A discrete quantum Drift-Diffusion model

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Over the last few decades electronic devices, as for example semiconductors, were downsized until reaching magnitudes in the nano-meter regime. This is where classical equations start to fail giving good descriptions for the behaviour of quantum particles and quantum effects need to be taken into account.

Density-matrix formalism of quantum mechanics

In quantum mechanics the state of a particle at time t and place $x \in \mathbb{R}^D$ is described by its wave vector $\psi(t,x) \in \mathbb{C}$ with $\psi(t,\cdot) \in L^2(\mathbb{R}^D,\mathbb{C})$. If the state is subject to a given potential $V(t,x)$, then the Hamiltonian $\mathcal{H}$, which operates on ψ as follows:

$$\mathcal{H}\psi = -\frac{\hbar^2}{2}\Delta\psi + V\psi \tag{1}$$

corresponds to the total energy of the system, and a state ψ evolves according to the Schrödinger equation

$$i\hbar\partial_t\psi = \mathcal{H}\psi. \tag{2}$$

A mixed state is then modelled by a trace-class, positive and hermitian operator $\rho_t : L^2(\mathbb{R}^D,\mathbb{C}) \to L^2(\mathbb{R}^D,\mathbb{C})$, the so called **density operator**.

The modified quantum Liouville equation

The density operator ρ then fulfills the quantum Liouville Equation

$$\partial_t\rho = -\frac{i}{\hbar}[\mathcal{H},\rho], \tag{3}$$

where $[\mathcal{H},\rho] = \mathcal{H}\rho - \rho\mathcal{H}$ denotes the commutator of $\mathcal{H}$ and ρ. To moreover include the interaction between particles and themselves as well as their environment one adds a **collision operator** $\mathcal{Q}$. Finally we gain the **modified Quantum Liouville Equation**:

$$\partial_t\rho = -\frac{i}{\hbar}[H,\rho] + \mathcal{Q}(\rho). \tag{4}$$

Choice of the collision operator

To carry out a diffusion approximation we postulate properties for the collision operator, like e.g.:

- *Decay of a quantum entropy*

  A convenient entropy concept in the description of quantum systems in a thermal bath of fixed background temperature $1/\beta$ is defined by the **relative quantum entropy**

$$\tilde{H}_{cont}(\rho) = \mathrm{Tr}\left\{\rho(\log\rho - 1 + \beta\mathcal{H})\right\}.$$

- *Local conservation of the density*

  Hereby the **density** n at a point x is given by $\utilde{\rho}(x,x)$ where $\utilde{\rho}$ denotes the integral kernel associated to ρ.

Since it gets to complex to model each particle collision if they are very frequent, it is common to choose a very simple form for $\mathcal{Q}$, the **Bhatnagar–Gross–Krook (BGK)** operator:

$$\mathcal{Q}(\rho) = \mathcal{M}_\rho - \rho \tag{5}$$

where the **quantum Maxwellian** $\mathcal{M}_\rho$ is defined as

$$\mathcal{M}_\rho = \min\{\tilde{H}_{cont}(\tilde{\rho}) \big| \utilde{\rho}(x,x) = \utilde{\tilde{\rho}}(x,x)\ \forall x \in \mathbb{R}^D\}.$$

Expansion in powers of $\hbar$

The semiclassical limit $\hbar \to 0$ leads to the classical Drift-Diffusion equation. To get an better insight on how the quantum effects affect the classical part in the QDD model we further derive a leading order correction to the classical equation, i.e. an expansion of the QDD model up to order $\hbar^2$ while passing to the limit $\delta \to 0$.

Theorem. *In the limit $\delta \to 0$, after expanding the discrete quantum Maxwellian, the first order correction of the QDD in powers of $\hbar^2$, called* **Gradient-Density model***, is given by*

$$\partial_t n = \frac{1}{\beta}\Delta n + \nabla\cdot(n\nabla(V + V_B[n])) + \mathcal{O}(\hbar^4)$$

with the so called Bohm-potential

$$V_B[n] = -\frac{\hbar^2}{6}\nabla\left(\frac{\Delta\sqrt{n}}{\sqrt{n}}\right).$$

Recovery of the continuous QDD

Theorem. *In the limit $\delta \to 0$ we recover the* **continuous quantum Drift-Diffusion** *equation*

$$\partial_t n = \nabla\cdot\left(n\nabla\left(V + \frac{A}{\beta}\right)\right) \tag{6}$$

from the DQDD model.

Idea of the proof:

With y as fixed element of the mesh we can look at the following system of ODEs

$$\partial_t G^t(x,y) = A(x)G^t(x,y) + \frac{\hbar^2\beta}{2\delta^2}(G^t(x+\delta,y) + G^t(x-\delta,y) - 2G^t(x,y))$$
$$G^0(x,y) = \delta_{xy}.$$

which yields another representation of the quantum Maxwellian:

$$\mathcal{M}_{kl} = G^1(\delta(k-1),\delta(l-1)).$$

Applying a discretized version of the Variations of Constants Formula one sees that a solution to the differential equation above is given by

$$G^t(x,y) = \delta K^t(x-y) + \int_0^t \sum_{z\in\mathbb{T}_{\delta N}} \delta K^{t-s}(x-z)A(z)G^s(z,y)\,ds,$$

where $K^t(x)$ describes a discrete heat kernel. With Gronwall-type inequalities we then can derive necessary bounds in orders of δ for $\mathcal{M}_{k,k} + \mathcal{M}_{k+1,k+1} - 2\mathcal{M}_{k,k+1}$.

