Quantum Diffusion models derived from the entropy principle

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Summary

1. Introduction

Classical Drift-Diffusion models

$$\partial_t n + \nabla_x \cdot j = 0$$

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$$j = -D\, n\, \nabla_x (\mu + V)$$
$$\mu = \ln n + \mathrm{Cst}$$

Quantum extension (Ancona, Iafrate)

The Density-Gradient model

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$$\partial_t n + \nabla_x \cdot nu = 0$$
$$\partial_t u + u \cdot \nabla_x u = -\nabla_x(V + 3V_B)$$

Other approach (Sacco et al)

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and change the relation between n and μ

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Classical case:

$$g(\varepsilon) = C\sqrt{\varepsilon}$$

Other quantum extension (Sacco et al)

Quantum case:

$$g(\varepsilon) = \sum_k \delta(\varepsilon - E_k) \, |\psi_k(x)|^2$$

where (E_k, ψ_k) eigen-elements of the Hamiltonian

$$H = -\frac{\hbar^2}{2}\Delta + V$$

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Our goal (and model)

Propose (and justify) a different reconstruction:

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where $(\lambda_k[\mu], \psi_k[\mu])$ eigen-elements of the modified 'Hamiltonian'

$$H_{-\mu} = -\frac{\hbar^2}{2}\Delta - \mu$$

2. Derivation of classical Drift-Diffusion

Boltzmann equation

- phase-space density $f(x, p, t)$: Boltzmann-BGK equation

$$\partial_t f + p \cdot \nabla_x f - \nabla_x V \cdot \nabla_p f = Q(f)$$

$$Q(f) = -\nu(f - M_f)$$

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- M_f = Maxwellian:

$$\begin{aligned} M_f &= \frac{n}{(2\pi)^{3/2}} \exp\left(-\frac{|p|^2}{2}\right) \qquad n = \int f \, dp \\ &= \exp\left(\mu - \frac{|p|^2}{2}\right) \end{aligned}$$

Diffusion scaling:

- Rescaling:

$$Q \longrightarrow \frac{1}{\varepsilon} Q \qquad t \longrightarrow \frac{1}{\varepsilon} t$$

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- When $\varepsilon \to 0$:

$$f \to M_f$$

where n satisfies Drift-Diffusion model with $D = \frac{1}{3\nu}$.

Characterization of the Maxellian

- Free energy

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- Density n given. Maxwellian is the solution of

$$\min\{\,\mathcal{F}[f] \mid \int f\,dp = n\}$$

Extension to quantum systems:

- Quantum kinetic equation

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- Quantum Maxwellian

3. Quantum kinetic equation

Density operator

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$$\mathrm{Tr}\rho = 1$$

- Typically:

$$\rho\psi = \sum_{s\in S} \rho_s(\psi, \phi_s)\,\phi_s$$

for a complete orthonormal system $(\phi_s)_{s\in S}$ and real numbers $(\rho_s)_{s\in S}$ such that $0 \le \rho_s \le 1$, $\sum \rho_s = 1$

Quantum Liouville equation

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- $$i\hbar\partial_t\rho = [H,\rho] + Q(\rho)$$

- $H =$ Hamiltonian:

$$H\psi = -\frac{\hbar^2}{2}\Delta\psi + V(x,t)\psi$$

- $Q(\rho)$ to be specified later

Wigner Transform

➠ $\underline{\rho}(x, x')$ integral kernel of ρ:

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- $W[\rho](x, p)$ Wigner transform of ρ:

$$W[\rho](x, p) = \int \underline{\rho}(x - \frac{1}{2}\xi, x + \frac{1}{2}\xi)\, e^{i\frac{\xi \cdot p}{\hbar}}\, d\xi$$

Inverse Wigner transform (Weyl quantization)

- Let $w(x,p)$. $\rho = W^{-1}(w)$ is the operator defined by:

$$W^{-1}(w)\psi = \frac{1}{(2\pi)^d} \int w(\frac{x+y}{2}, \hbar k)\, \psi(y) e^{ik(x-y)}\, dk\, dy$$

w= Weyl symbol of ρ.

