

Multiscale analysis and mean field asymptotics

Francis Nier, LAGA, Univ. Paris 13
Joint work with Z. Ammari and S. Breteaux

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Outline

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- Wick observables
- Reduced density matrices
- Multiscale measures
- Multiscale analysis of reduced density matrices
- Examples

Wick observables

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\mathcal{Z} complex separable Hilbert space.

$$\Gamma_{\pm}(\mathcal{Z}) = \bigoplus_{n \in \mathbb{N}} \mathcal{S}_{\pm}^n \mathcal{Z}^{\otimes n}$$
$$\mathcal{S}_{\pm}^n(f_1 \otimes \cdots \otimes f_n) = \frac{1}{n!} \sum_{\sigma \in \mathfrak{S}_n} s_{\pm}(\sigma) f_{\sigma(1)} \otimes \cdots \otimes f_{\sigma(n)}.$$

$s_+(\sigma) = +1$ (bosons) $s_-(\sigma) = \text{signature of } \sigma$ (fermions).

Definition

For $\tilde{b} \in \mathcal{L}(\mathcal{S}_{\pm}^p \mathcal{Z}^{\otimes p}; \mathcal{S}_{\pm}^q \mathcal{Z}^{\otimes q})$,

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

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Examples:

$$\blacksquare a_{\pm}(f) = (\langle f | : \mathcal{Z} \rightarrow \mathbb{C})^{Wick} ; a_{\pm}^*(f) = (|f\rangle : \mathbb{C} \rightarrow \mathcal{Z})^{Wick} ;$$

$$[a_{\pm}(f_1), a_{\pm}(f_2)]_{\pm} = [a_{\pm}^*(f_1), a_{\pm}^*(f_2)]_{\pm} = 0$$

$$[a_{\pm}(f_1), a_{\pm}^*(f_2)]_{\pm} = \varepsilon \langle f_1, f_2 \rangle .$$

$$\blacksquare A \in \mathcal{L}(\mathcal{Z}), d\Gamma_{\pm}(A) = A^{Wick} .$$

$$d\Gamma_{\pm}(A) = i \frac{d}{dt} \Gamma_{\pm}(-i\varepsilon t A) \quad \text{when } A = A^*$$

$$\mathbf{N}_{\pm} = (\text{Id}_{\mathcal{Z}})^{Wick} = d\Gamma(\text{Id}_{\mathcal{Z}}) \quad \mathbf{N}_{\pm}|_{S_{\pm}^n \mathcal{Z}^{\otimes n}} = \varepsilon n .$$

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Consequences:

- Mean field asymptotics $n \rightarrow \infty$ same as considering $\mathbf{N}_{\pm} = \mathcal{O}(1)$ and $\varepsilon \rightarrow 0$.
- In the bosonic setting, mean field asymptotics = infinite semiclassical analysis with small parameter " \hbar " = $\frac{\varepsilon}{2}$.

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Some properties when $p = q$, $\tilde{b} \in \mathcal{L}(S_{\pm}^p \mathcal{Z}^{\otimes p})$, $\tilde{b}_1 \in \mathcal{L}(\mathcal{Z})$.

- $(\tilde{b} = \tilde{b}^*) \Rightarrow (\tilde{b}^{Wick} \text{ symmetric})$
- $(\tilde{b} \geq 0) \Rightarrow (\tilde{b}^{Wick} \geq 0)$
- Number estimates, $m + m' \geq p$

$$\|(1 + \mathbf{N}_{\pm})^{-m} \tilde{b}^{Wick} (1 + \mathbf{N}_{\pm})^{-m'}\| \leq C_{m,m'} \|\tilde{b}\|$$

$$\|(1 + \mathbf{N}_{\pm})^{-m} [d\Gamma_{\pm}(\tilde{b}_1)^p - (\tilde{b}_1^{\otimes p})]^{Wick} (1 + \mathbf{N}_{\pm})^{-m'}\| \leq \varepsilon B_p \|\tilde{b}_1\|^p$$

- finite ε -expansion for composition formulas.

Reduced density matrices

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Non normalized reduced density matrices

Definition

Assume $\varrho_\varepsilon \in \mathcal{L}^1(\Gamma_\pm(\mathcal{Z}))$, $\text{Tr} [\varrho_\varepsilon] = 1$ and $\text{Tr} [\varrho_\varepsilon e^{c\mathbf{N}^\pm}] < +\infty$.

