# Entropic discretization of a 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 recently derived. In a first step, we introduce an implicit semi-discretization in time which possesses some interesting properties: this system is well-posed, it preserves the positivity of the density, the total charge is conserved, and it is entropic (a free energy is dissipated). Then, after a discretization of the space variable, we define a numerical scheme which has the same properties and is equivalent to a convex minimization problem. Moreover, we show that this discrete solution converges for long times to the solution of a discrete Schrödinger-Poisson system. These results are illustrated by some numerical simulations.

**Key words :** Quantum drift-diffusion, Schrödinger-Poisson, entropic scheme, convex minimization, long-time behavior.

# 1 Introduction

Recently, Degond and Ringhofer [15, 16] have explored a new direction for quantum hydrodynamic models by extending Levermore's moment approach [33] to the context of quantum mechanics. Their strategy consists in 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 relation between the thermodynamic quantities (such as the chemical potential or the temperature) and the extensive quantities (the densities) in a non local way. In [15], quantum hydrodynamic (QHD) models have been derived from quantum kinetic equations by moment expansions closed by these quantum equilibria. In this reference, Degond and Ringhofer have also sketched an important program related to these QHD models, including namely the setting up of a rigourous framework to this formal modeling, the inclusion of other quantum effects (Pauli exclusion principle, spin effects,...), or the numerical discretization and simulation. Following the same approach, these authors have then introduced in [17] a family of ad-hoc collision operators which decrease the quantum entropy and relax to the equilibria. Afterwards, this strategy was applied in [13] in order to derive quantum diffusive models: a quantum drift-diffusion model (QDD)

and a quantum energy-transport model (QET). In a work in progress [8], other diffusive models of the type of the Spherical Harmonic Expansion (SHE) model are also constructed in the quantum framework.

All 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 and make these systems difficult to analyze (these papers [15, 13] remained at a formal level). 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.

In this paper, we are interested in the quantum drift-diffusion (QDD) model, with two objectives. Firstly, the present work is a first step in the rigourous analysis of this system, coupled to the Poisson equation. Secondly, we study the discretization of this system and its numerical simulation.

Let us now describe the main results of this paper. The QDD system is given by (2.7)–(2.9). Actually, we are not able yet to answer the question of the well-posedness of this system. Nevertheless, we introduce, instead, and analyze rigourously a semi-discretized (in time) version of this model, defined by (3.1)–(3.3), and which presents the same entropy dissipation property as the QDD system. This first set of results is given in Theorem 3.1. Next, concerning the second objective of the paper, the implicit numerical scheme (4.1)–(4.3) is defined. This scheme is well-posed and equivalent to a problem of convex minimization. Then, we show that this scheme is stable in the sense of a discrete entropy. Finally, we analyze the long-time behavior of its discrete solution and we show that it converges to a discrete steady state. All these results concerning the numerical scheme are stated in Theorem 4.1.

We end this introduction with bibliographical notes on quantum transport modeling. The quantum drift-diffusion system applies to the modeling of nanoscale semiconductor devices. In the semiconductor industry, the classical drift-diffusion model has been a valuable tool for many years [11, 28, 35, 37, 48]. Currently, the ongoing miniaturization of electronic devices to the nanometer scale creates the need of models which take into account quantum effects. To this aim, two strategies can be followed.

The first approach, with a radical change in the level of description, consists in choosing full quantum models such as the Schrödinger equation, the von Neumann equation or the Wigner equation [4, 9, 12, 18, 19, 32, 38, 45, 46]. These models are well fitted for very small devices but they lead to the resolution of huge numerical systems at the intermediate scale which is currently considered by electronic engineers. Another reason why this approach is limited to very small devices is that the question of describing collisions in quantum transport models is extremely difficult and has not received a completely satisfactory answer yet. Therefore, full quantum models are still mainly reserved to ballistic transport in small devices.

The opposite strategy consists in introducing quantum correction terms in the classical drift-diffusion model. The most common quantum correction involves the

Bohm potential, which naturally appears in quantum hydrodynamics, thanks to an analogy between the Schrödinger equation and the pressureless Euler system corrected with the Bohm potential. This analogy can be seen thanks to the Madelung transformation [34, 50], by considering the equations satisfied by the amplitude and the phase of a wavefunction solving the Schrödinger equation (see e.g. [13] for more details). Next, assuming that adding this Bohm potential enables to model quantum effects in classical macroscopic systems, several models with corrective terms have been written. In a fluid context, hydrodynamics models with quantum corrections have been studied in [22, 23, 24, 25, 26, 27, 29, 44, 51]. In a diffusive context, and closest to the QDD model studied in this paper, one can find the drift-diffusion model corrected with the Bohm potential, called density-gradient model (it is also sometimes called quantum drift-diffusion model, but in this paper we shall refer it as density-gradient model, in order to avoid any confusion with the QDD model presented here). This model was introduced in [1, 2], then mathematically and numerically studied in [3, 7, 29, 30, 41, 42]. An advantage of such an approach is that it takes into account collisions, at least heuristically. Another strength is that, as this method is based on an evolution of the classical drift-diffusion model, the numerical codes currently employed in semiconductor industry can be adapted by following this evolution. Nevertheless, one has to insist on the fact that the justification of these models is far from obvious in the case of statistical mixtures (several attempts were made to address this issue, see for instance [22, 23, 24, 27]). Moreover, quantum corrections involving the Bohm potential produce high order terms in these systems and make their resolution difficult, from the mathematical and from the numerical point of view. To conclude this description, one can also cite two other recent attempts to model quantum effects in diffusive models [6, 43]. The models presented in these works are different but both take the form of a drift-diffusion equation, coupled to the Poisson equation, and where the quantum phenomena are taken into account by a modification of the link between the density and the quasi-Fermi potential, via the resolution of a quasistatic Schrödinger equation.

As a compromise, the quantum drift-diffusion (QDD) model studied in the present paper tries to conciliate these two approaches: this model is really quantum and non local, while the length scales are macroscopic and collisions are modelled. Indeed, as it is shown in Section 2.3, the steady states of the QDD model solve the Schrödinger-Poisson system studied in [31, 39, 40]: this shows the quantum character of this model. Besides, it has been shown in [13] that, at least formally, the limit of the QDD model as $\hbar$ goes to zero is the classical drift-diffusion model, while the leading order correction term in an $\hbar$ expansion is the Bohm potential: this shows a clear link between the QDD model and the density-gradient model described above.

The paper is organized as follows: in Section 2, we write a formulation of the QDD model in a bounded domain and give some of its properties. Then, in Section 3, we define the semi-discretization in time of the QDD system and show that this new system is well-posed and entropic. In Section 4, the numerical scheme is constructed and we analyze its properties (well-posedness, stability, long-time behavior). Finally, in Section 5 we illustrate these properties by some numerical simulations.

# 2 The quantum drift-diffusion model

This section is devoted to the presentation of the quantum drift-diffusion model (QDD). It is not clear which precise functional framework would be adapted to a rigourous analysis of this system. Nevertheless, we can still state some properties satisfied by any smooth solution of this system. This enables to put into perspective the results of Section 3. Indeed, we shall see in Section 3 that similar properties are satisfied by the solutions of the semi-discretized QDD system (3.1)–(3.3), whereas their existence can be rigourously proved.

## 2.1 Notations: the QDD model on a bounded domain

Let us first give a formulation of the quantum drift-diffusion model in the case of bounded domains. This model, which describes the evolution of a quantum system of electrons, was derived in [13] and a most convenient equivalent form of this model was written in the review paper [14]. The first equation is the equation of mass conservation:

$$\partial_t n + \operatorname{div} j = 0. \tag{2.1}$$

The second equation of the model is the constitutive equation which gives the expression of the current:

$$j = n\nabla(A - V). \tag{2.2}$$

In this equation, $V(t,x)$ is the selfconsistent potential (modeling the interactions between the electrons) and $A(t,x)$ is the *quantum chemical potential*, linked to the density by a relation which is non local in space and which is the key of this quantum model. In order to make this relation explicit, let us introduce the operator

$$H[A] = -\hbar^2\Delta + A + V^{ext},$$

where $\hbar$ is a positive dimensionless parameter ($\hbar^{-2}$ is proportional to the temperature of the system), whose domain $D(H)$ will be precised below. Here, $V^{ext}(x)$ is an external potential applied to the system (assumed independent of time for simplicity). In the QDD model, the electron system is at any time in a *local quantum equilibrium* (see [15, 13]) and its density matrix is

$$\varrho = \exp\left(-H[A]\right), \tag{2.3}$$

where exp denotes here the exponential of the operator. Remark that when the chemical potential $A$ differs from the electrical potential, the operator $H[A]$ is not the Hamiltonian and $\varrho$ is not the density matrix of a global quantum equilibria as defined usually [5]. A consequence of this formula (2.3) is the relation between the density and the chemical potential, given in a weak sense by:

$$\forall\phi \qquad \int n\,\phi\,dx = \operatorname{tr}\ \left(\exp\left(-H[A]\right)\ \phi\right) \tag{2.4}$$

(here we used the usual convention where, implicitely in the right-hand side of this expression, $\phi$ stands for the operator of multiplication by $\phi$). Finally, the last equation of the model is the Poisson equation, which links the density and the selfconsistent potential:

$$-\alpha\Delta V = n. \tag{2.5}$$

In this equation, $\alpha$ is a positive dimensionless parameter (which is proportional to the square of the Debye length of the system); a given background charge density may be taken into account in this model, for instance, by a modification of the external potential $V^{ext}$ and a shift of the chemical potential $A$.