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- Isometries between $\mathcal{L}^2$ (Operators s.t. $\rho\rho^\dagger$ is trace-class) and $L^2(\mathbb{R}^{2d})$:

$$\mathrm{Tr}\{\rho\sigma^\dagger\} = \int W[\rho](x,p)\overline{W[\sigma](x,p)}\, \frac{dx\, dp}{(2\pi\hbar)^d}$$

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$$\Theta^{\hbar}[V]w = -\frac{i}{(2\pi)^d \hbar} \int \left(V(x + \frac{\hbar}{2}\eta) - V(x - \frac{\hbar}{2}\eta)\right) \times w(x,q)\, e^{i\eta\cdot(p-q)}\, dq\, d\eta$$

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- $\Theta^\hbar[V]w \xrightarrow{\hbar \to 0} -\nabla_x V \cdot \nabla_p w$
- $Q(w)$ collision operator (to be specified later)

4. Quantum equilibria and BGK operator

Entropy principle

- Entropy = free energy

$$\mathcal{F}[\rho] = \mathrm{Tr}\{\rho(\ln \rho - 1 + H)\}$$

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- Density $n(x)$ given. Minimize $\mathcal{F}$ under the constraint of given density $n(x)$, i.e.

$$\min\{\mathcal{F}[\rho] \mid \int W[\rho](x,p)\,dp = n(x)\}$$

Quantum equilibria

- Solution of the entropy minimization problem

$$\rho_\mu = \exp W^{-1}(\mu - \frac{|p|^2}{2})$$

or

$$f_\mu(x,p) = \mathcal{E}\mathrm{xp}(\mu - \frac{|p|^2}{2}) \qquad \mathcal{E}\mathrm{xp} = W \exp W^{-1}$$

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- μ related to n by the density constraint:

$$\int f_\mu(x,p)\, dp = n$$

Quantum BGK operator

$$Q(f) = -\nu(f - \mathcal{M}_f)$$

$$\mathcal{M}_f = \mathcal{E}\text{xp}(\mu - \frac{|p|^2}{2})$$

where μ is related with f by:

$$\int (f - \mathcal{M}_f)\, dp = 0$$

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$$\int (f - \mathcal{M}_f)\, dp = 0$$

➠ Q decreases the quantum entropy:

$$\text{Tr}\{W^{-1}(Q(f)) \ln \rho\} \leq 0$$

5. Derivation of new quantum Drift-Diffusion model

Rescaling of Quantum Kinetic Equation

- Same as for Classical Bolzmann equation gives

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$$n = \int \mathcal{E}\mathrm{xp}(\mu - \frac{|p|^2}{2})\, dp$$

(only change from Classical DD)

Bounded domain

- bounded domain Ω

$$H_{-\mu} \; = \; \frac{p^2}{2} - \mu \; = \; -\frac{\hbar^2}{2}\Delta - \mu$$

with $\psi = 0$ or $\partial\psi/\partial n = 0$ on $\partial\Omega$.

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- $\mu \in L^2 \Longrightarrow H_{-\mu}$ has compact resolvent
  $(\lambda_k[\mu], \psi_k[\mu](x))$ discrete eigenvalues and vectors

$$\mathcal{E}\mathrm{xp}(\mu - \frac{|p|^2}{2}) = \sum_k e^{-\lambda_k[\mu]} \psi_k[\mu] \psi_k^*[\mu]$$

Reconstruction of n

$$n(x) = \sum_k e^{-\lambda_k[\mu]} |\psi_k[\mu]|^2(x)$$

The result previously stated

6. Properties

Poisson eq. and equilibria

- Coupling with Poisson eq.

