Diffusion in quantum fluid models for semiconductors

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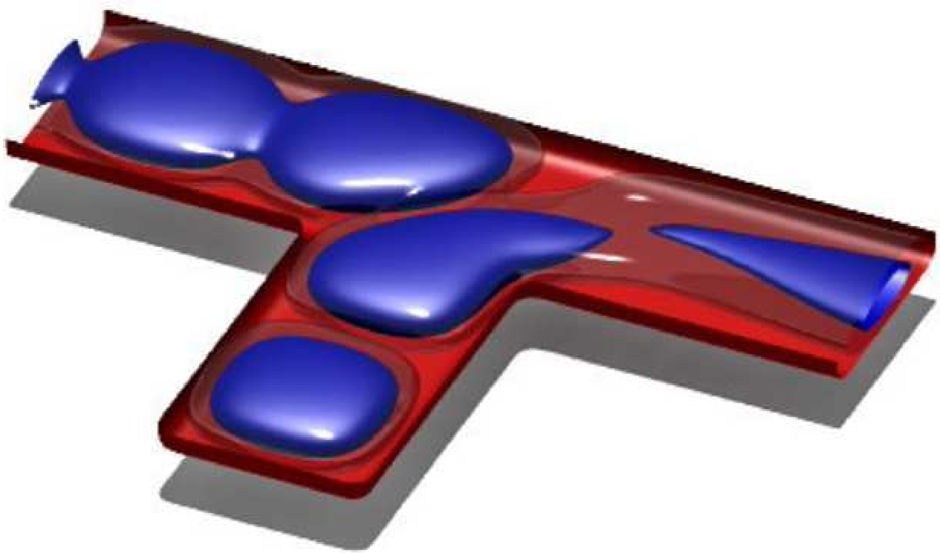
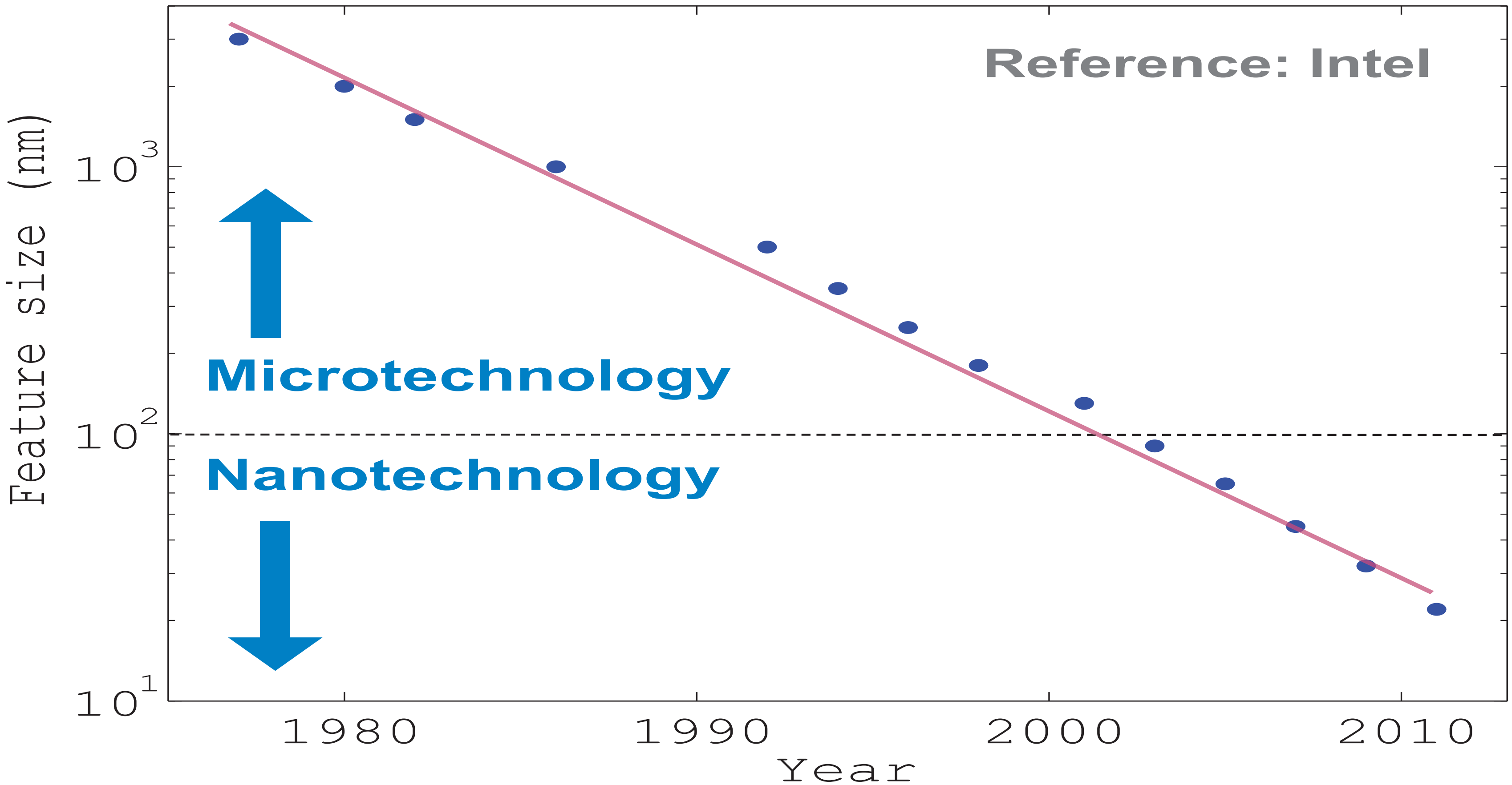
- Introduction
- Quantum diffusion model of fourth order
- Quantum Navier-Stokes model