Let $\Omega \in \mathbb{R}^d$ be a regular bounded domain ($d \leq 3$). Its boundary is denoted by $\partial\Omega$ and $\nu(x)$ is the outward unit normal vector at $x \in \partial\Omega$. All the unknowns of the system $n(t,x)$, $j(t,x)$, $A(t,x)$, $V(t,x)$ are defined for $t \geq 0$ and $x \in \Omega$. Now we need to precise the boundary conditions for this system. The most simple ones, that will be studied in this paper, prescribe a vanishing current at the boundary. This no-flux boundary condition takes the form of the Neumann condition:

$$\nabla(A - V) \cdot \nu = 0 \qquad \text{on } \partial\Omega.$$

For the selfconsistent potential, we consider a Dirichlet boundary condition

$$V = 0 \qquad \text{on } \partial\Omega.$$

It remains to fix the domain of the Hamiltonian $H[A]$. In the Note [21], the QDD model was written with Dirichlet boundary conditions for the wavefunctions, as well as its discrete version. Here, for technical reasons which will be explained further (at the end of the proof of Lemma 2.4), Neumann boundary conditions are chosen:

$$D(H) = \left\{\phi \in H^2(\Omega) \,:\, \nabla\phi \cdot \nu = 0 \qquad \text{on } \partial\Omega\right\}.$$

Hence, if $A$ belongs to –say– $L^2(\Omega)$, then the operator $H[A]$ is bounded from below and has a compact resolvent. Let us denote by $(\chi_p[A])_{p=1,\cdots,\infty}$ an orthogonal basis of eigenfunctions, associated to the eigenvalues $\lambda_1[A] \leq \lambda_2[A] \leq \cdots \leq \lambda_p[A] \leq \cdots$. The non local relation (2.4) between $n$ and $A$ takes a more explicit form:

$$n[A] = \sum_{p\geq 1} e^{-\lambda_p[A]} \, |\chi_p[A]|^2. \tag{2.6}$$

To summarize this part, one can write the quantum drift-diffusion model including self-consistent effects as follows:

$$\partial_t n + \operatorname{div}\ (n\nabla(A - V)) = 0, \tag{2.7}$$

$$-\alpha\Delta V = n, \tag{2.8}$$

$$n = \sum_{p} e^{-\lambda_p[A]} \, |\chi_p[A]|^2, \tag{2.9}$$

where $(\lambda_p[A], \chi_p[A])_p$ denote the eigenvalues and the eigenfunctions of the Hamiltonian $H[A] = -\hbar^2\Delta + A + V^{ext}$ whose domain is $D(H) = \{\psi \in H^2(\Omega) : \partial_\nu \psi = 0\}$. The unknowns of this system are subject to the following no-flux boundary conditions on $\partial\Omega$:

$$V = 0 \quad ; \quad \partial_\nu (A - V) = 0 \qquad\qquad (\partial\Omega) \tag{2.10}$$

and to a Cauchy datum $n^0(x)$.

In this paper, the assumptions on the data will be the following ones:

**Assumption 2.1** *The initial datum $n^0$ is continuous and positive on $\overline{\Omega}$.*

**Assumption 2.2** *The external potential $V^{ext}$ is nonnegative and belongs to $L^\infty(\Omega)$.*

## 2.2 Technical lemmas: the relation between $n$ and $A$

In this subsection, we gather some technical lemmas that are used in this paper. The first lemma, which is given without proof, is directly adapted from [40] (the only difference lies in the domain $D(H)$; in [40], a Dirichlet boundary condition was considered instead of our Neumann boundary condition).

**Lemma 2.3** *The map $F$ defined by*

$$A \in H^1(\Omega) \mapsto F[A] := \mathrm{tr}\ \left(e^{-H[A]}\right) = \int n[A]\, dx \tag{2.11}$$

*is well-defined, Fréchet $C^\infty$ and strictly convex. Its first derivative in the direction $\phi \in H^1(\Omega)$ reads*

$$d_A F \cdot \phi = -\mathrm{tr}\ \left(e^{-H[A]}\, \phi\right) = -\int n[A]\, \phi\, dx \tag{2.12}$$

*and its second derivative reads*

$$d_A^2 F \cdot \phi \cdot \phi = -\sum_{p=1}^{\infty} \sum_{q=1}^{\infty} \frac{e^{-\lambda_p[A]} - e^{-\lambda_q[A]}}{\lambda_p[A] - \lambda_q[A]} \left| \int \phi\, \chi_p\, \overline{\chi_q}\, dx \right|^2, \tag{2.13}$$

*where $\frac{e^{-\lambda_p[A]} - e^{-\lambda_q[A]}}{\lambda_p[A] - \lambda_q[A]}$ conventionally equals $-e^{-\lambda_p[A]}$ if $\lambda_p[A] = \lambda_q[A]$.*

Remark that this lemma gives a sense to the formula (2.6) as soon as $A$ belongs to $H^1(\Omega)$.

**Lemma 2.4** *Let $A \in H^1(\Omega)$. Then the function $n[A]$ defined by (2.6) is a continuous function on $\overline{\Omega}$. If in addition we have $A \in L^\infty(\Omega)$ then $n[A]$ does not vanish on $\overline{\Omega}$.*

**Proof.** Again, the first part of this lemma is proved in [40]. Let us nevertheless give a sketch of the argument. For any $n \in \mathbb{N}^*$, the operator $(1 + H[A]^2)^{n/2} e^{-H[A]}$ is trace class (with a bound depending only on the $H^1$ norm of $A$). Moreover, the following estimate holds for the eigenfunctions:

$$\|\chi_p[A]\|_{H^2(\Omega)} \leq C(A)\,(1 + \lambda_p[A]^2)^{1/2},$$

where $C(A)$ is a constant which depends only on the $H^1$ norm of $A$. Since $H^2(\Omega)$ is an algebra (in the considered dimension $d \leq 3$), the series (2.6) defining $n[A]$ converges in $H^2(\Omega)$ and, by Sobolev embedding, $n[A]$ is continuous.

The second part of the lemma is a direct consequence of Krein-Rutman's theorem [10]. Here we use the fact that $A + V^{ext}$ is bounded from below, thanks to $A \in L^\infty(\Omega)$ and thanks to Assumption 2.2. It is important to precise that we have chosen the Neumann boundary conditions for the $\chi_p$'s (instead of Dirichlet boundary conditions) in order to garantee the fact that $n$ does not vanish on the closed domain $\overline{\Omega}$. □

**Remark 2.5** *The assumptions of this Lemma* 2.4 *are sufficient for a use in our context, since the chemical potential $A$ will always belong to $H^2(\Omega)$, but one has to say that these assumptions are not optimal and can be weakened. For instance, $A \in L^2(\Omega)$ would lead to the same result, as it can be seen from [31] and [47].*

**Lemma 2.6** *Let $A$ and $\widetilde{A}$ belong to $H^1(\Omega)$ and, using the notation* (2.6)*, let $n = n[A]$, $\widetilde{n} = n[\widetilde{A}]$. Then we have*

$$\int \left( n(A - \widetilde{A}) + n - \widetilde{n} \right) dx \leq 0. \tag{2.14}$$

**Proof.** The functional $F[A]$ defined in Lemma 2.3 is convex, thus we have the inequality:

$$F[\widetilde{A}] - F[A] \geq d_A F \cdot (\widetilde{A} - A).$$

The desired result is a consequence of the expression (2.12) of $d_A F$. □

## 2.3 Steady states and entropy dissipation

The steady states of the QDD system are well-known: these are the solutions of the Schrödinger-Poisson system studied by Nier in [40]. Following this reference, the following Proposition can be proved (its proof is left to the reader):

**Proposition 2.7** *Let $N > 0$ and let $(n, A, V)$ be a steady state of* (2.7)–(2.9) *such that $\int n(x)\,dx = N$. Assume that $n$ is continuous and positive on $\overline{\Omega}$. Then there*

*exists a constant $\epsilon_F$ such that $A = V - \epsilon_F$ and $(n, V, \epsilon_F)$ is the unique solution of the Schrödinger-Poisson system under a constraint of total charge:*

$$\begin{cases} -\hbar^2 \Delta \chi_p + (V + V^{ext})\, \chi_p = \lambda_p\, \chi_p \qquad (p = 1, \cdots, \infty) \\ \chi_p \in D(H) \quad ; \quad \displaystyle\int \chi_p\, \overline{\chi_q} = \delta_{pq}\,, \end{cases} \tag{2.15}$$

$$-\alpha \Delta V = n = \sum_p e^{\epsilon_F - \lambda_p}\, |\chi_p|^2, \qquad V \in H^1_0(\Omega), \tag{2.16}$$

$$\int n(x)\, dx = N. \tag{2.17}$$

Next, the following formal result shows that the QDD system coupled with the Poisson equation is entropic:

**Proposition 2.8** *Let $(n, A, V)$ be a smooth solution of (2.7)–(2.9). Then the following properties hold:*
*(i) The following free energy $S(t)$ is a decreasing function of time and is bounded from below (by a negative constant depending only on $\Omega$ and $\hbar$):*

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

*(ii) If $(n^\infty, A^\infty, V^\infty)$ is the solution of (2.15)–(2.17) corresponding to $N = \int n(0,x)\, dx$, then the following relative entropy $\Sigma(t)$ is the sum of two nonnegative terms and is a decreasing function of time:*

$$\Sigma(t) = -\int \left(n\,(A - A^\infty) + n - n^\infty\right) dx + \frac{\alpha}{2} \int |\nabla (V - V^\infty)|^2 dx.$$

**Proof.** By applying (2.14) with $\widetilde{A} \equiv 0$, we get

$$-\int n\,(A+1) \geq -\int n[0]\, dx.$$

Assumption 2.2 gives $V^{ext} \geq 0$. Hence, by the min-max formula, the eigenvalues $\lambda_p[0]$ of $H[0] = -\hbar^2\Delta + V^{ext}$ satisfy $\lambda_p[0] \geq \lambda_p^\Delta$, where $\lambda_p^\Delta$ are the eigenvalues of $-\hbar^2\Delta$ with Neumann boundary conditions on $\partial\Omega$. Thus we have

$$\int n[0]\, dx \leq \sum_p e^{-\lambda_p^\Delta}$$

and $S$ is bounded from below by a constant which depends only on $\Omega$ and $\hbar$.

