

Phase-space approach to the bosonic mean field dynamics: review, new developments

Francis Nier,
LAGA, Univ. Paris 13
Joint works with Z. Ammari
cont'd with
S. Breteaux, M. Falconi,
Q. Liard, B. Pawilowski,
M. Zerzeri

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- Semiclassical and mean field asymptotics
- Wigner (semiclassical) measures
- Wick quantization, (PI)-condition, BBGKY hierarchy
- Propagation results
- Order of convergence
- Other developments

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Wigner measures

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Wick calculus

Reconsider the old program: Bosonic QFT=infinite dimensional microlocal analysis (see e.g. Kree's seminar in the 70's).
Mean field=Semiclassical (easier).

Check the mean field convergence for dynamical problems with general initial data.

While doing so find assumptions and results which are invariant by the N -body and mean-field dynamics (when defined).

In the spirit of (semiclassical) propagation of singularities.

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Finite dimensional semiclassical asymptotics

For $w \in \mathcal{Z} = \mathbb{C}^d$ set $a(w) = \sum_j \bar{w}_j a_j$, $a^*(w) = \sum_j w_j a_j^*$,

$$[a(w), a^*(w')] = 2h \langle w, w' \rangle_{\mathcal{Z}} = \varepsilon \langle w, w' \rangle_{\mathcal{Z}} \quad , \quad \varepsilon = 2h$$

The Wick (resp. anti-Wick) quantization associates with the polynomial

$$b(z) = \sum_{\substack{|\beta| = p \\ |\alpha| = q}} b_{\alpha, \beta} \bar{z}^\alpha z^\beta = \langle z^{\otimes q}, \tilde{b} z^{\otimes p} \rangle \quad , \quad \tilde{b} = \frac{1}{q!p!} \partial_{\bar{z}}^q \partial_z^p b$$

the operator $b^{Wick} = \sum_{\alpha, \beta} b_{\alpha, \beta} a^{*\alpha} a^\beta$, (Wick)

Weyl operator $W(f)$:

$$\Phi(f) = \frac{a(f) + a^*(f)}{\sqrt{2}} = \sqrt{2} \operatorname{Re} \langle f, z \rangle^{Wick} \quad , \quad W(f) = e^{i\Phi(f)} .$$

Semiclassical annihilation-creation operators:

$$(PDE) \quad a_j = \hbar \partial_{\nu_j} + \nu_j \quad , \quad a_j^* = -\hbar \partial_{\nu_j} + \nu_j \quad , \quad \nu \in \mathbb{R}^d$$

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Example: $\mathbf{N} = (|z|^2)^{Wick} = \sum_j a_j^* a_j = \varepsilon \mathbf{N}_{\varepsilon=1}$, $\mathbf{N} \varphi_\alpha = \varepsilon |\alpha| \varphi_\alpha$ when φ_α is the α -th Hermite function $\alpha \in \mathbb{N}^d$, $|\alpha| = \sum_j \alpha_j$. $\mathbf{N} = \mathcal{O}(1) \leftrightarrow |\alpha| = \mathcal{O}(\frac{1}{\varepsilon})$.

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If $\hat{b}(\zeta) = \int_{\mathcal{Z}} b(z) e^{-2i\pi \operatorname{Re} \langle \zeta, z \rangle} dL_{\mathcal{Z}}(z)$ then $b(z) = \int_{\mathcal{Z}} \hat{b}(\zeta) e^{2i\pi \operatorname{Re} \langle \zeta, z \rangle} dL_{\mathcal{Z}}(\zeta)$

$$\text{and } b^{Weyl} = b^{Weyl}(\sqrt{h\nu}, \sqrt{h}D_{\nu}) = \int_{\mathcal{Z}} \hat{b}(\zeta) W(\sqrt{2\pi}\zeta) dL_{\mathcal{Z}}(\zeta) .$$

Bosonic mean field asymptotics

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Bosonic Fock space: Consider now the one particle (separable) complex Hilbert space $\mathcal{Z} = L^2(\mathbb{R}^D, dx; \mathbb{C})$.