Discretization

The discretization process is applied to the space variable x, which should be element of a grid $\mathbb{T}_{\delta N}$ with $N+1$ equidistant points on the 1-torus $[0,1]$, where $\delta := 1/N$ denotes the mesh size.

Step 1: Discretize the quantum Liouville equation

The following relations for the discrete representation are defined:

wave-vector	$\psi \rightsquigarrow z \in \mathbb{C}^N$
density matrix	$\rho \rightsquigarrow R \in \mathfrak{D}_N$
integral kernel	$\utilde{\rho} \rightsquigarrow \utilde{R} = R/\delta$

with $\mathfrak{D}_N := \{R \in \mathbb{C}^{N\times N} | R = R^*, \mathrm{Tr}\{R\} = 1, R \geq 0\}$. For the discretization H of the Hamiltonian $\mathcal{H}$ we find by approximating derivatives through difference quotients:

$$H = -\frac{\hbar^2}{2}\frac{1}{\delta^2}D + V$$

with the discrete Laplace operator D given by

$$D = \begin{pmatrix} -2 & 1 & & & 1 \\ 1 & -2 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & 1 & -2 & 1 \\ 1 & & & 1 & -2 \end{pmatrix} \quad \text{and} \quad V = \begin{pmatrix} V(t,0) & & & \\ & V(t,\delta) & & \\ & & \ddots & \\ & & & V(t,1-\delta) \end{pmatrix}$$

indicating the discrete multiplication operator given through a underlying continuous potential with periodic boundary conditions. The discrete quantum Liouville equation for a density matrix $R \in \mathfrak{D}_N$ is then written as

$$\partial_t R = -\frac{i}{\hbar}[H,R]. \tag{7}$$

Step 2: Discretize the BGK-collision operator

To define the **discrete quantum Maxwellian** $\mathcal{M}_R$ corresponding to a density matrix R we consider the minimization problem

$$\min\left\{\tilde{H}[\tilde{R}] \,\middle|\, \tilde{R} \in \mathfrak{D}_N,\ \utilde{R}_{kk} = \utilde{\tilde{R}}_{kk}\ \forall k \in [N]\right\} \tag{8}$$

for the **discrete relative quantum entropy**

$$\tilde{H}[R] = \mathrm{Tr}\left\{\tilde{R}(\log\tilde{R} - \mathbb{1} + \beta H)\right\}.$$

Theorem. *The solution of* (8) *is given by*

$$\mathcal{M}_R = \exp\left(A + \frac{\beta\hbar^2}{2\delta^2}\left[N + N^T - 2\mathbb{1}\right]\right),$$

under the assumption that there exists a unique diagonal matrix $A \in \mathbb{C}^{N\times N}$, which is the suitable Lagrange multiplier to fulfill the constraint $\utilde{\mathcal{M}}_{kk} = \mathcal{M}_{kk}/\delta = \utilde{R}_{kk}$.

Step 3: Diffusive limit

To derive a macroscopic equation, whose solutions only depend on time and space, we look at a diffusive scaling of the QDD equation, obtained by $t \mapsto t/\varepsilon$ and $\mathcal{Q} \mapsto \mathcal{Q}/\varepsilon$:

$$\varepsilon\partial_t R^\varepsilon = -\frac{i}{\hbar}[H,R^\varepsilon] + \frac{1}{\varepsilon}(\mathcal{M}_{R^\varepsilon} - R^\varepsilon). \tag{9}$$

and let $\varepsilon \to 0$. Hence what becomes important are the effects of the collision operator on a larger time scale.

Theorem 1. *Let R^ε be the solution of (9). Then the formal limit $\varepsilon \to 0$ yields $R^\varepsilon \to R^0$, where R^0 is a quantum Maxwellian $R^0 = \mathcal{M}_{R^0}$ which solves*

$$\partial_t R^0_{kk} = -\frac{1}{\hbar^2}\left([H,[H,R^0]]\right)_{kk} \tag{10}$$

for all $k \in [N]$.

We call the system

$$\begin{cases} \partial_t[\mathcal{M}_R]_{kk} = -\frac{1}{\hbar^2}([H,[H,\mathcal{M}_R]])_{kk} \\ \mathcal{M}_R = \exp\left(A + \frac{\beta\hbar^2}{2\delta^2}\left[N + N^T - 2\mathbb{1}\right]\right) \end{cases}$$

discrete quantum Drift-Diffusion (DQDD) model. Note that this system describes the evolution of A or respectively, through the non-local closure relation $\utilde{\mathcal{M}}_{kk} = \utilde{R}_{kk} = n_k$, of the density n.

Entropy dissipation

Theorem. *Let $\mathcal{M} = \mathcal{M}_{R^0}$ be given as in Theorem 1. Then the quantum fluid entropy satisfies:*

$$\frac{d}{dt}\mathrm{Tr}\left\{\mathcal{M}(\log\mathcal{M} - \mathbb{1} + \beta H)\right\} \leq \beta\,\mathrm{Tr}\left\{\mathcal{M}\partial_t V\right\}. \tag{11}$$

References

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