

Matrix-valued Quantum Boltzmann Methods

joint work with Jianfeng Lu, Martin L.R. Fürst, Herbert Spohn

Christian B. Mendl

Stanford University, USA

November 29, 2016



Stanford
University



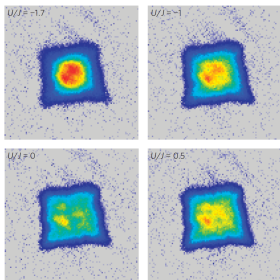
Alexander von Humboldt
Stiftung/Foundation

KI-Net Workshop

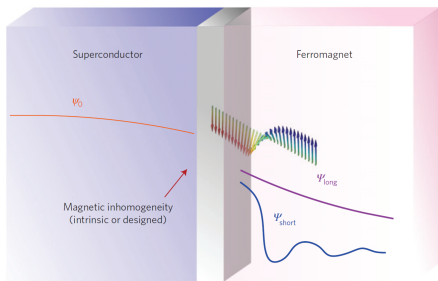
Stochastic and deterministic methods in kinetic theory

Duke University, NC, USA

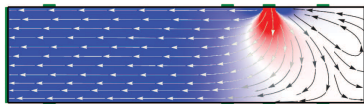
Introduction: Boltzmann equations for quantum systems



(a) ultracold atoms in an optical lattice (Schneider et al., Science 2012)

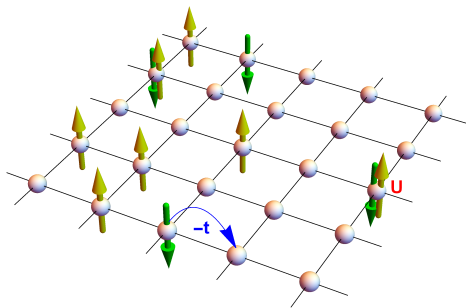


(b) superconducting spintronics (Linder and Robinson, Nat. Phys. 2015)



(c) Viscous electron backflow (Bandurin et al., Science 2016)

Quantum Boltzmann derived from the Hubbard model



Second order time-dependent perturbation theory for $U \ll 1 \rightsquigarrow$

$$\frac{\partial}{\partial t} W(k, t) = \mathcal{C}_{\text{cons}}[W](k, t) + \mathcal{C}_{\text{diss}}[W](k, t) = \mathcal{C}[W](k, t)$$

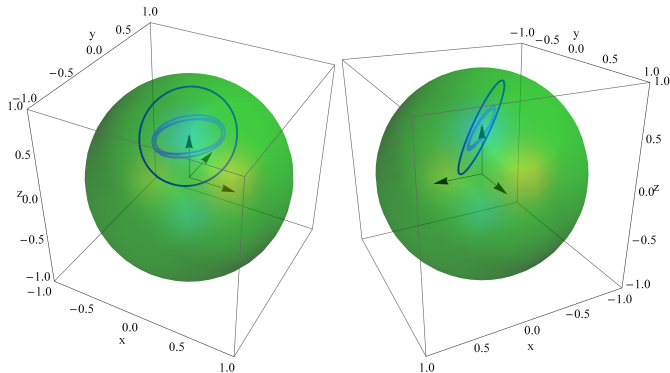
Wigner function $W(k, t)$ is the 2×2 matrix-valued “spin density matrix”.

Fürst, Lukkarinen, Mei, Spohn, J. Phys. A 46, 485002 (2013)

Bloch sphere representation

Bloch sphere representation $\vec{r}(k, t) \in \mathbb{R}^3$ of $W(k, t)$:

$$W(k, t) = \frac{1}{2} (\alpha \mathbb{1} + \vec{r}(k, t) \cdot \vec{\sigma}), \quad \vec{\sigma} = (\sigma_x, \sigma_y, \sigma_z).$$



$k \in \mathbb{T} = [-\frac{1}{2}, \frac{1}{2})$ parametrizes a closed path within the Bloch sphere.

Conservative collision operator $\mathcal{C}_{\text{cons}}[W]$

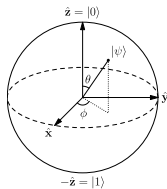
Vlasov type commutator:

$$\mathcal{C}_{\text{cons}}[W](k, t) = -i[H_{\text{eff}}(k, t), W(k, t)],$$

with an effective Hamiltonian $H_{\text{eff}}(k, t)$ itself depending on $W(\cdot, t)$.

\rightsquigarrow k -dependent **rotations** on the Bloch sphere.

Denoted “conservative” since $\text{tr}[W]$
does not change, and entropy does not increase.



Dissipative collision operator $\mathcal{C}_{\text{diss}}[W]$

Notation: $\tilde{W} = \mathbb{1} - W$,

$\underline{k} = k_1 + k_2 - k_3 - k_4 \pmod{1}$,

$\underline{\omega} = \omega(k_1) + \omega(k_2) - \omega(k_3) - \omega(k_4)$.

$$\mathcal{C}_{\text{diss}}[W](k_1) = \pi \int_{\mathbb{T}^3} \delta(\underline{k}) \delta(\underline{\omega}) (\mathcal{A}[W]_{1234} + \mathcal{A}[W]_{1234}^\dagger) dk_2 dk_3 dk_4,$$

Dissipative collision operator $\mathcal{C}_{\text{diss}}[W]$

Notation: $\tilde{W} = \mathbb{1} - W$,

$\underline{k} = k_1 + k_2 - k_3 - k_4 \pmod{1}$,

$\underline{\omega} = \omega(k_1) + \omega(k_2) - \omega(k_3) - \omega(k_4)$.