Let us now remark that, due to the no-flux boundary conditions (2.10), an integration of the first equation of (2.7)–(2.9) yields the conservation of the total charge:

$$\forall t \geq 0 \qquad \int n(t,x)\, dx = \int n(0,x)\, dx. \tag{2.18}$$

Independently, by differentiating with respect to time the functional $F[A]$ defined by (2.11), and recalling that $V^{ext}$ is independent of time, we get

$$\frac{d}{dt}\int n(t,x)\,dx = \frac{d}{dt}F[A(t)] = d_A F\cdot\partial_t A = -\int n(t,x)\,\partial_t A(t,x)\,dx,$$

thus we have

$$\frac{d}{dt}\int n\,(A+1)\,dx = \int (\partial_t n) A\,dx.$$

To prove Item *(i)*, it remains to remark that the Poisson equation with Dirichlet boundary conditions yields

$$\frac{d}{dt}\frac{\alpha}{2}\int |\nabla V|^2\,dx = \int (\partial_t n)\,V\,dx.$$

Consequently we obtain

$$\frac{d}{dt}S(t) = -\int (\partial_t n)(A-V)dx = -\int n\,|\nabla(A-V)|^2\,dx \le 0, \tag{2.19}$$

which proves *(i)*. Let us now prove *(ii)*. The fact that the first term of $\Sigma(t)$ is nonnegative stems from (2.14). Besides, since we have $A^\infty = V^\infty - \epsilon_F$, we deduce the equivalent expression:

$$\begin{aligned}\Sigma(t) &= -\int (n\,(A+\epsilon_F) + n - n^\infty)\,dx \\ &\quad +\alpha\int \nabla V\cdot\nabla V^\infty\,dx + \frac{\alpha}{2}\int |\nabla(V-V^\infty)|^2 \\ &= S(t) - \epsilon_F\int n\,dx + \int n^\infty\,dx + \frac{\alpha}{2}\int |\nabla V^\infty|^2\,dx,\end{aligned}$$

where we used the Poisson equation $-\alpha\Delta V = n$. Therefore, by using (2.18), we deduce

$$\frac{d}{dt}\Sigma(t) = \frac{d}{dt}S(t) \le 0.$$

□

**Remark 2.9** *Eq.* (2.19) *gives the expression of the entropy dissipation. This term indicates that, in long time,* $A - V$ *should converge towards a constant. Thus any transient solution of the QDD model should converge to the (unique) corresponding steady state. In order to prove rigourously this convergence, we need to control* $n$ *from below. This is an open problem in the continuous case* (2.7)–(2.9)*, but this question finds an answer in the discrete model presented in Section* 4 *(see Theorem* 4.1*,* (iv)*).*

# 3 Semi-discretization in time

As announced in the introduction, this section is devoted to the study of a semi-discrete version of (2.7)–(2.9), which presents the advantage to be rigourous analyzed (existence and uniqueness, entropy dissipation). Notice that this part also appears as a first step towards the numerical scheme that is presented in Section 4.

Let $\Delta t > 0$ be the time step. For $k \in \mathbb{N}$, the semi-discretized model is written:

$$\frac{n^{k+1} - n^k}{\Delta t} + \text{div}\,\left(n^k \nabla (A^{k+1} - V^{k+1})\right) = 0, \tag{3.1}$$

$$-\alpha \Delta V^{k+1} = n^{k+1}, \tag{3.2}$$

$$n^{k+1} = \sum_p e^{-\lambda_p[A^{k+1}]}\, |\chi_p[A^{k+1}]|^2, \tag{3.3}$$

subject to the boundary conditions

$$V^{k+1} = 0 \quad ; \quad \partial_\nu (A^{k+1} - V^{k+1}) = 0. \tag{3.4}$$

Recall that, in this system, $\lambda_p[\cdot]$ and $\chi_p[\cdot]$ denote the whole sequence of eigenvalues and eigenfunctions of the operator $H[\cdot]$ defined in Section 2.1. The unknowns are the functions $n^k(x)$, $A^k(x)$, $V^k(x)$, for $k \in \mathbb{N}^*$. For $k = 0$, the density $n^0$ is given satisfying Assumption 2.1. Then the Poisson equation enables to define $V^0$. Concerning the initial chemical potential $A^0$, since it is not clear whether (2.6) can be inverted, we choose to let $A^0$ undetermined. Remark that $A^0$ is not required in this model to compute $(n^k, A^k, V^k)$ for $k \geq 1$. An alternative choice for the initial conditions would be to take an initial datum $A^0$, then to deduce $n^0$ by (2.6) and $V^0$ by the Poisson equation. However, it seems more interesting, for physical reasons, to start from an initial density $n^0$.

The main result of this section is the

**Theorem 3.1** *Under Assumptions* 2.1 *and* 2.2*, we have the following properties:*
*(i) The semi-discretized model* (3.1)–(3.3) *is well-posed. For all $k \in \mathbb{N}^*$, the functions $A^k \in H^1(\Omega)$, $V^k(\Omega) \in H^1_0(\Omega)$ and $n^k \in C(\overline{\Omega})$ are uniquely defined. Moreover, for all $k$ we have $n^k > 0$ on $\overline{\Omega}$ and the total charge is conserved:*

$$\int n^k \, dx = \int n^0 \, dx. \tag{3.5}$$

*(ii) The following free energy $S^k$, defined for $k \geq 1$, is bounded from below and decreases as $k$ increases:*

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

*(iii) If $(n^\infty, A^\infty, V^\infty)$ is the solution of the Schrödinger-Poisson system* (2.15)–(2.17) *corresponding to $N = \int n^0 \, dx$, then the following relative entropy $\Sigma^k$ is the sum of two nonnegative terms and decreases as $k$ increases:*

$$\Sigma^k = -\int \left(n^k \, (A^k - A^\infty) + n^k - n^\infty\right) dx + \frac{\alpha}{2} \int |\nabla (V^k - V^\infty)|^2.$$

**Proof.** *(i)* Let us proceed by induction. Let $n^k$ be a given function, positive and continuous on $\overline{\Omega}$. Inspired by [39, 40], we introduce the following functional, defined for $A \in H^1(\Omega)$ and $V \in H^1_0(\Omega)$:

$$J(A,V) = \frac{\Delta t}{2} \int n^k \, |\nabla(A-V)|^2 \, dx + \frac{\alpha}{2} \int |\nabla V|^2 \, dx + F[A] + \int n^k \, (A-V) \, dx,$$

where $F[A]$ is defined by (2.11). This functional is continuous, Frchet differentiable, and its derivative is given by

$$\begin{aligned} d_{A,V} J \cdot (\delta A, \delta V) = \; & \Delta t \int n^k \, \nabla(A-V) \cdot \nabla(\delta A - \delta V) \, dx \\ & + \alpha \int \nabla V \cdot \nabla \delta V \, dx \\ & - \int n[A] \, \delta A \, dx + \int n^k \, (\delta A - \delta V) \, dx, \end{aligned}$$

where we have applied Lemma 2.3. Therefore it is readily seen that the critical points of $J$ satisfy (3.1)–(3.3), (3.4). To prove the existence and uniqueness of $A^{k+1}$ and $V^{k+1}$, it suffices to show that $J$ is strictly convex and coercive, since its unique minimizer will be $(A^{k+1}, V^{k+1})$. The strict convexity is a consequence of Lemma 2.3 (which states that $F$ is strictly convex), of the strict convexity of the functional

$$V \in H^1_0(\Omega) \longmapsto \int |\nabla V|^2 \, dx$$

and of the convexity of the functional

$$(A,V) \in H^1(\Omega) \times H^1_0(\Omega) \longmapsto \int n^k \, |\nabla(A-V)|^2 \, dx.$$

It remains to prove the coercivity with respect to $A \in H^1(\Omega)$ and $V \in H^1_0(\Omega)$. Let $(A^\varepsilon, V^\varepsilon)$ be a sequence in $H^1(\Omega) \times H^1_0(\Omega)$, parametrized by $\varepsilon > 0$, such that $J(A^\varepsilon, V^\varepsilon)$ has an upper bound independent of $\varepsilon$. To prove the coercivity of $J$, it suffices to show that $\|A^\varepsilon\|_{H^1} + \|V^\varepsilon\|_{H^1}$ can be bounded independently of $\varepsilon$.