For $p \in \mathbb{N}$, $\gamma_\varepsilon^{(p)}$ is defined by

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

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Properties:

- In the bosonic case, if $\varrho_\varepsilon = |\varphi^{\otimes n}\rangle\langle\varphi^{\otimes n}|$, $\|\varphi\| = 1$,
 $\gamma_\varepsilon^{(p)} = 1_{[0:n]}(p) \varepsilon^p \frac{n!}{(n-p)!} |\varphi^{\otimes p}\rangle\langle\varphi^{\otimes p}|$.
- Symmetrization: $\gamma_\varepsilon^{(p)}$ is completely determined by the quantities
 $\text{Tr} [\varrho_\varepsilon (\tilde{b}_1^{\otimes p})^{\text{Wick}}]$, $\tilde{b}_1 \in \mathcal{L}(\mathcal{Z})$ (or $\tilde{b}_1 \in \mathcal{L}^\infty(\mathcal{Z})$).
- The sequence $(\gamma_\varepsilon^{(p)})_{p \in \mathbb{N}}$ is determined by the family of
generating functions $z \mapsto \text{Tr} [\varrho_\varepsilon \Gamma_\pm(e^{\varepsilon z \tilde{b}_1})]$, $|z| < \frac{c}{\|\tilde{b}_1\|}$.

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Asymptotics of $\gamma_\varepsilon^{(p)}$ as $\varepsilon \rightarrow 0$: Assume $\lim_{\varepsilon \rightarrow 0} \text{Tr} \left[\varrho_\varepsilon \mathbf{N}_\pm^{(p)} \right] = c_p$.

1) **Bosonic case:** Wigner measure = probability measure μ on \mathcal{Z} such that after extraction $\varepsilon \in \mathcal{E}$, $0 \in \overline{\mathcal{E}}$,

$$\forall f \in \mathcal{Z}, \quad \lim_{\substack{\varepsilon \rightarrow 0 \\ \varepsilon \in \mathcal{E}}} \text{Tr} \left[W(\sqrt{2\pi}f) \varrho_\varepsilon \right] = \int e^{2i\pi \text{Re}\langle f, z \rangle} d\mu(z).$$

Then the weak*-limit of $\gamma_\varepsilon^{(p)}$ is

$$\gamma_0^{(p)} = \int_{\mathcal{Z}} |z^{\otimes p}\rangle \langle z^{\otimes p}| d\mu(z).$$

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But $\text{Tr} [\gamma_0^{(p)}] = \int_{\mathcal{Z}} d\mu < c_p = \lim_{\varepsilon \rightarrow 0} \text{Tr} [\varrho_\varepsilon \mathbf{N}_+^p]$ may happen.

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But $\text{Tr} [\gamma_0^{(p)}] = \int_{\mathcal{Z}} d\mu < c_p = \lim_{\varepsilon \rightarrow 0} \text{Tr} [\varrho_\varepsilon \mathbf{N}_+^p]$ may happen.

Example: $\varrho_\varepsilon = |\varphi_\varepsilon^{\otimes n_\varepsilon}\rangle \langle \varphi_\varepsilon^{\otimes n_\varepsilon}|$ with $\|\varphi_\varepsilon\| = 1$, $\lim_{\varepsilon \rightarrow 0} \varepsilon n_\varepsilon = 1$,
 $w\text{-}\lim_{\varepsilon \rightarrow 0} \varphi_\varepsilon = 0$. Then $\mu = \delta_0$ while $\lim_{\varepsilon \rightarrow 0} \text{Tr} [\varrho_\varepsilon \mathbf{N}_+^p] = 1$.

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Asymptotics of $\gamma_\varepsilon^{(p)}$ as $\varepsilon \rightarrow 0$: Assume $\lim_{\varepsilon \rightarrow 0} \text{Tr} \left[\varrho_\varepsilon \mathbf{N}_\pm^{(p)} \right] = c_p$.

2) Fermionic case:

For any fixed $p \in \mathbb{N}$, the weak* limit of $\gamma_\varepsilon^{(p)}$ is always 0 while $\lim_{\varepsilon \rightarrow 0} \text{Tr} \left[\gamma_\varepsilon^{(p)} \right] = c_p$.

