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The relaxation-time limit of the quantum hydrodynamics equations for semiconductors

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Prague, Sep 23, 2024, MPDE Conference

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QHD system with damping

$$\begin{cases} \partial_t \rho + \operatorname{div} J = 0 \\ \partial_t J + \operatorname{div}\left(\dfrac{J \otimes J}{\rho}\right) + \nabla P(\rho) + \rho \nabla V = \dfrac{1}{2} \rho \nabla\left(\dfrac{\Delta\sqrt{\rho}}{\sqrt{\rho}}\right) - \dfrac{1}{\tau} J \\ -\Delta V = \rho - C \end{cases}$$

$\mathcal{E} = -\nabla V$ electrostatic force

$\rho \geq 0$ charge, $J = \rho u$ current, $u \to$ velocity field

$0 < \tau \ll 1 \to$ momentum relaxation time [Baccarani, Wordeman, '85]

$$E = \int \frac{1}{2} \frac{|J|^2}{\rho} + f(\rho) + \frac{1}{2}|\nabla V|^2 + \frac{1}{2}|\nabla\sqrt{\rho}|^2 \, dx$$

$$f(\rho) = \rho \int_{\rho_*}^{\rho} \frac{P(s) - P(\rho_*)}{s^2} \, ds$$

$$\frac{d}{dt} E(t) = -\frac{1}{\tau} \int \frac{|J|^2}{\rho} \, dx$$

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Finite energy weak solutions

$$\underbrace{\int \frac{1}{2}\rho|u|^2 + f(\rho) + \frac{1}{2}|\nabla V|^2 + \frac{1}{2}|\nabla\sqrt{\rho}|^2 \, dx}_{E(t)} + \frac{1}{\tau}\int_0^t\!\!\int \rho|u|^2 \, dx\, dt' \leq E(0)$$

$\frac{J}{\sqrt{\rho}} = \sqrt{\rho}\, u \in L^\infty(0,T;L^2)$, $\sqrt{\rho} \in L^\infty(0,T;H^1)$, $M(t) = \int \rho(t,x)\,dx = M_0$

$$\frac{1}{2}\rho\nabla\left(\frac{\Delta\sqrt{\rho}}{\sqrt{\rho}}\right) = \operatorname{div}\left(\frac{1}{4}\rho\nabla^2\log\rho\right) = \operatorname{div}\left(\frac{1}{4}\nabla^2\rho - \nabla\sqrt{\rho}\otimes\nabla\sqrt{\rho}\right)$$

Def (ρ, J) is a f.e.w.s. if there exists $\sqrt{\rho} \in L^2_t H^1_x$, $\Lambda \in L^\infty_t L^2_x$ s.t. $\rho = (\sqrt{\rho})^2$, $J = \sqrt{\rho}\,\Lambda$ &

$$\begin{cases} \partial_t \rho + \operatorname{div} J = 0 \\ \partial_t J + \operatorname{div}(\Lambda\otimes\Lambda) + \nabla P(\rho) + \rho\nabla V = \operatorname{div}\left(\frac{1}{4}\nabla^2\rho - \nabla\sqrt{\rho}\otimes\nabla\sqrt{\rho}\right) - \frac{1}{\tau}J \end{cases}$$

Th. (A., Marcati CMP 2009 & ARMA 2012)

$d=2,3$, $f(\rho)\sim\rho^{\gamma}$, $1<\gamma<\frac{d}{(d-2)_+}$, (ρ_0, J_0) be s.t.

there exists $\psi_0 \in H^1$ s.t. $\rho_0 = |\psi_0|^2$, $J_0 = \mathrm{Im}(\bar{\psi}_0 \nabla \psi_0)$.

