\mathcal{Z}} |z|^{r(p+q)} d\mu(z) < \infty$ and,

$$\text{for all } n \in \mathbb{N}, \text{ for all } z \in \mathcal{Z}, \quad |b(z) - b_n(z)|^r \leq (2|b|_{\mathcal{P}_{p,q}})^r |z|^{r(p+q)},$$

Lebesgue's convergence theorem yields

$$\lim_{n \rightarrow \infty} \int_{\mathcal{Z}} |b - b_n|^r d\mu = 0 \quad (35)$$

for $r \in \{1, 2\}$. Combining (33), (34) and (35) proves (P) for any $b \in \mathcal{P}_{p,q}(\mathcal{Z})$. $\square$

Appendix C. The composition formula of Wick quantized operators

We give an algebraic proof for the composition formula (4) of two Wick quantized operators on a finite- or infinite-dimensional separable complex Hilbert space $\mathcal{Z}$. This proof holds in both the bosonic and fermionic cases. It uses only the definition of the Wick quantization, and it involves neither creation and annihilation operators, nor the canonical commutation or anticommutation relations.

We define $\llbracket m, n \rrbracket := \{m, \dots, n\}$ for $m \leq n \in \mathbb{N}$. The action of the symmetric group $\mathfrak{S}_{\llbracket 1, n \rrbracket}$ on product vectors in $\mathcal{Z}^{\otimes n}$, $\sigma \cdot (z_1 \otimes \dots \otimes z_n) = z_{\sigma_1} \otimes \dots \otimes z_{\sigma_n}$, $z_j \in \mathcal{Z}$, is extended to $\mathcal{Z}^{\otimes n}$ by linearity and density. With this notation,

$$\mathcal{S}_{\pm}^n = \frac{1}{n!} \sum_{\sigma \in \llbracket 1, n \rrbracket} s_{\pm}(\sigma) \sigma \cdot .$$

We begin with a preliminary lemma on a special set of permutations.

Lemma C.1. *Let $k, p, q, K \in \mathbb{N}$ such that $k \in \llbracket \max\{0, p + q - K\}, \min\{p, q\} \rrbracket$, and*

$$\mathfrak{S}(k) := \{\sigma \in \mathfrak{S}_{\llbracket 1, K \rrbracket} \mid \text{card}(\sigma(\llbracket p - k + 1, p - k + q \rrbracket) \cap \llbracket 1, p \rrbracket) = k\}.$$

(1) *The cardinal of $\mathfrak{S}(k)$ is*

$$\text{card } \mathfrak{S}(k) = \binom{q}{k} \binom{p}{k} k! \frac{(K - q)!(K - p)!}{(K - (q + p - k))!}.$$

(2) *Any permutation $\sigma \in \mathfrak{S}(k)$ can be factorized as $\sigma = \sigma^{(1)} \sigma^{(2)} \sigma^{(3)} \sigma^{(4)}$, where*

$$\begin{aligned} \sigma^{(1)} &\in \mathfrak{S}_{\llbracket 1, p \rrbracket}, & \sigma^{(3)} &\in \mathfrak{S}_{\llbracket p - k + 1, p - k + q \rrbracket}, \\ \sigma^{(2)} &\in \mathfrak{S}_{\llbracket p + 1, K \rrbracket}, & \sigma^{(4)} &\in \mathfrak{S}_{\llbracket 1, K \rrbracket \setminus \llbracket p - k + 1, p - k + q \rrbracket}. \end{aligned}$$

Note that:

- There is no uniqueness of such a decomposition.
- For $A \subset B$ an element of $\mathfrak{S}_A$ is identified with the corresponding element of $\mathfrak{S}_B$ which is the identity on $B \setminus A$.
- The permutations $\sigma^{(1)}$ and $\sigma^{(2)}$ commute, and so do $\sigma^{(3)}$ and $\sigma^{(4)}$.