Multiscale measures

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$$\gamma_h \in \mathcal{L}^1(L^2(\mathbb{R}^d)),$$
$$x \in \mathbb{R}^D, X = (x, \xi) \in \mathbb{R}^{2D}, \text{ used with } D = pd \text{ when } \gamma_h = \gamma_{\varepsilon(h)}^{(p)}.$$

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Double scale class of symbols $a \in \mathcal{S}^{(2)}$: $a \in \mathcal{C}^\infty(\mathbb{R}^{2D} \times \mathbb{R}^{2D})$,

- $\exists C_a > 0, \forall Y \in \mathbb{R}^{2D}, a(\cdot, Y) \in \mathcal{C}_0^\infty(B(0, C_a))$.
- There exists $a_\infty \in \mathcal{C}^\infty(\mathbb{R}^{2D} \times \mathbb{S}^{2D-1})$ such that $a(X, R\omega) \xrightarrow{R \rightarrow \infty} a_\infty(X, \omega)$ in $\mathcal{C}^\infty(\mathbb{R}^{2D} \times \mathbb{S}^{2D-1})$.

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Quantization:

$$a^{(2),h} = a^{\text{Weyl}}(\sqrt{h}x, \sqrt{h}D_x, x, D_x) = [a(\cdot, h^{-1/2} \cdot)]^{\text{Weyl}}(\sqrt{h}x, \sqrt{h}D_x).$$

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Quantization:

$$a^{(2),h} = a^{Weyl}(\sqrt{h}x, \sqrt{h}D_x, x, D_x) = [a(\cdot, h^{-1/2} \cdot)]^{Weyl}(\sqrt{h}x, \sqrt{h}D_x).$$

Multiscale measures: Assume $\text{Tr} [\gamma_h] = 1$ there exists a subset \mathcal{E} , $0 \in \bar{\mathcal{E}}$, two non negative measures ν on \mathbb{R}^{2D} , ν_l on \mathbb{S}^{2D-1} and a trace class operator γ_0 such that

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

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Notations: Wigner measures $\nu \in \mathcal{M}(\gamma_h, h \in \mathcal{E})$.
Multiscale measures $(\nu, \nu_I, \gamma_0) \in \mathcal{M}^{(2)}(\gamma_h, h \in \mathcal{E})$.

Definition

The scaling $a^{Weyl}(\sqrt{h}x, \sqrt{h}D_x)$, $h \rightarrow 0$, is said adapted to the family $(\gamma_h)_{h \in \mathcal{E}}$, $\gamma_h \in \mathcal{L}^1(L^2(\mathbb{R}^D))$, $\gamma_h \geq 0$, if for some $\chi \in \mathcal{C}_0^\infty(\mathbb{R}^{2D})$, $0 \leq \chi \leq 1$, $\chi(0) = 1$,

$$\lim_{R \rightarrow \infty} \limsup_{\substack{h \rightarrow 0 \\ h \in \mathcal{E}}} \text{Tr} [(1 - \chi(R^{-1} \cdot))^{Weyl, h} \gamma_h] = 0.$$

After extraction one can assume $c = \lim_{h \rightarrow 0} \text{Tr} [\gamma_h]$ and if the scale is adapted all Wigner measures have the total mass c .

Definition

The scale $h \rightarrow 0$ is said separating if for all $(\nu, \nu_I, \gamma_0) \in \mathcal{M}^{(2)}(\gamma_h, h \in \mathcal{E})$, $\nu_I = 0$.

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When the scale is adapted, the separating property can be checked by a simple mass argument: After extraction assume that γ_0 is the weak* limit of γ_h and $\mathcal{M}(\gamma_h, h \in \mathcal{E}) = \{\nu\}$. Then the scale h is separating iff $\nu(\{0\}) = \text{Tr} [\gamma_0]$ and then $\mathcal{M}^{(2)}(\gamma_h, h \in \mathcal{E}) = \{(\nu, 0, \gamma_0)\}$.

Multiscale analysis of reduced density matrices

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We shall consider $\varepsilon = \varepsilon(h)$ with $\lim_{h \rightarrow 0} \varepsilon(h) = 0$ and $\varepsilon(h)$ -Wick quantization of h -dependent semiclassical observables, $\tilde{b} = a^{\text{Weyl}}(\sqrt{h}X, \sqrt{h}D_x)$, $a \in \mathcal{C}_0^\infty(\mathbb{R}^{2d})$ or $\tilde{b} = a^{(2)}$, when $a \in \mathcal{S}^{(2)}$.

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Assumptions: $\varrho_{\varepsilon(h)} \in \mathcal{L}^1(\Gamma_\pm(\mathcal{Z}))$, $\varrho_{\varepsilon(h)} \geq 0$.