$$\mathcal{H} = \Gamma_b(\mathcal{Z}) = \bigoplus_{n=0}^{\infty} \mathcal{S}_n \mathcal{Z}^{\otimes n} = \bigoplus_{n=0}^{\infty} \bigvee^n \mathcal{Z} \quad , \quad \bigvee^n \mathcal{Z} = L^2_{sym}((\mathbb{R}^D)^n; \mathbb{C})$$

Energy: $\mathcal{E}(z, \bar{z}) = \langle z, -\Delta z \rangle + \frac{1}{2} \iint_{\mathbb{R}^{2D}} V(x-y) |z(x)|^2 |z(y)|^2 dx dy$

Nonlinear Hamiltonian dynamics: $i \partial_t z = \partial_{\bar{z}} \mathcal{E}$

Wick quantized Hamiltonian : Take $a = \sqrt{\varepsilon} a_{\varepsilon=1}$ with $\varepsilon > 0$ and set

$$H_\varepsilon = \mathcal{E}(z)^{Wick} = \langle z, -\Delta z \rangle^{Wick} + \frac{1}{2} \langle z^{\otimes 2}, V(x-y) z^{\otimes 2} \rangle^{Wick}$$

n-body evolution: For $\Psi_0 \in L^2_{sym}((\mathbb{R}^D)^n; \mathbb{C}) = \bigvee^n \mathcal{Z}$

$\Psi(t) = e^{-i \frac{t}{\varepsilon} H_\varepsilon} \Psi_0 = \Psi(x_1, \dots, x_n, t)$ solves

Formally "mean field limit" = "semiclassical limit" with $\varepsilon = \frac{1}{n}$

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$$\mathcal{S}_n(f_1 \otimes \cdots \otimes f_n) = \frac{1}{n!} \sum_{\sigma \in \mathfrak{S}_n} f_{\sigma(1)} \otimes \cdots \otimes f_{\sigma(n)}.$$

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Formally "mean field limit" = "semiclassical limit" with $\varepsilon = \frac{1}{n}$

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Hartree (NLS) equation: $i\partial_t z = -\Delta z + (V * |z|^2)z$

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$$H_\varepsilon = \underbrace{\int_{\mathbb{R}^D} \nabla a^*(x) \nabla a(x) dx}_{d\Gamma(-\Delta)} + \frac{1}{2} \int_{\mathbb{R}^{2D}} V(x-y) a^*(x) a^*(y) a(x) a(y) dx dy .$$

$$d\Gamma(A) = \varepsilon d\Gamma_{\varepsilon=1}(A) \quad , \quad d\Gamma(\text{Id}) = \mathbf{N} = \varepsilon \mathbf{N}_{\varepsilon=1} .$$

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Definition of infinite dimensional Wigner measures

Remember: \mathcal{Z} is a separable complex Hilbert space (1 part. space)

$$\begin{aligned}\mathcal{H} &= \Gamma_b(\mathcal{Z}) = \bigoplus_{n=0}^{\infty} \bigvee^n \mathcal{Z} \quad , \quad \mathbf{N}_{\mathcal{Z}}^{\otimes n} = \varepsilon n z^{\otimes n} \text{ ,} \\ a(f) z^{\otimes n} &= \sqrt{\varepsilon n} \langle f, z \rangle z^{\otimes n-1} \quad , \quad a^*(f) z^{\otimes n} = \sqrt{\varepsilon(n+1)} \mathcal{S}_{n+1}[f \otimes z^{\otimes n}] \text{ ,} \\ \Phi(f) &= \frac{a(f) + a^*(f)}{\sqrt{2}} \quad , \quad W(f) = e^{i\Phi(f)} \text{ .}\end{aligned}$$

Consider a normal state in \mathcal{H} , $\varrho_\varepsilon \in \mathcal{L}^1(\mathcal{H})$, $\varrho_\varepsilon \geq 0$, $\text{Tr} [\varrho_\varepsilon] = 1$.

