Mean field limit of quantum dynamics for general bosonic states.
In collaboration with F. Nier

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Many body system

- Schrödinger Hamiltonian:

$$H_N = -\sum_{i=1}^{N} \frac{\hbar^2}{2m} \Delta_{x_i} + \varepsilon(N) \sum_{1 \leq i < j \leq N} V(x_i - x_j)$$

$(x_1, \cdots, x_N) \in \mathbb{R}^{3N}$ and H_N is an operator on $L^2_s(\mathbb{R}^{3N})$.

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- Time-dependent Schrödinger equation:

$$\begin{cases} i\hbar\partial_t \psi^N = H_N \psi^N \\ \psi^N_{|t=0} = \psi^N_0 . \end{cases} \tag{1}$$

(1) admits a unique solution for any $\psi^N_0 \in L^2_s(\mathbb{R}^{3N})$.

Energy per particle

$\hbar = 2m = 1$

- Let $\psi_0^N = \varphi_0^{\otimes N} \in L^2_s(\mathbb{R}^{3N}), \varphi_0 \in H^1(\mathbb{R}^3)$, $||\varphi_0||_{L^2(\mathbb{R}^3)} = 1$.

$$\begin{aligned}\frac{\langle \psi^N, H_N \psi^N \rangle}{N} &= \int_{\mathbb{R}^3} |\nabla \varphi_0|^2(x)\, dx \\ &+ \varepsilon(N) \frac{N-1}{2} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} V(x-y) |\varphi_0(x)|^2 \, |\varphi_0(y)|^2 \, dx\, dy\end{aligned}$$

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- Hartree Equation:

$$\begin{cases} i\partial_t \varphi = -\Delta \varphi + V * |\varphi|^2 \varphi & \text{on } \mathbb{R}_t \times \mathbb{R}^3_x \\ \varphi_{|t=0} = \varphi_0 \,. \end{cases} \tag{2}$$

A standard result

Theorem

Let $A : L^2_s(\mathbb{R}^{3k}) \to L^2_s(\mathbb{R}^{3k})$ bounded. Then for any $t \in \mathbb{R}$

$$\lim_{N\to\infty} \langle \psi_t^N, A \otimes 1^{N-k} \psi_t^N \rangle = \langle \varphi_t^{\otimes k}, A \varphi_t^{\otimes k} \rangle$$

where ψ_t^N is a solution of (1) with $\psi_0^N = \varphi_0^{\otimes N}$ and φ_t is a solution of (2).

Some references:
- Spohn (1980), Bardos-Golse-Mauser (2000), Erdös-Yau (2001), Erdös-Schlein-Yau... [BBGKY hierarchy, chaos states, BEC]

- Hepp (1974), Ginibre-Velo (1987) [Second quantization, coherent states]

- Fröhlich-Graffi-Schwarz (2007), Fröhlich-Knoles-Pizzo (2007)

- Pickl (2009), Knowles-Pickl (2010), Rodnianski-Schlein (2007),...

- The classical limit of the one particle Schrödinger equation

$$i\varepsilon\frac{\partial\psi}{\partial t} = P(\varepsilon)\psi \quad \text{with} \quad P(\varepsilon) = -\frac{\varepsilon^2}{2}\Delta_x + V(x)$$

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- Egorov's theorem:

$$e^{it/\varepsilon P(\varepsilon)} a^w(x,\varepsilon D_x) e^{-it/\varepsilon P(\varepsilon)} = (a \circ \Phi_t)^w(x,\varepsilon D_x) + \mathcal{O}(\varepsilon)$$

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- Or semi-classical measures (Wigner):
For any bounded sequence (ψ_ε) in $L^2(\mathbb{R}^d)$, there exists a subsequence $\psi_{\varepsilon_j}, \varepsilon_j \to 0$ and a Radon measure μ on $\mathbb{R}^d \times \mathbb{R}^d$ such that

$$\lim_{j\to\infty} \langle \psi_{\varepsilon_j}, a^w(x, \varepsilon_j D_x)\psi_{\varepsilon_j}\rangle = \int_{\mathbb{R}^d\times\mathbb{R}^d} a(x,\xi)\, d\mu\,.$$