Why quantum fluid models?



- Feature size of transistors $< 100\,\mathrm{nm}$: quantum effects
- Need for physically accurate models whose numerical solution is cheap

Why quantum fluid models?

- Very rich mathematical structure
- Develop mathematical theory for higher-order equations

① Quantum diffusion model of 4th order: (n: particle density)

$$n_t + \operatorname{div}\left(n\nabla\left(\frac{\Delta\sqrt{n}}{\sqrt{n}}\right)\right) = 0$$

② Quantum Navier-Stokes model: (u: velocity, ε: Planck const.)

$$n_t + \operatorname{div}(nu) = 0, \quad D(u) = \frac{1}{2}(\nabla u + \nabla u^\top)$$

$$(nu)_t + \operatorname{div}(nu \otimes u) + \nabla p(n) - \frac{\varepsilon^2}{6} n\nabla\left(\frac{\Delta\sqrt{n}}{\sqrt{n}}\right) = 2\nu\operatorname{div}(nD(u))$$

Mathematical challenges:

- How to prove positivity of n? No maximum principle!
- How to derive a priori estimates? Highly nonlinear!

Derivation (Degond/Ringhofer 2003)

- Wigner-BGK equation for $w(x,p,t)$: moment method

$$n = \int_{\mathbb{R}^3} w dp, \quad nu = \int_{\mathbb{R}^3} wp dp$$

- Collisions: $Q(w) = M[w] - w$
- Quantum equilibrium $M[w]$:

$$M[w] = \exp(A + \tfrac{1}{2}|p|^2)\Big(1 + \tfrac{\varepsilon^2}{8}(\Delta A + \tfrac{1}{3}|\nabla A|^2 - \tfrac{1}{3}p^\top(\nabla^2 A)p)\Big) + O(\varepsilon^4)$$

Chapman-Enskog expansion:

- $Q(w)$ conserves mass, zero mean-free path limit $\alpha \to 0$: gives nonlocal evolution equation for particle density n
- $Q(w)$ conserves mass and momentum, $\alpha > 0$: gives nonlocal evolution equation for n and nu
- Expansion of $M[w]$ in powers of ε^2: gives local models

Fourth-order quantum diffusion equation

Simplified quantum diffusion model:

- No pressure, constant electric potential, $\varepsilon^2/6 = 1$
- Retain quantum term with Bohm potential $\Delta\sqrt{n}/\sqrt{n}$ only
- Periodic boundary conditions, $\mathbb{T}^d$: torus

$$n_t + \operatorname{div}\left(n\nabla\left(\frac{\Delta\sqrt{n}}{\sqrt{n}}\right)\right) = 0, \quad n(0) = n_0 \text{ in } \mathbb{T}^d$$

Mathematical results:

- Local-in-time existence in 1D: Bleher et al. 1994
- Global-in-time existence in 1D: A.J.-Pinnau, *SIMA* 2000
- Global-in-time existence in 3D: Gianazza-Savaré-Toscani 2009, A.J.-Matthes, *SIMA* 2008

Fourth-order quantum diffusion equation

$$n_t + \mathrm{div}\left(n\nabla\left(\frac{\Delta\sqrt{n}}{\sqrt{n}}\right)\right) = 0, \quad n(\cdot,0) = n_0 \text{ in } \mathbb{T}^d$$

Entropy: $E_1[n] = \int_{\mathbb{T}^d}(n(\log n - 1) + 1)dx$

Theorem: (A.J.-Matthes, *SIMA* 2008)

Let $d \le 3$ and $E_1[n_0] < \infty$.