Definition

For $\hat{E} \in (0, +\infty)$, $0 \in \overline{\hat{E}}$, and a family $(\varrho_\varepsilon)_{\varepsilon \in \hat{E}}$ of normal states in \mathcal{H} , $\mathcal{M}(\varrho_\varepsilon, \varepsilon \in \hat{E})$ is the set of Borel probability measures μ on \mathcal{Z} for which there exists $\hat{E}' \subset \hat{E}$ such that

$$\begin{aligned}0 &\in \overline{\hat{E}'} \text{ ,} \\ \forall f \in \mathcal{Z} \text{ ,} \quad \lim_{\varepsilon \rightarrow 0, \varepsilon \in \hat{E}'} \text{Tr} \left[\varrho_\varepsilon W(\sqrt{2\pi}f) \right] &= \int_{\mathcal{Z}} e^{2i\pi \text{Re} \langle f, z \rangle} d\mu(z)\end{aligned}$$

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Example: $\varrho_\varepsilon = |\Psi_\varepsilon\rangle\langle\Psi_\varepsilon|$, $\Psi_\varepsilon \in \mathcal{H}$,

Mean field coherent state $\Psi_\varepsilon = E(f) = W(\frac{\sqrt{2}}{i\varepsilon}f)|\Omega\rangle$

Mean field Hermite (atomic coherent) state: $\Psi_\varepsilon = \varphi^{\otimes n}$ with $\varepsilon = \frac{1}{n}$.

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Wigner measures: Existence

Phase-space approach to the bosonic mean field dynamics: review, new developments

Francis Nier, LAGA, Univ. Paris 13
Joint works with Z. Ammari cont'd with S. Breteaux, M. Falconi, Q. Liard, B. Pawilowski, M. Zerzeri

Semiclassical and mean field asymptotics

Wigner measures

Wick calculus

Th. (Ammari-N. AHP 08)

If there exists $\delta > 0$ and $C_\delta > 0$ s.t.

$$\forall \varepsilon \in \hat{E}, \quad \text{Tr} \left[\varrho_\varepsilon \langle \mathbf{N} \rangle^\delta \right] \leq C_\delta \quad (2.1)$$

then $\mathcal{M}(\varrho_\varepsilon, \varepsilon \in \hat{E}) \neq \emptyset$ and every $\mu \in \mathcal{M}(\varrho_\varepsilon, \varepsilon \in \hat{E})$ satisfies

$$\int_{\mathcal{Z}} (1 + |z|^2)^\delta d\mu(z) \leq C_\delta.$$

Definition

$b \in \mathcal{S}_{\text{cyl}}(\mathcal{Z})$ if there exist a finite rank orth. proj. p and $a \in \mathcal{S}(p\mathcal{Z})$ s.t. $b = a \circ p$.

Corollary

Under the condition (2.1) with $\mathcal{M}(\varrho_\varepsilon, \varepsilon \in \hat{E}) = \{\mu\}$,

$$\forall b \in \mathcal{S}_{\text{cyl}}(\mathcal{Z}), \quad \lim_{\varepsilon \rightarrow 0, \varepsilon \in \hat{E}} \text{Tr} \left[\varrho_\varepsilon b^{\text{Weyl}} \right] = \int_{\mathcal{Z}} b(z) d\mu(z).$$

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Main ideas of the proof:

1 Separation of variables:

$$\begin{array}{llll}
\mathcal{Z} & = & \mathcal{Z}_1 & \overset{\perp}{\oplus} & \mathcal{Z}_2 \\
\mathcal{H} & = & \mathcal{H}_1 & \otimes & \mathcal{H}_2, & \mathcal{H}_* = \Gamma_b(\mathcal{Z}_*) \\
W(f_1 \oplus f_2) & = & W(f_1) & \otimes & W(f_2) & = W(f_1) \otimes \text{Id}_{\mathcal{H}_2} \quad \text{if } f_2 = 0.
\end{array}$$

2 \mathcal{Z} is separable \rightarrow Borel σ -set and diagonal extraction.