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- Propagation of those measures:

$$\lim_{j\to\infty}\langle e^{-it/\varepsilon_j P(\varepsilon_j)}\psi_{\varepsilon_j}, a^w(x,\varepsilon_j D_x)e^{-it/\varepsilon_j P(\varepsilon_j)}\psi_{\varepsilon_j}\rangle = \int_{\mathbb{R}^d\times\mathbb{R}^d} a\circ\Phi_t(x,\xi)d\mu\,.$$

- 1-Schrödinger representation: The quantization of the canonical variables $(x,\xi) \in \mathbb{R}^d \times \mathbb{R}^d$ are $q_j = x_j, p_j = -i\partial_{x_j}$ acting on $L^2(\mathbb{R}^d, dx)$, and satisfying

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- Symbol-operator association:

$$x_j^\alpha \xi_j^\beta \longrightarrow ((q_j^\alpha p_j^\beta)) \text{ symmetric product}$$

Weyl quantization

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- Creation-annihilation operators :
$$a_j^* = \frac{1}{\sqrt{2}}(q_j - ip_j) \quad \text{et } a_j = \frac{1}{\sqrt{2}}(q_j + ip_j).$$
  The vacuum: $h_0(x) = \frac{1}{\pi^{d/4}} \mathrm{e}^{-|x|^2/2}$; where $a_j h_0 = 0$.
- We have: $L^2(\mathbb{R}^d, dx) = \oplus_{n=0}^\infty \mathrm{Vect}\{a_\alpha^* h_0, |\alpha| = n\}$, où $a_\alpha^* = a_1^{*\,\alpha_1} \cdots a_d^{*\,\alpha_d}$.

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- Correspondence: Let $\{e_j\}$ a basis of $\mathbb{C}^d$,

$$a_\alpha^* h_0 \leftrightarrow e_1^{\alpha_1} \otimes_s \cdots \otimes_s e_d^{\alpha_d} \in \otimes_s^{|\alpha|} \mathbb{C}^d. \tag{3}$$

$L^2(\mathbb{R}^d, dx) \simeq \oplus_{n=0}^{\infty} \otimes_s^n \mathbb{C}^d$ (Symmetric Fock space).

2- Fock representation: Let $\mathcal{Z}$ be a separable Hilbert . The symmetric Fock space over $\mathcal{Z}$ is

$$\mathcal{H} = \oplus_{n=0}^{\infty} \otimes_s^n \mathcal{Z} \,.$$

where $\otimes_s^n \mathcal{Z}$ is the symmetric tensor of n copy of $\mathcal{Z}$.
Annihilation operator:

$$a(f) f_1 \otimes_s \cdots \otimes_s f_n = \sqrt{\varepsilon n}\; \frac{1}{n!} \sum_{\sigma \in \mathfrak{S}_n} \langle f, f_{\sigma_1} \rangle \, f_{\sigma_2} \otimes \cdots \otimes f_{\sigma_n} \,,$$

Creation operator:

$$a^*(f) f_1 \otimes_s \cdots \otimes_s f_n = \sqrt{\varepsilon(n+1)}\; f \otimes_s f_1 \cdots \otimes_s f_n .$$

$$[a(f), a^*(g)] = \varepsilon \langle f, g \rangle I .$$

Wick operators:

$$b^{Wick}_{|\otimes_s^N \mathcal{Z}} = \frac{\sqrt{(N-p+q)!N!}}{(N-p)!} \, \varepsilon^{\frac{p+q}{2}} \; b \otimes_s 1^{N-p}$$

where $b : \otimes_s^p \mathcal{Z} \to \otimes_s^q \mathcal{Z}$ is a bounded operator. For instance, the number operator is $\hat{N} = (I)^{Wick}$ with $I : \mathcal{Z} \to \mathcal{Z}$ is the identity.

