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Numerical approximation of a quantum drift-diffusion model

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Abstract

This Note is devoted to the discretization and numerical simulation of a new quantum drift-diffusion model that was recently derived. We define an implicit numerical scheme which is equivalent to a convex minimization problem and which preserves the physical properties of the continuous model: charge conservation, positivity of the density and dissipation of an entropy. We illustrate these results by some numerical simulations. ***To cite this article: S. Gallego, F. Méhats, C. R. Acad. Sci. Paris, Ser. I 339 (2004).***

Résumé

Approximation numérique d'un modèle de dérive-diffusion quantique. Cette Note est consacrée à la discrétisation et à la simulation numérique d'un modèle de dérive-diffusion quantique qui a été dérivé récemment. Nous définissons un schéma numérique implicite dont la résolution se ramène à un problème de minimisation convexe. Par ailleurs, ce schéma préserve les propriétés physiques vérifiées par le modèle continu : conservation de la charge totale, positivité de la densité et dissipation d'une entropie. Enfin, nous illustrons ces propriétés à l'aide de simulations numériques. ***Pour citer cet article : S. Gallego, F. Méhats, C. R. Acad. Sci. Paris, Ser. I 339 (2004).***

Version française abrégée

L'objet de cette Note est la discrétisation numérique et la simulation d'un modèle dérivé récemment dans [3] (voir aussi l'article de revue [4]), le modèle de dérive-diffusion quantique. Ce modèle décrit le transport quantique de charges en forte interaction avec le milieu environnant. Il est constitué d'une équation de conservation de la charge (1), couplée avec l'équation constitutive (2) qui donne l'expression du courant $j(t,x)$ en fonction de la densité $n(t,x)$ et de deux quantités : le potentiel électrostatique $V(t,x)$ et le potentiel chimique quantique $A(t,x)$,

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sur lequel repose le caractère quantique du modèle. En effet, ce dernier est relié à la densité n par le bias de la relation non locale (3), qui fait elle-même intervenir une procédure de diagonalisation d'un Hamiltonien modifié $H[A] = -\hbar^2\Delta + A + V^{\text{ext}}$, via l'Éq. (4) (ici V^{ext} désigne un potentiel extérieur donné). Enfin, pour compléter ce modèle, l'équation de Poisson (5) est prise en compte afin de décrire les interactions électrostatiques autoconsistantes.

Nous donnons dans la proposition suivante quelques propriétés formellement satisfaites par ce modèle posé sur un domaine borné Ω, soumis aux conditions aux limites isolantes (6), (7) :

Proposition 0.1. *Soit (n, A, V) une solution régulière de* (1)–(5) *soumis à* (6), (7). *Alors la densité vérifie $n > 0$ sur Ω, la charge totale $\int n(t,x)\,\mathrm{d}x$ est indépendante du temps et l'énergie libre $S(t)$ définie par* (8) *est décroissante.*

Les résultats principaux de cette Note concernent la discrétisation de ce modèle (1)–(7) en une dimension d'espace. Introduisant une grille spatiale $x_i = i\Delta x$ ($i = 0, \ldots, N+1$, où $\Delta x = \frac{1}{N+1}$) et une grille temporelle $t^k = k\Delta t$, on définit le schéma numérique aux différences finies implicite (9)–(11). Dans ce schéma, $\ell_p[A]$, $X_p[A]$ désignent respectivement les valeurs propres et les vecteurs propres d'une matrice $M[A]$ de discrétisation par différences finies de l'opérateur $H[A]$. Les deux théorèmes suivants énoncent le fait que ce schéma est bien posé, se ramène à un problème d'optimisation convexe (de la même manière que le système de Schrödinger–Poisson a une structure variationnelle [11,12]) et préserve les propriétés du modèle continu :

Théorème 0.2. *Soit $n_i^0 > 0$ pour $1 \leqslant i \leqslant N$. Alors, pour tout $k \in \mathbb{N}$, la solution (n^k, A^k, V^k) du schéma numérique* (9)–(11) *est définie de manière unique. Pour tout $k \in \mathbb{N}$, (A^{k+1}, V^{k+1}) est l'unique minimiseur de la fonctionnelle J_1 strictement convexe, coercive et définie par* (12). *Par ailleurs, le potentiel chimique au temps initial A^0 se définit comme l'unique minimiseur de la fonctionnelle J_2 strictement convexe, coercive et définie par* (13).