3 Condition (2.1) is a tightness condition (see Prokhorov criterion)

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Remark: After a subsequence extraction we can assume $\mathcal{M}(\varrho_\varepsilon, \varepsilon \in \hat{E}) = \{\mu\}$.

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Wigner measures: Examples

Corollary

Assume $\mathcal{M}(\varrho_\varepsilon, \varepsilon \in \hat{E}) = \{\mu\}$ and

$$\forall k \in \mathbb{N}, \exists C_k > 0, \forall \varepsilon \in \hat{E}, \operatorname{Tr} [\varrho_\varepsilon \mathbf{N}^k] \leq C_k,$$

then for any cylindrical polynomial and with $Q = \text{Weyl, Wick or anti-Wick}$

$$\lim_{\varepsilon \rightarrow 0, \varepsilon \in \hat{E}} \operatorname{Tr} [\varrho_\varepsilon b^Q] = \int_{\mathcal{Z}} b(z) d\mu(z).$$

Examples

Coherent states: $f \in \mathcal{Z}, |f|_{\mathcal{Z}} = 1, E(f) = W(\frac{\sqrt{2}}{i\varepsilon} f)|\Omega\rangle = e^{\frac{a^*(f) - a(f)}{\varepsilon}} |\Omega\rangle,$
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Wigner measures: Examples

Corollary

Assume $\mathcal{M}(\varrho_\varepsilon, \varepsilon \in \hat{E}) = \{\mu\}$ and

$$\forall k \in \mathbb{N}, \exists C_k > 0, \forall \varepsilon \in \hat{E}, \operatorname{Tr} [\varrho_\varepsilon \mathbf{N}^k] \leq C_k,$$

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Definition

Fixed degrees: we say that $b(z) = \langle z^{\otimes q}, \tilde{b}z^{\otimes p} \rangle$ belongs to $\mathcal{P}_{p,q}(\mathcal{Z})$, if

$$\tilde{b} = \frac{1}{q!} \frac{1}{p!} \partial_z^q \partial_z^p b \in \mathcal{L}\left(\bigvee^p \mathcal{Z}; \bigvee^q \mathcal{Z}\right),$$

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Wick calculus, (PI)-condition, reduced density matrices

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Proposition

Assume $\mathcal{M}(\varrho_\varepsilon, \varepsilon \in \hat{E}) = \{\mu\}$ and

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then $\lim_{\varepsilon \rightarrow 0, \varepsilon \in E} \text{Tr} [\varrho_\varepsilon b^{Wick}] = \int_{\mathcal{Z}} b(z) d\mu(z)$ for all $b \in \mathcal{P}^\infty(\mathcal{Z})$.

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A counter-example with \tilde{b} not compact: Take $\varepsilon = \frac{1}{n}$, $\hat{E} = \{\frac{1}{n}, n \in \mathbb{N}^*\}$ and consider a normalized sequence $(f_n)_{n \in \mathbb{N}^*}$ converging weakly to 0. Then

$$\mathcal{M}(\varrho_\varepsilon^C(f_n), \varepsilon \in \hat{E}) = \{\delta_0\},$$

$$\text{Tr} \left[\varrho_\varepsilon^C(f_n) (|z|^{2p})^{Wick} \right] = |f_n|^{2p} = 1 \neq 0 = \int_{\mathcal{Z}} |z|^{2p} \delta_0(z).$$

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Wick calculus, (PI) condition, reduced density matrices

Phase-space approach to the bosonic mean field dynamics: review, new developments

Francis Nier,
LAGA,
Univ.