Correspondence

Fock representation	Schrödinger representation $\mathbb{R}^d$
$a(z)$	$a(z) = \sum_j \overline{z_j} \frac{\sqrt{\varepsilon}(\partial_{x_j} + x_j)}{\sqrt{2}}$
$a^*(z)$	$a^*(z) = \sum_j z_j \frac{\sqrt{\varepsilon}(-\partial_{x_j} + x_j)}{\sqrt{2}}$
$\Phi(z) = \frac{1}{\sqrt{2}}(a(z) + a^*(z))$	$Re(z)\sqrt{\varepsilon}x + Im(z)\sqrt{\varepsilon}D_x$
$W(z) = e^{i\Phi(z)}$	$\tau_{(-\sqrt{\varepsilon}Im(z),\sqrt{\varepsilon}Re(z))}$
$W(\frac{\sqrt{2}}{i\varepsilon}z)\Omega$	$\tau_{(\sqrt{\frac{2}{\varepsilon}}Re(z),\sqrt{\frac{2}{\varepsilon}}Im(z))}(\frac{1}{\pi^{d/4}}e^{-\frac{x^2}{2}})$
$z^{\otimes n}, \lvert z\rvert = 1$	$\varepsilon/2$ − *Hermite functions.*

The mean field problem

- We consider a Wick operator

$$H_\varepsilon = (A)^{Wick} + \sum_{j=2}^{r} Q_j^{Wick}$$

where $Q_j : \otimes_s^j \mathcal{Z} \to \otimes_s^j \mathcal{Z}$ bounded and $A : D(A) \subset \mathcal{Z} \to \mathcal{Z}$ a self-adjoint operator.

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- If $\mathcal{Z} = L^2(\mathbb{R}^3)$, $r = 2$, $A = -\Delta$ and $Q_2 = V(x-y)$, then

$$\varepsilon^{-1} H_{\varepsilon}{}_{|L_s^2(\mathbb{R}^{3N})} = H_N \text{ with } \varepsilon = \frac{1}{N}.$$

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- The problem of convergence of the quantum dynamics in the mean field scaling can be stated as

$$\lim_{\varepsilon \to 0} \mathrm{Tr}\left[\rho_\varepsilon \; e^{i\frac{t}{\varepsilon}H_\varepsilon} \; \mathcal{O}_\varepsilon \; e^{-i\frac{t}{\varepsilon}H_\varepsilon}\right] = ?$$

where $\mathcal{O}_\varepsilon$ is a scaled observable (Wick, Weyl, Anti-Wick,...) on $\mathcal{H}$ and ρ_ε is a family of density operators.

projective observable

We define Weyl and Anti-Wick quantized operators as projective observables on the symmetric Fock space $\mathcal{H} = \oplus_{n=0}^{\infty} \otimes_s^n \mathcal{Z}$.
We denote by $\mathbb{P}$ the set of all orthogonal projection of finite rank on $\mathcal{Z}$. Let $p \in \mathbb{P}$,

Weyl quantized operator:

$$\mathcal{F}[f](z) = \int_{p\mathcal{Z}} f(\xi) \;\; e^{-2\pi i \,\mathrm{Re}\langle z,\xi\rangle} \; L_p(d\xi),$$

$$b^{Weyl} = \int_{p\mathcal{Z}} \mathcal{F}[b](z) \;\; W(\sqrt{2}\pi z) \; L_p(dz)\,.$$

A-Wick quantized operator:

$$b^{A-Wick} = \int_{p\mathcal{Z}} \mathcal{F}[b](\xi) \;\; W(\sqrt{2}\pi \xi) \;\; e^{-\frac{\varepsilon\pi^2}{2}|\xi|^2_{p\mathcal{Z}}} \; L_p(d\xi)\,.$$

