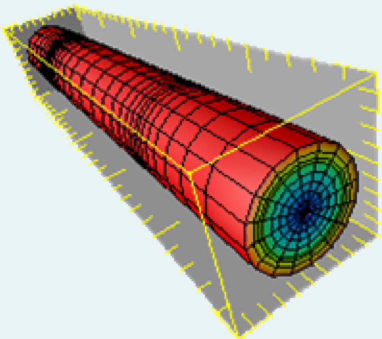

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QUANTUM HYDRODYNAMICS: MODELING AND ASYMPTOTICS

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HIERARCHY of QUANTUM SEMICONDUCTOR MODELS

- Quantum Dynamics
  - *Many Particle Schrödinger Equation*
  - *Heisenberg Equation*
  - *Schrödinger Equation*
- Quantum Kinetics
  - *Quantum Liouville Equation*
  - *Quantum Vlasov Equation*
  - *Quantum Boltzmann Equation*
- Quantum Hydrodynamics
  - *Quantum Hydrodynamic Equations*
  - *Energy-Transport Equations*
  - *Quantum Drift-Diffusion Equations*

THE QUANTUM KINETIC MODEL

The linear Wigner equation provides a kinetic description of the evolution of a quantum system, under the effect of an external potential $V = V(x), \quad x \in \mathbb{R}^d$

$$\frac{\partial w}{\partial t} + v \cdot \nabla_x w - \Theta[V]w = 0$$

Here the (real-valued) potential V enters through the pseudo-differential operator defined by

$$(\Theta[V]w)(x,v,t) = \frac{i}{(2\pi)^{d/2}} \int_{\mathbb{R}^d} \delta V(x,\eta) \mathcal{F}w(x,\eta,t) e^{iv\cdot\eta}\, d\eta$$

where

$$\delta V(x,\eta) := \frac{1}{\hbar}\left[V\left(x + \frac{\hbar\eta}{2m}\right) - V\left(x - \frac{\hbar\eta}{2m}\right)\right]$$

DERIVATION OF QUANTUM HYDRODYNAMIC EQUATIONS

FIRST STEP

Introduce dissipative interactions

SECOND STEP

Derive evolution equations with unknown the following moments of the Wigner functions

$$n(x,t) \quad := \quad \int_{R_v^d} w(x,v,t)\,dv$$

Particle density

$$nu(x,t) \quad := \quad \int_{R_v^d} v\,w(x,v,t)\,dv$$

Current density

$$e(x,t) \quad := \quad \int_{R_v^d} \frac{1}{2} m|v|^2\,w(x,v,t)\,dv$$

Energy density

For the derivation of a fluid-dynamical model, the conservative dynamics of the isolated quantum system has to be broken, by taking into account dissipative interactions.

REVERSIBILE EVOLUTION OF QUANTUM SYSTEM

Quantum-physically consistent description of a quantum model

Von Neumann equation

density matrix operators

Wigner transform

Kinetic version

Wigner equation

IRREVERSIBILE EVOLUTION OF QUANTUM SYSTEM

Von Neumann equation with dissipative term in Lindblad form →

Wigner transform

Modified Wigner equation

For the derivation of a fluid-dynamical model, the conservative dynamics of the isolated quantum system has to be broken, by taken into account dissipative interactions.

REVERSIBILE EVOLUTION OF QUANTUM SYSTEM

Quantum-physically consistent description of a quantum model

Von Neumann equation

density matrix operators

Wigner transform

Kinetic version

Wigner equation

IRREVERSIBILE EVOLUTION OF QUANTUM SYSTEM

Von Neumann equation (Fokker-Planck)

Von Neumann-BGK equation

Wigner transform

Wigner-Fokker-Planck eq.