- $\exists$ weak solution satisfying $n(\cdot,t) \ge 0$ and

$$n \in W^{1,1}_{\mathrm{loc}}(0,\infty; H^{-2}),\ \sqrt{n} \in L^2_{\mathrm{loc}}(0,\infty; H^2)$$

- Exponential convergence to constant steady state n_∞:

$$\|n(\cdot,t) - n_\infty\|_{L^1(\mathbb{T}^d)} \le \sqrt{2E_1[n_0]}e^{-8\pi^4\kappa t},\ \kappa = \frac{4d-1}{d(d+2)}$$

- Nonuniqueness: $\exists$ two solutions in $L^1_{\mathrm{loc}}(0,\infty; H^2)$
- Positivity: $\exists$ weak solution with $n(x_0,t) = 0$ for some x_0

Fourth-order quantum diffusion equation

$$n_t + \operatorname{div}\left(n\nabla\left(\frac{\Delta\sqrt{n}}{\sqrt{n}}\right)\right) = 0, \quad n(\cdot,0) = n_0 \text{ in } \mathbb{T}^d$$

How to prove nonnegativity? Idea: Define $n = e^y$ solving

$$(e^y)_t + \nabla^2 : (e^y \nabla^2 y) = 0$$

Advantage: symmetric PDE, y bounded $\Rightarrow n = e^y > 0$

How to derive a priori estimates? Multiply equation by $\log n$ and integrate by parts

$$\frac{d}{dt}\int_{\mathbb{T}^d} n \log n dx = \int_{\mathbb{T}^d} \operatorname{div}\left(n\nabla\left(\frac{\Delta\sqrt{n}}{\sqrt{n}}\right)\right)\log n dx$$

$$= \int_{\mathbb{T}^d} \nabla\left(\frac{\Delta\sqrt{n}}{\sqrt{n}}\right)\cdot\nabla n dx = -\int_{\mathbb{T}^d}\frac{\Delta\sqrt{n}}{\sqrt{n}}\Delta n dx \le 0?$$

Idea: systematic integration by parts

Systematic integration by parts

(A.J.-Matthes, *Nonlinearity* 2006)

- To prove (we simplify): find $c > 0$ such that

$$Q_c = \int_{\mathbb{T}} \frac{(\sqrt{n})_{xx}}{\sqrt{n}} n_{xx} dx - c \int_{\mathbb{T}} (\sqrt{n})_{xx}^2 dx \geq 0$$

- Formalize integration by parts:

$$I_1 = \int_{\mathbb{T}} n \left(3 \left(\frac{n_x}{n} \right)^2 \frac{n_{xx}}{n} - 2 \left(\frac{n_x}{n} \right)^4 \right) dx = \int_{\mathbb{T}} \left(\frac{n_x^3}{n^2} \right)_x dx = 0$$

$$I_2 = \int_{\mathbb{T}} n \left(\left(\frac{n_x}{n} \right)^2 \frac{n_{xx}}{n} + \left(\frac{n_{xx}}{n} \right)^2 - \frac{n_x}{n} \frac{n_{xxx}}{n} \right) dx = 0$$

- These are all (useful) independent integrations by parts

Objective: show that $\exists\ c > 0,\ c_1, c_2 \in \mathbb{R}$:

$$Q_c = Q_c + c_1 I_1 + c_2 I_2 \geq 0$$

Systematic integration by parts

Main idea: identify $\frac{u_x}{u} \triangleq \xi_1$, $\frac{u_{xx}}{u} \triangleq \xi_2$ etc.

- Formalisation with polynomials:

  Q_c becomes $S_c(\xi) = (8-c)\xi_1^4 - 4(4-c)\xi_1^2\xi_2 + 8\xi_1\xi_3 - 4c\xi_2^2$

  I_1 becomes $T_1(\xi) = -2\xi_1^4 + 3\xi_1^2\xi_2$

  I_2 becomes $T_2(\xi) = \xi_1^2\xi_2 - \xi_2^2 + \xi_1\xi_3$

Nonnegativity of ...

$$\exists c > 0,\, c_1,\, c_2 \in \mathbb{R} : \mathcal{Q}_c = Q_c + c_1 I_1 + c_2 I_2 \geq 0$$

... is a consequence of decision problem:

$$\exists c > 0,\, c_1,\, c_2 \in \mathbb{R} : \forall \xi \in \mathbb{R}^3 : \; (S_c + c_1 T_1 + c_2 T_2)(\xi) \geq 0$$