Wick symbolic calculus

For $b_1 \in \mathcal{P}_{p_1,q_1}(\mathcal{Z})$, $b_2 \in \mathcal{P}_{p_2,q_2}(\mathcal{Z})$, $k \in \mathbb{N}$ we have $\partial_z^k b_1(z) \in \mathcal{L}(\bigvee^k \mathcal{Z};\mathbb{C})$ and $\partial_{\bar z}^k b_2(z) \in \bigvee^k \mathcal{Z}$. We define the Poisson multiple brackets:

$$\{b_1, b_2\}^{(k)} = \partial_z^k b_1.\partial_{\bar z}^k b_2 - \partial_z^k b_2.\partial_{\bar z}^k b_1, \quad k \in \mathbb{N},$$
$$\{b_1, b_2\} = \{b_1, b_2\}^{(1)}.$$

Proposition

Let $b_1 \in \mathcal{P}_{p_1,q_1}(\mathcal{Z})$ et $b_2 \in \mathcal{P}_{p_2,q_2}(\mathcal{Z})$.
Then for any $k \in \{0,\dots,\min\{p_1,q_2\}\}$, $\partial_z^k b_1.\partial_{\bar z}^k b_2 \in \mathcal{P}_{p_2-k,q_1-k}(\mathcal{Z})$. Moreover

$$(i) \qquad b_1^{Wick} \circ b_2^{Wick} = \left(\sum_{k=0}^{\min\{p_1,q_2\}} \frac{\varepsilon^k}{k!} \partial_z^k b_1.\partial_{\bar z}^k b_2\right)^{Wick},$$

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

Theorem

Consider a sequence of density operators $(\varrho_{\varepsilon_n})_{n\in\mathbb{N}}$ *with* $\lim_n \varepsilon_n = 0$ *satisfying for some* $\delta > 0$, $\mathrm{Tr}\left[\varrho_{\varepsilon_n}\hat{N}^\delta\right] \leq C_\delta < \infty$ *for any* $n \in \mathbb{N}$.
Then there exist a subsequence $(\varepsilon_n)_{n\in\mathbb{N}}$ *and a Borel probability measure over* $\mathcal{Z}$, *such that*

$$\lim_{n\to\infty} \mathrm{Tr}\left[\varrho_{\varepsilon_n}\, b^{Weyl}\right] = \int_{\mathcal{Z}} b(z)\; d\mu(z)$$

for any $b \in \mathcal{C}_0^\infty(p\mathcal{Z})$, $p \in \mathbb{P}$. *Moreover*

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

Proof:
1-Bochner theorem: characteristic function of a probability distribution iff positive definite + continuity over all finite dimensional subspaces.
2-Prokhorov criterion: a probability distribution μ on separable Hilbert space $\mathcal{Z}$ is a Borel probability measure iff $\forall\eta > 0$, $\exists R_\eta > 0$ such that

$$\forall p \in \mathbb{P}, \quad \mu\left(\{z \in \mathcal{Z},\; |pz| \leq R_\eta\}\right) \geq 1 - \eta\,.$$

.

Corollaire

Let μ a Wigner measure associated to the sequence of density operators $(\varrho_{\varepsilon_n})_{n\in\mathbb{N}}$. Then for any $b \in C_0^\infty(p\mathcal{Z})$, $p \in \mathbb{P}$

$$\lim_{n\to\infty} \mathrm{Tr}\left[\varrho_{\varepsilon_n}\, b^{A-Wick}\right] = \int_{\mathcal{Z}} b(z)\, d\mu(z)$$

Proposition

Let μ *be a Wigner associated to the sequence of density operators* $(\varrho_{\varepsilon_n})_{n\in\mathbb{N}}$ *satisfying for any* $s \in \mathbb{N}$, $\mathrm{Tr}[\hat{N}^s \varrho_{\varepsilon_n}] < \infty$. *Then, for any* $b \in \mathcal{L}(\otimes_s^k \mathcal{Z}, \otimes_s^m \mathcal{Z})$ *compact*

$$\lim_{n\to\infty} \mathrm{Tr}\left[\varrho_{\varepsilon_n}\, b^{Wick}\right] = \int_{\mathcal{Z}} \langle z^{\otimes m}, b z^{\otimes k}\rangle \, d\mu(z)\,.$$