Wigner-BGK equation

Let us modify the Wigner equation by adding a collisional term which mimics the dissipative interaction of the quantum system with the environment.
The simpler model is a BGK relaxation-time operator, which say that after a time $1/\nu$ *the system will relax to a state* w_{eq}

$$\frac{\partial w}{\partial t} + v \cdot \nabla_x w - \Theta[V]w \;=\; -\nu(w - w_{\mathrm{eq}})$$

We shall describe the thermodynamical equilibrium state by

$$w_{\mathrm{eq}}(x,v,t) = n(x,t)\left(\frac{\beta m}{2\pi}\right)^{d/2} e^{-\beta m v^2/2}$$
$$\times\left\{1 + \hbar^2\frac{\beta^2}{24}\left[-\frac{1}{m}\Delta V(x) + \beta\sum_{r,s=1}^{d} v_r v_s \frac{\partial^2 V(x)}{\partial x_r x_s}\right] + O(\hbar^4)\right\}$$

This is obtained by inserting in the Wigner thermodinamical equilibrium (1932) the two parameters $n = n(x,t), \quad T = T(x,t)$ *(the reciprocal of* β *) and then by assuming*

$$\int w_{\mathrm{eq}}(x,v,t)\,dv \;=\; \int w(x,v,t)\,dv \;=:\; n[w](x,t) \equiv n(x,t)\,.$$

This corresponds to say that the equilibrium determined by the collisions depends on time both through the density n and through the temperature T.

The external potential coexists with the collisions.Thus the relaxation-time state is determined by considering the joint actions of collisions and of external field.

The subject of next section is the individuation of the state that annihilates jointly both effects. The corresponding distribution function shall be adopted to close our system.

THE SCALED EQUATION

Let $\varepsilon = l / x_0$ *be the Knudsen number. We consider the case in which the external potential and the interactions are dominant in the evolution.*

$$\epsilon \frac{\partial w}{\partial t} + \epsilon v \cdot \nabla_x w - \Theta[V]\, w \;=\; -\nu \left(w - w_{\mathrm{eq}} \right)$$

We rewrite the right-hand side as

$$\Omega w(x,v) = \nu\, n[w](x) \left[F(v) + \hbar^2 F^{(2)}(x,v) \right]$$

where

$F(v)$ is the classical Maxwellian $\left(\frac{\beta m}{2\pi}\right)^{d/2} e^{-\beta m v^2/2}$

$F^{(2)}$ is the $O(\hbar^2)-$ term

$$F^{(2)}[V](x,v) = \frac{\beta^2}{24} \left[-\frac{1}{m} \Delta V + \beta \sum_{r,s=1}^{d} v_r v_s \frac{\partial^2 V}{\partial x_r x_s} \right] F(v)$$

The solution of the problem with $\varepsilon = 0$ is the distribution function at relaxation -time

$$\theta[V]w + Qw = 0$$

Proposition

If V is sufficiently smooth, for a fixed $x \in \mathbb{R}^d$, in a suitable Hilbert space (see later), there exists a unique solution M with

$$\int M(x,v,t)\,dv = \int w(x,v,t)$$

given by

$$M(x,v,t) = \nu n(x,t)\mathcal{F}^{-1}\left(\frac{\mathcal{F}(F + \hbar^2 F^{(2)})}{\nu - i\delta V(x,\eta)}\right)(x,v)$$

We use the relaxation-time distribution function M to close the system of the moments.

Let us compute the moments of the function M

M is not the equilibrium state

$$\int v M(x,v)\,dv = -n\frac{\nabla V}{\nu\, m}$$

$$\int v\otimes m v M(x,v)\,dv = n\frac{\mathcal{I}}{\beta} + 2mn\frac{\nabla V}{\nu\, m}\otimes\frac{\nabla V}{\nu\, m} + \frac{\beta\hbar^2}{12m} n\nabla\otimes\nabla V$$

$$\int \frac{1}{2} m|v|^2 M(x,v)\,dv = n\frac{d}{2\beta} + mn\frac{|\nabla V|^2}{\nu^2 m^2} + \frac{\beta\hbar^2}{24m} n\Delta V$$

$$\int m v|v|^2 M(x,v)\,dv = \frac{\hbar^2}{4}\Delta\frac{\nabla V}{\nu\, n} + \frac{\nabla V}{\nu\, m}\int v\otimes m v M\,dv + \frac{\nabla V}{\nu\, m}\int \frac{1}{2} m|v|^2 M\,dv \quad (4.7)$$