Setting $a^\varepsilon = \frac{1}{|\Omega|} \int A^\varepsilon \, dx$ (where $|\Omega|$ denotes the measure of $\Omega$), we introduce the function $B^\varepsilon = A^\varepsilon - a^\varepsilon$. We have

$$\begin{aligned} J(A^\varepsilon, V^\varepsilon) = \; & \frac{\Delta t}{2} \int n^k \, |\nabla(B^\varepsilon - V^\varepsilon)|^2 \, dx + \frac{\alpha}{2} \int |\nabla V^\varepsilon|^2 \, dx \\ & + e^{-a^\varepsilon} \sum_p e^{-\lambda_p[B^\varepsilon]} + \int n^k \, (B^\varepsilon - V^\varepsilon) \, dx + a^\varepsilon \int n^k \, dx \le C, \end{aligned}$$

where $C$ does not depend on $\varepsilon$. We recall that there exist two constants $\underline{n} > 0$ and $\overline{n} > 0$, independent of $\varepsilon$, such that

$$\underline{n} \le n^k(x) \le \overline{n} \qquad \text{on } \overline{\Omega}.$$

Hence the Cauchy-Schwarz inequality gives

$$\frac{\Delta t}{2}\,\underline{n}\int|\nabla(B^\varepsilon-V^\varepsilon)|^2\,dx+\frac{\alpha}{2}\int|\nabla V^\varepsilon|^2\,dx-\overline{n}\,|\Omega|^{1/2}\left(\|B^\varepsilon\|_{L^2(\Omega)}+\|V^\varepsilon\|_{L^2(\Omega)}\right)$$
$$+e^{-a^\varepsilon}\sum_p e^{-\lambda_p[B^\varepsilon]}+a^\varepsilon\int n^k\,dx\le J(A^\varepsilon,V^\varepsilon)\le C. \tag{3.6}$$

Besides, denoting by $\widetilde{H^1}(\Omega)$ the space of $H^1(\Omega)$ functions which have a vanishing integral on $\Omega$, a classical compactness argument shows that, for any $a_1>0$ and $a_2>0$, the norm

$$(B,V)\in\widetilde{H^1}(\Omega)\times H^1_0(\Omega)\quad\longmapsto\quad\left(a_1\|\nabla(B-V)\|^2_{L^2(\Omega)}+a_2\|\nabla V\|^2_{L^2(\Omega)}\right)^{1/2}$$

is equivalent on this space $\widetilde{H^1}(\Omega)\times H^1_0(\Omega)$ to the standard $H^1(\Omega)\times H^1(\Omega)$ norm. Hence there exist two constants $C_0>0$ and $C_1>0$ independent of $\varepsilon$ such that

$$\frac{\Delta t}{2}\,\underline{n}\int|\nabla(B^\varepsilon-V^\varepsilon)|^2\,dx+\frac{\alpha}{2}\int|\nabla V^\varepsilon|^2\,dx-\overline{n}\,|\Omega|^{1/2}\left(\|B^\varepsilon\|_{L^2(\Omega)}+\|V^\varepsilon\|_{L^2(\Omega)}\right)$$
$$\ge C_0\|B^\varepsilon\|^2_{H^1(\Omega)}+C_0\|V^\varepsilon\|^2_{H^1(\Omega)}-C_1,$$

thus (3.6) gives

$$C_0\|B^\varepsilon\|^2_{H^1(\Omega)}+C_0\|V^\varepsilon\|^2_{H^1(\Omega)}+e^{-a^\varepsilon}\sum_p e^{-\lambda_p[B^\varepsilon]}+a^\varepsilon\int n^k\,dx\le C. \tag{3.7}$$

Let us now recall that the first eigenvalue of $H[B^\varepsilon]$ is defined by

$$\lambda_1[B^\varepsilon]=\min_{\substack{\phi\in H^1(\Omega)\\ \|\phi\|_{L^2(\Omega)}=1}}\left(\hbar^2\int|\nabla\phi|^2\,dx+\int(B^\varepsilon+V^{ext})\,\phi^2\,dx\right).$$

By choosing the test function $\phi(x)\equiv 1/\sqrt{|\Omega|}$ in this formula, we deduce from $\int B^\varepsilon\,dx=0$ that

$$\lambda_1[B^\varepsilon]\le\frac{1}{|\Omega|}\int V^{ext}\,dx.$$

There exists consequently a constant $C_2>0$ independent of $\varepsilon$ such that

$$e^{-a^\varepsilon}\sum_p e^{-\lambda_p[B^\varepsilon]}\ge C_2\,e^{-a^\varepsilon}$$

and (3.7) implies

$$C_0\|B^\varepsilon\|^2_{H^1(\Omega)}+C_0\|V^\varepsilon\|^2_{H^1(\Omega)}+C_2e^{-a^\varepsilon}+a^\varepsilon\int n^k\,dx\le C.$$

Since $\int n^k\,dx > 0$, it is clear then that $\|B^\varepsilon\|_{H^1(\Omega)}$, $\|V^\varepsilon\|_{H^1(\Omega)}$ and $|a^\varepsilon|$ are bounded independently of $\varepsilon$. Thus $\|A^\varepsilon\|_{H^1(\Omega)}$ is bounded, which completes the proof of coercivity.

As soon as $(A^{k+1}, V^{k+1})$ is defined as the unique minimizer of $J$, we define $n^{k+1}$ thanks to (2.6). The first part of Lemma 2.4 shows that $n^{k+1}$ is continuous on $\overline{\Omega}$. Hence, (3.1)–(3.3) and standard elliptic regularity estimates imply that $V^{k+1} \in H^2(\Omega)$ and $A^{k+1} \in H^2(\Omega)$. The Sobolev embedding $H^2(\Omega) \hookrightarrow C(\overline{\Omega})$ yields $A^{k+1} \in L^\infty(\Omega)$, which implies, thanks to the second part of Lemma 2.4, that $n^{k+1} > 0$ on $\overline{\Omega}$. Consequently, $A^{k+2}$ and $\Phi^{k+2}$ can be constructed and, by induction, all the sequence $(A^k, \Phi^k)_{k\geq 1}$ (thanks to Assumption 2.1 which enables the first step of the construction).

To complete the proof of *(i)*, it remains to integrate (3.1) on $\Omega$, which gives, thanks to the boundary conditions (3.4):

$$\int n^{k+1}\,dx = \int n^k\,dx. \tag{3.8}$$

This yields the charge conservation (3.5).

*(ii)* Let us adapt to the semi-discrete case the proof of Proposition 2.8. By using Lemma 2.6, we have

$$\int \left(n^k(A^k - A^{k+1}) + n^k - n^{k+1}\right)\,dx \leq 0,$$

thus

$$\begin{aligned} -\int (n^{k+1}\,A^{k+1} - n^k\,A^k + n^{k+1} - n^k)\,dx \;&= -\int (n^{k+1} - n^k)\,A^{k+1}\,dx \\ &\quad + \int \left(n^k(A^k - A^{k+1}) + n^k - n^{k+1}\right)\,dx \\ &\leq -\int (n^{k+1} - n^k)\,A^{k+1}\,dx. \end{aligned} \tag{3.9}$$

Besides, by using the Poisson equation (3.2), we obtain

$$\begin{aligned} \frac{\alpha}{2}\int \left(|\nabla V^{k+1}|^2 - |\nabla V^k|^2\right)\,dx \;&= \frac{1}{2}\int (n^{k+1}\,V^{k+1} - n^k\,V^k)\,dx \\ &= \frac{1}{2}\int (n^{k+1} - n^k)\,V^{k+1}\,dx + \frac{1}{2}\int n^k(V^{k+1} - V^k)\,dx \\ &= \frac{1}{2}\int (n^{k+1} - n^k)\,V^{k+1}\,dx + \frac{1}{2}\int V^k(n^{k+1} - n^k)\,dx. \end{aligned}$$

By remarking that

$$0 \leq \alpha\int |\nabla(V^{k+1} - V^k)|^2 dx = \int (n^{k+1} - n^k)(V^{k+1} - V^k),$$

we deduce that

$$\frac{1}{2}\int V^k(n^{k+1}-n^k)\,dx \le \frac{1}{2}\int V^{k+1}(n^{k+1}-n^k)\,dx$$

and get

$$\frac{\alpha}{2}\int \left(|\nabla V^{k+1}|^2 - |\nabla V^k|^2\right)\,dx \le \int V^{k+1}(n^{k+1}-n^k)\,dx.$$

By combining this inequality and (3.9), we obtain

$$\begin{aligned} S^{k+1}-S^k &\le -\int (n^{k+1}-n^k)(A^{k+1}-V^{k+1})\,dx \\ &= \Delta t \int (A^{k+1}-V^{k+1})\,\mathrm{div}\,\left(n^k\nabla(A^{k+1}-V^{k+1})\right)\,dx, \end{aligned}$$

thanks to (3.1). An integration by parts, using (3.4), gives finally

$$S^{k+1}-S^k \le -\Delta t \int n^k\,|\nabla(A^{k+1}-V^{k+1})|^2\,dx \le 0.$$

This proves *(ii)*. Finally, to prove *(iii)*, it suffices to remark as for Proposition 2.8 that

$$\Sigma^{k+1}-\Sigma^k = S^{k+1}-S^k \le 0.$$

□

# 4 The fully discretized system: construction and analysis

We complete the construction of a numerical scheme for the QDD model (2.7)–(2.9) by now discretizing the system (3.1)–(3.3) with respect to the space variable. In the following section, we construct the scheme and give in Theorem 4.1 its main properties: well-posedness, charge conservation, entropy dissipation and long-time stability. These properties are proved in Sections 4.2, 4.3 and 4.4.