Then there exists global in time f.e.w.s., with

$$\int \frac{1}{2}|\Lambda|^2 + \frac{1}{2}|\nabla\sqrt{\rho}|^2 + f(\rho) + \frac{1}{2}|\nabla V|^2 dx + \frac{1}{2}\int_0^t\int |\Lambda|^2 dx dt' \leq C E(0)$$

Th. (A., Marcati, Zheng, 2024+)

$d=1$, $1<\gamma<\infty$, (ρ_0, J_0) be finite energy, then global in time f.e.w.s.

strategy of proof

- exploit relation w. nonlinear Schrödinger eqn. through Madelung transform $\psi = \sqrt{\rho}\, e^{iS}$, $u = \nabla S$
- use fractional step method
- compactness by dispersive estimates

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Relaxation-time limit $\tau \to 0$

$$\rho^\tau(t,x) = \rho\left(\frac{t}{\tau},x\right), \quad J^\tau(t,x) = \frac{1}{\tau} J\left(\frac{t}{\tau},x\right)$$

$$\begin{cases} \partial_t \rho^\tau + \operatorname{div} J^\tau = 0 \\ \tau^2\left(\partial_t J^\tau + \operatorname{div}(\Lambda^\tau \otimes \Lambda^\tau)\right) + \nabla P(\rho^\tau) + \rho^\tau \nabla V^\tau = \operatorname{div}\left(\frac{1}{4}\nabla \rho^\tau - \nabla\sqrt{\rho^\tau} \otimes \nabla\sqrt{\rho^\tau}\right) - J^\tau \end{cases}$$

$$\underbrace{\int \frac{\tau^2}{2}|\Lambda^\tau|^2 + \frac{1}{2}|\nabla\sqrt{\rho^\tau}|^2 + f(\rho^\tau) + \frac{1}{2}|\nabla V^\tau|^2 dx}_{E^\tau(t)} + \int_0^t\int |\Lambda^\tau|^2 dx\,dt \leq C E^\tau(0)$$

$\rightarrow$ quantum drift-diffusion (QDD) eqn.

$$\begin{cases} \partial_t \bar\rho + \operatorname{div} \bar J = 0 \\ \bar J = \frac{1}{2}\bar\rho \nabla\left(\frac{\Delta\sqrt{\bar\rho}}{\sqrt{\bar\rho}}\right) - \nabla P(\bar\rho) - \bar\rho \nabla \bar V \end{cases}$$

[Jüngel, Matthes, 2008]

[Gianazza, Savaré, Toscani, 2009]

main obstruction $\sqrt{\rho^\tau} \in L^\infty_t H^1_x$

Quantum Navier-Stokes (qNS) eqns. $\rightsquigarrow$ viscosity helps

$x \in \mathbb{T}^3$

$$\begin{cases} \partial_t \rho + \operatorname{div} J = 0 \\ \tau^2 \left(\partial_t J + \operatorname{div}(\Lambda \otimes \Lambda) \right) + \nabla P(\rho) + \rho \nabla V = \frac{1}{2} \rho \nabla \left(\frac{\Delta \sqrt{\rho}}{\sqrt{\rho}} \right) + \nu \tau \operatorname{div}(\rho D u) - J \end{cases}$$

$$E^\tau(t) + \int_0^t \!\! \int |\Lambda^\tau|^2 \, dx\, dt' + \underbrace{\nu \tau \int_0^t \!\! \int \rho |Du|^2 \, dx\, dt'} \leq E^\tau(0)$$

$\hookrightarrow$ not rigorously correct, see for instance [Li, Xin, arXiv:1504.06826]

BD-entropy estimates

$w = \tau u + \nabla \log \rho$

$$\underbrace{\int \frac{1}{2} \rho |w|^2 + \frac{1}{2} |\nabla \sqrt{\rho}|^2 + f(\rho) + \frac{1}{2} |\nabla V|^2 + \frac{1}{\tau} \rho (\log \rho - 1) \, dx}_{E_{BD}(t)}$$

$$+ \tau \int_0^t \!\! \int \rho |\nabla^A u|^2 \, dx\, dt' + \frac{1}{\tau} \int_0^t \!\! \int \rho |\nabla^2 \log \rho|^2 \, dx\, dt' \leq E_{BD}(0)$$

Relaxation-time limit of qNS

Thus $\int \rho_0(\log\rho_0 - 1)\,dx < \infty \Rightarrow \int_0^t\int \rho^\tau |\nabla^2 \log\rho^\tau|^2\,dx\,dt' < \infty$.