DERIVATION OF THE HIGH-FIELD QHD SYSTEM

We multiply the scaled equation by $1, \quad mv, \quad \frac{1}{2}m|v|^2$, *we integrate in* dv , *we use the properties of the operator* $\theta[V]+Q$, *obtaining*

$$
\begin{aligned}
\partial_t n + \nabla_x \cdot (nu) &= 0\,, \\
\partial_t (mnu) + \nabla_x \cdot \int mv \otimes vw\, dv &= 0\,, \\
\partial_t e + \nabla_x \cdot \int \frac{1}{2} mv|v|^2 w\, dv &= 0\,.
\end{aligned}
$$

the velocity momentum can be expressed in terms of the deviation from the relaxation-time velocity (fluid velocity at relaxation-time)

DERIVATION OF THE HIGH-FIELD QHD SYSTEM

We multiply the scaled equation by $1, \quad mv, \quad \frac{1}{2}m|v|^2$*, we integrate in* dv *, we use the properties of the operator* $\theta[V]+Q$ *, obtaining*

$$\partial_t n + \nabla_x \cdot (nu) = 0\,,$$
$$\partial_t (mnu) + \nabla_x \cdot \int mv \otimes vw\, dv = 0\,,$$
$$\partial_t e + \nabla_x \cdot \int \frac{1}{2} mv|v|^2 w\, dv = 0\,.$$

$$\mathrm{P} = \int m(v-u) \otimes (v-u)dv$$

This can be expressed in terms of the pressure tensor $\mathcal{P}$

$$\int mv \otimes vw = mnu \otimes u - \mathcal{P}\,,$$
$$e := \int \frac{1}{2} m|v|^2 w\, dv = \frac{1}{2} mn|u|^2 - \frac{1}{2}\mathrm{tr}\mathcal{P}$$

DERIVATION OF THE HIGH-FIELD QHD SYSTEM

We multiply the scaled equation by $1, \quad mv, \quad \frac{1}{2}m|v|^2$*, we integrate in* dv *, we use the properties of the operator* $\theta[V]+Q$ *, obtaining*

$$\begin{aligned} \partial_t n + \nabla_x \cdot (nu) &= 0\,, \\ \partial_t (mnu) + \nabla_x \cdot \int mv \otimes vw\, dv &= 0\,, \\ \partial_t e + \nabla_x \cdot \int \frac{1}{2} mv|v|^2 w\, dv &= 0\,. \end{aligned}$$

We use the relaxation-time distribution function M to close the system

$$\int \frac{1}{2} mv|v|^2 w\, dv = q + (e\mathcal{I} - \mathcal{P})u\,.$$

Summarising

diagonal part:
classical temperature

Pressure tensor

$$\mathcal{P} = -n\frac{\mathcal{I}}{\beta} - \frac{n}{\nu^2\, m}\nabla V \otimes \nabla V - \frac{\beta\hbar^2}{12m} n\nabla \otimes \nabla V$$

Heat flux

$$q \;=\; \frac{\hbar^2}{8m} n\Delta\frac{\nabla V}{\nu\, m} - n\frac{\nabla V}{\nu^3 m^2}\nabla V \otimes \nabla V\,.$$

Summarising

due to the strong field

Pressure tensor

$$\mathcal{P} = -n\frac{\mathcal{I}}{\beta} - \frac{n}{\nu^2\, m}\nabla V \otimes \nabla V - \frac{\beta\hbar^2}{12m} n \nabla \otimes \nabla V$$