## 4.1 Notations and main results

For simplicity, the space dimension is now $d = 1$. The domain is $\Omega = (0,1)$ and the space gridstep is $\Delta x = 1/(N+1)$. The grid is composed of the points $x_i = i\Delta x$ for $i = 0, \cdots, N+1$, where $N \in \mathbb{N}$. In order to write the fully discretized finite difference numerical scheme, let us introduce the following $N \times N$ matrices of discrete derivative:

$$D^- = \frac{1}{\Delta x}\begin{pmatrix} 0 & 0 & \cdots & \\ -1 & 1 & 0 & \cdots \\ 0 & \ddots & \ddots & 0 \\ \vdots & 0 & -1 & 1 \end{pmatrix}, \qquad D^+ = \frac{1}{\Delta x}\begin{pmatrix} -1 & 1 & 0 & \dots \\ 0 & -1 & 1 & \cdots \\ 0 & \ddots & \ddots & 1 \\ \vdots & \cdots & 0 & 0 \end{pmatrix},$$

$$\widetilde{D^-} = \frac{1}{\Delta x}\begin{pmatrix} 1 & 0 & \cdots & \\ -1 & 1 & 0 & \cdots \\ 0 & \ddots & \ddots & 0 \\ \vdots & 0 & -1 & 1 \end{pmatrix}, \qquad \widetilde{D^+} = \frac{1}{\Delta x}\begin{pmatrix} -1 & 1 & 0 & \dots \\ 0 & -1 & 1 & \cdots \\ 0 & \ddots & \ddots & 1 \\ \vdots & \cdots & 0 & 1 \end{pmatrix},$$

$$\Delta_{Dir} = \frac{1}{\Delta x^2}\begin{pmatrix} -2 & 1 & 0 & \dots \\ 1 & -2 & \ddots & 0 \\ 0 & \ddots & \ddots & 1 \\ \vdots & \cdots & 1 & -2 \end{pmatrix}, \qquad \Delta_{Neu} = \frac{1}{\Delta x^2}\begin{pmatrix} -1 & 1 & 0 & \dots \\ 1 & -2 & \ddots & 0 \\ 0 & \ddots & \ddots & 1 \\ \vdots & \cdots & 1 & -1 \end{pmatrix}.$$

Remark that $\Delta_{Neu} = \widetilde{D^-}D^+ = \widetilde{D^+}D^-$. The unknowns are the following sequences of vectors in $\mathbb{R}^N$: $n^k = (n_i^k)_{1\le i\le N}$, $A^k = (A_i^k)_{1\le i\le N}$, $V^k = (V_i^k)_{1\le i\le N}$ and the scheme is written:

$$\frac{n^{k+1}-n^k}{\Delta t} + \frac{1}{2}\widetilde{D^-}\left(n^k\, D^+(A^{k+1}-V^{k+1})\right) + \frac{1}{2}\widetilde{D^+}\left(n^k\, D^-(A^{k+1}-V^{k+1})\right) = 0, \quad (4.1)$$

$$-\alpha\,\Delta_{Dir}V^k = n^k, \quad (4.2)$$

$$n^k = \sum_p \exp\left(-\ell_p[A^k]\right)(X_p[A^k])^2 \quad (4.3)$$

for $k \in \mathbb{N}$ (here and in the sequel, for any $(X,Y) \in \mathbb{R}^N \times \mathbb{R}^N$, $XY$ denotes the direct product $(X_iY_i)_{1\le i\le N}$). In this discretized system, the definitions of $\ell_p[A]$ and $X_p[A]$ are the discrete analogue of those of $\lambda_p[A]$, $\chi_p[A]$ for the continuous problem. These quantities are the eigenvalues and the normalized eigenvectors of the discretized Hamiltonian with Neumann boundary conditions:

$$M[A] = -\hbar^2\Delta_{Neu} + \mathrm{Diag}(A + V^{ext}),$$

where $\mathrm{Diag}(A)$ denotes the diagonal matrix of coefficients $(A_i)_{1\le i\le N}$ and where the components of the vector $V^{ext}$ are $V_i^{ext} = \frac{1}{\Delta x}\int_{x_{i-1/2}}^{x_{i+1/2}} V^{ext}(x)\,dx$. Of course, the index $p$ of the eigenvalues and eigenvectors belongs now to $\{1,\cdots,N\}$. Moreover, the eigenvectors are normalized with respect to the euclidean norm $\|\cdot\|_N$ associated to the scalar product on $\mathbb{R}^N$:

$$(U,V)_N = \Delta x \sum_{i=1}^N U_i\, V_i\,.$$

Remark that the boundary conditions are already taken into account in this scheme, the values of the unknowns for $i = 0$ or $i = N+1$ being implicitely defined. To complete (4.1)–(4.3), it suffices to add an initial condition. If a Cauchy data for the continuous problem $n^0$ is given, the vector $n^0 \in \mathbb{R}^N$ is chosen as follows:

$$n_i^0 = \frac{1}{\Delta x}\int_{x_{i-1/2}}^{x_{i+1/2}} n^0(x)\,dx \qquad \text{for } i = 1,\cdots,N. \quad (4.4)$$

The numerical scheme (4.1)–(4.3) is clearly consistent with the QDD system (2.7)–(2.10). Its properties are listed in the following Theorem, whose proof is developed in the three next subsections:

**Theorem 4.1** *If Assumptions* 2.1 *and* 2.2 *are satisfied, the numerical scheme* (4.1)–(4.4) *is consistent with* (2.7)–(2.10) *and has the following properties:*
*(i)* (well-posedness) *For all $k \in \mathbb{N}$, its numerical solution $(n^k, A^k, V^k)$ is uniquely defined. Moreover, for all $k \in \mathbb{N}$, $(A^{k+1}, V^{k+1})$ is the unique minimizer of the strictly convex and coercive functional*

$$\begin{aligned}\widehat{J}(A,V) = \ & \frac{\Delta t\,\Delta x}{4}\sum_{i=1}^{N} n_i^k \left(D^+(A-V)\right)_i^2 + \frac{\Delta t\,\Delta x}{4}\sum_{i=1}^{N} n_i^k \left(D^-(A-V)\right)_i^2 \\ & + \frac{\alpha\,\Delta x}{2}\sum_{i=1}^{N}(D^+V)_i^2 + \frac{\alpha}{2\,\Delta x}(V_1)^2 + \frac{\alpha}{2\,\Delta x}(V_N)^2 \\ & + \sum_{p=1}^{N}\exp\left(-\ell_p[A]\right) + \Delta x\sum_{i=1}^{N} n_i^k\,(A_i - V_i)\,.\end{aligned} \tag{4.5}$$

*(ii)* (charge conservation) *For all $k$ and for all $i$ we have $n_i^k > 0$ and the (discrete) total charge is conserved:*

$$\forall k \in \mathbb{N} \qquad \Delta x\sum_{i=1}^{N} n_i^k = \Delta x\sum_{i=1}^{N} n_i^0\,. \tag{4.6}$$

*(iii)* (entropy dissipation) *The sequence of (discrete) free energies defined by*

$$S^k = -\Delta x\sum_{i=1}^{N} n_i^k\,(A_i^k + 1) + \frac{\alpha\Delta x}{2}\sum_{i=1}^{N}(D^+V^k)_i^2 + \frac{\alpha}{2\,\Delta x}(V_1^k)^2 + \frac{\alpha}{2\,\Delta x}(V_N^k)^2 \tag{4.7}$$

*is decreasing and belongs to $\ell^\infty$. Moreover there exists a constant $C > 0$ (depending only on $\Omega$ and $\hbar$) such that, for any $K \in \mathbb{N}$, we have*

$$\begin{aligned}-C \le S^K + & \frac{\Delta t\Delta x}{2}\sum_{k=1}^{K}\sum_{i=1}^{N} n_i^{k-1}\left(D^+(A^k - V^k)\right)_i^2 \\ & + \frac{\Delta t\Delta x}{2}\sum_{k=1}^{K}\sum_{i=1}^{N} n_i^{k-1}\left(D^-(A^k - V^k)\right)_i^2 \le S^0.\end{aligned} \tag{4.8}$$

*(iv)* (long-time behavior) *The numerical solution of* (4.1)–(4.3), (4.4) *converges, as $k$ tends to $+\infty$, to the unique solution of the discrete Schrödinger-Poisson system:*

$$\forall i \in \{1, \cdots, N\} \qquad A_i = V_i - \epsilon_F\,, \qquad \epsilon_F \in \mathbb{R}, \tag{4.9}$$

$$\begin{cases} -\hbar^2\Delta_{Neu}X_p + (V + V^{ext})\,X_p = \ell_p\,X_p \qquad (p = 1, \cdots, N) \\ \forall (p,q) \qquad (X_p, X_q)_N = \delta_{pq}\,, \end{cases} \tag{4.10}$$

$$-\alpha\Delta_{Dir}V = n = \sum_p e^{\epsilon_F-\ell_p}\,(X_p)^2, \tag{4.11}$$

$$\Delta x\sum_{i=1}^{N} n = \Delta x\sum_{i=1}^{N} n^0. \tag{4.12}$$

## 4.2 Proof of well-posedness and entropy dissipation

For the sake of conciseness, we shall not develop the proofs of the first three items, *(i)*, *(ii)* and *(iii)* of Theorem 4.1. Indeed, it suffices to adapt to the discrete case the proof of Theorem 3.1. These results are based on formulas of discrete integration by parts and on technical results concerning matrix analysis which are the discrete equivalents of the technical results stated in Section 2.2, and that we have listed in Lemma 4.2 below.

It is worthwhile to precise that the similarity between the functional $J(A,V)$, introduced in the proof of Theorem 3.1, and the functional $\widehat{J}(A,V)$ of this Theorem 4.1 is due to two useful formulas of discrete integration by parts: for any pair of vectors $(U,V)\in\mathbb{R}^N\times\mathbb{R}^N$, we have

$$\begin{aligned} -\left(\Delta_{Neu}U,V\right)_N &= -\left(\widetilde{D^-}D^+U,V\right)_N = \left(D^+U,D^+V\right)_N \\ &= -\left(\widetilde{D^+}D^-U,V\right)_N = \left(D^-U,D^-V\right)_N \end{aligned} \tag{4.13}$$

and

$$-\left(\Delta_{Dir}U,V\right)_N = \left(D^+U,D^+V\right)_N + \frac{U_1V_1+U_NV_N}{\Delta x}. \tag{4.14}$$

Next, we gather in the following lemma some classical but useful technical results on matrices:

**Lemma 4.2** *Let $A\in\mathbb{R}^N$. Then the eigenvalues $\ell_p[A]$ of the matrix $M[A] = -\hbar^2\Delta_{Neu} + \mathrm{Diag}(A+V^{ext})$ are simple. (Up to a multiplication by -1), its first eigenvector $X_1[A]$ has positive components. The derivatives of the eigenvalues and eigenvectors of $M[A]$ with respect to $A$, in the direction $\delta A$, are given by*

$$d\ell_p[A]\cdot\delta A = \left(\delta A\,X_p[A],X_p[A]\right)_N,$$

$$dX_p[A]\cdot\delta A = \sum_{q\neq p}\frac{1}{\ell_p[A]-\ell_q[A]}\left(\delta A\,X_p[A],X_q[A]\right)_N X_q[A].$$

**Proof.** The simplicity of the eigenvalues of $M[A]$ is a general classical result for Hessenberg matrices [49], *i.e* matrices $M=(m_{i,j})_{1\leq i,j\leq N}$ such that

$$m_{i,j}=0 \text{ for } j<i-1 \qquad \text{and} \qquad m_{i,i-1}\neq 0 \text{ for } 2\leq i\leq N.$$

This simplicity enables to differentiate $\ell_p$ and $X_p[A]$ by using classical perturbation theory.