$$V = V_{ext} + V_{sc} \qquad -\Delta V_{sc} = n \qquad V_{ext} \text{ given}$$

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$$V = V_{ext} + V_{sc} \qquad -\Delta V_{sc} = n \qquad V_{ext} \text{ given}$$

- Equilibria: $j = 0 \qquad \mu = -V$

$$-\Delta V_{sc} = \sum_k e^{-\lambda_k[-(V_{ext}+V_{sc})]} |\psi_k|^2(x)$$

Schrödinger-Poisson problem

Entropy decay

- Free energy: V independent of t

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- V coupled with Poisson

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- The relative entropy to the equilibrium decreases.
$\Rightarrow$ convervence to equilibrium if n bounded from below

Discrete models

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- The implicit semi-discretized model (coupled w Poisson) is well-posed and has a variational formulation [Gallego, Méhats]
- The fully (space and time) discretized problem converges in time towards a solution of a discrete Schrödinger-Poisson problem [GM]

$\hbar^2$ expansions of QDD

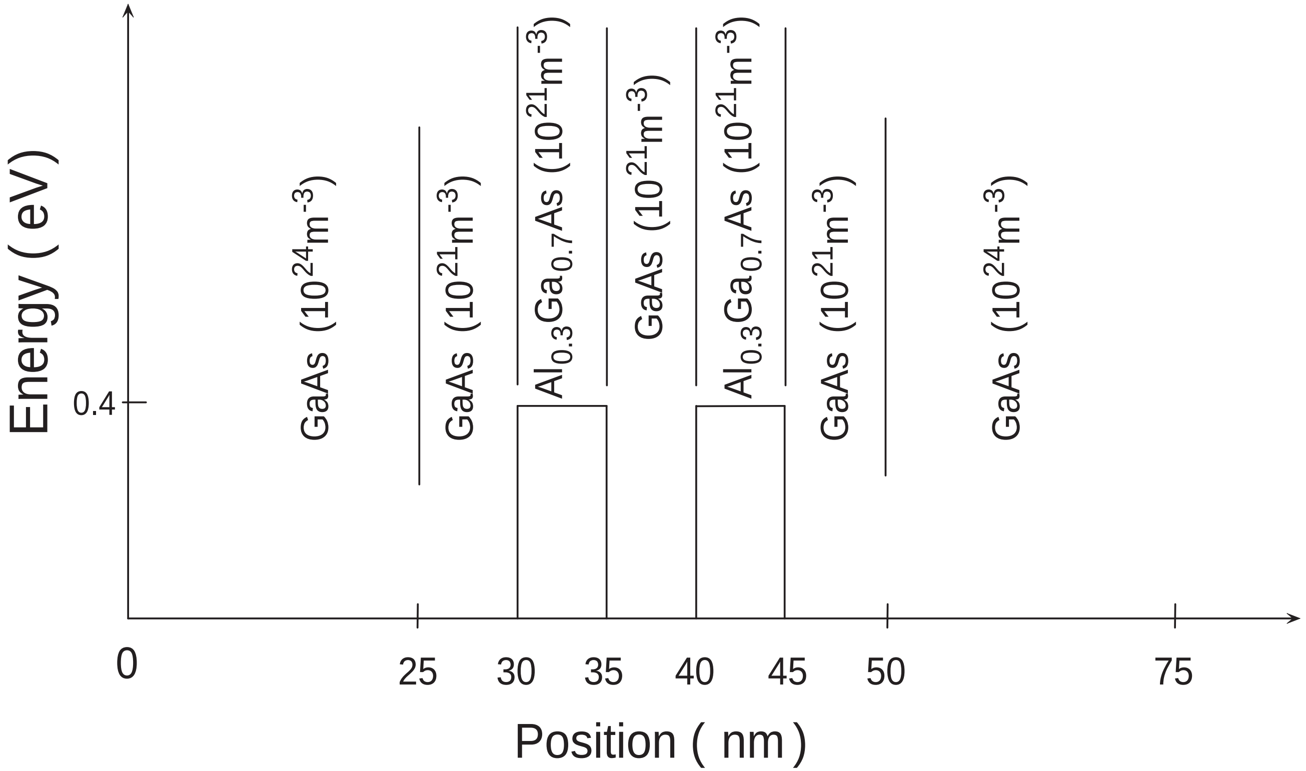
- $\hbar \to 0$ gives classical DD model