Heat flux

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Summarising

Pressure tensor

$$\mathcal{P} = -n\frac{\mathcal{I}}{\beta} - \frac{n}{\nu^2\, m}\nabla V \otimes \nabla V - \frac{\beta\hbar^2}{12m} n\nabla \otimes \nabla V$$

quantum correction part of second order in ħ

Heat flux

$$q \;=\; \frac{\hbar^2}{8m} n\Delta\frac{\nabla V}{\nu\, m} - n\frac{\nabla V}{\nu^3 m^2}\nabla V \otimes \nabla V\,.$$

QUANTUM HYDRODINAMIC SYSTEM with strong field

$$\begin{aligned} \frac{\partial n}{\partial t} + \nabla_x \cdot (nu) &= 0\,, \\ \frac{\partial (mnu)}{\partial t} + \nabla_x \cdot mnu \otimes u - \nabla_x \cdot \mathcal{P} &= 0\,, \\ \frac{\partial e}{\partial t} + \nabla_x \cdot (eu) - \nabla_x \cdot (\mathcal{P} u) + \nabla_x \cdot q &= 0\,. \end{aligned}$$

Pressure tensor

Heat flux

Introducing the temperature, taking the trace of the first pressure tensor term

$$\frac{\partial (nT)}{\partial t} + \nabla_x \cdot (nTu) + \frac{2}{3} nT \nabla_x \cdot u + \frac{2}{3} \nabla_x \cdot q = 0\,.$$

The second part of my talk will be devoted to the

RIGOROUS DERIVATION of the QUANTUM DRIFT-DIFFUSION EQUATION in presence of a STRONG FIELD

We consider the Wigner-BGK equation in the scaled form

$$\epsilon \frac{\partial w}{\partial t} + \epsilon v \cdot \nabla_x w - \Theta[V]\, w \;=\; -\nu \left(w - w_{\mathrm{eq}} \right)$$

- *We derive the quantum drift-diffusion using the compressed Chapman-Enskog method*
- *We prove that the QDD solution approximates the solution to the Wigner-BGK equation up to the second order in* ε

THE PROBLEM IN ABSTRACT FORM

Let X_k be the space $L^2(\mathbb{R}^{2d}, (1+|v|^{2k})dx\,dv; \mathbb{R})$ and X_k^v the Hilbert space $L^2(\mathbb{R}^d, (1+|v|^{2k})dv; \mathbb{R})$

$$\begin{cases} \epsilon \dfrac{dw}{dt} = \epsilon\, Sw + Aw + Cw, \\ \lim_{t\to 0^+} \|w(t) - w_0\|_{X_k} = 0 \end{cases}$$

with

- streaming operator $Su := -v \cdot \nabla_x$,
- field operator $Aw := \Theta[V]w,$
- collision operator $Cw := -(\nu\, w - \Omega\, w)$,

where the collision operator Ω is defined by

$$\Omega w(x,v) = \nu n[w](x) \left[F(v) + \hbar^2 F^{(2)}(x,v) \right]$$

where $F^{(2)}$ is the $O(\hbar^2)$ correction.

We shall apply the compressed Chapman-Enskog procedure, as proposed by J.Mika and J.Banasiak (1995).

Accordingly, it is necessary to study the problem with $\varepsilon = 0$, i.e. the equation $(\mathcal{A}+\mathcal{C})f = 0$ in the space X_k^v for any fixed

Proposition

If V is sufficiently smooth, for a fixed $x \in \mathbb{R}^d$

$$\ker(\mathcal{A}+\mathcal{C}) = \{cM(v), c \in \mathbb{R}\} \subset X_k^v$$

The previous *M* differs by the factor *n*

with

$$M(x,v) := \nu \mathcal{F}^{-1}\left\{ \frac{\mathcal{F}F(\eta)}{\nu - i\delta V(x,\eta)} \left(1 - \frac{\beta\hbar^2}{24m^2} \sum_{r,s=1}^{d} \eta_r \eta_s \frac{\partial^2 V(x)}{\partial x_r x_s} \right) \right\}(x,v)$$