Let $\lambda = 1 + \max_i |A_i|$. Then it is clear that the matrix $M[A] + \lambda I$ is invertible and satisfies the discrete maximum principle:

$$\forall Y \in \mathbb{R}^N \backslash \{0\} \qquad Y \geq 0 \quad \Longrightarrow \quad (M[A] + \lambda I)^{-1} Y > 0,$$

where, for any vector $X \in \mathbb{R}^N$, the notation $X \geq 0$ (resp. $X > 0$) stands for $X_i \geq 0$ (resp. $X_i > 0$), for all $i = 1, \cdots, N$. Hence Perron-Frobenius theorem (see [49]) applies to the matrix $(M[A] + \lambda I)^{-1}$: the spectral radius of this matrix is an eigenvalue and, up to a multiplication by $-1$, the corresponding eigenvector has positive components. This vector is the ground state $X_1[A]$ of $M[A]$. □

**Remark 4.3** *A special care has to be taken for the initial step of the scheme. In the semi-discrete case of system* (3.1)–(3.3)*, the question of the initial step was left unsolved: for a given initial density $n^0(x)$, can we define a unique corresponding chemical potential $A^0$ such that* (3.3) *holds ? In the fully discrete case, this question finds a positive answer, as stated in Theorem* 4.1*,* (i)*. Section* 4.3 *is devoted to this particular point of the theorem.*

## 4.3 Initialization of the chemical potential

As noted above in Remark 4.3, one question has not been addressed yet concerning the numerical scheme (4.1)–(4.4): the computation of the initial chemical potential $A^0$ corresponding to the initial data $n^0$. While, in the continuous problem, we do not know whether (or in which functional framework) the non local relation (2.6) linking $n$ to $A$ is invertible, this operation is possible with its discrete analogous (4.3). The aim of this section is to establish this property: we show that this problem is again equivalent to a convex minimization problem. Remark that this enables to deduce a practical method to solve numerically this problem, by writing an algorithm for this optimization problem (see [20] for details). Note also that the possibility of inverting the constitutive relation $A \mapsto n[A]$, interesting for itself, is not mandatory for the other steps of the scheme (see Theorem 4.1 *(i)*): the minimization of $J$ for the computation of $(A^{k+1}, V^{k+1})$ does not require the knowledge of $A^k$. The following Proposition is the main result of this subsection:

**Proposition 4.4** *Let $n \in (\mathbb{R}_+^*)^N$. Then there exists a unique $A \in \mathbb{R}^N$ such that*

$$n = \sum_{p=1}^{N} \exp\left(-\ell_p[A]\right) \, (X_p[A])^2, \tag{4.15}$$

*where $\ell_p[A]$ and $X_p[A]$ are the eigenvalues and the eigenvectors of the discrete Hamiltonian $M[A] = -\hbar^2 \Delta_{Neu} + \mathrm{Diag}(A + V^{ext})$.*

**Proof.** Consider the functional

$$\Phi(A) = \sum_{p} \exp\left(-\ell_p[A]\right) + (n, A)_N \, . \tag{4.16}$$

Straightforward calculations using Lemma 4.2 lead to the expression of its first and second derivatives:

$$d\Phi_A \cdot \delta A = \left( n - \sum_p \exp(-\ell_p[A])\,(X_p[A])^2, \delta A \right)_N$$

and

$$\begin{aligned} d^2\Phi_A \cdot \delta A \cdot \delta A = & \sum_{p=1}^{N} \exp(-\ell_p[A])\,(\delta A\, X_p[A]\,,\, X_p[A])_N^2 \\ & - \sum_p \sum_{q \neq p} \frac{\exp(-\ell_p[A]) - \exp(-\ell_q[A])}{\ell_p[A] - \ell_q[A]}\,(\delta A\, X_p[A]\,,\, X_q[A])_N^2\,. \end{aligned}$$

It is clear then that this functional $\Phi$ is strictly convex and that its unique minimizer satisfies (4.15). To prove the existence of a solution to the problem, the major task is to prove the coercivity of this functional.

Recall that

$$\ell_1[A] = \min_{\|\phi\|_N = 1} \left( (-\hbar^2 \Delta_{Neu}\phi, \phi)_N + (\mathrm{Diag}(A + V^{ext})\phi, \phi)_N \right). \tag{4.17}$$

Let $i_0 \in \{1, \cdots, N\}$. By choosing the $i_0$-th normalized basis vector as $\phi$ in (4.17) (*i.e.* $\phi_i = \delta_{i,i_0}/\sqrt{\Delta x}$), we obtain

$$\ell_1[A] \leq A_{i_0} + \frac{2\hbar^2}{\Delta x^2} + V_{i_0}^{ext}\,. \tag{4.18}$$

Hence, there exists a constant $C > 0$ depending only on $\Delta x$, $\hbar$ and $V^{ext}$ such that

$$\Phi[A] \geq C \sum_i \exp\left(-A_i\right) + \Delta x \sum_i n_i\, A_i\,. \tag{4.19}$$

Since for all $i$ we have $n_i > 0$, it is clear that

$$\lim_{\|A\| \to \infty} \Phi[A] = +\infty.$$

This proves the coercivity of $\Phi$.

Remark that, since $A$ realizes the minimum of $\Phi$, we have in particular the following inequality, which will be used later on:

$$\Phi[A] \leq \Phi[-V^{ext}] \leq \sum_p \exp\left(-\ell_p^{\Delta}\right) \leq C, \tag{4.20}$$

where $(\ell_p^{\Delta})_{p=1,\cdots,N}$ denote the eigenvalues of $-\hbar^2\Delta_{Neu}$ and $C$ is independent of $\Delta x$.

□

## 4.4 Proof of long-time behavior

This subsection is devoted to the proof of Item *(iv)* of Theorem 4.1. The study of the long-time behavior of the model is an interesting issue which is addressed here in the fully discrete case (Theorem 4.1) but was not solved in the semi-discrete case (Theorem 3.1). As will be seen later on, it is possible here to control the density from below, while this crucial question is still open for the continuous QDD problem (2.7)–(2.9) or the semi-discrete QDD problem (3.1)–(3.3).

From the positivity of the $n_i^k$'s and from (4.6), it is first deduced that, for any $i$, the sequence $(n_i^k)_{k\in\mathbb{N}}$ is bounded :

$$\forall k,\, \forall i \qquad 0 < n_i^k \leq C_0. \tag{4.21}$$

In this proof, $C_j$ $(j = 0, \cdots, 9)$ denote positive constants independent of $i$ and $k$ and which only depend on $\Delta x$. After extraction of a subsequence, we get

$$\forall i \in \{1, \cdots, N\} \qquad\qquad n_i^k \longrightarrow n_i^\infty \quad \text{as } k \to +\infty.$$

*Step 1: finding a bound from below for the density.* The crucial step in this proof consists in proving that for all $i$ we have $n_i^\infty > 0$. Let us introduce the set

$$\mathcal{I} = \{i \in \{1, \cdots, N\} \,:\, n_i^\infty > 0\}\,.$$

By passing to the limit in (4.6), we deduce that $\sum_i n_i^\infty = \sum_i n_i^0 > 0$, thus $\mathcal{I} \neq \emptyset$.

In the proof of Proposition 4.4, we have obtained the estimate (4.19), which, together with (4.20), implies

$$C_1 \sum_i \exp\left(-A_i^k\right) + \Delta x \sum_i n_i^k\, A_i^k \leq C_2.$$

From this inequality, two facts are deduced. Firstly, thanks to (4.21), we obtain the lower bound

$$\forall k,\, \forall i \qquad A_i^k \geq -C_3.$$

Secondly, the inequality

$$n_i^k\, A_i^k \leq \frac{C_2 + C_0 C_3}{\Delta x}$$

provides an upper bound for the sequence $(A_i^k)_{k\in\mathbb{N}}$ for each $i \in \mathcal{I}$.

