Quantum fluid-dynamical models
for semiconductors in high-field regime

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joint work with

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Motivation

- Goal: provide macroscopic models for semiconductor nanodevice simulation.

- Many devices work at high-field regimes: Drift-Diffusion models fail. Huge literature about "corrected" models (F. Poupaud, P. Degond, N. Ben Abdallah, I.M. Gamba, A. Jüngel and many others).

  Common point: semi-classical approach, i.e. Boltzmann equation for semiconductors.

- Boltzmann equation has proved suitable for including diverse mechanisms, physical regimes,. . . .

  BUT advance in semiconductor technology requires to consider **quantum effects** at quasi-ballistic regimes

  $\Longrightarrow$ **quantum macroscopic models**.

Wigner-BGK equation

$w = w(x,v,t)$, $(x,v) \in \mathbb{R}^{2d}, t \geq 0$ quasi-distribution function for an electron ensemble with d degrees of freedom. $1/k\beta$ phonon temperature, V applied potential (also self-consistent).

$$\partial_t w + v \cdot \nabla_x w - \Theta[V]w = -\nu(w - w_{\text{eq}}), \quad t > 0, \qquad w(t=0) = w_0,$$

$$\Theta[V]w(x,v) := i\,\mathcal{F}^{-1}\left\{\frac{1}{\hbar}\left(V\left(x + \frac{\hbar\eta}{2m}\right) - V\left(x - \frac{\hbar\eta}{2m}\right)\right)\mathcal{F}w(x,\eta)\right\}$$

$$w_{\text{eq}}(x,v,t) = n(x,t)C\,e^{-\beta m v^2/2}\left\{1 + \hbar^2\left[-\frac{\beta^2\,\Delta V(x)}{24m} + \frac{\beta^3}{24}\sum_{r,s=1}^{d} v_r v_s \frac{\partial^2 V(x)}{\partial x_r x_s}\right]\right\}$$

with ν inverse relaxation-time, m effective mass, and $\mathcal{F} = \mathcal{F}_{v\to\eta}$ Fourier transform.
$w_{\text{eq}}(x,v,t)$, $\mathcal{O}(\hbar^2)$-accurate local thermal equilibrium distribution function (with β, V assigned),

$$\int w_{\text{eq}}(x,v,t)\,dv \;=\; n(x,t) \;:=\; \int w(x,v,t)\,dv\,, \quad \text{electron position density.}$$

Wigner equation: semiclassical limit

In the Fourier space (η dual variable)

$$\mathcal{F}\left(\Theta[V]w(x,v)\right) := \frac{i}{\hbar}\left(V\left(x+\frac{\hbar\eta}{2m}\right) - V\left(x-\frac{\hbar\eta}{2m}\right)\right)\mathcal{F}(w)$$

$$\frac{1}{\hbar}\left(V\left(x+\frac{\hbar\eta}{2m}\right) - V\left(x-\frac{\hbar\eta}{2m}\right)\right) \xrightarrow{\hbar\to 0} \frac{1}{m}\eta\cdot\nabla_x V(x)$$

where

$$\mathcal{F}\Big(\nabla_x V(x)\cdot\nabla_v w\Big) = i\,\eta\cdot\nabla_x V(x)\,\mathcal{F}(w)$$

then

$$\Theta[V]w \xrightarrow{\hbar\to 0} -\frac{1}{m}\nabla_x V(x)\cdot\nabla_v w \qquad \text{Vlasov operator.}$$

$$\Theta[V]w = -\frac{1}{m}\nabla_x V(x)\cdot\nabla_v w + \mathcal{O}(\hbar^2)\,.$$

Fact: the v-moments of $\Theta[V]$ and of $-(1/m)\,\nabla_x V(x)\cdot\nabla_v$ coincide up to 2^{nd}-order moments. Instead,

$$\int v^3\,\Theta[V]w\,dv = -\frac{1}{m}\int v^3\,\nabla_x V(x)\cdot\nabla_v w\,dv + \frac{\hbar^2}{4m^3} n\,\nabla_x\Delta_x V\,.$$

Derivation of quantum macroscopic models

Questions:

- what are the differences in using $-(1/m)\,\nabla_x V(x)\cdot\,\nabla_v$ in spite of $\Theta[V]$ for the derivation of quantum macroscopic models?