Moreover, for all $h \in X_k^v$, $(\mathcal{A}+\mathcal{C})u = h$ has a solution if and only if

$$\int_{\mathbb{R}^d} h(v)\, dv = 0 .$$

FORMAL EXPANSION

We decompose the space X_k as follows

$$X_k = (X_k)_M \oplus (X_k)^0$$

where $(X_k)_M$ is the eigenspace spanned by $M(x,v)$ and

$$(X_k)^0 = \left\{ f \in X_k \,\middle|\, \int f(v)dv = 0 \right\}$$

We define the corresponding spectral projections

$$\mathcal{P}f = M \int f(v)dv$$

$$\mathcal{Q} = \mathcal{I} - \mathcal{P}.$$

We decompose the function w as $w = \mathcal{P}w + \mathcal{Q}w.$

$$w = \mathcal{P}w + \mathcal{Q}w.$$

φ is called the hydrodynamic part

ψ is called the kinetic part of w.

Our strategy is

to find the evolution equations for the hydrodynamic and kinetic parts

to expand the kinetic part in series of $\mathcal{E}$

to correct the solution of the hydrodynamic equation up to the first order

Operating formally on both sides of the evolution equation for the function w with the projections $\mathcal{P}$ and Q, we obtain the following system of equations

$$\begin{cases} \dfrac{\partial \varphi}{\partial t} = \mathcal{PSP}\varphi + \mathcal{PSQ}\psi \\ \dfrac{\partial \psi}{\partial t} = \mathcal{QSP}\varphi + \mathcal{QSQ}\psi + \dfrac{1}{\epsilon}\mathcal{Q}(\mathcal{A}+\mathcal{C})\mathcal{Q}\psi \end{cases}$$

with initial conditions

$$\begin{cases} \varphi(0) = \varphi_0 = \mathcal{P}f_0 \\ \psi(0) = \psi_0 = \mathcal{Q}f_0. \end{cases}$$

Applying the compressed asymptotic expansion, we split the solutions φ and ψ into the sums of the

"bulk" parts $\bar{\varphi}$ and $\bar{\psi}$

and the "initial-layer" parts $\tilde{\varphi}$ and $\tilde{\psi}$

which take account of the rapid changes of w for small times.

$\bar{\varphi}$ is left unexpanded

$$\varphi(t) = \bar{\varphi}(t) + \tilde{\varphi}\left(\frac{t}{\epsilon}\right)$$

$$\psi(t) = \bar{\psi}(t) + \tilde{\psi}\left(\frac{t}{\epsilon}\right)$$

$\tilde{\varphi}$, $\bar{\psi}$, $\tilde{\psi}$ are expanded in series of ε

The expansion up to the second order gives

$$\begin{cases} \dfrac{\partial \bar{\varphi}}{\partial t} = \mathcal{PSP}\bar{\varphi} + \mathcal{PSQ}\bar{\psi}_0 + \epsilon \mathcal{PSQ}\bar{\psi}_1 \\ 0 = \mathcal{Q}(\mathcal{A}+\mathcal{C})\mathcal{Q}\bar{\psi}_0 \\ 0 = \mathcal{QSP}\bar{\varphi} + \mathcal{Q}(\mathcal{A}+\mathcal{C})\mathcal{Q}\bar{\psi}_1 \end{cases}$$

Thus, concerning the kinetic parts

$$\bar{\psi}_0 \equiv 0$$

$$\bar{\psi}_1 = -(\mathcal{Q}(\mathcal{A}+\mathcal{C})\mathcal{Q})^{-1}\mathcal{QSP}\bar{\varphi}\,,$$

and inserting in the first equation, we get

$$\frac{\partial \bar{\varphi}}{\partial t} = \mathcal{PSP}\bar{\varphi} - \epsilon \mathcal{PSQ}(\mathcal{Q}(\mathcal{A}+\mathcal{C})\mathcal{Q})^{-1}\mathcal{QSP}\bar{\varphi}$$