In this proof, we denote $\ell_p^k = \ell_p[A^k]$ and $X_p^k = X_p[A^k]$. Recall that $\mathcal{I} \neq \emptyset$. In other terms, we have $n_{i_0}^\infty > 0$ for a certain $i_0$. Consequently, $A_{i_0}^k$ is bounded from above independently of $k$ and, by (4.18), there exists a constant $C_4$ such that

$$\ell_1^k \leq C_4. \tag{4.22}$$

Furthermore, (4.1)–(4.3) yields

$$\forall i \qquad \exp\left(-\ell_1^k\right) (X_{1,i}^k)^2 \leq n_i^k\,. \tag{4.23}$$

Since the vector $X_1^k$ is normalized, we have

$$N\Delta x \max_i (X_{1,i}^k)^2 \geq \|X_1^k\|_N^2 = 1,$$

thus, from (4.21) and (4.23), we deduce

$$\exp\left(-\ell_1^k\right) \leq \frac{C_0}{\max_i (X_{1,i}^k)^2} \leq C_0\, N\Delta x \leq C_0,$$

which gives

$$\ell_1^k \geq -C_5. \tag{4.24}$$

Next, from (4.22) and (4.23), we deduce that there exists a constant $C$ such that

$$\forall i \qquad 0 < X_{1,i}^k \leq C\sqrt{n_i^k} \tag{4.25}$$

(the first eigenvector $X_1^k$ is implicitly chosen with positive components). Besides, since this vector $X_1^k$ is normalized, it converges as $k \to \infty$ (up to another extraction of subsequence) to a normalized vector $X^\infty$ :

$$\forall i \in \{1, \cdots, N\} \qquad\qquad X_{1,i}^k \longrightarrow X_i^\infty \geq 0 \quad \text{as } k \to +\infty.$$

Thanks to (4.25), we get

$$\forall i \in \{1, \cdots, N\} \backslash \mathcal{I}, \qquad X_i^\infty = 0.$$

Let us show that $\mathcal{I} = \{1, \cdots, N\}$ by using a contradiction argument. We assume that there exists $i_0 \in \{1, \cdots, N\} \backslash \mathcal{I}$. Since we know that $X^\infty \neq 0$, one can choose in fact $i_0$ such that $X_{i_0+1}^\infty > 0$ or $X_{i_0-1}^\infty > 0$. For instance and with no loss of generality, assume that $X_{i_0+1}^\infty > 0$, which gives $n_{i_0+1}^\infty > 0$ with (4.25) (due to the symmetric form of the finite difference scheme (4.1), a similar argument can be used in the case $X_{i_0-1}^\infty > 0$). We deduce from

$$M[A^k]\, X_1^k = \ell_1^k\, X_1^k$$

the identity

$$\left(\frac{2\hbar^2}{\Delta x^2} + A_{i_0}^k + V_{i_0}^{ext} - \ell_1^k\right) X_{1,i_0}^k = \frac{\hbar^2}{\Delta x^2}\left(X_{1,i_0+1}^k + X_{1,i_0-1}^k\right)$$

(actually, this equality holds only if $i_0 > 1$; if $i_0 = 1$ the term $2\hbar^2$ in the left-hand side has to be replaced by $\hbar^2$, which does not affect the rest of the proof). Thus, for $k$ large enough, we deduce from (4.24) that

$$\left(A_{i_0}^k + \frac{2\hbar^2}{\Delta x^2} + V_{i_0}^{ext} + C_5\right) X_{1,i_0}[A^k] \geq \frac{\hbar^2}{2\Delta x^2} X_{i_0+1}^\infty > 0.$$

Since $X^k_{1,i_0}$ converges to 0 as $k$ goes to $+\infty$, this yields

$$A^k_{i_0} \longrightarrow +\infty \qquad \text{as } k \to +\infty.$$

The contradiction will now come from the entropy estimate (4.8). Indeed, one can deduce from this inequality that

$$\forall k,\, \forall i \qquad |V^k_i| \leq C_6 \tag{4.26}$$

and

$$\Delta t\, n^{k-1}_{i_0+1} \left(A^k_{i_0+1} - A^k_{i_0} - V^k_{i_0+1} - V^k_{i_0}\right)^2 \leq C_7.$$

This leads to a contradiction, since we have seen that, as $k \to +\infty$,

$$n^k_{i_0+1} \to n^\infty_{i_0+1} > 0, \qquad |A^k_{i_0+1}| + |V^k_{i_0+1}| + |V^k_{i_0}| \leq C_8 \quad \text{and} \quad A^k_{i_0} \to +\infty.$$

Consequently, we have $\mathcal{I} = \{1, \cdots, N\}$ and, for all $i$, we have $n^\infty_i > 0$.

*Step 2: passing to the limit.* Due to the fact that $n^\infty_i > 0$, for all $i$, we deduce the bound

$$\forall k,\, \forall i \qquad |A^k_i| \leq C_9$$

and, thanks to the bound (4.26), one can extract another subsequence such that

$$\forall i \in \{1, \cdots, N\} \qquad A^k_i \longrightarrow A^\infty_i \quad \text{and} \quad V^k_i \longrightarrow V^\infty_i \quad \text{as } k \to +\infty.$$

By using again the entropy estimate (4.8), we obtain

$$\frac{\Delta t}{2\Delta x} \sum_{k=1}^{\infty} \sum_{i=1}^{N-1} n^{k-1}_i \left(A^k_{i+1} - V^k_{i+1} - A^k_i + V^k_i\right)^2 \leq C,$$

which implies that $A^\infty_i - V^\infty_i$ does not depend on $i$. Denoting by $-\epsilon_F$ this constant, one can pass to the limit in (4.1)–(4.3) and obtain a solution of (4.9)–(4.12). To conclude that all the sequence converges (and not only a subsequence), it remains to prove the uniqueness of the solution for this discrete Schrödinger-Poisson system. This can be done by following the approach developed in [39]. Indeed, it is possible to show that the following functional is strictly convex and that its unique minimizer solves (4.9)–(4.12):

$$\begin{aligned} \widetilde{J}(\epsilon_F, V) = \; & \frac{\alpha\, \Delta x}{2} \sum_{i=1}^{N} (D^+ V)^2_i + \frac{\alpha}{2\, \Delta x} (V_1)^2 + \frac{\alpha}{2\, \Delta x} (V_N)^2 \\ & + \sum_{p=1}^{N} \exp\left(\epsilon_F - \ell_p[V]\right) - \epsilon_F \Delta x \sum_{i=1}^{N} n^0_i \,. \end{aligned}$$

□

# 5 Numerical results

In order to simulate the quantum drift-diffusion model, the numerical scheme (4.1)–(4.3) has been implemented by minimizing the functional $\widehat{J}$ defined by (4.5). Each strictly convex unconstrained minimization problem is solved by a Newton method (note that the Hessian matrix is explicit and always positive definite). The computation of the eigenelements of the discrete Hamiltonian $M[A]$ is performed by using the matlab function `eigs` [36]. For details concerning the practical implementation of the scheme, one can refer to [20].

The external potential is a discontinuous function playing the role of a double barrier structure potential and the initial density $n^0$ is concentrated on the left of the double barrier (see Figure 1). The initial step involves the inversion of the formula (4.15), *i.e.* the computation of the initial chemical potential $A^0$ corresponding to $n^0$. The calculation of $A^0$ is done by minimizing the strictly convex functional $\Phi$ defined in (4.16). Recall that $A^0$ is not used in the sequel of the algorithm.

On Figures 1, 2, 3, 4 and 5, we have represented, as functions of $x$, the density $n$, the total potential $V + V^{ext}$ and the electrochemical potential $A - V$ at the initial step and at different time steps: $k = 3$, 20, 100, 500. The parameters of these computations are the following ones:

| $\Delta x$ | $\Delta t$ | $\hbar^2$ | $\alpha$ |
|---|---|---|---|
| 0.01 | 0.005 | 0.02 | 0.1 |

On the right side of these figures, one can check that the electrochemical potential converges to a constant: at time $t = 500\Delta t$, one can consider that the system has converged to a steady state. On Figure 6, we show the evolution of the free energy $S^k$ defined by (4.7) and check that it is a decreasing function, converging to a constant. In these simulations, the initial total charge is equal to 1 and this quantity is conserved during the evolution, up to a relative error of $10^{-4}\,\%$.

# 6 Conclusion

We have introduced a semi-discrete (in time) version (3.1)–(3.3) of the quantum drift-diffusion model (2.7)–(2.9). We have proved that this system is well-posed and that its resolution amounts to minimizing a convex functional. Moreover, this semi-discrete model has the following interesting properties: it preserves the total charge and the positivity of the density and it dissipates the free energy. Then we have defined the numerical scheme (4.1)–(4.3) by discretizing the space variable in this system. As a consequence, this scheme possesses the same properties as the semi-discrete model. We have also studied the long-time behavior of the discrete solution: it converges to the solution of a discrete Schrödinger-Poisson system. Finally, we have given some results of numerical simulations which have been performed with this scheme.

A lot of open questions arise naturally. Let us list a few of them. By passing formally to the limit in the semi-discrete model as $\Delta t$ goes to zero, one obtains a

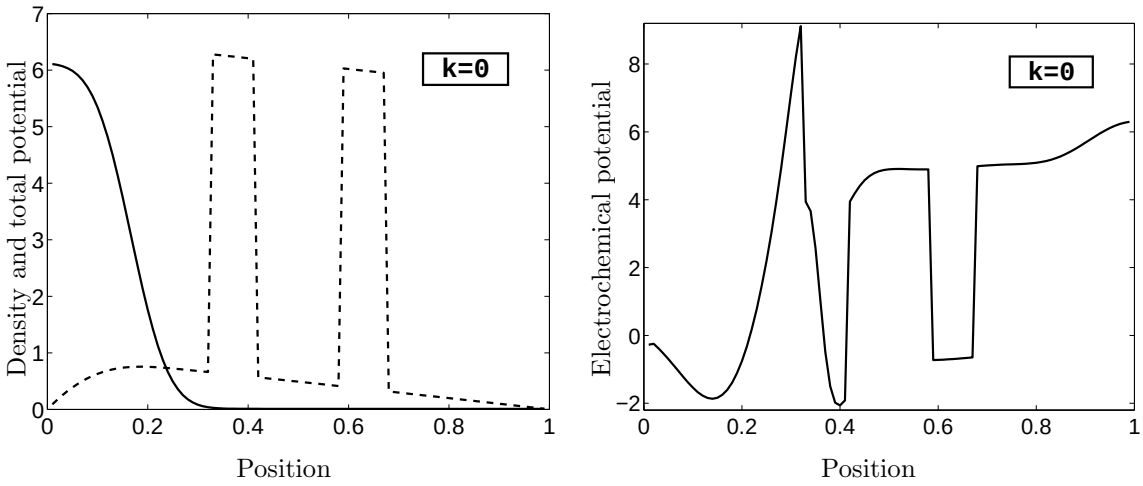


Figure 1: Numerical solution of the QDD model: initial step. Left: the density $n(x)$ (solid line) and the total potential $(V + V^{ext})(x)$(dashed line) as functions of the position $x$. Right: the electrochemical potential $(A - V)(x)$.