Proof. (1) We count the number of permutations in $\mathfrak{S}(k)$. We first choose k integers out of $\llbracket p - k + 1, p - k + q \rrbracket$ and k integers out of $\llbracket 1, p \rrbracket$. There are $\binom{q}{k} \binom{p}{k}$ such possible choices and $k!$ possible permutations for each of these choices. Then the remaining $q - k$ integers of $\llbracket p - k + 1, p - k + q \rrbracket$ have to be sent in $\llbracket p + 1, K \rrbracket$. There are $(q - k)! \binom{K - p}{q - k}$ possibilities for that. In the same way we have $(p - k)! \binom{K - q}{p - k}$ possibilities for the remaining integers of $\llbracket 1, p \rrbracket$ that come from $\llbracket 1, K \rrbracket \setminus \llbracket p - k + 1, p - k + q \rrbracket$. Finally the $K - k - (q - k) - (p - k)$ remaining integers on both sides can be permuted in $(K - q - p + k)!$ different ways, so that

$$\text{card } \mathfrak{S}(k) = \binom{q}{k} \binom{p}{k} k! (q - k)! \binom{K - p}{q - k} (p - k)! \binom{K - q}{p - k} (K - q - p + k)!$$

and this gives the result.

(2) Let $A = \sigma^{-1}(\llbracket 1, p \rrbracket) \cap \llbracket p - k + 1, p - k + q \rrbracket$. There exists $\sigma^{(3)} \in \mathfrak{S}_{\llbracket p - k + 1, p - k + q \rrbracket}$ such that $\sigma^{(3)}(A) = \llbracket p - k + 1, p \rrbracket$. Then

$$\sigma \sigma^{(3)-1}(\llbracket p - k + 1, p \rrbracket) = \sigma(A) \subseteq \llbracket 1, p \rrbracket.$$

Hence there exists $\sigma^{(1)} \in \mathfrak{S}_{\llbracket 1, p \rrbracket}$ such that $\sigma^{(1)}(j) = \sigma \sigma^{(3)-1}(j)$ on $\llbracket p - k + 1, p \rrbracket$. Similarly, there exists $\sigma^{(2)} \in \mathfrak{S}_{\llbracket p + 1, K \rrbracket}$ such that $\sigma^{(2)}(j) = \sigma \sigma^{(3)-1}(j)$ on $\llbracket p + 1, p - k + q \rrbracket$. Note that $\sigma^{(1)}$ and $\sigma^{(2)}$ commute. Finally, we set $\sigma^{(4)} = \sigma^{(2)-1} \sigma^{(1)-1} \sigma \sigma^{(3)-1}$. By construction, $\sigma^{(4)}(j) = j$ for $j \in \llbracket p - k + 1, p - k + q \rrbracket$, hence $\sigma^{(4)} \in \mathfrak{S}_{\llbracket 1, K \rrbracket \setminus \llbracket p - k + 1, p - k + q \rrbracket}$ and $\sigma = \sigma^{(1)} \sigma^{(2)} \sigma^{(3)} \sigma^{(4)}$ (as $\sigma^{(4)}$ and $\sigma^{(3)}$ commute). $\square$

Notation 1. On $\mathcal{L}(\mathcal{X}^{\otimes p}; \mathcal{X}^{\otimes q})$, the equivalence relation $\cong$ is defined by

$$A \cong B \iff S_{\pm}^q A S_{\pm}^{p,*} = S_{\pm}^q B S_{\pm}^{p,*}.$$

Lemma C.2. Let $\tilde{b}_j \in \mathcal{L}(S_{\pm}^{p_j} \mathcal{X}^{\otimes p_j}; S_{\pm}^{q_j} \mathcal{X}^{\otimes q_j})$ and n_j such that $n_1 + p_1 = n_2 + q_2 =: K$. Then

$$\begin{aligned} (\tilde{b}_1 \otimes \text{Id}^{\otimes n_1}) S_{\pm}^{K,*} S_{\pm}^K (\tilde{b}_2 \otimes \text{Id}^{\otimes n_2}) \\ \cong \sum_k (\pm 1)^{(p_2 + q_2)(k - p_1)} \frac{n_2! n_1!}{K'! K! k!} (\tilde{b}_1 \sharp^k \tilde{b}_2) \otimes \text{Id}^{\otimes K'}, \end{aligned}$$

where $k \in \llbracket \max\{0, p_1 + q_2 - K\}, \min\{p_1, q_2\} \rrbracket$, and $K' = K - q_2 - p_1 + k$.