The unexpanded function $\bar{\varphi}(x,v,t)$ can be written as the product

$$\bar{\varphi}(x,v,t) = n(x,t)\, M(x,v)$$

particle density

solution of the problem with $\varepsilon = 0$

$$(\mathcal{A} + \mathcal{C})f = 0$$

The "diffusion-like" equation takes the form

$$\frac{\partial n}{\partial t} = -\nabla_x \left(n \int vM\,dv \right) + \epsilon \nabla_x \cdot \left[\left(\int v \otimes D_2\, dv \right) \cdot \nabla_x n + n \int v D_1\, dv \right]$$

with the initial condition truncated at first order in ε

$$n(x,0) = n_0(x) + \epsilon n_1(x)$$

The "diffusion-like" equation takes the form

$$\frac{\partial n}{\partial t} = -\nabla_x \left(n \int v M dv \right) + \epsilon \nabla_x \cdot \left[\left(\int v \otimes D_2 dv \right) \cdot \nabla_x n + n \int v D_1 dv \right]$$

with the initial condition truncated at first order in ε

$$n(x,0) = n_0(x) + \epsilon \int v \cdot \nabla_x D_3(x,v) dv$$

where

$D_1(x,v)$ and $D_2(x,v) \equiv (D_2)_i(x,v)$

and

$D_3 = D_3(x,v)$

are solutions of auxiliary problems,
related to the invertibility of the operator $\mathcal{Q}(\mathcal{A}+\mathcal{C})\mathcal{Q}$

We can prove that all terms of the bulk part of the expansion are well-defined.

$$J = J^{(0)} + \epsilon J^{(1)} := n \int vM\,dv + \epsilon \int v\bar{\psi}_1\,dv$$

Lemma. The first term in $J^{(1)}$ is D$\cdot \nabla_x$n where the tensor D is given by

$$\mathsf{D} = \frac{1}{\nu}\left(\frac{\mathcal{I}}{\beta m} + \frac{1}{\nu^2 m^2}\nabla V \otimes \nabla V + \frac{\beta\hbar^2}{12 m^2}(\nabla \otimes \nabla)\,V\right) + O(\hbar^4)\,.$$

Lemma. The second term in $J^{(1)}$ is given by n times $\int v D_1(x,v)\,dv =$

$$= \frac{1}{\nu}\left(\frac{2}{\nu^2 m^2}(\nabla \otimes \nabla)\,V\,\nabla V + \frac{1}{\nu^2 m^2}\Delta V \nabla V + \frac{\beta\hbar^2}{12 m^2}\nabla_x \cdot (\nabla \otimes \nabla)\,V\right) + O(\hbar^4)\,.$$

Correction from the kinetic part

THE HIGH-FIELD QUANTUM DRIFT-DIFFUSION EQUATION

$$\frac{\partial n}{\partial t} - \frac{1}{\nu m}\nabla\cdot(n\nabla V) - \frac{\epsilon}{\nu\beta m}\nabla\cdot\nabla n$$

$$- \frac{\epsilon}{\nu^3 m^2}\left[\nabla\cdot(n(\nabla\otimes\nabla)V\nabla V) + \nabla\cdot\nabla\cdot(n\nabla V\otimes\nabla V)\right]$$

$$- \frac{\epsilon\beta\hbar^2}{12\nu m^2}\nabla\cdot\nabla\cdot(n\nabla\otimes\nabla V) = 0$$

THE HIGH-FIELD QUANTUM DRIFT-DIFFUSION EQUATION

$$\frac{\partial n}{\partial t} - \frac{1}{\nu m}\nabla\cdot(n\nabla V) - \frac{\epsilon}{\nu\beta m}\nabla\cdot\nabla n$$

$$- \frac{\epsilon}{\nu^3 m^2}\left[\nabla\cdot(n(\nabla\otimes\nabla)V\nabla V) + \nabla\cdot\nabla\cdot(n\nabla V\otimes\nabla V)\right]$$

$$- \frac{\epsilon\beta\hbar^2}{12\nu m^2}\nabla\cdot\nabla\cdot(n\nabla\otimes\nabla V) = 0$$