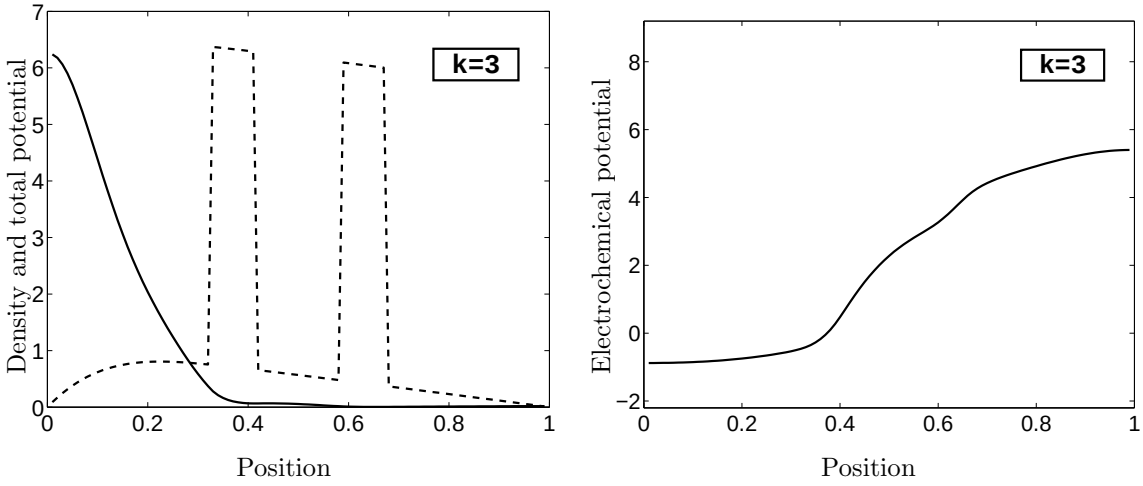


Figure 2: Numerical solution of the QDD model, after 3 iterations. The same quantities as on Fig. 1 are represented.

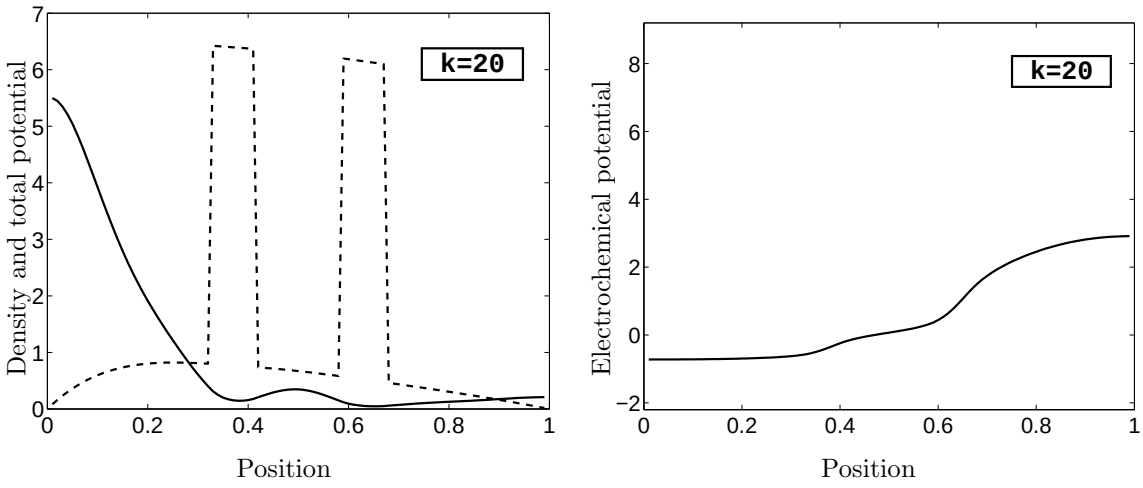


Figure 3: Numerical solution of the QDD model, after 20 iterations. The same quantities as on Fig. 1 are represented.

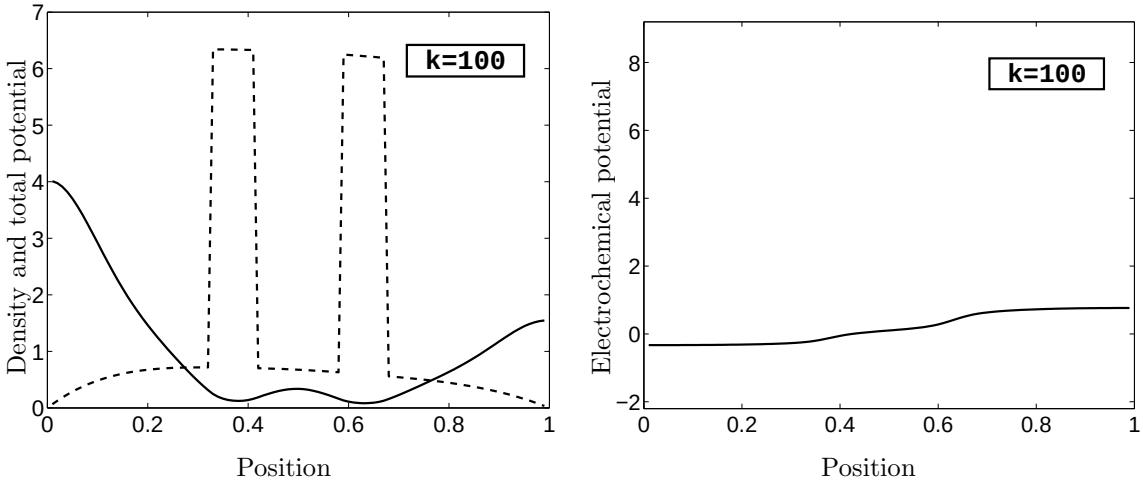


Figure 4: Numerical solution of the QDD model, after 100 iterations. The same quantities as on Fig. 1 are represented.

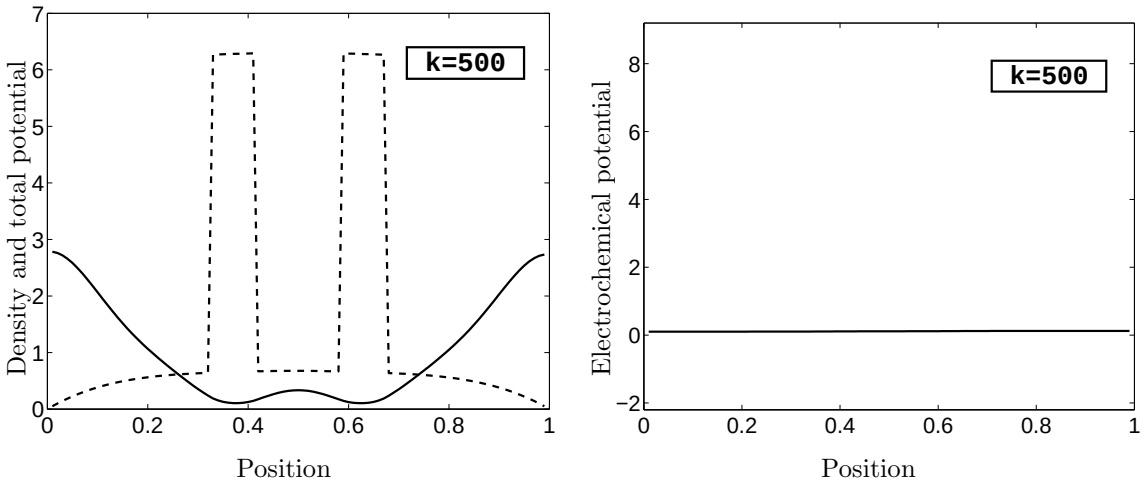


Figure 5: Numerical solution of the QDD model, after 500 iterations. The same quantities as on Fig. 1 are represented.

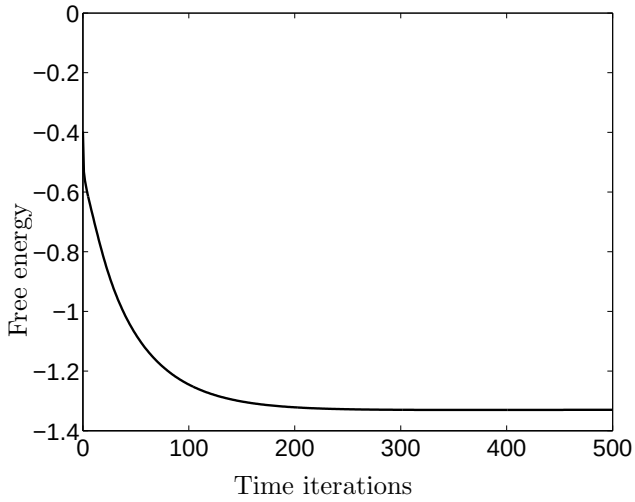


Figure 6: Free energy $S^k$ as a function of the time step $k$

solution of the initial QDD model. To make this statement rigourous, one of the most difficult points to be solved seems to find a bound from below for the density (this was possible with the fully discrete case as seen in Subsection 4.4). Studying the long-time behavior of the semi-discrete model or the continuous model is also an interesting challenge: do their solutions converge to the solution of the Schrödinger-Poisson system studied in [39, 40] ? Another important question is concerned with boundary conditions. We have chosen no-flux boundary conditions, but for pratical use it is necessary to enable a current flow through the boundary. This issue will be investigated in a future work.

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