Moreover, [Jüngel, Matthes, 2008]

$$\int_0^t\int |\nabla\rho^{\frac{1}{4}}|^2 + |\nabla^2\sqrt{\rho}|^2\,dx\,dt' \lesssim \int_0^t\int \rho\,|\nabla^2\log\rho|^2\,dx\,dt$$

<u>Th.</u> (A., Cianfarani Carnevale, Lattanzio, Spirito, J. Nonlin. Sci. 2021)

Let $(\sqrt{\rho^\tau}, \Lambda^\tau)$ be a global in time f.e.w.s. of qNS, with uniformly bounded energy. Then $\sqrt{\rho^\tau} \to \sqrt{\bar\rho}$ $L^2_t H^1_x$, where $\bar\rho$ solves QDD.

Need further estimates for the inviscid model

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GCP solutions for QHD # [A., Marcati, Zheng, CMP 2021]

$d=1, \ \frac{1}{\tau}=0$

$$\begin{cases} \partial_t \rho + \partial_x(\rho u) = 0 \\ \partial_t(\rho u) + \partial_x(\rho u^2 + p(\rho)) = \frac{1}{2}\rho\partial_x\left(\frac{\partial_{xx}\sqrt{\rho}}{\sqrt{\rho}}\right) \end{cases} \Rightarrow \begin{cases} \partial_t \rho = -\partial_x(\rho u) \\ \partial_t u = -\partial_x\left(\frac{u^2}{2} + f'(\rho) - \frac{1}{2}\frac{\partial_{xx}\sqrt{\rho}}{\sqrt{\rho}}\right) \end{cases}$$

$$\Downarrow$$

$$E = \int \frac{1}{2}\rho|u|^2 + f(\rho) + \frac{1}{2}(\partial_x\sqrt{\rho})^2 dx \Rightarrow \begin{cases} \partial_t \rho = -\partial_x \frac{\delta E}{\delta u} \\ \partial_t u = -\partial_x \frac{\delta E}{\delta \rho} \end{cases}$$

Hamilton eqns. with symplectic struct. given by ∂_x

$$\mu = \frac{\delta E}{\delta \rho} = \frac{1}{2}|u|^2 + f'(\rho) - \frac{1}{2}\frac{\partial_{xx}\sqrt{\rho}}{\sqrt{\rho}}$$ chemical potential

$$I(t) = \int \frac{1}{2}\rho\mu^2 + \underbrace{\frac{1}{2}\rho\sigma^2}_{\frac{1}{2}(\partial_t\sqrt{\rho})^2} dx, \quad \sigma = \frac{\partial_x(\rho u)}{2\rho} = -\partial_t \log\sqrt{\rho}$$

$I(t) \le C(t, E_0, M_0)\, I(0)$

$$I(t) = \int \frac{1}{2}\underbrace{\rho\mu^2}_{\lambda^2} + \frac{1}{2}(\partial_t\sqrt{\rho})^2 \, dx \quad , \quad \mu = \frac{1}{2}|u|^2 + f'(\rho) - \frac{1}{2}\frac{\partial_{xx}\sqrt{\rho}}{\sqrt{\rho}}$$

$\lambda = \sqrt{\rho}\mu$ generalized chemical potential

$$\sqrt{\rho}\lambda = \rho\mu = -\frac{1}{4}\partial_{xx}\rho + \frac{1}{2}\Lambda^2 + \frac{1}{2}(\partial_x\sqrt{\rho})^2 + \rho f'(\rho)$$