Proof. Using the partition $\mathfrak{S}_{\llbracket 1, K \rrbracket} = \bigsqcup_k \tilde{\mathfrak{S}}(k)$ into subsets

$$\tilde{\mathfrak{S}}(k) := \{\sigma \in \mathfrak{S}_{\llbracket 1, K \rrbracket} \mid \text{card}(\sigma(\llbracket 1, q_2 \rrbracket) \cap \llbracket 1, p_1 \rrbracket) = k\}$$

for $k \in \llbracket \max\{0, p_1 + q_2 - K\}, \min\{p_1, q_2\} \rrbracket$ yields

$$(\tilde{b}_1 \otimes \text{Id}^{\otimes n_1}) S_{\pm}^{K,*} S_{\pm}^K (\tilde{b}_2 \otimes \text{Id}^{\otimes n_2}) = \frac{1}{K!} \sum_k \sum_{\tilde{\sigma} \in \tilde{\mathfrak{S}}(k)} (\tilde{b}_1 \otimes \text{Id}^{\otimes n_1})_{s_{\pm}(\tilde{\sigma})} \tilde{\sigma} \cdot (\tilde{b}_2 \otimes \text{Id}^{\otimes n_2}).$$

We fix k and $\tilde{\sigma} \in \tilde{\mathfrak{S}}(k)$. A cyclic permutation $\tau_r := (1\ 2\ 3 \cdots r)$ acting on $\mathcal{Z}^{\otimes r}$ defines the shift operator $\tau_r \cdot = (1\ 2\ 3 \cdots r) \cdot$ and then $\sigma := \tilde{\sigma} \tau_K^{k-p_1}$ is in $\mathfrak{S}(k)$ (with $p = p_1$ and $q = q_2$) and

$$\begin{aligned} & (\tilde{b}_1 \otimes \text{Id}^{\otimes n_1})_{s_{\pm}(\tilde{\sigma})} \tilde{\sigma} \tau_K^{k-p_1} \tau_K^{p_1-k} \cdot (\tilde{b}_2 \otimes \text{Id}^{\otimes n_2}) \tau_{p_2+n_2}^{k-p_1} \tau_{p_2+n_2}^{p_1-k} \cdot \\ & \cong (\tilde{b}_1 \otimes \text{Id}^{\otimes n_1})_{s_{\pm}(\sigma)} \sigma \cdot (\pm 1)^{K(k-p_1)} (\text{Id}^{\otimes p_1-k} \otimes \tilde{b}_2 \otimes \text{Id}^{\otimes K'}) (\pm 1)^{(p_2+n_2)(k-p_1)} \\ & \cong (\pm 1)^{(K+p_2+n_2)(k-p_1)} (\tilde{b}_1 \otimes \text{Id}^{\otimes n_1})_{s_{\pm}(\sigma)} \sigma \cdot (\text{Id}^{\otimes p_1-k} \otimes \tilde{b}_2 \otimes \text{Id}^{\otimes K'}) \end{aligned}$$

holds for operators in $\mathcal{L}(\mathcal{X}^{\otimes q_1+n_1}; \mathcal{X}^{\otimes p_2+n_2})$. We used

$$s_{\pm}(\sigma) = s_{\pm}(\tilde{\sigma}) s_{\pm}(\tau_K^{k-p_1}) = s_{\pm}(\tilde{\sigma}) (\pm 1)^{K(k-p_1)}$$

and

$$(\tau_{p_2+n_2}^{p_1-k} \cdot) \circ \mathcal{S}_{\pm}^{p_2+n_2} = (\pm 1)^{(p_2+n_2)(p_1-k)} \mathcal{S}_{\pm}^{p_2+n_2}.$$