Théorème 0.3. *Le schéma numérique* (9)–(11) *satisfait les propriétés suivantes : pour tout k et $1 \leqslant i \leqslant N$, on a $n_i^k > 0$ et la charge totale discrète $\Delta x \sum_{i=1}^N n_i^k$ ne dépend pas de k. De plus, l'énergie libre définie par* (14) *est décroissante.*

Le premier théorème a une importance pratique et nous avons implémenté ce schéma numérique en programmant une méthode de Newton pour résoudre les problèmes d'optimisation convexe associés à J_1 et J_2. Sur les Figs. 1 et 2 sont donnés des résultats de simulation numérique sur un cas test simple : l'évolution de la densité et du potentiel total sont représentés, ainsi que la décroissance de l'énergie libre.

1. Introduction

This Note is concerned with the discretization and the numerical simulation of a quantum drift-diffusion (QDD) model. This model was derived in [3] (see also the review paper [4]) and describes the transport of quantum charge-species in strong interaction with a surrounding medium at a given temperature. It 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 *quantum chemical potential*. The originality of this model is that this chemical potential is linked to the density by a relation which is

nonlocal in space. In a classical setting, we would have a local relation such as $n(t,x) = \mathrm{e}^{-A(t,x)}$ (which induces diffusive effects) whereas, in this quantum model we have instead

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

where $(\lambda_p[A], \chi_p[A])_p$ denotes the whole sequence of eigenvalues and eigenfunctions of the modified Hamiltonian $H[A] = -\hbar^2\Delta + A + V^{\mathrm{ext}}$ (the domain of this unbounded operator is made precise in Section 2), i.e. satisfy

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

To complete the model, selfconsistent interactions are taken into account by the mean of the Poisson equation, satisfied by the selfconsistent potential $V(t,x)$:

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

In this system, V^{ext} denotes an applied external potential in $L^\infty(\Omega)$ and $\hbar$ and α are two dimensionless parameters.

Let us briefly describe the approach which led to the derivation of the QDD model. Initially, Degond and Ringhofer [5] have set up a formalism for extending Levermore's moments method [10] to the quantum framework, by introducing a notion of local quantum equilibria thanks to nonlocal entropy principles, in order to derive quantum hydrodynamic models. They have then applied this idea in [6] to generalize the Boltzmann collision operator, while keeping a quantum analogue to the H-theorem. Similarly, a relaxation operator of BGK type was defined in [3], presenting the same property of quantum entropy dissipation, and a quantum kinetic equation was written by plugging this operator in the right-hand side of the Wigner equation. The QDD model studied in this Note was then obtained in [3] by performing a diffusion approximation of this Wigner-BGK equation and, as in the classical case, satisfies an entropy principle inherited from the underlying quantum kinetic model. Note also that the QDD model has an interesting link with another quantum diffusive model which has been widely studied [1,2,8,13]: the so-called density-gradient model (also referred to as quantum drift-diffusion model), which consists of the classical drift-diffusion model corrected by the Bohm potential. Indeed, in [3] it was shown that the density-gradient model can be obtained as an approximation of the QDD model in a semiclassical asymptotics.

Despite the interesting physical properties of the QDD model, presented in Section 2, its analysis is still at a very early stage. As a first step, we present in Section 3 an implicit discretization of this system and obtain a discrete version of the QDD model, which is easier to study and enjoys the same properties as the continuous model: its preserves the total charge and the positivity of the density and it dissipates the entropy. In particular we address an important subproblem: at the discrete level, it is possible to invert the constitutive relation $A \mapsto n$ given by (3) (see the last part of Theorem 3.1) while, in the continuous case, this question is still open. Finally, in Section 4 we illustrate these results by some numerical simulations. For more details about the present work, we refer the reader to [7].

2. Basic properties of the QDD model

Let $\Omega \subset \mathbb{R}^d$ $(d \leqslant 3)$ be a regular bounded domain. We need to complement the QDD model (1)–(5) with boundary conditions on $\partial\Omega$. Among the most simple ones are the isolating boundary conditions, i.e. Dirichlet boundary conditions for the wavefunctions χ_p and for the selfconsistent potential:

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

In other terms, for each function $A \in L^2(\Omega)$, the Hamiltonian $H[A]$ is chosen with the domain $D = \{\phi \in H^2(\Omega):\ \phi = 0 \text{ on } \partial\Omega\}$. This operator is selfadjoint, bounded from below and has a compact resolvent [14]. With this choice, it is required to supplement the following no-flux boundary condition:

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

where $\nu(x)$ denotes the normal vector at $x \in \partial\Omega$. Indeed, if we expect a solution to this system, such that, e.g., A belongs to $H^1(\Omega)$, then it can be proved (see [12,9,14] and also [7]) that we have $n > 0$ in Ω and $n = 0$ on $\partial\Omega$. Hence, since (1), (2) reads as a transport equation for n, it is clear that the characteristic curves associated to this equation cannot intersect $\partial\Omega$, which yields the Neumann condition (7).

