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 function $\psi(x,t) \in C$. If the state is subject to a given potential $V(t,x)$, then the Hamiltonian $H$, which operates on $\psi$, as follows:

$$H\psi = \frac{-\hbar^2}{2m} \Delta \psi + V\psi$$

(1)

corresponds to the total energy of the system, and a state $\psi$ evolves according to the Schrödinger equation

$$i\hbar \frac{d\psi}{dt} = H\psi.$$ 

(2)

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

The modified quantum Liouville equation

The density operator $\rho$ then fulfills the quantum Liouville Equation

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

(3)

where $[H, \rho] = H\rho - \rho H$ denotes the commutator of $H$ and $\rho$. 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:

$$\partial_t \rho = \frac{1}{\hbar}[H, \rho] + \mathcal{Q}(\rho).$$ 

(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

$$\tilde{H}_{rel}(\rho) = \text{Tr}(\rho \ln(\rho - 1 + \beta H)).$$

- Local conservation of the density

Hereby the density $n$ at a point $x$ is given by $\rho(x, z)$ where $\rho$ denotes the integral kernel associated to $\rho$. Since it gets to complex to model each particle variation if they are very particle, it is common to choose a very simple form for $\mathcal{Q}$, the Bhattacharyya-Gross-Krook (BGK) operator:

$$\mathcal{Q}(\rho) = \mathcal{M}_\beta \rho - \rho,$n

where the quantum Maxwellian $M_\beta$ is defined as

$$M_\beta = \min\{\tilde{H}_{rel}(\rho)|\rho(x, z) = \tilde{\rho}(x)|\forall x \in \mathbb{R}^d\}.$$

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 $\hbar \to 0$.

Theorem. In the limit $\hbar \to 0$, the continuous quantum Liouville model

$$\partial_t \rho = \nabla \cdot (v \nabla \rho + \frac{\rho}{\beta} \nabla V) + \mathcal{Q}(\rho),$$

with the so-called Bohm-potential

$$V_B(n) = \frac{1}{2} \frac{x^2}{\hbar^2} \sqrt{\nabla \rho \nabla \rho},$$

Recovery of the continuous QDD

Theorem. In the limit $\hbar \to 0$, the continuous quantum Liouville model

$$\partial_t \rho = \nabla \cdot (v \nabla \rho + \frac{\rho}{\beta} \nabla V) + \mathcal{Q}(\rho),$$

(5)

does not lead to the classical Drift-Diffusion equation.

Idea of the proof:

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

$$\partial_t G^i(x,y) = A_i(x)G^i(x, y) + \frac{\beta}{2M} G^i(x, y)$$

$$+ G^i(x, y) - 2G^i(x, y),$$

which yields another representation of the quantum Maxwellian:

$$\mathcal{M}_\beta = G^i \delta t \left(\frac{1}{\hbar^2} \frac{x^2}{\beta} \sqrt{\nabla \rho \nabla \rho} \right)$$

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

$$G^i(x,y) = \delta(kx - y) + \int_0^x \sum_{k} \delta(k^2(x-y))A_i(x) \mathcal{G}^i(x, y) ds,$n

where $\mathcal{G}^i(x,y)$ describes a discrete heat kernel. With Gronwall-type inequalities we then can derive necessary bounds in orders of $\hbar$ for $\mathcal{M}_\beta = M_\beta \delta \mathcal{M}_\beta = M_\beta \delta \mathcal{M}_\beta$.

Discretization

The discretization process is applied to the space variable $x$, which should be element of a grid $\mathcal{T}_{h_N}$ 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 $\psi \to \zeta \in C^N$.
- density matrix $\rho \to \rho \in \mathbb{D}_N$.
- integral kernel $\rho \to R = R/\delta$.

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

$$\mathcal{H}_D = \frac{1}{\hbar^2} D + V,$n

with the discrete Laplace operator $D$ given by

$$D = \begin{pmatrix} 2 & -1 & & & \\ -1 & 2 & -1 & & \\ & \ddots & \ddots & \ddots \\ & & -1 & 2 & -1 \\ & & & -1 & 2 \end{pmatrix}$$

and $V = \begin{pmatrix} V(x) & & & \\ & V(x) & & \\ & & \ddots & \ddots \\ & & & V(x) \end{pmatrix}$

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

$$\partial_t \rho = \frac{1}{\hbar^2} [H, \rho] + \mathcal{Q}(\rho).$$

Step 2: Discretize the BGK-collision operator

To define the discrete quantum Maxwellian $M_\beta$ corresponding to a density matrix $\rho$ we consider the minimization problem

$$\min R \in \mathbb{D}_N \big\{ \text{Tr}(R) \big\},$$

for the discrete relative quantum entropy

$$H[R] = \text{Tr}(R \log R - 1 + \beta R).$$

Theorem. The solution of (8) is given by

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

under the assumption that there exists a unique diagonal matrix $A \in C^{N \times N}$, which is the suitable Lagrange multiplier to fulfill the constraint $M_\beta = M_\beta \delta M_\beta = M_\beta$.

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 $\delta t \to 1/t$ and $\mathbb{Q} \to \mathbb{Q}/\epsilon$:

$$\epsilon \partial_t R = \frac{1}{\hbar^2} [H, R] \epsilon + \frac{1}{\hbar^2} [M_\beta - R].$$

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

Theorem 1. Let $\tilde{R}$ be the solution of (9). Then, the formal limit $\epsilon \to 0$ yields $\tilde{R}^\delta \to \tilde{R}^\delta$, where $\tilde{R}^\delta$ is a quantum Maxwellian $R^\delta = M_\beta^\delta$ which solves

$$\partial_t M_\delta = \frac{1}{\hbar^2} [H, M_\delta] + \frac{1}{\hbar^2} [M_\delta - R],$$

for all $k \in [N]$. We call the system

$$\mathcal{M}_\delta \exp \left( A + \frac{\beta}{2M} \left[ N + \delta T - 21 \right] \right),$$

discrete quantum Drift-Diffusion (QDD) model. Note that this system describes the evolution of $A$ or, respectively, of the non-local closure relation $\mathcal{M}_\delta = \mathcal{M}_\delta = \mathcal{M}_\delta$, of the density $n$. Entropy dissipation

Theorem. Let $M = M_\delta$ be given as in Theorem 1. Then the quantum fluid entropy satisfies

$$\frac{d}{dt} \text{Tr}(M \log M + 1 + \beta H) \leq \beta \text{Tr}(M \nabla V).$$. (11)

References