Paris 13
Joint works with
Z. Ammari
cont'd
with

S. Breteaux,
M. Falconi,
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B. Pawilowski,
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Semiclassical and mean field asymptotics

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Remember $(|z|^{2p})^{Wick} = (\langle z^{\otimes p}, \text{Id } z^{\otimes p} \rangle)^{Wick} = \mathbf{N}(\mathbf{N} - \varepsilon) \cdots (\mathbf{N} - \varepsilon(p - 1)) \sim \mathbf{N}^p$

Theorem Ammari-N. (JMPA 11)

Assume $\mathcal{M}(\varrho_\varepsilon, \varepsilon \in \hat{E}) = \{\mu\}$, with

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with (assuming $\mu \neq \delta_0$)

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Remark: When $\varrho_\varepsilon \in \mathcal{L}^1(L_{sym}^2((\mathbb{R}^D)^n))$, $\varepsilon = \frac{1}{n}$,

$$\gamma_\varepsilon^p(x_1, \dots, x_p; y_1, \dots, y_p) = \int_{(\mathbb{R}^D)^{N-p}} \varrho_\varepsilon(x_1, \dots, x_p, X; y_1, \dots, y_p, X) dX$$

Mean field propagation of Wigner measures

Problem: After composition with a nonlinear flow, cylindrical (resp. polynomial symbols) do not remain cylindrical (resp. polynomials).

Take $\mathcal{E}(z) = \langle z, Az \rangle + Q(z)$ with A self-adjoint and $Q \in \mathcal{P}(\mathcal{Z})$ and set $H_\varepsilon = \mathcal{E}^{Wick}$ while Φ is the hamiltonian flow associated with \mathcal{E} .

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Assume $\mathcal{M}(\varrho_\varepsilon, \varepsilon \in \hat{E}) = \{\mu\}$ and the condition (PI), then

$$\mathcal{M}(e^{-i\frac{t}{\varepsilon}H_\varepsilon} \varrho_\varepsilon e^{i\frac{t}{\varepsilon}H_\varepsilon}, \varepsilon \in \hat{E}) = \{\Phi(t)_*\mu\}$$

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Theorem Ammari-N. (Ann. della Sc. Norm. Pisa 15)

With $A = -\Delta$ and $V(x) = \frac{\alpha}{|x|}$, $x \in \mathbb{R}^3$, $\alpha \in \mathbb{R}$.

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Method: Truncated Dyson expansion after (Fröhlich-Graffi-Schwarz 07 and Fröhlich-Knowles-Schwarz 09) combined with a priori information on $\mu(t)$.

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Method: Measure transportation adapted from Ambrosio-Gigli-Savaré (book 05).

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Some compactness is needed either on the interaction or on the initial data. In the 3D-Coulombic case, we used the compactness of $(1 - \Delta)^{-1/2} \frac{1}{|x|} (1 - \Delta)^{-1/2}$.

Propagation: Improvement by Q. Liard

In our last work with Z. Ammari for singular interactions, the assumptions on the interaction potential were

$$V(-x) = V(x) \quad V(1 - \Delta)^{-1/2} \in \mathcal{L}(L^2) \quad (1 - \Delta)^{-1/2} V(1 - \Delta)^{-1/2} \text{ compact.}$$

While the usual assumptions for $-\Delta + V(x)$ are expressed in term of $V(1 - \Delta)^{-1}$.

With a similar strategy but significant new ideas Q. Liard is able to treat one particle hamiltonians $H_0 = -\Delta + U(x)$ with assumptions on the interaction potential $V(x)$ similar to the one for the KLMN perturbative theorem for $H_0 + V$.

Significant difference: Infinite dimensional method of characteristics.

Z. Ammari, N.: Quadratic Wasserstein distance

$$W^p(\mu_1, \mu_2) = \inf_{\pi_j \mu = \mu_j} \int \int |x - y|^p d\mu(x, y), \text{ quadratic means } p = 2.$$

Q. Liard: Use of $W^1(\mu_1, \mu_2)$, inspired by finite dimensional results of Maniglia.

Tightness for families of probability measures on phase-space (tightness \rightarrow weak compactness) less obvious (coercivity replaced by Dunford-Pettis type arguments).