  Remark: quantum corrections due to $w_{\rm eq}$, which is $\mathcal{O}(\hbar^2)$-accurate, appear already in $2^{\rm nd}$-order moments:

$$\int v \otimes v \, w_{\rm eq} \, dv \;=\; \frac{nI}{\beta m} + \frac{\beta \hbar^2}{12 m^2} \, n \, \nabla_x \otimes \nabla_x V \; .$$

- And in high-field regimes?

High-field Wigner-BGK equation

$$\epsilon^{\alpha} w_t + \epsilon\, v \cdot \nabla_x w - \Theta[V]w = -\nu(w - w_{\mathrm{eq}})\,, \quad t > 0\,, \qquad w(t=0) = w_0\,,$$

with $\alpha = 1, 2$. $\alpha = 2$ is the diffusive scaling.

$$\frac{t_V}{t_0} \approx \frac{t_C}{t_0} \approx \epsilon$$

with t_V, t_C, t_0 characteristic times, is the high-field scaling (cf. [Poupaud 91], semiclassical case).

External potential *and* interaction with phonons are the dominant mechanisms in the evolution and balance each other.

At the leading order, $\epsilon = 0$, the solution of $\quad (\nu - \Theta[V])w = \nu w_{\mathrm{eq}} \quad$ is

$$w^{(0)} \;:=\; (\nu\mathcal{I} - \Theta[V])^{-1}\nu w_{\mathrm{eq}} \;=\; \nu\mathcal{F}^{-1}\left(\frac{\mathcal{F}w_{\mathrm{eq}}}{\nu - i\,\delta V}\right)$$

by using the Vlasov operator, the solution of $(\nu + \nabla_x V/m\cdot \nabla_v)f = \nu w_{\mathrm{eq}}$ is

$$f^{(0)} \;:=\; \left(\nu\mathcal{I} + \frac{\nabla_x V}{m}\cdot \nabla_v\right)^{-1}\nu w_{\mathrm{eq}} \;=\; \nu\mathcal{F}^{-1}\left(\frac{\mathcal{F}w_{\mathrm{eq}}}{\nu +\, i\,\eta\cdot \nabla_x V/m}\right)\,.$$

High-field Wigner-BGK: leading order

- the moments up to 2^{nd}-order of $w^{(0)}$ and of $f^{(0)}$ are equal,

- the macroscopic velocity at the leading order is

$$\frac{1}{n}\int v\, w^{(0)}\, dv \;=\; \frac{1}{n}\int v\, f^{(0)}\, dv \;=\; -\frac{\nabla_x V}{\nu m}\,,$$

  i.e., is determined by the field (assigned),

- both quantum and high-field corrections appear in the 2^{nd}-moment tensor

$$\int v\otimes v\, w^{(0)}\, dv \;=\; \int v\otimes v\, f^{(0)}\, dv \;=\; \int v\otimes v\, w_{\mathrm{eq}}\, dv + 2\, n\frac{\nabla_x V}{\nu m}\otimes\frac{\nabla_x V}{\nu m}\,,$$

  where

$$\int v\otimes v\, w_{\mathrm{eq}}\, dv \;=\; \frac{nI}{\beta\nu} + \frac{\beta\hbar^2}{12m^2\nu} n\nabla_x\otimes\nabla_x V\,.$$

Remark: both with $\Theta[V]$ and when substituting it with $-(1/m)\,\nabla_x V\cdot\nabla_v$!!