- $\text{Tr} [\varrho_{\varepsilon(h)}] = 1$.
- $\text{Tr} [\varrho_{\varepsilon(h)} e^{c\mathbf{N}^\pm}] \leq C$.
- There exist $\chi \in \mathcal{C}_0^\infty(\mathbb{R}^{2D})$ and $0 < c' < c$, $0 \leq \chi \leq 1$, $\chi(0) = 1$, such that, with $\chi_\delta = \chi(\delta \cdot)$,

$$\lim_{\delta \rightarrow 0} \limsup_{h \rightarrow 0} \text{Tr} \left[\varrho_{\varepsilon(h)} (e^{c'\mathbf{N}^\pm} - e^{c'd\Gamma_\pm(\chi_\delta)^{W,h}}) \right] = 0.$$

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Proposition

The set \mathcal{E} can be chosen such that for all $p \in \mathbb{N}$,

$$\mathcal{M}(\gamma_{\varepsilon(h)}^{(p)}, h \in \mathcal{E}') = \{\nu^{(p)}\} \text{ with } \int_{\mathbb{R}^{2dp}} d\nu^{(p)} = \lim_{h \rightarrow 0} \text{Tr} \left[\gamma_h^{(p)} \right].$$

Moreover for any $a \in \mathcal{C}_0^\infty(\mathbb{R}^{2d})$, there exists $r_a > 0$ such that

$$\Phi_{a,h}(s) = \text{Tr} \left[\varrho_{\varepsilon(h)} e^{sd\Gamma \pm (a^{W,h})} \right] \text{ is uniformly bounded in } H^\infty(\{|s| < r_a\}) \text{ and}$$

$$\lim_{\substack{h \rightarrow 0 \\ h \in \mathcal{E}'}} \Phi_{a,h}(s) = \Phi_{a,0}(s) = \sum_{p=0}^{\infty} \frac{s^p}{p!} \int_{\mathbb{R}^{2dp}} a^{\otimes p}(X) d\nu^{(p)}(X).$$

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Proposition

For all $K \in \mathcal{L}^\infty(L^2(\mathbb{R}^d))$, there exists $r_K > 0$ such that $\Psi_{K,h}(s) = \text{Tr} [\varrho_{\varepsilon(h)} e^{sd\Gamma_\pm(K)}]$ is uniformly bounded in $H^\infty(\{|s| < r_K\})$. The pointwise convergence (or any weak convergence) of $\Psi_{K,h}$ to $\Psi_{K,0}$ for all $K \in \mathcal{L}^\infty(L^2(\mathbb{R}^d))$ is equivalent to $w^ - \lim_{h \rightarrow 0} \gamma_{\varepsilon(h)}^{(p)} = \gamma_0^{(p)}$ with*

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

The above convergence can always be achieved after some extraction $h \in \mathcal{E}'$, $0 \in \overline{\mathcal{E}'}$, $\mathcal{E}' \subset \mathcal{E}$.

Examples: Gibbs states

Multiscale
analysis and
mean field
asymptotics

Francis Nier,
LAGA, Univ.
Paris 13

Joint work with
Z. Ammari and
S. Breteaux

$\alpha(X) = |X|^2 = x^2 + \xi^2$ or $\alpha(X)$ like $|X|^2$ at infinity with a non degenerate minimum at $X = 0$.

$$H = \alpha^{Weyl}(\sqrt{h}X, \sqrt{h}D_x) - \lambda_0(\alpha^{Weyl}(\sqrt{h}X, \sqrt{h}D_x)),$$

$$\varepsilon = \varepsilon(h) = h^d, \quad \mu(\varepsilon) = -\frac{\varepsilon}{\beta\nu_C}, \nu_C, \beta > 0$$

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

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1) Fermionic case: For all $p \in \mathbb{N}$,

$\mathcal{M}^{(2)}(\gamma_{\varepsilon(h)}^{(p)}, h \in (0, h_0)) = \{\nu^{(p)}, 0, 0\}$ with

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

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2) **Bosonic case with Bose-Einstein condensation:** Assume $d \leq 2$.

Then for all $p \in \mathbb{N}$, $\mathcal{M}^{(2)}(\gamma_{\varepsilon(h)}^{(p)}, h \in (0, h_0)) = \{(\nu^{(p)}, 0, \gamma_0^{(p)})\}$ with

$$\gamma_0^{(p)} = p! n_C^p |\psi_0^{\otimes p}\rangle \langle \psi_0^{\otimes p}|, \quad \psi_0(x) = U_T \left[\frac{e^{-x^2/2}}{\pi^{d/4}} \right]$$

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

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