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Order of convergence and numerics

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Ammari-Falconi-Pawilowski: Assume $\|\gamma_\varepsilon^{(p)} - \gamma_0^{(p)}\|_{\mathcal{L}^1} = C(\varepsilon)C^p$ for all $p \in \mathbb{N}$ with

$$\gamma_0^{(p)} = \frac{\int_{\mathcal{Z}} |z^{\otimes p}\rangle \langle z^{\otimes p}| d\mu_0(z)}{\int_{\mathcal{Z}} |z|^{2p} d\mu_0(z)} \quad \text{with } C(\varepsilon) \geq C^{-1}\varepsilon$$

then $\|\gamma_\varepsilon^{(p)}(t) - \gamma_0^{(p)}(t)\|_{\mathcal{L}^1} = C_T C^p C(\varepsilon)$ for all $p \in \mathbb{N}$ and all $t \in [-T, T]$.

Example of numerical results obtained by B. Pawilowski:

- $\mathcal{Z} = \ell^2(\mathbb{Z}/K\mathbb{Z}) \sim \mathbb{C}^K$, H_0 periodic discrete Laplacian.
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- Heavy accurate computation of the quantum N -body problem $N \leq 20$

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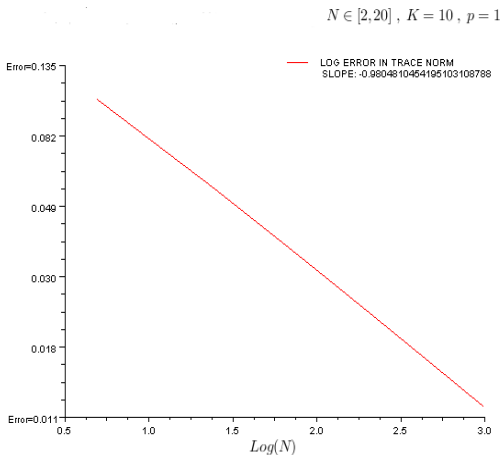
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Order of convergence for $\sup_{t \in [0, T]} \|\gamma_\varepsilon^{(p)}(t) - \gamma_0^{(p)}(t)\|_{\mathcal{L}^1}$, here $p = 1$

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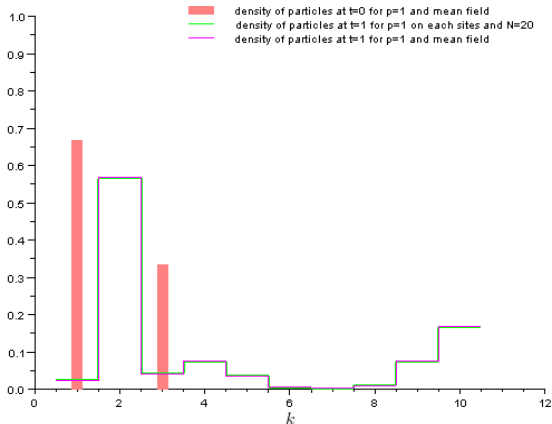
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Particle density: red=mean field $t = 0$,
green and purple = 20-body and mean field $t = 1$

Semiclassical analysis is easier than microlocal analysis: It is possible to reconsider classical problems of bosonic quantum field theory by introducing scales and a semiclassical parameters.

- Z. Ammari, M. Zerzeri: $P(\Phi)_2$ and Hoegh-Krohn model.
- Z. Ammari, M. Falconi: Nelson model.

Work in progress with Z. Ammari and S. Breteaux: Use of multiscale (2nd microlocalized see e.g. C. Fermanian) semiclassical analysis for a more accurate description of all the $\gamma_\varepsilon^{(p)}$.
Observable looking like $\langle z^{\otimes p}, [K + a^{W,h}]z^{\otimes p} \rangle^{Wick}$ with K compact $\varepsilon = \varepsilon(h)$, $h \rightarrow 0$, $\varepsilon(h) \rightarrow 0$.

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Motivations:

- Mixture of BEC and non condensate phase
- Approach valid for the bosonic and fermionic case
- Another way of refining the mean field analysis, as compared with Bogoliubov 2nd order approximation.
- Possibly combine Ammari-N. propagation result (quantum part) with the recent result by Golse-Paul (macroscopic part).
- Double scales appear in random homogenization problems (see Breteaux' PhD).

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Thank you for your attention !