- Such problems are well known in real algebraic geometry
- Solve decision problem by quantifier elimination

Intermezzo: entropy construction method

Decision problem:

$$\exists c > 0,\ c_1,\ c_2 \in \mathbb{R} : \forall \xi \in \mathbb{R}^3 : \ (S_c + c_1 T_1 + c_2 T_2)(\xi) \geq 0$$

- Tarski 1930: Such quantified statements can be reduced to quantifier-free statement in an algorithmic way
- Quantifier elimination: `Mathematica`, QEPCAD
- Advantage: complete, exact answer
- Drawback: algorithms are doubly exponential in no. of ξ_i, c_i

Coming back to the quantum diffusion model: to show

$$\int_{\mathbb{T}^d} \left(\frac{\Delta\sqrt{n}}{\sqrt{n}} \Delta n - \kappa |\nabla^2 \sqrt{n}|^2 \right) dx \geq 0 \quad \text{for some } \kappa > 0$$

- Write as polynomial in scalar variables $|\nabla n|^2$, Δn etc.
- Choose particular shift polynomials (compare Δn and $\nabla^2 n$)
- Solve quantifier elimination problem "by hand"

Fourth-order quantum diffusion equation

Ideas of existence proof:

- Entropy estimate: from entropy construction method:

$$\frac{d}{dt}\int_{\mathbb{T}^d} n \log n dx = -\int_{\mathbb{T}^d} \frac{\Delta\sqrt{n}}{\sqrt{n}} \Delta n dx \leq -\kappa \int_{\mathbb{T}^d} |\nabla^2\sqrt{n}|^2 dx$$

  $\Rightarrow$ gives H^2 bound for $\sqrt{n}$

- Solve semi-discrete equation: $n_k = e^{y_k} \approx n(\cdot, k\triangle t)$

$$\frac{1}{\triangle t}(e^{y_k} - e^{y_{k-1}}) + \underbrace{\nabla^2 : (e^{y_k}\nabla^2 y_k)}_{\text{may degenerate}} + \underbrace{\delta(\Delta^2 y_k + y_k)}_{\text{ensures ellipticity}} = 0$$

- Use Leray-Schauder fixed-point theorem for fixed $(\triangle t, \delta)$
- Compactness allows for limit $\triangle t \to 0$, $\delta \to 0$, we loose positivity of $n = e^y$ in the limit

Quantum Navier-Stokes equations

Derivation: (Brull/Méhats 2009)

- Chapman-Enskog expansion in Wigner-BGK equation
- Assumptions: nearly irrotational case, expansion in scaled Planck constant

Equations: (n: particle density, u: velocity)

$$n_t + \operatorname{div}(nu) = 0$$

$$(nu)_t + \operatorname{div}(nu \otimes u) + \nabla p(n) - 2\varepsilon^2 n \nabla\left(\frac{\Delta\sqrt{n}}{\sqrt{n}}\right) = 2\nu \operatorname{div}(nD(u))$$

- Viscosity: $\mu(n) = \nu n$, Planck constant: ε
- Pressure: $p(n) = n^\gamma$ ($\gamma \geq 1$), $D(u) = \frac{1}{2}(\nabla u + \nabla u^\top)$

Relation to other models:

- $\varepsilon = \nu = 0$: hydrodynamic (Euler) equations
- $\nu = 0$: quantum hydrodynamic equations

Quantum Navier-Stokes equations

Energy estimate: $H(n) = n^\gamma/(\gamma-1)$

$$\frac{d}{dt}\int_{\mathbb{T}^d}\left(\tfrac{n}{2}|u|^2 + H(n) + 2\varepsilon^2|\nabla\sqrt{n}|^2\right)dx + \nu\int_{\mathbb{T}^d} n|D(u)|^2 dx = 0$$

Mathematical challenges:

- Positivity of n
- Energy estimate gives H^1 bound for $\sqrt{n}$ only

Idea:

- Define new velocity variable $w = u + \nu\nabla\log n$
- New entropy estimate gives H^2 bound for $\sqrt{n}$ if $\varepsilon > \nu$

$$\frac{d}{dt}\int_{\mathbb{T}^d}\left(\tfrac{n}{2}|w|^2 + H(n) + 2\varepsilon^2|\nabla\sqrt{n}|^2\right)dx$$
$$+\nu\int_{\mathbb{T}^d}\left(n|\nabla w|^2 + (\varepsilon^2-\nu^2)n|\nabla^2\log n|^2\right)dx \le 0$$

