Numerical discretization of a fully quantum drift-diffusion model

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Abstract

This paper is devoted to the discretization and numerical simulation of a new quantum drift-diffusion model that was derived recently. We define an implicit numerical scheme that is equivalent to a convex minimization problem and that preserves the physical properties of the continuous model: charge conservation, positivity of the density and dissipation of an entropy. We illustrate these results with some numerical simulations.

Keywords: Quantum hydrodynamic models; Quantum drift-diffusion

1. Introduction

Recently [1], a new direction for quantum hydrodynamic models was explored by extending Levermore's moment approach [2] to the context of quantum mechanics. The strategy consists of defining a notion of 'local' quantum equilibrium as the minimizer of an entropy functional under local moment constraints. Such equilibria are defined thanks to a relationship between the thermodynamic quantities (such as the chemical potential or the temperature) and the extensive quantities (the densities) in a non-local way. Quantum hydrodynamic (QHD) models have been derived from quantum kinetic equations by moment expansions closed by these quantum equilibria[1]. Following the same approach, a family of ad-hoc collision operators has been introduced [3], which decrease the quantum entropy and relax to the equilibria. This strategy has been applied [4] in order to derive quantum diffusive models: a quantum drift-diffusion (QDD) model and a quantum energy-transport (QET) model. These works have been reviewed [5]. Other diffusive models of the type of the spherical harmonic expansion (SHE) model are also constructed in the quantum framework[6].

All of these fluid models are written as conservation laws coupled to constitutive equations. The quantum character of these models lies in these constitutive equations, which are non-local in space, making these systems difficult to analyse. However, an interesting property of these models is that – at least formally – a fluid entropy functional is dissipated. This feature gives an indication of the well-posedness of these systems; besides, it is interesting to recall that the entropic property is obtained as a by-product of the strategy of entropy minimization.

We are interested here in the QDD model. This consists of a mass balance equation for the density of particles $n(t, x)$

$$\partial_t n + \operatorname{div} j = 0, \tag{1}$$

supplemented with a constitutive equation for the charge flux $j(t,x)$

$$j = n\nabla(A - V), \tag{2}$$

describing the combined effects of the potential $V(t, x)$ and of a quantity A (t, x) called the *quantum chemical potential*. The originality of this model is that this chemical potential is linked to the density by a relationship that is non-local in space. In a classical setting, we would have a local relation such as $n(t, x) = e^{-A(t,x)}$ (which induces diffusive effects), whereas in this quantum model we have instead

$$n = \sum_p e^{-\lambda_p[A]} \left|\chi_p[A]\right|^2, \tag{3}$$

where $(\lambda_p[A], \chi_p[A])_p$ denotes the whole sequence of eigenvalues and eigenfunctions of the modified Hamiltonian $H[A] = -\hbar^2 \Delta + A + V^{ext}$, i.e. satisfy

$$-\hbar^2 \Delta \chi_p + (A + V^{ext})\chi_p = \lambda_p \chi_p \qquad (p \in \mathbb{N}^*). \tag{4}$$

To complete the model, self-consistent interactions

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are taken into account by the mean of the Poisson equation, satisfied by the self-consistent potential $V(t, x)$:

$$-\alpha \Delta V = n. \tag{5}$$

In this system, V^{ext} denotes an applied external potential and $\hbar$ and α are two dimensionless parameters. These equations are set on a bounded domain $\Omega \subset \mathbb{R}^d$ ($d \leq 3$), subject to the following boundary conditions on $\partial\Omega$:

$$V = 0 \quad \text{and} \quad \chi_p = 0 \quad (\forall p \in \mathbb{N}^*) \quad \text{on} \quad \partial\Omega, \tag{6}$$

$$\nabla(A - V) \cdot \nu = 0 \quad \text{on} \quad \partial\Omega, \tag{7}$$

where $\nu(x)$ denotes the normal vector at $x \in \partial\Omega$. Among other properties [4,7], one can show that the following free energy is dissipated by this model, i.e. is a decreasing function of time:

$$S(t) = -\int n(A+1)\,dx + \frac{\alpha}{2}\int |\nabla V|^2\,dx.$$

2. Entropic discretization of the model

In dimension 1, an implicit numerical scheme for this system was introduced [7,8], consistent with the entropy dissipation. The domain is $\Omega = (0, 1)$. In order to discretize the QDD system (Eqs (1)–(7)), we introduce a time gridstep $\Delta t > 0$, a space gridstep $\Delta x = 1/(N+1)$ (where $N \in \mathbb{N}^*$), and we set $t^k = k\Delta t$ for $k \in \mathbb{N}$ and $x_i = i\Delta x$ for $i = 0, \ldots, N+1$.

Let us define the discrete equivalents of the operator $H[A]$ and of its eigenelements $\lambda_p[A]$, $\chi_p[A]$. To this aim, we first introduce the matrix Δ_{Dir} of discretization of the operator $\frac{d^2}{dx^2}$ on (0, 1) with Dirichlet boundary conditions by a centred finite difference method. Then, for any vector $(A_i)_{1\leq i\leq N}$, we define the matrix $M[A] = -\hbar^2\Delta_{Dir} + \mathrm{Diag}\,(A + V^{ext})$, where $Diag(A + V^{ext})$ denotes the diagonal matrix of coefficients $\mathrm{A}_i + \frac{1}{\Delta x}\int_{x_{i-1/2}}^{x_{i+1/2}} \mathrm{V}^{ext}(x)dx$. This matrix is the discretization of the operator $H[A]$ and, for $1 \leq p \leq N$, we denote, respectively, by $\ell_p[A]$ and $X_p[A]$ the eigenvalues and eigenvectors of $M[A]$. The eigenvectors $X_p[A]$ are normalized, such that $\Delta x \sum_{i=1}^N (X_p[A]_i)^2 = 1$.

Let us now describe the numerical scheme. The unknowns n_i^k, A_i^k and V_i^k of the discrete model approximate the corresponding functions at the point (t^k, x_i). For $k \in \mathbb{N}$ and $i \in 1, \ldots, N$, the implicit finite difference numerical scheme is written

$$\frac{n_i^{k+1} - n_i^k}{\Delta t} + \frac{n_i^k\left(A_{i+1}^{k+1} - V_{i+1}^{k+1} - A_i^{k+1} + V_i^{k+1}\right)}{\Delta x^2}$$

$$-\frac{n_{i-1}^k\left(A_i^{k+1} - V_i^{k+1} - A_{i-1}^{k+1} + V_{i-1}^{k+1}\right)}{\Delta x^2} = 0, \tag{8}$$

$$n_i^k = \sum_p \exp\left(-\ell_p[A^k]\right)\left(X_p[A^k]_i\right)^2, \tag{9}$$

$$-\alpha\frac{V_{i+1}^k - 2V_i^k + V_{i-1}^k}{\Delta x^2} = n_i^k, \tag{10}$$

and we set $n_i^o = n^o(x_i)$. In order to take into account the boundary conditions in Eqs (6) and (7), we define the unknowns for $i = 0$ and $i = N+1$ by

$$n_0^k = n_{N+1}^k = V_0^k = V_{N+1}^k = 0, \tag{11}$$

$$A_0^k - V_0^k = A_1^k - V_1^k, \qquad A_{N+1}^k - V_{N+1}^k = A_N^k - V_N^k. \tag{12}$$

From Eq. (9), it is clear that this scheme preserves the positivity of the density. Moreover, the conservative form of Eq. (8) and the no-flux boundary conditions show that the total mass is independent of time. One can show that each iteration of this scheme (the calculation of (A^{k+1}, V^{k+1}) for a given n^k) is equivalent to the minimization of the following convex functional:

$$J(A,V) = \frac{\Delta t}{2\Delta x}\sum_{i=1}^N n_i^k(A_{i+1} - V_{i+1} - A_i + V_i)^2 +$$

$$\frac{\alpha}{2\Delta x}\sum_{i=0}^N (V_{i+1} - V_i)^2$$

$$+\sum_{p=1}^N \exp\left(-\ell_p[A]\right) + \Delta x\sum_{i=1}^N n_i^k(A_i - V_i).$$

Notice that the variational structure of this problem is similar to that of the stationary Schrödinger–Poisson system studied in the works of Nier [9,10].