Classical pressure tensor

High-field pressure tensor

Quantum pressure tensor

The second line

$$-\quad\frac{\epsilon}{\nu^3 m^2}\left[\nabla\cdot\left(n(\nabla\otimes\nabla)V\nabla V\right)+\nabla\cdot\nabla\cdot\left(n\nabla V\otimes\nabla V\right)\right]$$

is peculiar of the strong-field assumption and it is a correction of order ε and consists of the additional terms

$$\frac{1}{\nu}\frac{\nabla V\otimes\nabla V}{\nu^2 m^2}$$

→ in the pressure tensor

$$\frac{1}{\nu}\left(\frac{\nabla\otimes\nabla)V\nabla V}{\nu^2 m^2}\right)$$

→ in the drift term

It can be written also as (Poupaud, Runaway paper 1992)

$$-\frac{\epsilon}{\nu^3 m^2}\nabla\cdot\left(\nabla V\otimes\nabla V\nabla n+n\left(2\nabla\otimes\nabla V\nabla V+\Delta V\nabla V\right)\right)$$

RIGOROUS RESULTS

The rigorous asymptotic analysis can be found in Frosali-Manzini (2006) (submitted)

- *Existence and regularity of the initial layer functions*
- *Strong differentiability of the first order correction to bulk function*
- *Well-posedness and regularity of the QDD with a given external potential V*
- *Estimates of the evolution semigroups*
- *Estimate of error*

The main result consists in proving that the asymptotic expansion up to the first order gives an approximations of order ε^2 to the quantum Wigner equation.

$$\|\varphi(t) + \psi(t) - [\bar{\varphi}(t) + \epsilon\tilde{\varphi}_1(\tau)] - [\epsilon\bar{\psi}_1(t) + \tilde{\psi}_0(\tau) + \epsilon\tilde{\psi}_1(\tau)\|_{X_k} \leq C\epsilon^2$$

Thanks for your attention !!!!!

Under the approximation $-\beta\nabla V = \nabla \log n$ the second order term

$$-\frac{\epsilon\beta\hbar^2}{12\nu m^2}\nabla\cdot\nabla\cdot(n\nabla\otimes\nabla V) = 0$$

becomes

Quantum pressure term

$$-\frac{\varepsilon\hbar^2}{6\nu m^2} n\nabla\left(\frac{\Delta\sqrt{n}}{\sqrt{n}}\right)$$

Bohm potential

$$-\frac{\varepsilon\hbar^2}{12\nu m^2} n(\nabla\otimes\nabla)\log n$$

Nondiagonal pressure tensor

LINDBLAD FORM

Open quantum system: model evolution of small quantum system S coupled to large reservoir R:
S = electrons - R = phonon bath (environment)

Postulates:
- *R stays in thermodynamic equilibrium*
- *Open system S described by density matrix formulation*
- *S: Markovian dynamics (completely positive quantum dynamical semigroup (QDS)*

STRUCTURE of QDS-GENERATORS (Lindblad 1976)

The bounded QDS-generator G(t) (in terms of the Hamiltonian and the Lindblad operators) is in Lindblad form when the dual map G(t)* is completely positive, i.e. G(t)* tensor-times the unit matrix is positivity preserving

E. Wigner , Phys. Rev. 40, 749 (1932)

Following Wigner 1932, the quantum correction of the classical equilibrium distribution function on the phase space is

$$w_{\mathrm{W}}(x,v) := \left(\frac{m}{2\pi\hbar}\right)^{d} e^{-\beta E}$$

$$\times \left\{1 + \hbar^2 \frac{\beta^2}{24}\left[-\frac{3}{m}\Delta V(x) + \frac{\beta}{m}|\nabla V|^2(x) + \beta \sum_{r,s=1}^{d} v_r v_s \frac{\partial^2 V(x)}{\partial x_r \partial x_s}\right] + O(\hbar^4)\right\}$$

where $E = \frac{1}{2}mv^2 + V(x)$ Is the total energy of the system