Proposition

Let μ be a Wigner associated to the sequence of density operators $(\varrho_{\varepsilon_n})_{n\in\mathbb{N}}$ satisfying for any $s\in\mathbb{N}$, $\mathrm{Tr}[\hat{N}^s\varrho_{\varepsilon_n}]<\infty$. Then, for any $b\in\mathcal{L}(\otimes_s^k\mathcal{Z},\otimes_s^m\mathcal{Z})$ compact

$$\lim_{n\to\infty}\mathrm{Tr}\left[\varrho_{\varepsilon_n}\,b^{Wick}\right]=\int_{\mathcal{Z}}\langle z^{\otimes m},bz^{\otimes k}\rangle\;d\mu(z)\,.$$

<u>Counter-example</u>: Let

$$\Psi_\varepsilon=e^{1/\varepsilon[a^*(\varphi_\varepsilon)-a(\varphi_\varepsilon)]}\Omega_0$$

be a family of coherent states such that $\varphi_\varepsilon\rightharpoonup 0$, $|\varphi_\varepsilon|=1$. Then the Wigner measure associated to $|\Psi_\varepsilon\rangle\langle\Psi_\varepsilon|$ is the Dirac measure δ_0 however

$$\lim_{\varepsilon\to 0}\langle\Psi_\varepsilon,b^{Wick}\Psi_\varepsilon\rangle\neq\int_{\mathcal{Z}}\langle z^{\otimes m},bz^{\otimes k}\rangle\;d\delta_0(z)\,.$$

Theorem

Let $(\varrho_\varepsilon)_{\varepsilon\in(0,\bar\varepsilon)}$ *be a sequence of density operators with a unique Wigner measure* μ_0 *such that*

$$\forall\alpha\in\mathbb{N},\quad \lim_{\varepsilon\to0}\mathrm{Tr}[\varrho_\varepsilon\hat N^\alpha]=\int_{\mathcal{Z}}|z|^{2\alpha}\,d\mu_0(z)<+\infty\,. \tag{4}$$

Then for any $t\in\mathbb{R}$, *the family* $(\varrho_\varepsilon(t)=e^{-i\frac{t}{\varepsilon}H_\varepsilon}\varrho_\varepsilon e^{i\frac{t}{\varepsilon}H_\varepsilon})_{\varepsilon\in(0,\bar\varepsilon)}$ *admits a unique Wigner measure* $\mu_t=(\mathbf{F}_t)_*\mu_0$, *which is the initial measure* μ_0 *pushed forward by the flow of the Hartree equation (2)). Moreover, for any* $b\in\mathcal{L}(\otimes_s^k\mathcal{Z},\otimes_s^m\mathcal{Z})$

$$\lim_{\varepsilon\to0}\mathrm{Tr}\left[\varrho_\varepsilon(t)b^{Wick}\right]=\int_{\mathcal{Z}}\langle z^{\otimes m},bz^{\otimes k}\rangle\,d\mu_t(z)=\int_{\mathcal{Z}}b(z_t)\,d\mu_0(z)\,.$$

Proof: 1- Approximation by states ϱ_ε^R asymptotically localized on a ball of radius $R>0$.
2- Existence of Wigner measures μ_t^R for all times associated to $e^{-i\frac{t}{\varepsilon}H_\varepsilon}\varrho_\varepsilon^R e^{i\frac{t}{\varepsilon}H_\varepsilon}$.
3- Passing from Weyl observables to Wick observables in the construction of Wigner measures.
4- Polynomial approximation of the classical Hartree flow.
5- Identification of the measures μ_t as the push-forwarded measures $\mathbf{F}_{t*}\mu_0$.

Corollaire

We consider $(\rho_{\varepsilon_n})_{n\in\mathbb{N}}$ *as above. Then for any* $b \in C_0^\infty(p\mathcal{Z}), p \in \mathbb{P}$, *we have*

$$\lim_{\varepsilon_n \to 0} \mathrm{Tr}[\rho_{\varepsilon_n} \; e^{i\frac{t}{\varepsilon_n}H_{\varepsilon_n}} \; b^{A-Wick} \; e^{-i\frac{t}{\varepsilon_n}H_{\varepsilon_n}}] = \int_{\mathcal{Z}} b(z_t) \; d\mu \,, \tag{5}$$

for all $t \in \mathbb{R}$, *with* z_t *solving the Hartree equation* (2).