3. Numerical results

Since this scheme is equivalent to a convex minimization problem, its implementation can be achieved efficiently by Newton iterations. Let us present some numerical results that were obtained thanks to this scheme. The external potential V^{ext} is a discontinuous function playing the role of a double barrier structure potential and the initial density is concentrated on the left of the double barrier. In Figs 1–3, we have represented the density $n(x)$ and the total potential $V + V^{ext}$ as functions of the position x, at the initial step and then after 60 and 600 iterations. One observes numerically the convergence to a steady state where a part of the total charge is trapped inside the double barrier and the rest is distributed equally outside the barriers. The study of this long-term behaviour is given by Gallego and Méhats [7].

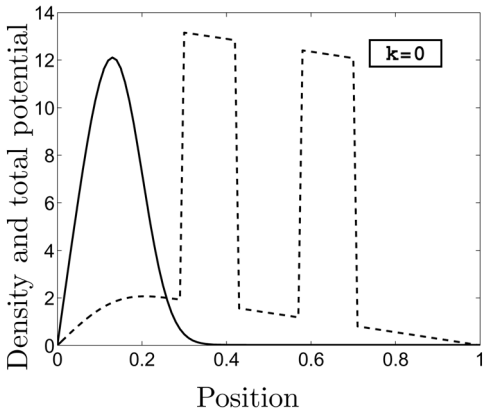

Fig. 1. Initial density $n(x)$ (solid line) and total potential ($V + V^{ext}$) (x) (dashed line).

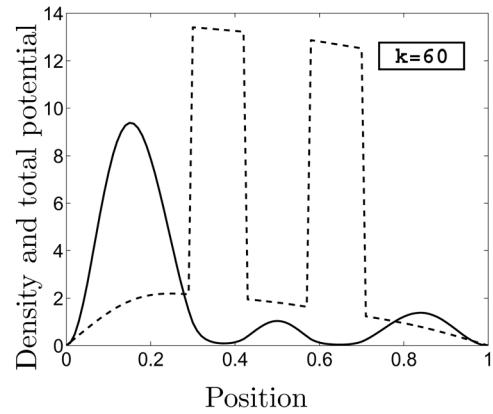

Fig. 2. Density and potential after 60 iterations.

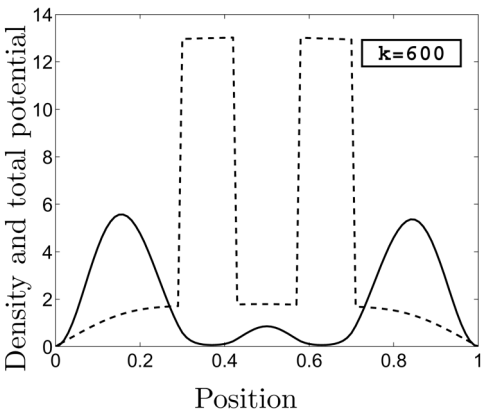

Fig. 3. Density and potential after 600 iterations.

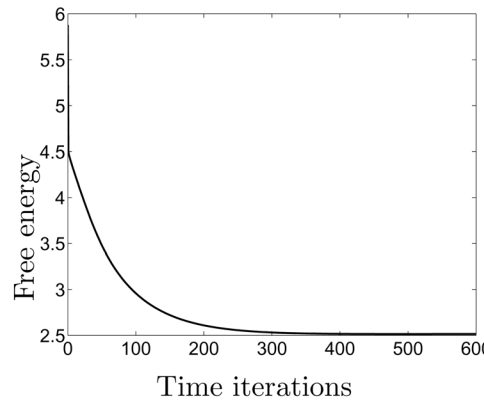

Fig. 4. Evolution of free energy.

In Fig. 4, we have represented the free energy as a function of time and shown that it is a decreasing function converging to a constant.

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