CIME

Quantum transport: modelling, analysis and asymptotics

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New Quantum Hydrodynamic Models for Semiconductors

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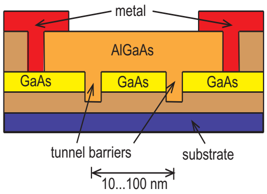
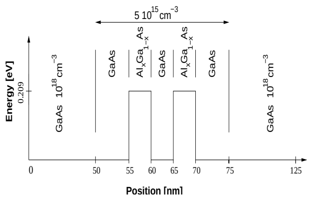
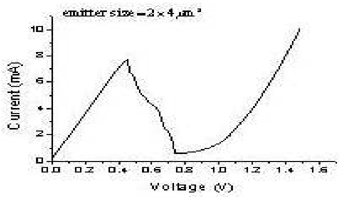
Semiconductor devices

- Resonant tunneling diode





- Applications
  - logic devices
  - laser diodes
  - oscillator circuits



Quantum entropy minimization

For the Wigner distribution function $f:\mathbb{R}^d_x\times\mathbb{R}^d_p\to\mathbb{R}$ define

- Quantum relative entropy

$$H(f)=\int\int f(\mathrm{Log}\, f-1+\frac{1}{2}|p|^2+V(x))dxdp$$

where $\mathrm{Log}\, f$ is the operator logarithm

- Moments
$(n,nu,ne)=m[f](x,t)=\int f(x,p,t)\chi(p)dp$
with weight $\chi(p)=(1,p,\frac{1}{2}|p|^2)$
- Quantum Maxwellian
M_f is the solution to the constrained minimization

$$H(M_f)=\min\left\{H(f):\int f(p)\chi(p)dp=m[f]\right\}$$

From kinetic to fluid models

- Wigner-BGK equation

$$\partial_t f_\alpha+p\cdot\nabla_x f_\alpha+\Theta_\varepsilon[V]f_\alpha=\frac{1}{\alpha}(M_{f_\alpha}-f_\alpha,)$$

$\Theta_\varepsilon[V]$ pseudo-diff. operator, $\Theta_\varepsilon[V]f\to\nabla_x V\cdot\nabla_p f$ as $\varepsilon\to 0$

- Hydrodynamic limit
limit $\alpha\to 0$ yields $f_\alpha\to f=M_f$, the Quantum Maxwellian
- Moment equations
multiply by moments χ and integrate over $p\in\mathbb{R}^d$

$$\partial_t m[M_f]+\nabla_x\cdot\int p\chi(p)M_f\,dp+\int\chi(p)\Theta_\varepsilon[V]M_f\,dp=0$$

- General Quantum hydrodynamic (QHD) equations

$$\begin{aligned}\partial_t n+\mathrm{div}(nu)&=0\\ \partial_t(nu)+\mathrm{div}\left(\frac{nu\otimes u}{n}\right)+\mathrm{div}P-n\nabla V&=0\\ \partial_t(ne)+\mathrm{div}\Big((P+neT)u\Big)+\mathrm{div}S-nu\cdot\nabla V&=0\end{aligned}$$

n particle density, nu momentum, ne energy density
$P=\int(p-u)\otimes(p-u)M_f\,dp$ stress tensor
$S=\frac{1}{2}\int(p-u)|p-u|^2M_f\,dp$ correction flux

- Expansion in powers of ε^2
Neglect terms $O(\varepsilon^4)$ and smaller, assume $\nabla\log T=O(\varepsilon^2)$

$$ne=\frac{d}{2}nT+\frac{1}{2}n|u|^2-\frac{\varepsilon^2}{24}n\left(\Delta\log n-\frac{\mathrm{tr}(R^{\mathrm{T}}R)}{T}\right)$$

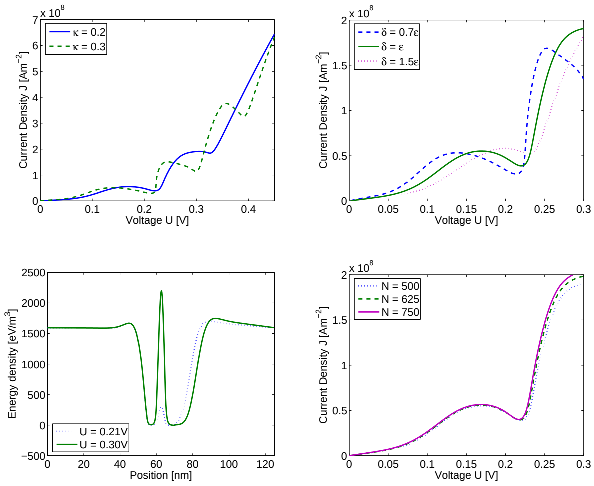
$$P=nTI-\frac{\varepsilon^2}{12}n\left((\nabla\otimes\nabla)\log n-\frac{R^{\mathrm{T}}R}{T}\right)$$

$$S=-\frac{\varepsilon^2}{8}(\mathrm{div}(n\Delta u)+f(R,\mathrm{div}R,n,\nabla n))$$

with the vorticity $R=\nabla u-(\nabla u)^{\mathrm{T}}$

Numerical results

- Genuine quantum hydrodynamical simulations



- CFD discretization, Newton iteration, heat conduction
- new dispersive velocity term has regularizing effect in CV-curve and stabilizes the numerical scheme

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