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for all $t \in \mathbb{R}$, *with* z_t *solving the Hartree equation* (2).

Remark: Let (ρ_{ε_n}) as before and μ_t the Wigner measure associated with he sequence $e^{-it/\varepsilon H_\varepsilon}\rho_{\varepsilon_n}e^{it/\varepsilon H_\varepsilon}$. Then the map $t \in \mathbb{R} \mapsto \mu_t$ solves the following transport equation:

$$\mu_t(b) = \mu_t^0(b) + i\int_0^t \mu_s(\{Q, b_{t-s}\})\, ds\,, \tag{6}$$

for any $b : \otimes_s^m \mathcal{Z} \to \otimes_s^k \mathcal{Z}$. Here $\mu_t^0(B) = \mu(e^{-itA}B)$, for any Borel set B .

- For a density operator $\varrho_N \in \mathcal{L}^1(\bigvee^N \mathcal{Z})$ with $\mathcal{Z} = L^2(\mathbb{R}^3)$, we define the reduced density matrices:

$$\gamma_N^{(p)}(x,y) = \int_{\mathbb{R}^{6(N_\varepsilon - p)}} \varrho_N(x,X,y,X)\; dX\,, \quad p \leq N\,,$$

Let $\gamma_N^{(p)}(t)$ be the reduced density matrices associated to

$$\varrho_N(t) = e^{-itH_N} \varrho_N e^{itH_N}\,.$$

Corollaire

The convergence of the BBGKY hierarchy

$$\lim_{N\to\infty} \gamma_N^{(p)}(t) = \frac{1}{\int_{\mathcal{Z}} |z|^{2p}\; d\mu_t(z)} \int_{\mathcal{Z}} |z^{\otimes p}\rangle\langle z^{\otimes p}|\; d\mu_t(z) =: \gamma_\infty^{(p)}(t)\,,$$

holds in the trace norm for all $p \in \mathbb{N}$. *Here* $\mu_t = (\mathbf{F}_t)_*\mu_0$ *and* μ_0 *is the Wigner measure associated with* ϱ_N.

The Hartree-Von Neumann limit

Let ϱ_0 be a density operator on $L^2(\mathbb{R}^d)$ and $\varrho^{\otimes N} = \varrho \otimes \cdots \otimes \varrho$. The von Neumann equation for a N particle system is given by

$$\begin{cases} i\partial_t \varrho_N(t) & = & [\mathbb{H}_N, \varrho_N(t)] \\ \varrho_N(0) & = & \varrho_0^{\otimes N}, \end{cases} \tag{7}$$

with $\varrho_N(t)$ trace class operator on $L^2(\mathbb{R}^{dN})$ and $\mathbb{H}_N$ is the Hamiltonian of the N particles system (without specific statistics)

$$\mathbb{H}_N = -\sum_{i=1}^{N} \Delta_{x_i} + \frac{1}{N}\sum_{i\neq j} V(x_i - x_j)\,,$$

where $V \in L^\infty(\mathbb{R}^d)$ real. Using the propagation of Wigner measures, we prove

$$\lim_{N\to\infty} \mathrm{Tr}\left[\varrho_N(t)(B \otimes I_{L^2(\mathbb{R}^{d(N-k)})})\right] = \mathrm{Tr}[\varrho(t)^{\otimes k} B] \tag{8}$$

for any $t \in \mathbb{R}$ with $\varrho(t)$ a solution of the Hartree-von Neumann equation

$$\begin{cases} i\partial_t \varrho(t) & = & [-\Delta + (V * n_{\varrho(t)}), \varrho(t)] \\ \varrho(0) & = & \varrho_0\,, \end{cases} \tag{9}$$

where $n_\varrho(x,t) := \varrho(x;x,t)$ is the charge density.