$$\mathcal{C}_{\text{diss}}[W](k_1) = \pi \int_{\mathbb{T}^3} \delta(\underline{k}) \delta(\underline{\omega}) (\mathcal{A}[W]_{1234} + \mathcal{A}[W]_{1234}^\dagger) dk_2 dk_3 dk_4,$$

with

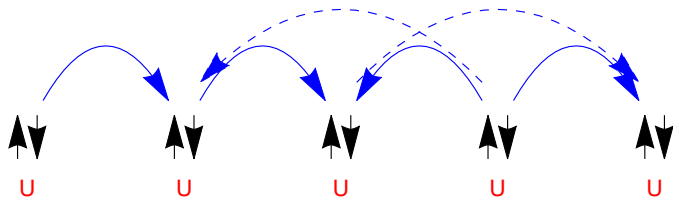
$$\begin{aligned} \mathcal{A}[W]_{1234} = & -W_4 \tilde{W}_2 W_3 + W_4 \operatorname{tr}[\tilde{W}_2 W_3] \\ & - (\tilde{W}_4 W_3 - \tilde{W}_4 W_2 - \tilde{W}_2 W_3 + \tilde{W}_4 \operatorname{tr}[W_2] \\ & - \tilde{W}_4 \operatorname{tr}[W_3] + \operatorname{tr}[W_3 \tilde{W}_2]) W_1 \end{aligned}$$

with **gain term (+ h.c.)** and **loss term (+ h.c.)**. The gain term is always positive definite since

$$A \operatorname{tr}[BC] + C \operatorname{tr}[BA] - ABC - CBA \geq 0$$

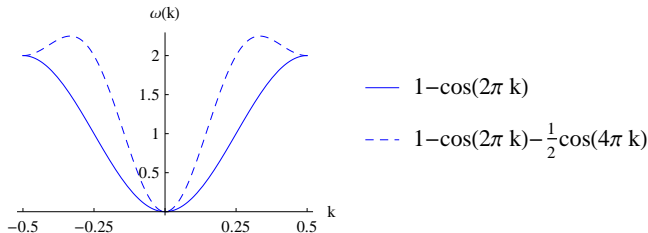
for any positive definite matrices A, B, C .

(Next-)nearest neighbor hopping model (1D)



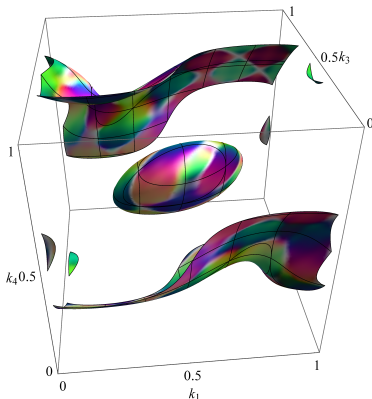
Nearest neighbor hopping: $\omega(k) = 1 - \cos(2\pi k)$

Next-nearest neighbor: $\omega_\eta(k) = 1 - \cos(2\pi k) - \eta \cos(4\pi k)$



Collision channels for next-nearest neighbor hopping (1D)

Simultaneous non-trivial solutions of momentum and energy conservation constraints, here $\omega_\eta(k) = 1 - \cos(2\pi k) - \eta \cos(4\pi k)$ with $\eta = \frac{1}{2}$:



Discretization of the collision manifold which preserves discrete (finite k -grid) conservation laws exactly.

Mollification of $\mathcal{C}_{\text{diss}}[W]$

Conservative collision operator

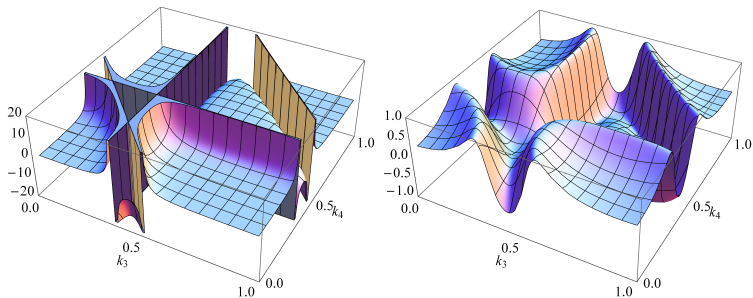
$$\mathcal{C}_{\text{cons}}[W](k, t) = -i [H_{\text{eff}}(k, t), W(k, t)],$$

integral defining $H_{\text{eff}}(k, t)$ contains principal value term $\mathcal{P}\left(\frac{1}{\underline{\omega}}\right)$.

“Mollification”:

$$\frac{1}{\underline{\omega}} \rightarrow \frac{\underline{\omega}}{\underline{\omega}^2 + \epsilon^2}$$

with finite $\epsilon > 0$ (here $\epsilon = \frac{1}{2}$):



Invariances and conservation laws

- SU(2) invariance of H :

$$\mathcal{C}[U^\dagger W U] = U^\dagger \mathcal{C}[W] U$$

for all $U \in \text{SU}(2)$. Hermiticity is propagated in time

- Fermi property $0 \leq W(k, t) \leq 1$ (eigenvalues) is propagated in time
- spin density conservation

$$\frac{d}{dt} \int_{\mathbb{T}^d} W(k, t) dk = 0$$

- energy conservation

$$\frac{d}{dt} \int_{\mathbb{T}^d} \omega(k) \text{tr}[W(k, t)] dk = 0$$

Entropy and H-theorem

Entropy of a state $W(k)$:

$$S[W] = - \int_{\mathbb{T}^d} \text{tr}[W(k) \log W(k)] + \text{tr}[\tilde{W}(k) \log \tilde{W}(k)] dk,$$

and corresponding entropy production

$$\sigma[W] = \frac{d}{dt} S[W] = - \int_{\mathbb{T}^d} \text{tr}[(\log W(k) - \log \tilde{W}(k)) \mathcal{C}[W](k)] dk.$$