If it exists, a solution of the QDD system must satisfy the following properties (a proof of this proposition can be found in [7]):

Proposition 2.1. *Let (n, A, V) be a smooth solution of* (1)–(5) *subject to* (6), (7). *Then we have $n > 0$ on Ω, the charge $\int n(t,x)\,\mathrm{d}x$ is independent of time and the following free energy $S(t)$ is a decreasing function of time*:

$$S(t) = -\int n(A+1)\,\mathrm{d}x + \frac{\alpha}{2}\int |\nabla V|^2\,\mathrm{d}x. \tag{8}$$

3. The numerical scheme and its properties

The space dimension is now $d = 1$ and the domain is $\Omega = (0,1)$. In order to discretize the QDD system (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 $\frac{\mathrm{d}^2}{\mathrm{d}x^2}$ on $(0,1)$ with Dirichlet boundary conditions by a centered finite difference method. Then, for any vector $(A_i)_{1\leqslant i\leqslant N}$, we define the matrix $M[A] = -\hbar^2\Delta_{\mathrm{Dir}} + \mathrm{Diag}(A + V^{\mathrm{ext}})$, where $\mathrm{Diag}(A + V^{\mathrm{ext}})$ denotes the diagonal matrix of coefficients $A_i + \frac{1}{\Delta x}\int_{x_{i-1/2}}^{x_{i+1/2}} V^{\mathrm{ext}}(x)\,\mathrm{d}x$. This matrix is the discretization of the operator $H[A]$ and, for $1 \leqslant p \leqslant N$, 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 $\Delta x \sum_{i=1}^N (X_p[A]_i)^2 = 1$. By classical results of matrix analysis [15], we know that these eigenvalues are always simple and infinitely differentiable with respect to A. In particular, we have the useful formula:

$$\forall W \in \mathbb{R}^N \quad \mathrm{d}\ell_p[A]\cdot W = \Delta x \sum_{i=1}^N \big(X_p[A]_i\big)^2 W_i.$$

Let us now describe our numerical scheme. The unknowns n_i^k, A_i^k, 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 can be written

$$\frac{n_i^{k+1} - n_i^k}{\Delta t} + \frac{n_i^k(A_{i+1}^{k+1} - V_{i+1}^{k+1} - A_i^{k+1} + V_i^{k+1}) - n_{i-1}^k(A_i^{k+1} - V_i^{k+1} - A_{i-1}^{k+1} + V_{i-1}^{k+1})}{\Delta x^2} = 0, \tag{9}$$

$$n_i^k = \sum_p \exp\big(-\ell_p[A^k]\big)\big(X_p[A^k]_i\big)^2, \qquad -\alpha\,\frac{V_{i+1}^k - 2V_i^k + V_{i-1}^k}{\Delta x^2} = n_i^k, \tag{10}$$

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

$$n_0^k = n_{N+1}^k = V_0^k = V_{N+1}^k = 0, \qquad A_0^k - V_0^k = A_1^k - V_1^k, \qquad A_{N+1}^k - V_{N+1}^k = A_N^k - V_N^k. \tag{11}$$

The numerical scheme (9)–(11) is clearly consistent with the QDD system (1)–(7). Its properties are listed in the following theorems, whose proofs are developed in [7]. The formulation of this scheme under a variational problem was inspired by the works of Nier [11,12].