$\hbar^2$ expansions of QDD

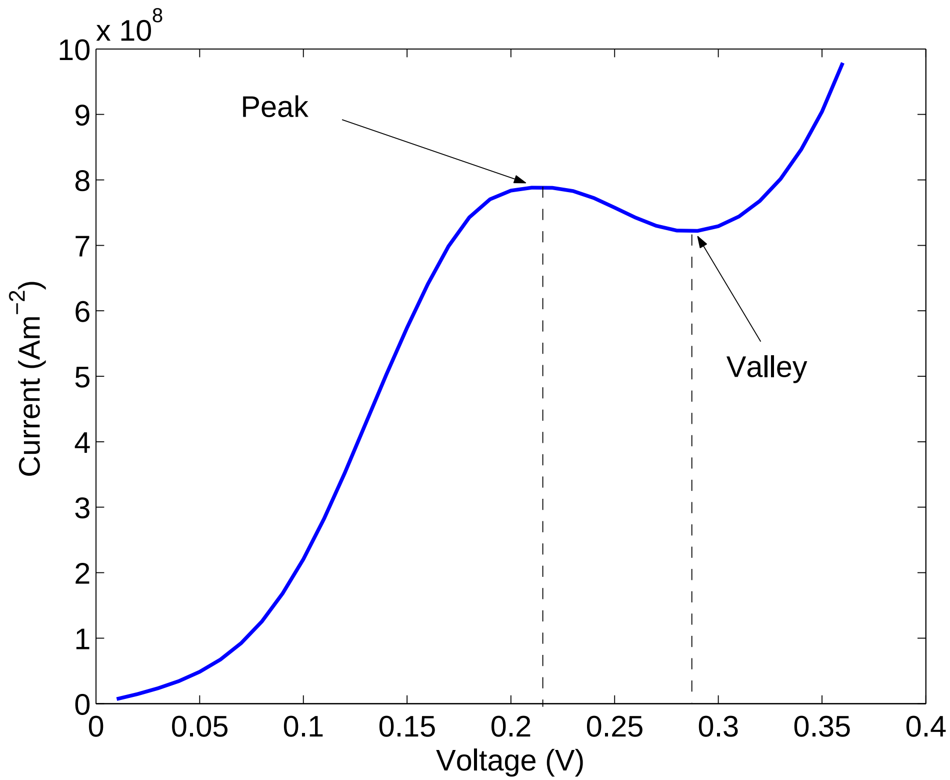
- $\hbar \longrightarrow 0$ gives classical DD model
- $O(\hbar^2)$ corrections to classical DD: recover the Density-Gradient Drift-Diffusion model (with the Bohm potential) of [Ancona, Iafrate]