Entropy and H-theorem

Entropy of a state $W(k)$:

$$S[W] = - \int_{\mathbb{T}^d} \text{tr}[W(k) \log W(k)] + \text{tr}[\tilde{W}(k) \log \tilde{W}(k)] dk,$$

and corresponding entropy production

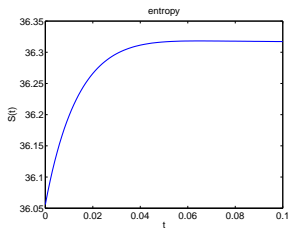
$$\sigma[W] = \frac{d}{dt} S[W] = - \int_{\mathbb{T}^d} \text{tr}[(\log W(k) - \log \tilde{W}(k)) \mathcal{C}[W](k)] dk.$$

The *H-theorem* asserts that

$$\sigma[W] \geq 0 \quad \text{for all } W \text{ with } 0 \leq W \leq 1$$

(We prove the H-theorem by writing $\sigma[W]$ as an integral of non-negative terms times $(x - y) \log(x/y) \geq 0$.)

Fürst, Mendl, Spohn, Phys. Rev. E 86, 031122 (2012)



(Thermal) Stationary states

Stationarity $\leftrightarrow \mathcal{C}[W] = 0$

In particular, entropy production $\sigma[W] = 0$. Physically, thermal equilibrium (Fermi-Dirac) states should be stationary:

$$W_{\text{FD}}(k) = \sum_{\sigma \in \{\uparrow, \downarrow\}} \left(e^{\beta(\omega(k) - \mu_{\sigma})} + 1 \right)^{-1} |\sigma\rangle\langle\sigma|,$$

$W_{\text{FD}}(k)$ indeed fulfills $\mathcal{C}[W_{\text{FD}}] = 0$.

(Thermal) Stationary states

Stationarity $\leftrightarrow \mathcal{C}[W] = 0$

In particular, entropy production $\sigma[W] = 0$. Physically, thermal equilibrium (Fermi-Dirac) states should be stationary:

$$W_{\text{FD}}(k) = \sum_{\sigma \in \{\uparrow, \downarrow\}} \left(e^{\beta(\omega(k) - \mu_\sigma)} + 1 \right)^{-1} |\sigma\rangle\langle\sigma|,$$

$W_{\text{FD}}(k)$ indeed fulfills $\mathcal{C}[W_{\text{FD}}] = 0$.

Conservation laws uniquely define $W_{\text{FD}}(k)$, can map initial $W(k, 0)$ to asymptotic $W(k, t)$ as $t \rightarrow \infty$

All stationary states of this form? \rightsquigarrow depends on dispersion relation!

Simulation example (1D): initial state

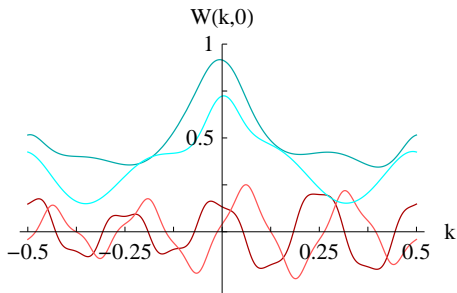
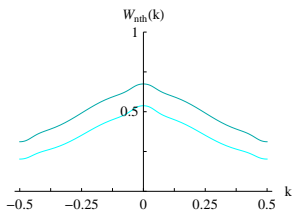


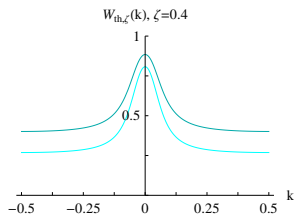
Figure: Cyan (upper) curves: real diagonal entries, darker and lighter red curves: real and imaginary parts of the off-diagonal $|\uparrow\rangle\langle\downarrow|$ entry, respectively

Fürst, Mendl, Spohn, Phys. Rev. E 88, 012108 (2013)

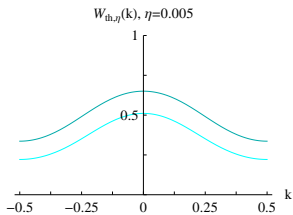
Simulation example (1D): asymptotic ($t \rightarrow \infty$) states



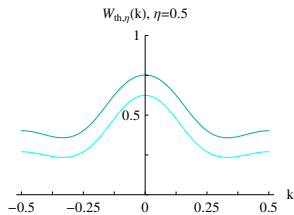
(a) non-thermal stationary state (nearest neighbor)



(b) thermal equilibrium state (exponential, $\zeta = \frac{2}{5}$)



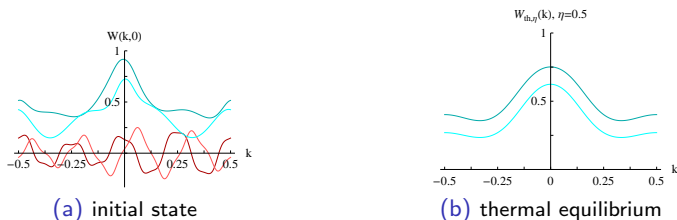
(c) thermal equilibrium state (next-nearest neighbor hopping with $\eta = \frac{1}{200}$)



