Numerical Analysis

An asymptotic preserving scheme for the Schrödinger equation in the semiclassical limit

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Abstract

This Note is devoted to the discretization of the fluid formulation of the Schrödinger equation (the Madelung system). We explore both the discretization of the system in Eulerian coordinates and Lagrangian coordinates. We propose schemes for these two formulations which are implicit in the mass flux term. This feature allows us to show that these schemes are asymptotic preserving i.e. they provide discretizations of the semi-classical Hamilton–Jacobi equation when the scaled Planck constant ε tends to 0. An analysis performed on the linearized systems also shows that they are asymptotically stable i.e. their stability condition remains bounded as ε tends to 0. Numerical simulations are given; they confirm that the considered schemes allow us to numerically bridge the quantum and semi-classical scales. *To cite this article: P. Degond et al., C. R. Acad. Sci. Paris, Ser. I 345 (2007).*
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Résumé

Un schéma AP pour l'équation de Schrödinger dans la limite semi-classique. Cette Note est consacrée à la discrétisation de la formulation fluide de l'équation de Schrödinger (le système de Madelung) en formulations eulerienne et lagrangienne. Nous proposons des schémas pour ces deux formulations qui sont implicites dans le terme de flux de masse. Cette caractéristique nous permet de montrer que ces schémas sont asymptotiquement préservatifs, c'est à dire qu'ils fournissent une discrétisation des équations de Hamilton–Jacobi semi-classiques lorsque la constante de Planck adimensionnée ε tend vers 0. De plus, une analyse linéarisée permet de montrer que ces schémas sont asymptotiquement stables, c'est à dire que leur contrainte de stabilité reste bornée lorsque ε tend vers 0. Des simulations numériques sont proposées ; elles confirment que les schémas considérés permettent de fournir une passerelle numérique entre les échelles quantiques et semi-classiques. *Pour citer cet article : P. Degond et al., C. R. Acad. Sci. Paris, Ser. I 345 (2007).*
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On sait depuis Madelung [5] que l'équation de Schrödinger a une formulation fluide équivalente qui consiste en un système d'Euler sans pression où un terme quantique additionnel est ajouté : le potentiel de Bohm (1). Ces équations

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sont non linéaires contrairement à l'équation de Schrödinger mais leur avantage est que les inconnues macroscopiques ne développent pas d'oscillations d'ordre ε (dans cette Note, ε est la constante de Planck adimensionnée), ce qui est le cas de la fonction d'onde dans la formulation de Schrödinger. Ceci est un avantage sérieux dans la limite semi-classique où ε tend vers 0. Différentes stratégies de maillage ont été adoptées dans plusieurs articles sur des schémas pour l'équation de Schrödinger [6,7,1] mais même la meilleure méthode nécessite de prendre pour pas d'espace et de temps $\Delta x = \mathrm{o}(\varepsilon)$ et $\Delta t = \mathrm{O}(\varepsilon)$. Plus proche de cette Note et en chimie quantique, des méthodes particulaires dans une formulation lagrangienne ont été employées pour résoudre le système de Madelung [2,4,8–11].

Dans cette Note, nous proposons d'utiliser un schéma semi-implicite qui a le même coût que le schéma explicite pour résoudre le système de Madelung en formulation eulerienne (2)–(4) et lagrangienne. Pour un potentiel extérieur nul, l'analyse du schéma pour le système linéarisé autour d'une densité constante et d'un courant nul montre qu'un critère de stabilité est donné par $\Delta t < \frac{\Delta x^2}{\varepsilon \pi^2}$. Pour palier l'hypothèse de faible courant et au vu de la même analyse linéaire, le système de Madelung en coordonnées lagrangiennes (5) est discrétisé de manière analogue.

Les résultats numériques pour le schéma en formulation eulerienne (Figs. 1 et 2) et lagrangienne (Figs. 2 et 3) avec des potentiels extérieurs constants nous confirment que les schémas sont asymptotiquement stables et que pour un pas d'espace Δx fixé, on peut augmenter le pas de temps comme $1/\varepsilon$. L'inconvénient de ces schémas réside dans leur instabilité lorsque la densité est très proche de zéro. Par ailleurs le schéma en formulation eulerienne est instable lorsque le courant est trop fort alors que le schéma en formulation lagrangienne dont les coordonnées bougent avec le fluide reste stable comme le montre la figure 3. L'étude de problèmes plus complexes faisant intervenir l'apparition de caustiques et/ou faisant intervenir des potentiels extérieurs non constants est en cours.