High-field Quantum Drift-Diffusion [Manzini, Frosali 06]

$$\epsilon\, w_t + \epsilon\, v \cdot \nabla_x w - \Theta[V]w = -\nu(w - w_{\mathrm{eq}})\,, \quad t > 0\,, \qquad w(t=0) = w_0\,,$$

- by a “modified” Chapman-Enskog expansion [Mika, Banasiak] up to 1^{st}-order in ϵ, obtain a Quantum Drift-Diffusion equation with unknown n and field-dependent corrections,
- prove *rigorously* high-field QDD is $\mathcal{O}(\epsilon^2)$-accurate approximation of high-field Wigner-BGK,
- treat at the same time the *initial layer* part that provides initial datum for high-field QDD.

Remark: coincides with [Poupaud 91], apart from quantum correction: depends on the use of $\mathcal{O}(\hbar^2)$-accurate equilibrium function w_{eq}

$$\frac{\partial n}{\partial t} - \nabla \cdot \nabla(\mathsf{D}n) - \nabla \cdot (\mathsf{E}\, n) = 0\,,$$

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

$$\mathsf{E} := \frac{\nabla V}{m\nu}\left(I + \frac{\epsilon}{\nu}\,\frac{\nabla \otimes \nabla V}{m\nu}\right).$$

Derivation of quantum macroscopic models (continued)

Questions and Answers:

- what are the differences in using $-(1/m)\,\nabla_x V(x)\cdot\,\nabla_v$ in spite of $\Theta[V]$ for the derivation of quantum macroscopic models? And in high-field regimes?

  In macroscopic models that involve only $2^{\rm nd}$-order moments, there is NO difference, also in the high-field regime.

New goal: derivation of macroscopic models involving higher order moments with high-field and quantum corrections.
Since at the leading order in ϵ holds

$$\frac{1}{n}\int v\,w^{(0)}\,dv \;=\; -\frac{\nabla_x V}{\nu m}\,,$$

i.e., the fluid velocity is determined by the (high) field, we consider as fluid unknown functions position density n and energy $\mathcal{W}$.

High-field Quantum Fluid-dynamical model (in progress)

$$\epsilon^2 w_t + \epsilon\, v \cdot \nabla_x w + \epsilon\, \nu_1 (w - w_{\rm eq}) - \Theta[V] w = -\nu_2 (w - w_{\rm eq}) \,, \quad t > 0 \,,\ w(t=0) = w_0 \,.$$

We add an unbalanced BGK term with inverse relaxation-time ν_1 and set in $w_{\rm eq}$

$$1/k\beta \;=:\; T(x,t) \,.$$

Via a Chapman-Enskog expansion up to the $1^{\rm st}$-order in ϵ, we write $w = w^{(0)} + \epsilon w^{(1)}$ with

$$\begin{aligned} w^{(0)} &:= (\nu_2 \mathcal{I} - \Theta[V])^{-1} \nu_2\, w_{\rm eq} \;=\; \nu_2\, \mathcal{F}^{-1} \left(\frac{\mathcal{F} w_{\rm eq}}{\nu_2 - i\,\delta V} \right) \\ w^{(1)} &:= (\nu_2 \mathcal{I} - \Theta[V])^{-1} \Big(-v \cdot \nabla_x w^{(0)} - \nu_1 (w^{(0)} - w_{\rm eq}) \Big) \;. \end{aligned}$$

We recover evolution equations for the fluid unknown $n, \mathcal{W}$, defined by

$$\begin{aligned} n(x,t) &:= \int w^{(0)}\, dv \,, \\ \mathcal{W}(x,t) &:= \int \frac{v^2}{2}\, w^{(0)}\, dv \;=\; \frac{d\, k\, nT}{2\nu_2} + \frac{\hbar^2}{24 m^2 \nu_2 k T} n\, \Delta_x V + n \frac{|\nabla_x V|^2}{(\nu_2 m)^2} \end{aligned}$$