Owing to the factorization $\sigma = \sigma^{(1)} \sigma^{(2)} \sigma^{(3)} \sigma^{(4)}$ of Lemma C.1 with $\sigma^{(i)} \sigma^{(i+1)} = \sigma^{(i+1)} \sigma^{(i)}$ for $i \in \{1, 3\}$, we get

$$\begin{aligned} & (\tilde{b}_1 \otimes \text{Id}^{\otimes n_1})_{s_{\pm}(\sigma)} \sigma \cdot (\text{Id}^{\otimes p_1-k} \otimes \tilde{b}_2 \otimes \text{Id}^{\otimes K'}) \\ & \cong (\tilde{b}_1 \otimes \text{Id}^{\otimes n_1})_{s_{\pm}(\sigma)} (\sigma^{(1)} \sigma^{(2)} \sigma^{(3)} \sigma^{(4)}) \cdot (\text{Id}^{\otimes p_1-k} \otimes \tilde{b}_2 \otimes \text{Id}^{\otimes K'}) \\ & \cong s_{\pm}(\sigma) ((b_1 \sigma^{(1)} \cdot) \otimes \text{Id}^{\otimes n_1} \sigma^{(2)} \cdot) \sigma^{(4)} \cdot (\text{Id}^{\otimes p_1-k} \otimes (\sigma^{(3)} \cdot \tilde{b}_2) \otimes \text{Id}^{\otimes K'}) \\ & \cong s_{\pm}(\sigma) (\tilde{b}_1 s_{\pm}(\sigma^{(1)}) \otimes s_{\pm}(\sigma^{(2)}) \text{Id}^{\otimes n_1})_{s_{\pm}(\sigma^{(4)})} (\text{Id}^{\otimes p_1-k} \otimes s_{\pm}(\sigma^{(3)}) \tilde{b}_2 \otimes \text{Id}^{\otimes K'}) \\ & \cong (\tilde{b}_1 \otimes \text{Id}^{\otimes n_1}) (\text{Id}^{\otimes p_1-k} \otimes \tilde{b}_2 \otimes \text{Id}^{\otimes K'}) \\ & \cong [(\tilde{b}_1 \otimes \text{Id}^{\otimes q_2-k}) (\text{Id}^{\otimes p_1-k} \otimes \tilde{b}_2)] \otimes \text{Id}^{\otimes K'} \\ & \cong \left(\frac{p_1!}{(p_1-k)!} \frac{q_2!}{(q_2-k)!} \right)^{-1} (\tilde{b}_1 \sharp^k \tilde{b}_2) \otimes \text{Id}^{\otimes K'}. \end{aligned}$$

We conclude with the first statement of Lemma C.1 which counts the terms in $\sum_{\tilde{\sigma} \in \tilde{\mathfrak{S}}(k)}$ because $\text{card}(\tilde{\mathfrak{S}}(k)) = \text{card}(\mathfrak{S}(k))$. $\square$

Proof of Proposition 2.2. For n_1, n_2 such that $n_1 + p_1 = n_2 + q_2 =: K$, using Lemma C.2,

$$\begin{aligned} & \varepsilon^{-\frac{p_1+q_1+p_2+q_2}{2}} \times \tilde{b}_1^{\text{Wick}} \tilde{b}_2^{\text{Wick}} \Big|_{\mathcal{S}_{\pm}^{n_2+p_2} \mathcal{X}^{\otimes n_2+p_2}} \\ & = \frac{\sqrt{K! (n_1+q_1)!}}{n_1!} \frac{\sqrt{(n_2+p_2)! K!}}{n_2!} \\ & \quad \cdot \mathcal{S}_{\pm}^{q_1+n_1} (\tilde{b}_1 \otimes \text{Id}^{\otimes n_1}) \mathcal{S}_{\pm}^{p_1+n_1,*} \mathcal{S}_{\pm}^{p_2+q_2} (\tilde{b}_2 \otimes \text{Id}^{\otimes n_2}) \mathcal{S}_{\pm}^{p_2+n_2,*} \end{aligned}$$