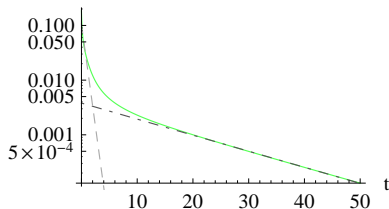
(d) thermal equilibrium state (next-nearest neighbor hopping with $\eta = \frac{1}{2}$)

Simulation example (1D): entropy convergence

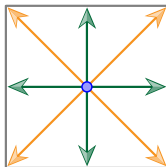
Entropy convergence for next-nearest neighbor hopping with $\eta = \frac{1}{2}$



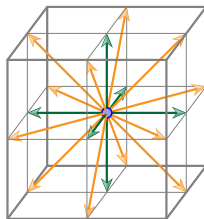
$S[W_{th,\eta}] - S[W(t)], \eta=0.5$



Quantum lattice Boltzmann methods (LBM)



D2Q9 model



D3Q19 model

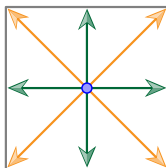
C. B. Mendl, Int. J. Mod. Phys. C 26, 1550113 (2015)

Spatially inhomogeneous version, using LBM

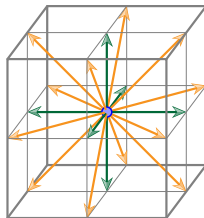
Spatially inhomogeneous case: Wigner function depends on position \mathbf{x} , Boltzmann equation is augmented by transport term:

$$\frac{\partial}{\partial t} W(\mathbf{x}, \mathbf{p}, t) + \nabla_{\mathbf{p}} \omega(\mathbf{p}) \cdot \nabla_{\mathbf{x}} W(\mathbf{x}, \mathbf{p}, t) = \mathcal{C}[W](\mathbf{x}, \mathbf{p}, t).$$

Discretization of momentum by the lattice Boltzmann method (LBM):



D2Q9 model



D3Q19 model

Figure: Illustration of the velocity vectors \mathbf{e}_i of the D2Q9 and D3Q19 models (adapted from Thürey 2006)

Quantum LBM: Quadrature rules

Idea: construct quadrature rules with **Fermi-Dirac weight** which are compatible with D2Q9 and D3Q19 discretizations:

$$\frac{1}{n_{2,\beta,\mu}} \int_{\mathbb{R}^2} h(\mathbf{p}) \left(e^{\beta(\frac{1}{2}\mathbf{p}^2 - \mu)} + 1 \right)^{-1} d\mathbf{p} \approx \sum_{i_1, i_2 \in \{-1, 0, 1\}} w_i h(\xi \mathbf{i})$$

(analogous in 3D) for smooth functions $h : \mathbb{R}^2 \rightarrow \mathbb{R}$, with equality for polynomials up to order 5.

Quantum LBM: Quadrature rules

Idea: construct quadrature rules with **Fermi-Dirac weight** which are compatible with D2Q9 and D3Q19 discretizations:

$$\frac{1}{n_{2,\beta,\mu}} \int_{\mathbb{R}^2} h(\mathbf{p}) \left(e^{\beta(\frac{1}{2}\mathbf{p}^2 - \mu)} + 1 \right)^{-1} d\mathbf{p} \approx \sum_{i_1, i_2 \in \{-1, 0, 1\}} w_i h(\xi \mathbf{i})$$

(analogous in 3D) for smooth functions $h : \mathbb{R}^2 \rightarrow \mathbb{R}$, with equality for polynomials up to order 5.

Analytic solution

$$w_{00} = 1 - 5a, \quad w_{01} = a, \quad w_{11} = \frac{a}{4},$$
$$a = \frac{F_1(\beta\mu)^2}{9 F_0(\beta\mu) F_2(\beta\mu)}, \quad \xi = \left(\frac{3 F_2(\beta\mu)}{\beta F_1(\beta\mu)} \right)^{1/2},$$

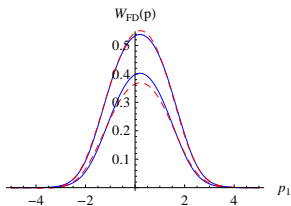
with $F_k(x)$ the complete Fermi-Dirac integral.

Quantum LBM: polynomial expansion of $W_{\text{FD}}(k)$

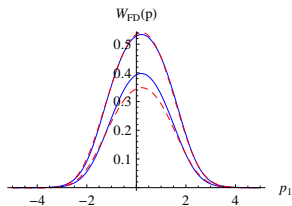
Goal: construct approximate equilibrium distribution function compatible with the quadrature formula, such that its moments agree with the exact Fermi-Dirac density, velocity and energy (analogous to “classical” LBM):

$$W^{(\text{eq})}(\mathbf{p}) = \frac{1}{n_{d,\beta_0,0}} \left(e^{\beta_0 \frac{1}{2} \mathbf{p}^2} + 1 \right)^{-1} U \begin{pmatrix} n_{d,\beta,\mu_\uparrow} & 0 \\ 0 & n_{d,\beta,\mu_\downarrow} \end{pmatrix} U^* \\ \times \underbrace{\left(\alpha_1 + \alpha_2 \beta_0 \frac{1}{2} \mathbf{p}^2 + \alpha_3 \beta_0 (\mathbf{p} \cdot \mathbf{u}) + \alpha_4 (\beta_0 \mathbf{p} \cdot \mathbf{u})^2 + \alpha_5 \beta_0 \frac{1}{2} \mathbf{u}^2 \right)}_{\text{polynomial in } \mathbf{p}},$$

with the coefficients α_j to be determined.