High-field Quantum Fluid-dynamical model (continued)

$$\frac{\partial n}{\partial t} - \frac{1}{\nu_2}\nabla\cdot\left(\nabla\int v\otimes v\, w^{(0)}\, dv - \frac{\nabla_x V}{m\nu_2}\nabla\cdot\int v\, w^{(0)}\, dv + 2\nu_1\int v\, w^{(0)}\, dv\right) = 0\,,$$

$$\frac{\partial n}{\partial t} - \nabla\cdot\nabla(\mathsf{D}_1 n) - \nabla\cdot(\mathsf{E}_1\, n) = 0\,,$$

$$\mathsf{D}_1 := \frac{1}{\nu_2}\left(\frac{kT}{m}\mathcal{I} + 3\,\frac{\nabla V}{m\nu_2}\otimes\frac{\nabla V}{m\nu_2} + \frac{\hbar^2}{12m^2kT}\nabla\otimes\nabla V\right)\,,$$

$$\mathsf{E}_1 := \frac{1}{\nu_2}\left(2\,\nu_1\,\mathcal{I} + \frac{\nabla\otimes\nabla V}{m\nu_2}\right)\left(-\frac{\nabla V}{m\nu_2}\right)\,.$$

Remarks:

- the first equation contains moments up to the 2^{nd}-order of $w^{(0)}$, thus the Vlasov operator can substitute $\Theta[V]$,
- high-field tensor differs from QDD model by $\mathsf{D}_1 = \mathsf{D} + 2\,\frac{\nabla V}{m\nu_2}\otimes\frac{\nabla V}{m\nu_2}\,.$

High-field Quantum Fluid-dynamical model (continued)

$$\frac{\partial \mathcal{W}}{\partial t} + \nabla \cdot \int v \, \frac{v^2}{2} \, w^{(1)} \, dv + \nu_1 \int \frac{v^2}{2} \, w^{(1)} \, dv = 0 \, ,$$

$$\frac{\partial n}{\partial t} - \nabla \cdot J_n = 0 \, , \qquad J_n := \nabla(\mathsf{D}_1 n) + (\mathsf{E}_1 \, n)$$

$$\frac{\partial \mathcal{W}}{\partial t} - \nu_1 J_n \cdot \left(-\frac{\nabla V}{m \nu_2} \right) - \nu_1 \nabla \cdot J_w^3 - \nabla \cdot J_w^4 = 0$$

$$J_w^3 := 2 \left(\mathcal{W} \left(-\frac{\nabla V}{m\nu_2} \right) + \left(\mathsf{D}_1 n + 2 \, \frac{\nabla V}{m\nu_2} \otimes \frac{\nabla V}{m\nu_2} n \right) \left(-\frac{\nabla V}{m\nu_2} \right) + 2 \frac{\hbar^2}{8m^3} n \, \nabla_x \Delta_x V \right)$$

Remarks:

- J_w^3 contains moments up to the 3^{rd}-order of $w^{(0)}$, thus the Vlasov operator can NOT substitute $\Theta[V]$ in the derivation,

High-field Quantum Fluid-dynamical model (continued)

- J_w^4 contains moments up to the 4^{th}-order of $w^{(0)}$ and also the energy flux, defined by

$$J_w^4 := \int v \otimes v\, v^2\, w_{\text{eq}}\, dv +$$

$$\nabla \cdot \nabla \left(\left(\mathcal{W} + \mathsf{D}_1 n + 3\, \frac{\nabla V}{m\nu_2} \otimes \frac{\nabla V}{m\nu_2} n \right) \left(\frac{\nabla V}{m\nu_2} \otimes \frac{\nabla V}{m\nu_2} n \right) + 2 \frac{\hbar^2}{8m^3} n\, \nabla_x \Delta_x V \frac{\nabla_x V}{\nu_2 m} \right)$$

$$+ \dots$$

Conclusions

- goal:derive macroscopic models for electron transport in semiconductor nanodevices,
- required feature of the model: capture quantum effects and high-field ones,
- in the derivation of drift-diffusion model the Vlasov operator can substitute $\Theta[V]$,
- in the derivation of of more accurate models (Energy-Transport, e.g.), $\Theta[V]$ is necessary to picture all the quantum effects.