$$\begin{aligned}
&= \sum_k (\pm 1)^{(p_2+q_2)(k-p_1)} \frac{\sqrt{(n_1+q_1)!(n_2+p_2)!}}{n_1!n_2!} K! \frac{n_2!n_1!}{K'!K!k!} \\
&\quad \cdot \mathcal{S}_{\pm}^{q_1+n_1}((\tilde{b}_1 \#^k \tilde{b}_2) \otimes \text{Id}^{\otimes K'}) \mathcal{S}_{\pm}^{p_2+n_2,*} \\
&= \sum_k (\pm 1)^{(p_2+q_2)(k-p_1)} \frac{\sqrt{(q_2+q_1-k+K')!(p_2+p_1-k+K')!}}{K'!k!} \\
&\quad \cdot \mathcal{S}_{\pm}^{q_1+n_1}((\tilde{b}_1 \#^k \tilde{b}_2) \otimes \text{Id}^{\otimes K'}) \mathcal{S}_{\pm}^{p_2+n_2,*},
\end{aligned}$$

where $K' := K - q_2 - p_1 + k$.

With $p_2 + n_2 = p_2 + p_1 - k + K'$ and $q_1 + n_1 = q_2 + q_1 - k + K'$, we thus obtain the equality of operators

$$\tilde{b}_1^{\text{Wick}} \tilde{b}_2^{\text{Wick}} = \sum_k (\pm 1)^{(p_2+q_2)(k-p_1)} \frac{\varepsilon^k}{k!} (\tilde{b}_1 \#^k \tilde{b}_2)^{\text{Wick}}$$

restricted to $\mathcal{S}_{\pm}^{n_2+p_2} \mathcal{L}^{\otimes n_2+p_2}$. □

Appendix D. A general formula for $\text{Tr}[\Gamma_{\pm}(C)]$

The following result about traces of the second quantized operator $\Gamma_{\pm}(C)$ is often presented for self-adjoint trace-class operators, although it is valid without self-adjointness. We recall here the general version for the sake of completeness. It relies on a simple holomorphy argument and can be compared with Lidskii's theorem, which says that for any trace-class operator T , we have $\text{Tr}[T] = \sum_{\lambda \in \sigma(T)} \lambda$.

Lemma D.1. *For any trace-class operator $C \in \mathcal{L}^1(\mathcal{H})$ (which is assumed to be a strict contraction in the bosonic case, $\pm = +$), its second quantized version $\Gamma_{\pm}(C)$ is trace-class in $\Gamma_{\pm}(\mathcal{H})$ and*

$$\text{Tr}[\Gamma_{\pm}(C)] = \exp(\mp \text{Tr}[\log(1 \mp C)]).$$

Proof. When $C = C^* \in \mathcal{L}^1(\mathcal{H})$ using an orthonormal basis of eigenvectors $(e_n)_{n \in \mathbb{N}}$ in $\mathcal{H}$ with the corresponding eigenvalues $(\lambda_n)_{n \in \mathbb{N}}$, and

$$\Gamma_{\pm}(\mathcal{H}) \cong \bigotimes_{n \in \mathbb{N}} \Gamma_{\pm}(\mathbb{C}e_n),$$

(the infinite tensor product of Hilbert spaces with a stabilizing sequence $u_n = \Omega_n$ with $\Omega_n \in \Gamma_{\pm}(\mathbb{C}e_n)$ the vacuum vector), we obtain

- in the bosonic case with $\|C\| < 1$,

$$\begin{aligned}
\text{Tr}[\Gamma_+(C)] &= \prod_{n \in \mathbb{N}} \text{Tr}[\Gamma_+(\lambda_n \text{Id}_{\mathbb{C}})] = \prod_{n \in \mathbb{N}} \frac{1}{1 - \lambda_n} = \exp\left(-\sum_{n \in \mathbb{N}} \log(1 - \lambda_n)\right) \\
&= \exp(-\text{Tr}[\log(1 - C)]),
\end{aligned}$$