(a) $d = 2, \beta_0 = 0.8$



(b) $d = 3, \beta_0 = 0.8$

Quantum LBM: Algorithm

time step $t \rightarrow t + \Delta t$:

- For each cell \mathbf{x} , compute local average density ρ , velocity \mathbf{u} and energy $\varepsilon \rightsquigarrow$ local equilibrium function

$$W_i^{(\text{eq})} = w_i \rho \left(\alpha_1 + \alpha_2 \beta_0 \frac{1}{2} \mathbf{e}_i^2 + \alpha_3 \beta_0 (\mathbf{e}_i \cdot \mathbf{u}) + \alpha_4 (\beta_0 \mathbf{e}_i \cdot \mathbf{u})^2 + \alpha_5 \beta_0 \frac{1}{2} \mathbf{u}^2 \right)$$

Quantum LBM: Algorithm

time step $t \rightarrow t + \Delta t$:

- For each cell \mathbf{x} , compute local average density ρ , velocity \mathbf{u} and energy $\varepsilon \rightsquigarrow$ local equilibrium function

$$W_i^{(\text{eq})} = w_i \rho \left(\alpha_1 + \alpha_2 \beta_0 \frac{1}{2} \mathbf{e}_i^2 + \alpha_3 \beta_0 (\mathbf{e}_i \cdot \mathbf{u}) + \alpha_4 (\beta_0 \mathbf{e}_i \cdot \mathbf{u})^2 + \alpha_5 \beta_0 \frac{1}{2} \mathbf{u}^2 \right)$$

- Collision: for each cell \mathbf{x} , apply discretized BGK collision operator:

$$W_i^{\text{coll}}(\mathbf{x}, t) = W_i(\mathbf{x}, t) + \frac{\Delta t}{\tau} \left(W_i^{(\text{eq})} - W_i(\mathbf{x}, t) \right)$$

Quantum LBM: Algorithm

time step $t \rightarrow t + \Delta t$:

- For each cell \mathbf{x} , compute local average density ρ , velocity \mathbf{u} and energy $\varepsilon \rightsquigarrow$ local equilibrium function

$$W_i^{(\text{eq})} = w_i \rho \left(\alpha_1 + \alpha_2 \beta_0 \frac{1}{2} \mathbf{e}_i^2 + \alpha_3 \beta_0 (\mathbf{e}_i \cdot \mathbf{u}) + \alpha_4 (\beta_0 \mathbf{e}_i \cdot \mathbf{u})^2 + \alpha_5 \beta_0 \frac{1}{2} \mathbf{u}^2 \right)$$

- Collision: for each cell \mathbf{x} , apply discretized BGK collision operator:

$$W_i^{\text{coll}}(\mathbf{x}, t) = W_i(\mathbf{x}, t) + \frac{\Delta t}{\tau} \left(W_i^{(\text{eq})} - W_i(\mathbf{x}, t) \right)$$

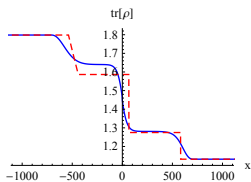
- Streaming:

$$W_i(\mathbf{x} + \Delta t \mathbf{e}_i, t + \Delta t) = W_i^{\text{coll}}(\mathbf{x}, t)$$

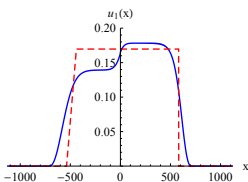
for all $i = 1, \dots, b$ and cells \mathbf{x} , to approximate transport term $\boldsymbol{\rho} \cdot \nabla_{\mathbf{x}} W(\mathbf{x}, \boldsymbol{\rho}, t)$

Quantum LBM: Validation

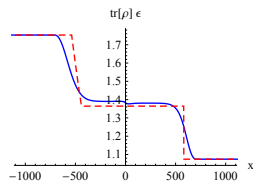
Comparison with analytic Riemann problem solution
(quasi-1D, 2048×2):



(a) density $\text{tr}[\rho]$



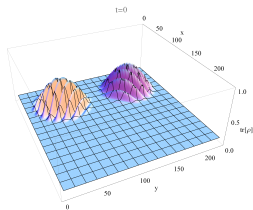
(b) velocity



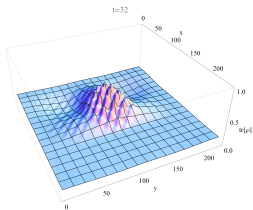
(c) pressure
 $P = (\gamma - 1) \text{tr}[\rho] \epsilon$