Theorem 3.1. *If $n_i^0 > 0$ for $1 \leqslant i \leqslant N$, then for any $k \in \mathbb{N}$ the solution (n^k, A^k, V^k) of the numerical scheme* (9)–(11) *is uniquely defined. For all $k \in \mathbb{N}$, (A^{k+1}, V^{k+1}) is defined as the unique minimizer of the strictly convex and coercive functional*

$$J_1(A,V) = \frac{\Delta t}{2\Delta x}\sum_{i=1}^{N} n_i^k (A_{i+1} - V_{i+1} - A_i + V_i)^2 + \frac{\alpha}{2\Delta x}\sum_{i=0}^{N}(V_{i+1} - V_i)^2 + \sum_{p=1}^{N}\exp\bigl(-\ell_p[A]\bigr) + \Delta x \sum_{i=1}^{N} n_i^k (A_i - V_i). \tag{12}$$

Moreover, the initial chemical potential A^0 is defined as the minimizer of the following strictly convex and coercive functional:

$$J_2(A) = \sum_{p}\exp\bigl(-\ell_p[A]\bigr) + \Delta x \sum_{i=1}^{N} n_i^0 A_i. \tag{13}$$

Theorem 3.2. *The numerical scheme* (9)–(11) *satisfies the following properties*: *for all k and $1 \leqslant i \leqslant N$, we have $n_i^k > 0$ and the* (*discrete*) *charge is conserved*: $\Delta x \sum_{i=1}^{N} n_i^k = \Delta x \sum_{i=1}^{N} n_i^0$. *Moreover, the sequence of* (*discrete*) *free energies defined as follows is decreasing*:

$$S^k = -\Delta x \sum_{i=1}^{N} n_i^k \bigl(A_i^k + 1\bigr) + \frac{\alpha}{2\Delta x}\sum_{i=1}^{N}\bigl(V_{i+1}^k - V_i^k\bigr)^2. \tag{14}$$

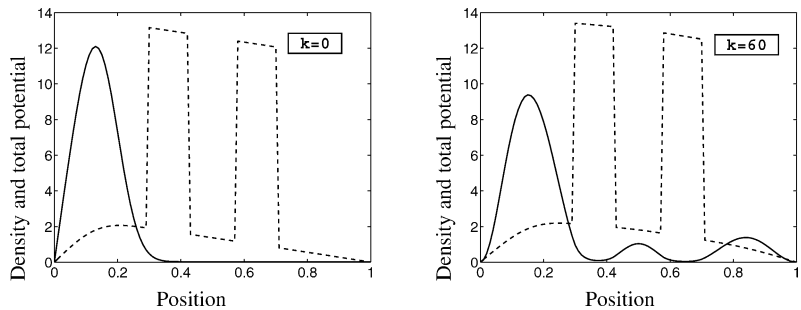

Fig. 1. Left: initial density $n(x)$ (solid line) and corresponding total potential $(V + V^{\text{ext}})(x)$ (dashed line). Right: density and potential after 60 iterations.

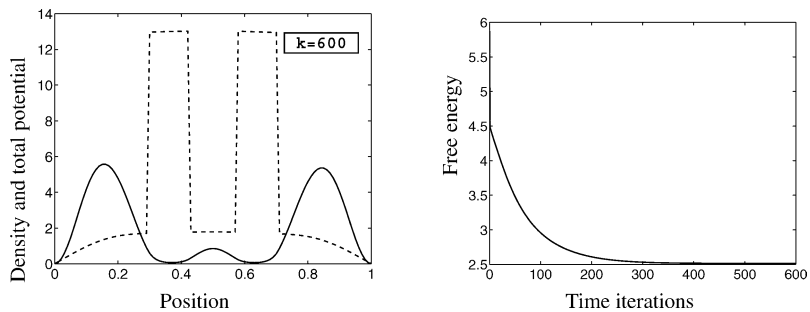

Fig. 2. Left: density $n(x)$ (solid line) and total potential $(V + V^{\text{ext}})(x)$ (dashed line) after 600 iterations. Right: evolution of the free energy S^k.

4. Numerical results

Let us now present some numerical results obtained with the scheme (9)–(11). A Newton method was implemented in order to solve the convex minimization problem for the time iterations (functional defined by (12)) as well as for the computation of the initial chemical potential (functional defined by (13)).

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. The grid steps are $\Delta x = 0.01$, $\Delta t = 0.005$, the dimensionless parameters are taken with the values $\hbar^2 = 0.02$, $\alpha = 0.1$.

On Fig. 1 and on the left of Fig. 2, we have represented the density $n(x)$ and the total potential $V + V^{\text{ext}}$ as functions of the position x, at the initial step, 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 equally distributed outside the barriers. The study of this long-time behavior goes beyond the objectives of this Note and is done in [7]. On the right of Fig. 2, we have represented the free energy S^k as a function of k and check that it is a decreasing function, converging to a constant.

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