- in the fermionic case,

$$\begin{aligned}\mathrm{Tr}[\Gamma_-(C)] &= \prod_{n \in \mathbb{N}} \mathrm{Tr}[\Gamma_-(\lambda_n \mathrm{Id}_{\mathbb{C}})] = \prod_{n \in \mathbb{N}} (1 + \lambda_n) = \exp\left(+ \sum_{n \in \mathbb{N}} \log(1 + \lambda_n)\right) \\ &= \exp(\mathrm{Tr}[\log(1 + C)]).\end{aligned}$$

The functoriality of $\Gamma_{\pm}$ for the polar decomposition $C = U|C|$ is given by $\Gamma_{\pm}(C) = \Gamma_{\pm}(U)\Gamma_{\pm}(|C|)$, while $\|C\| < 1 \Leftrightarrow \| |C| \| < 1$ in the bosonic case. Hence $\Gamma_{\pm}(C)$ is trace-class when $C \in \mathcal{L}^1(\mathcal{X})$ (and $\|C\| < 1$ in the bosonic case).

Set $\mathcal{C} = \mathcal{L}^1(\mathcal{X})$ in the fermionic case and $\mathcal{C} = \mathcal{L}^1(\mathcal{X}) \cap \{C \in \mathcal{L}(\mathcal{X}) : \|C\| < 1\}$ in the bosonic case. In both cases $\mathcal{C}$ is an open convex set on which the two sides of the equality are holomorphic functions. Actually the holomorphy of the left-hand side comes from series expansion

$$\mathrm{Tr}[\Gamma_{\pm}(C)] = \sum_{n=0}^{\infty} \mathrm{Tr}[S_{\pm}^n C^{\otimes n} S_{\pm}^{n,*}],$$

which converges uniformly in

$$B(C_0, \delta_{C_0}) = \{C \in \mathcal{L}^1(\mathcal{X}) : \|C - C_0\|_{\mathcal{L}^1(\mathcal{X})} < \delta_{C_0}\}$$

for $\delta_{C_0} > 0$ small enough, for any $C_0 \in \mathcal{L}^1(\mathcal{X})$ (satisfying additionally $\|C_0\| < 1$ in the bosonic case). Actually the estimate $\|C\|_{\mathcal{L}^1(\mathcal{X})} \leq A$ (and $\|C\| \leq \varrho$ with $\varrho < 1$ in the bosonic case) implies $\| |C| \|_{\mathcal{L}^1(\mathcal{X})} \leq A$ (and $\| |C| \| \leq \varrho$ in the bosonic case). Now the inequality

$$|\mathrm{Tr}[S_{\pm}^n C^{\otimes n} S_{\pm}^{n,*}]| \leq \mathrm{Tr}[S_{\pm}^n |C|^{\otimes n} S_{\pm}^{n,*}],$$

and the formula in the self-adjoint case with

$$\sum_{n=0}^{\infty} \mathrm{Tr}[S_{-}^n |C|^{\otimes n} S_{-}^{n,*}] \leq \exp(A) \quad (\text{fermions})$$

or

$$\sum_{n=0}^{\infty} \mathrm{Tr}[S_{+}^n |C|^{\otimes n} S_{+}^{n,*}] \leq \exp\left(\frac{A}{1-\varrho}\right) \quad (\text{bosons}),$$

ensures the uniform convergence of the series.

For any $C \in \mathcal{C}$, we know C and $\mathrm{Re} C = \frac{1}{2}(C + C^*)$ belong to $\mathcal{C}$ so that $C(s) = \mathrm{Re} C + is \mathrm{Im} C$ belongs to $\mathcal{C}$ when $s \in \omega_0 = (-\delta, \delta) + i(-\delta, \delta)$ and when $s \in \omega_1 = (1 - \delta, 1 + \delta) + i(-\delta, \delta)$ for $\delta > 0$ small enough. By the convexity of $\mathcal{C}$, we have $C(s) \in \mathcal{C}$ for all $s \in \omega = (-\delta, 1 + \delta) + i(-\delta, \delta)$. When $s \in i(-\delta, \delta)$, $C(s)$ is self-adjoint and the equality holds. The holomorphy of both sides with respect to $s \in \omega$ implies that the equality holds true for all $s \in \omega$, in particular when $s = 1$. $\square$

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