Adiabatic exponent $\gamma = 1 + \frac{2}{d} = 2$

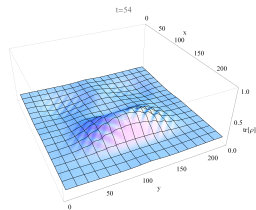
Quantum LBM simulation example



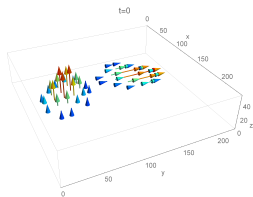
(a) $\text{tr}[\rho]$ at $t = 0$



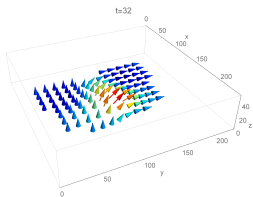
(b) $\text{tr}[\rho]$ at time step 32



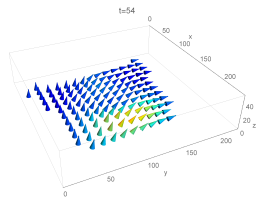
(c) $\text{tr}[\rho]$ at time step 54



(d) Bloch vectors at $t = 0$



(e) Bloch vectors at time step 32



(f) Bloch vectors at time step 54

C. B. Mendl, Int. J. Mod. Phys. C 26, 1550113 (2015)

Quantum LBM simulation example (animation)

Matrix-valued Quantum Lattice Boltzmann Method

Time evolution of the spin density matrix $\rho(x,t)$

Left: trace of density matrix

Right: Bloch vectors

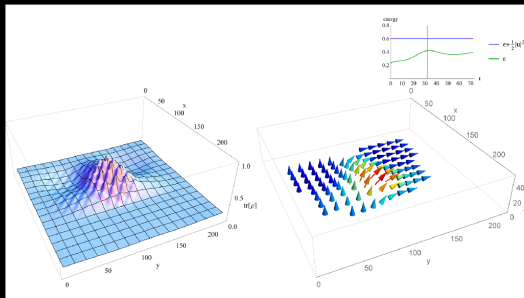
Inset: global energy

Simulation grid: 128 x 128

Relaxation time: 10

Christian B. Mendl

<http://christian.mendl.net>



Reference: Int. J. Mod. Phys. C 26, 1550113 (2015)

Spectral methods for the quantum Boltzmann equation

Lu and Mendl, J. Comput. Phys. 291, 303–316 (2015)

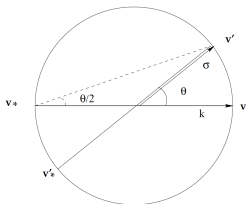
Spectral methods for the quantum Boltzmann equation

Idea: use fast Fourier spectral methods to evaluate the collision operators.

Carleman representation: perform a change of variables $p_1 \mapsto v$, $p_3 \mapsto v + u$, $p_4 \mapsto v + u'$, such that

$$p_2 = p_3 + p_4 - p_1 = v + u + u';$$

$$\underline{\omega} = \omega(p_1) + \omega(p_2) - \omega(p_3) - \omega(p_4) = u \cdot u'$$



Spectral methods for the quantum Boltzmann equation

Idea: use fast Fourier spectral methods to evaluate the collision operators.

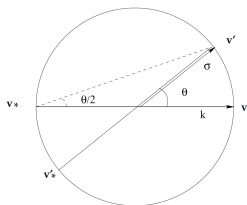
Carleman representation: perform a change of variables $p_1 \mapsto v, p_3 \mapsto v + u, p_4 \mapsto v + u'$, such that

$$p_2 = p_3 + p_4 - p_1 = v + u + u';$$

$$\underline{\omega} = \omega(p_1) + \omega(p_2) - \omega(p_3) - \omega(p_4) = u \cdot u'$$

\rightsquigarrow integral defining $\mathcal{C}_{\text{cons}}[W]$ can be written as

$$I_1(v) = \int_{B_R} \int_{B_R} \mathcal{P}\left(\frac{1}{u \cdot u'}\right) f(v+u)g(v+u+u')h(v) du du'$$



Spectral methods for the quantum Boltzmann equation

Idea: use fast Fourier spectral methods to evaluate the collision operators.

Carleman representation: perform a change of variables $p_1 \mapsto v, p_3 \mapsto v + u, p_4 \mapsto v + u'$, such that

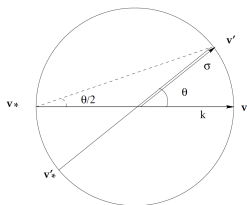
$$p_2 = p_3 + p_4 - p_1 = v + u + u';$$

$$\underline{\omega} = \omega(p_1) + \omega(p_2) - \omega(p_3) - \omega(p_4) = \mathbf{u} \cdot \mathbf{u}'$$

\rightsquigarrow integral defining $\mathcal{C}_{\text{CONS}}[W]$ can be written as

$$I_1(v) = \int_{B_R} \int_{B_R} \mathcal{P}\left(\frac{1}{\mathbf{u} \cdot \mathbf{u}'}\right) f(v+u)g(v+u+u')h(v) du du'$$

Next step: Fourier representation



Spectral methods: Fourier representation

Fourier representation:

$$\begin{aligned} I_1(v) &= \int_{B_R} \int_{B_R} \mathcal{P}\left(\frac{1}{u \cdot u'}\right) f(v+u)g(v+u+u')h(v) \, du \, du' \\ &\approx \sum_{\chi, \eta, \zeta} \hat{f}(\chi) \hat{g}(\eta) \hat{h}(\zeta) e^{j\frac{\pi}{L}v \cdot (\chi + \eta + \zeta)} G(\chi + \eta, \eta) \end{aligned}$$

with

$$G(\xi, \chi) = - \int_{S^1} \int_{S^1} \mathcal{P}\left(\frac{1}{\theta \cdot \theta'}\right) \phi_R(\xi \cdot \theta) \phi_R(\chi \cdot \theta') \, d\theta \, d\theta'.$$

Spectral methods: Fourier representation

Fourier representation:

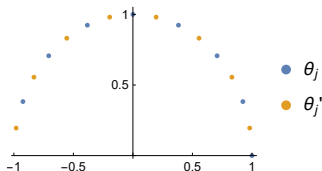
$$I_1(v) = \int_{B_R} \int_{B_R} \mathcal{P}\left(\frac{1}{u \cdot u'}\right) f(v+u)g(v+u+u')h(v) du du' \\ \approx \sum_{\chi, \eta, \zeta} \hat{f}(\chi) \hat{g}(\eta) \hat{h}(\zeta) e^{j\frac{\pi}{L}v \cdot (\chi + \eta + \zeta)} G(\chi + \eta, \eta)$$

with

$$G(\xi, \chi) = - \int_{S^1} \int_{S^1} \mathcal{P}\left(\frac{1}{\theta \cdot \theta'}\right) \phi_R(\xi \cdot \theta) \phi_R(\chi \cdot \theta') d\theta d\theta'.$$

Use numerical quadrature with uniform grid to approximate angular integrals:

$$G(\xi, \chi) \approx \sum_{j=1}^J \sum_{j'=1}^J \omega_{G,j,j'} \phi_{R,j}(\xi) \phi'_{R,j'}(\chi)$$



Spectral methods for the quantum Boltzmann equation

In summary, obtain the approximation

$$\begin{aligned}\hat{I}_1(\xi) &\approx \sum_{\substack{\chi, \eta, \zeta, \\ \chi + \eta + \zeta = \xi}} \sum_{j, j'} \omega_{G, j, j'} \hat{f}(\chi) \hat{g}(\eta) \hat{h}(\zeta) \phi_{R, j}(\chi + \eta) \phi'_{R, j'}(\eta) \\ &= \sum_{j, j'} \omega_{G, j, j'} \sum_{\zeta} \left[\sum_{\eta} \hat{f}(\xi - \zeta - \eta) (\phi'_{R, j'}(\eta) \hat{g}(\eta)) \right] \phi_{R, j}(\xi - \zeta) \hat{h}(\zeta).\end{aligned}$$

Overall cost: $\mathcal{O}(J^2 N^2 \log N)$

Spectral methods for the quantum Boltzmann equation

In summary, obtain the approximation

$$\begin{aligned}\hat{I}_1(\xi) &\approx \sum_{\substack{\chi, \eta, \zeta, \\ \chi + \eta + \zeta = \xi}} \sum_{j, j'} \omega_{G, j, j'} \hat{f}(\chi) \hat{g}(\eta) \hat{h}(\zeta) \phi_{R, j}(\chi + \eta) \phi'_{R, j'}(\eta) \\ &= \sum_{j, j'} \omega_{G, j, j'} \sum_{\zeta} \left[\sum_{\eta} \hat{f}(\xi - \zeta - \eta) (\phi'_{R, j'}(\eta) \hat{g}(\eta)) \right] \phi_{R, j}(\xi - \zeta) \hat{h}(\zeta).\end{aligned}$$

Overall cost: $\mathcal{O}(J^2 N^2 \log N)$

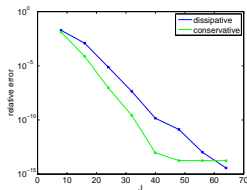
Similar approach for conservative collision operator, combined with

$$\frac{2}{\pi} \frac{\sin(\pi R \theta)}{\theta} = \int_{-R}^R e^{i\pi \theta \rho} d\rho \approx \sum_{m=1}^M \omega_m e^{i\pi \theta \rho_m}$$

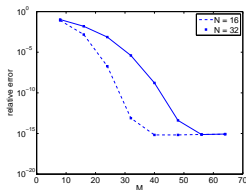
with $(\rho_m, \omega_m)_m$ the points and weights of a quadrature rule.

Hu and Ying, Commun. Math. Sci. 10, 989–999 (2012)

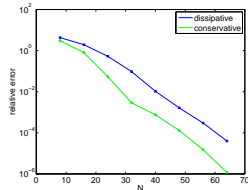
Spectral methods: Convergence test



(a) convergence with J



(b) convergence with M



(c) convergence with N

Figure: Exponential convergence of the dissipative $\mathcal{C}_{\text{diss}}$ and conservative $\mathcal{C}_{\text{cons}}$ collision operator calculation with respect to J , M and N

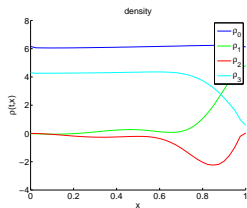
J : number of angular grid points

M : number of Gauss-Legendre quadrature points on $[-R, R]$

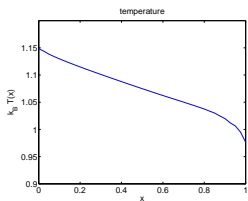
N : Fourier grid size in each direction

Spectral methods: Simulation example

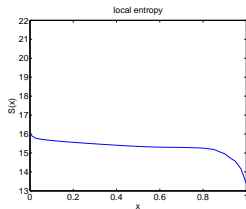
Dirichlet boundary conditions:



(a) stationary density



(b) $k_B T$



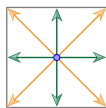
(c) local entropy

Summary and conclusions

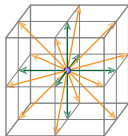
- Quantum Boltzmann equation derived from the Hubbard model, 2×2 matrix-valued due to spin
- Thermal equilibrium (Fermi-Dirac) states are stationary,

$$W_{\text{FD}}(k) = \sum_{\sigma \in \{\uparrow, \downarrow\}} \left(e^{\beta(\omega(k) - \mu_{\sigma})} + 1 \right)^{-1} |\sigma\rangle\langle\sigma|,$$