7. Numerical results

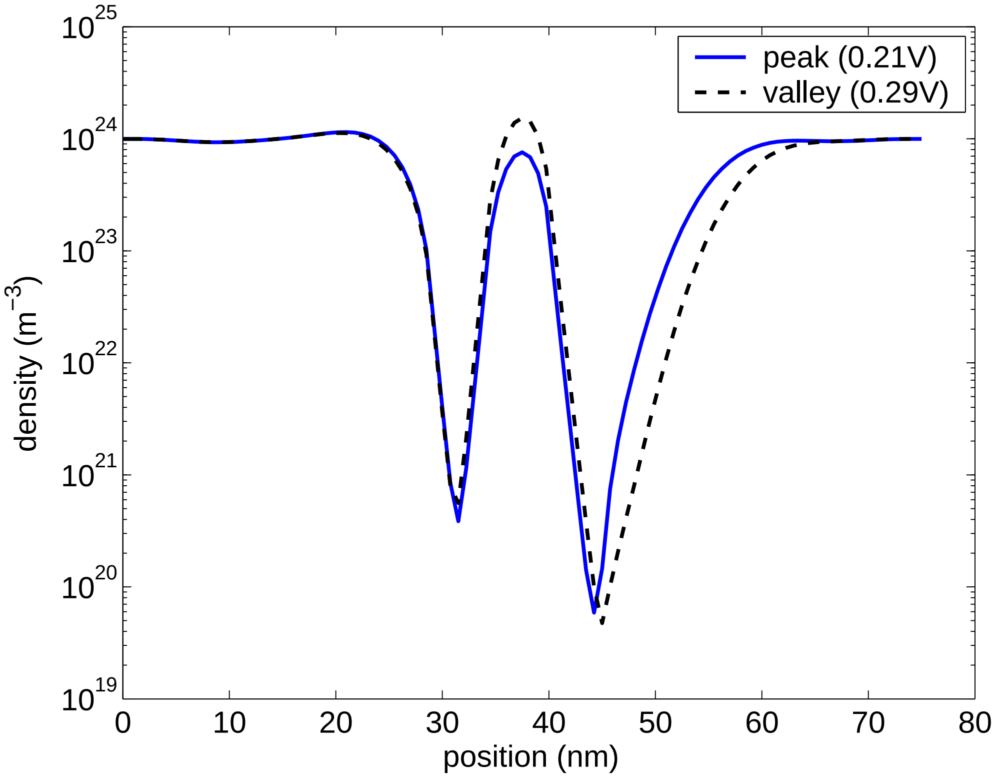
Resonant tunneling diode



$I - V$ curve


x 10^8
10
9
8
7
6
5
4
3
2
1
0
Current (Am^−2)
Peak
Valley
0
0.05
0.1
0.15
0.2
0.25
0.3
0.35
0.4
Voltage (V)

Densities


peak (0.21V)
valley (0.29V)
10^{25}
10^{24}
10^{23}
10^{22}
10^{21}
10^{20}
10^{19}
density (m^{-3})
0
10
20
30
40
50
60
70
80
position (nm)

8. Summary and conclusion

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- Developed a new concept of quantum equilibria as the minimizers of the quantum entropy subject to local constraints [D., Ringhofer]

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- Proposed a formulation of a quantum BGK operator
- Realized a diffusion approximation of the resulting Quantum Kinetic Equation which provides new Quantum Dift-Diffusion models

Comparison with existing approaches

- Differs from classical model by the reconstruction of the density from the chemical potential (through an eigenvalue problem)

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Comparison with existing approaches

- Differs from classical model by the reconstruction of the density from the chemical potential (through an eigenvalue problem)
- Recovers Density-Gradient (Bohm potential) models of [Ancona, Iafrate] as an $O(\hbar^2)$ approximation.
- Reconstruction bears similarities with but is different from Quantum Corrected Drift-Diffusion [Sacco et al]

Possible extensions

- Energy-Transport models. Classical:

$$\partial_t n + \nabla_x \cdot j_n = 0$$

$$\partial_t W + \nabla_x \cdot j_W + j_n \cdot \nabla_x V = 0$$

$$\begin{pmatrix} j_n \\ j_W \end{pmatrix} = -D \begin{pmatrix} \nabla_x n + n \frac{\nabla_x V}{T} \\ \nabla_x T \end{pmatrix}$$

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$$\begin{pmatrix} j_n \\ j_W \end{pmatrix} = -D \begin{pmatrix} \nabla_x n + n \frac{\nabla_x V}{T} \\ \nabla_x T \end{pmatrix}$$

- Extension of our approach written but not implemented yet
- Note: extension of Density-Gradient approach to Energy-Transport by [Chen, Liu]