New observation

Quantum Navier-Stokes equations . . .

$$n_t + \mathrm{div}(nu) = 0$$

$$(nu)_t + \mathrm{div}(nu \otimes u) + \nabla p(n) - 2\varepsilon^2 n \nabla \left(\frac{\Delta\sqrt{n}}{\sqrt{n}} \right) = 2\nu \mathrm{div}(nD(u))$$

. . . are equivalent to viscous quantum hydrodynamic eqs.

$$n_t + \mathrm{div}(nw) = \nu\Delta n, \quad \varepsilon_0^2 = \varepsilon^2 - \nu^2,$$

$$(nw)_t + \mathrm{div}(nw \otimes w) + \nabla p(n) - 2\varepsilon_0^2 n \nabla \left(\frac{\Delta\sqrt{n}}{\sqrt{n}} \right) = \nu\Delta(nw)$$

- $\varepsilon = \nu$ leads to viscous Euler system without quantum terms
- Velocity $w = u + \nu\nabla \log n$: viscous Korteweg models (Bresch-Desjardins), osmotic velocity $\nu\nabla \log n$: Nelson '67
- Existence for viscous quantum hydrodynamic model $\Rightarrow$ existence for quantum Navier-Stokes model

Quantum Navier-Stokes equations

$$n_t + \mathrm{div}(nu) = 0, \quad n(0) = n_0,\ u(0) = u_0 \quad \text{in } T^d$$

$$(nu)_t + \mathrm{div}(nu \otimes u) + \nabla p(n) - 2\varepsilon^2 n \nabla\left(\frac{\Delta\sqrt{n}}{\sqrt{n}}\right) = 2\nu \mathrm{div}(nD(u))$$

Theorem: (A.J., *SIMA* 2010)

Let $d \le 3$, $p(n) = n^\gamma$ with $\gamma > 3$. Then

$\exists$ weak solution (n, u) with $n(t) \ge 0$ and

$$\sqrt{n} \in L^2_{\mathrm{loc}}(0, \infty; H^2), \quad nu \in L^2_{\mathrm{loc}}(0, \infty; W^{1,3/2})$$

- Definition of weak solution: needs test functions $n^2\phi$
- $\gamma > 3$: energy estimate gives $n \in L^3$ but we need $n \in L^{3+\delta}$
- $\varepsilon \ge \nu$: combine estimates (Dong 2010, Jiang-Jiang 2010)

Ideas of proof:

- $n_t + \mathrm{div}(nw) = \nu\Delta n$: apply maximum principle
- Faedo-Galerkin method, entropy dissipation method

Extensions

Quantum diffusion model of 6th order: expansion up to $O(\varepsilon^6)$

$$n_t - \frac{\varepsilon^4}{360}\nabla^3 : \left(n\nabla^3 \log n\right) - 2\nabla^2 : \left(n(\nabla^2 \log n)^2\right) = 0$$

- Local existence and uniqueness of classical solutions
- Global existence of weak solutions (Bukal/A.J./Matthes 2010)

Full quantum Navier-Stokes model: collisions conserve energy

$$n_t + \mathrm{div}(nu) = 0$$

$$(nu)_t + \mathrm{div}(nu \otimes u) + \nabla(nT) - 2\varepsilon^2 \mathrm{div}(n\nabla^2 \log n) = \nu \mathrm{div}\, S$$

$$(ne)_t + \mathrm{div}((ne + nT)u) - \tfrac{\varepsilon^2}{12}\mathrm{div}(n(\nabla^2 \log n)u) = \nu \mathrm{div}(Su - q)$$

$$ne = \tfrac{3}{2}nT + \tfrac{1}{2}n|u|^2 - \tfrac{\varepsilon^2}{24}n\Delta \log n$$

$$S = nT\left(\nabla u + \nabla u^\top - \tfrac{2}{3}\mathrm{div}\, u\, \mathsf{Id}\right), \quad q = \tfrac{5}{2}nT\nabla T + \tfrac{\varepsilon^2}{24}n(\Delta u + 2\nabla \mathrm{div}\, u)$$

- Derivation and numerical solution (A.J./Milisic 2011)

Summary

Model	Global exist. 3D	Long-time asympt.	Positive solutions	Numerics
Fourth-order quantum diff.	✔	✔	✘	✔
Sixth-order quantum diff.	✔	✔	open	open
Quantum Navier-Stokes	✔	✔	open	✔
Full quantum Navier-Stokes	open	open	open	✔

New key ideas to derive a priori estimates:

- Systematic integration by parts
- New velocity variable (“‘osmotic velocity”)