- Numerically observe exponentially fast convergence to the predicted stationary state in 1D
- Generalization of the classical lattice Boltzmann method (LBM) to the quantum setting
- Fast evaluation of collision operator by spectral methods











D2Q9 model









D3Q19 model

References I

-  Bandurin, D. A. et al. (2016). “Negative local resistance caused by viscous electron backflow in graphene”. In: *Science* 351, pp. 1055–1058.
-  Erdős, L. et al. (2004). “On the quantum Boltzmann equation”. In: *J. Stat. Phys.* 116, pp. 367–380.
-  Fürst, M. L. R. et al. (2012). “Matrix-valued Boltzmann equation for the Hubbard chain”. In: *Phys. Rev. E* 86, p. 031122.
-  Fürst, M. L. R. et al. (2013a). “Derivation of a matrix-valued Boltzmann equation for the Hubbard model”. In: *J. Phys. A* 46, p. 485002.
-  Fürst, M. L. R. et al. (2013b). “Matrix-valued Boltzmann equation for the non-integrable Hubbard chain”. In: *Phys. Rev. E* 88, p. 012108.
-  – (2014). “Dynamics of the Bose-Hubbard chain for weak interactions”. In: *Phys. Rev. B* 89, p. 134311.
-  Hu, J. and Ying, L. (2012). “A fast spectral algorithm for the quantum Boltzmann collision operator”. In: *Commun. Math. Sci.* 10, pp. 989–999.
-  Linder, J. and Robinson, J. W. A. (2015). “Superconducting spintronics”. In: *Nat. Phys.* 11, pp. 307–315.

References II

-  Lu, J. and Mendl, C. B. (2015). “Numerical scheme for a spatially inhomogeneous matrix-valued quantum Boltzmann equation”. In: *J. Comput. Phys.* 291, pp. 303–316.
-  Lukkarinen, J. and Spohn, H. (2009). “Not to normal order – Notes on the kinetic limit for weakly interacting quantum fluids”. In: *J. Stat. Phys.* 134, pp. 1133–1172.
-  Mendl, C. B. (2015). “Matrix-valued quantum lattice Boltzmann method”. In: *Int. J. Mod. Phys. C* 26, p. 1550113.
-  Schneider, U. et al. (2012). “Fermionic transport and out-of-equilibrium dynamics in a homogeneous Hubbard model with ultracold atoms”. In: *Nat. Phys.* 8, pp. 213–218.
-  Spohn, H. (2006). “Collisional invariants for the phonon Boltzmann equation”. In: *J. Stat. Phys.* 124, pp. 1131–1135.
-  Thürey, N. (2006). “Physically based animation of free surface flows with the lattice Boltzmann method”. PhD thesis. Technische Fakultät der Universität Erlangen-Nürnberg.

Additional conservation laws for nearest neighbor hopping

Generalized energy conservation:

$$\frac{d}{dt} \int_{\mathbb{T}} dk g(k) \operatorname{tr}[W(k)] = 0$$

for any $g : \mathbb{T} \rightarrow \mathbb{R}$ with $g(k) = -g(\frac{1}{2} - k)$. It follows that

$$h(k) = \operatorname{tr}[W(k)] - \operatorname{tr}[W(\frac{1}{2} - k)]$$

is pointwise constant for each $k \in \mathbb{T}$. The additional conservation laws render the Hamiltonian *integrable*. By adding next-nearest neighbor hopping terms, these conservation laws disappear, and Hamiltonian becomes *non-integrable*.

Stationary states for nearest neighbor hopping (1D)

For pure nearest neighbor hopping, the general stationary states are

$$W_{\text{st}}(k) = \sum_{\sigma \in \{\uparrow, \downarrow\}} \left(e^{f(k) - a_{\sigma}} + 1 \right)^{-1} |\sigma\rangle\langle\sigma|, \quad \text{with}$$
$$f(k) = -f\left(\frac{1}{2} - k\right).$$

Adding higher order hopping terms destroys integrability, and only thermal (Fermi-Dirac) equilibrium states remain:

$$W_{\text{FD}}(k) = \sum_{\sigma \in \{\uparrow, \downarrow\}} \left(e^{\beta(\omega(k) - \mu_{\sigma})} + 1 \right)^{-1} |\sigma\rangle\langle\sigma|$$

Remark: conservation laws uniquely define stationary state, can map initial $W(k, 0)$ to asymptotic $W(k, t)$ as $t \rightarrow \infty$

Map from initial $W(0)$ to W_{st} (1D)

Generalized energy conservation:

$$\frac{d}{dt} \int_{\mathbb{T}} g(k) \operatorname{tr}[W(k)] dk = 0$$

for any $g : \mathbb{T} \rightarrow \mathbb{R}$ with $g(k) = -g(\frac{1}{2} - k)$. It follows that

$$h(k) = \operatorname{tr}[W(k)] - \operatorname{tr}[W(\frac{1}{2} - k)]$$

is pointwise constant for each $k \in \mathbb{T}$. Together with the spin conservation

$$\frac{d}{dt} \int_{\mathbb{T}^d} W(k, t) dk = 0$$

these conservation laws uniquely determine f and a_σ defining a stationary state. (The main ingredient of the proof is the Legendre transform.)