Def (GCP solutions)

(ρ, J) GCP solutions to QHD if they are

- finite energy, i.e. $(\sqrt{\rho}, \Lambda) \in L^\infty_t(H^1 \times L^2)_x$
- $\exists\ \lambda \in L^\infty_t L^2_x$ s.t. $\sqrt{\rho}\lambda = -\frac{1}{4}\partial_{xx}\rho + \frac{1}{2}\Lambda^2 + \frac{1}{2}(\partial_x\sqrt{\rho})^2 + \rho f'(\rho)$
- $\partial_t\sqrt{\rho} \in L^\infty_t L^2_x$

Th. (A., Marcati, Zheng, CMP 2021)

$\{(\rho_n, J_n)\}$ GCP solutions with

$$\|\sqrt{\rho_n}\|_{L^\infty_t H^1_x} + \|\Lambda_n\|_{L^\infty_t L^2_x} + \|\lambda_n\|_{L^\infty_t L^2_x} + \|\partial_t\sqrt{\rho_n}\|_{L^\infty_t L^2_x} \leq C.$$

then, $\sqrt{\rho_n} \to \sqrt{\rho}$ $L^2_t H^1_{x,loc}$, $\Lambda_n \to \Lambda$ $L^2_t L^2_{x,loc}$ & $(\rho, J) = ((\sqrt{\rho})^2, \sqrt{\rho}\Lambda)$ solves QHD

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GCP solutions for QHD w. damping

$$\begin{cases} \partial_t \rho + \partial_x(\rho u) = 0 \\ \partial_t u + \partial_x \mu + \frac{1}{\tau} u = 0 \end{cases}, \quad \mu = \frac{\delta E}{\delta \rho} = \frac{1}{2}u^2 + f'(\rho) - \frac{1}{2}\frac{\partial_{xx}\sqrt{\rho}}{\sqrt{\rho}}$$

velocity potential S, $u = \partial_x S \Rightarrow \partial_t S + \mu + \frac{1}{\tau} S = 0$

$$\nabla_{t,x} S = \begin{pmatrix} -\mu - \frac{1}{\tau}S \\ u \end{pmatrix} \quad \& \quad \nabla_{t,x} \times \begin{pmatrix} -\mu - \frac{1}{\tau}S \\ u \end{pmatrix} = \partial_t u + \partial_x \mu + \frac{1}{\tau} u = 0$$

Madelung transformation $\psi = \sqrt{\rho}\, e^{iS}$

(ρ, u) solns. to QHD w. damping $\Longleftrightarrow$ $i\partial_t \psi = -\frac{1}{2}\partial_{xx}\psi + f'(|\psi|^2)\psi + \frac{1}{\tau} S \psi$

rigorously: avoid vacuum
control fluctuations of ρ by total energy E

$x \in \mathbb{T}$, $\rho_0 \geq \delta$, $E_0 \leq \frac{1}{2}\left(M_0^{\frac{1}{2}} - \delta M_0^{-\frac{1}{2}}\right)^2$, $M_0 = \int \rho_0(x)\,dx$

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Th. (A., Marcati, Zheng, 2024+)

$x \in \mathbb{T}$, (ρ_0, J_0) be finite energy s.t.

- $\rho_0 \geq \delta > 0$
- $E_0 \leq \frac{1}{2}\left(M_0^{\frac{1}{2}} - \delta M_0^{-\frac{1}{2}}\right)^2$
- $I(0) < \infty$

Then, there exists global in time GCP solution of QHD w. damping.
Moreover, for the rescaled quantities (ρ^τ, J^τ) we have

$$\|\rho^\tau - \bar{\rho}\|_{L^\infty_t L^2_x} + \|J^\tau - \bar{J}\|_{L^1_{t,x}} \leq C(M_0, E_0, I_0, \delta)\,\tau,$$

with $(\bar{\rho}, \bar{J})$ sol. to QDD eqn.

Thank you!

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