1. Introduction

It is known since Madelung [5] that the Schrödinger equation $\mathrm{i}\varepsilon\partial_t\psi = -\frac{\varepsilon^2}{2}\Delta\psi + V\psi$ (ε is the scaled Planck constant) can be expressed equivalently in a fluid dynamical way using the Madelung Transform. This consists in writing the wave function in WKB form $\psi = \sqrt{n}\,\mathrm{e}^{\mathrm{i}\frac{S}{\varepsilon}}$ where n is the density and S is the phase. Inserting this ansatz in the Schrödinger equation and taking the real part and the gradient of the imaginary part, one obtains the following so-called Madelung system with unknowns the density n and the current $q = n\nabla S$:

$$\partial_t n + \nabla \cdot q = 0, \quad \partial_t q + \nabla \cdot \left(\frac{q \otimes q}{n}\right) + n\nabla(V - V^B) = 0, \quad V^B = \frac{\varepsilon^2}{2}\frac{\Delta\sqrt{n}}{\sqrt{n}}. \tag{1}$$

These equations consist in the classical pressureless Euler equations involving an additional quantum potential called the Bohm potential V^B.

These equations are nonlinear by contrast to the Schrödinger equation. In spite of this additional complexity (compared to the linear Schrödinger) the Madelung formulation can be useful from a numerical point of view. Indeed, in the semiclassical regime when the scaled Planck constant ε is small, the wave function develop oscillations of order ε and, in the Schrödinger formulation, the space discretization needs to resolve these oscillations. Since the values of the physical observables depend on the gradient of the phases, their accurate computation is often very difficult. Some schemes for the Schrödinger formulation have been analyzed by means of Wigner measures in the semiclassical limit such as e.g. the Crank–Nicolson scheme and the leap frog scheme in [6] and the Dufort–Frankel scheme in [7]. These analyses show that the space and time discretizations must satisfy $\Delta x = \mathrm{o}(\varepsilon)$ and $\Delta t = \mathrm{o}(\varepsilon)$. Time splitting spectral approximations are more efficient [1] but the constraints on the space and time discretizations are still very stringent: $\Delta t = \mathrm{O}(\varepsilon)$ and $\Delta x = \mathrm{o}(\varepsilon)$. In a closer spirit to this Note, the Madelung formulation (also called Bohmian mechanics or quantum trajectory methods) has been used for a long time and has recently been subject to a revived interest for quantum chemistry applications [10,2,4,8,9,11].

In this Note, we propose a semi-implicit scheme (which has the same cost as an explicit scheme) to solve the Madelung system in Eulerian and Lagrangian coordinates. The scheme is implicit in the mass flux term. The main advantage of this method is asymptotically stable and preserving when $\varepsilon \to 0$ i.e. the stability condition remains finite as $\varepsilon \to 0$ and in this limit, the scheme provides a discretization of the semi-classical Hamilton–Jacobi equations.

2. The method

2.1. Numerical schemes

We first propose a scheme for the one-dimensional Madelung system in Eulerian coordinates (1). Motivated by the linear analysis presented in next section, we choose a semi-implicit discretization in time and a centered finite discretization in space:

$$n_j^{k+1} = n_j^k - \frac{\Delta t}{2\Delta x}\left(q_{j+1}^{k+1} - q_{j-1}^{k+1}\right) = 0, \tag{2}$$

$$q_j^{k+1} = q_j^k - \frac{\Delta t}{2\Delta x}\left(\frac{q_{j+1}^k{}^2}{n_{j+1}^k} - \frac{q_{j-1}^k{}^2}{n_{j-1}^k}\right) + \frac{\Delta t}{2\Delta x}n_j^k\left(V_{j+1}^{B,k} - V_{j+1} - V_{j-1}^{B,k} + V_{j-1}\right) = 0, \tag{3}$$

$$V_j^{B,k} = \frac{\varepsilon^2}{2}\frac{\sqrt{n_{j+1}^k} - 2\sqrt{n_j^k} + \sqrt{n_{j-1}^k}}{\sqrt{n_j^k}\,\Delta x^2}. \tag{4}$$

This scheme is clearly asymptotic preserving. We show below that, at least for the linearized system, the scheme is also asymptotically stable.

This scheme has also a Lagrangian version. Let us transform the 1D Madelung system in Lagrangian coordinates. Suppose the total mass of the system is finite and equal to M. We introduce the new variables $m : \mathbb{R} \to [0, M], m(x) = \int_{-\infty}^x n(y, t)\,\mathrm{d}y$ and its inverse: $X : [0, M] \to \mathbb{R}, m \to X(m, t)$ such that $X(m(x, t), t) = x$. Let us also introduce the velocity and specific volume in Lagrangian coordinates $v(m, t) = q(X(m, t), t)/n(X(m, t), t)$ and $\tau(m, t) = 1/n(X(m, t), t)$. If we write the equations for the evolution of the system with unknowns τ and v with respect of the variables t and m, we obtain:

$$\partial_t \tau - \partial_m v = 0, \quad \partial_t v + \frac{1}{\tau}\partial_m(\overline{V} - \overline{V^B}) = 0, \quad \overline{V_B} = -\frac{\varepsilon^2}{4\sqrt{\tau}}\partial_m\left(\frac{\partial_m\tau}{\tau^{5/2}}\right), \quad \overline{V} = V\big(X(m, t), t\big), \tag{5}$$

with $\partial_t X = v$. Motivated by the same linear analysis as for the Madelung system in Eulerian coordinates, we choose a semi-implicit discretization in time and a centered finite discretization in mass. The interpolations for the passage from the Lagrangian to the Eulerian coordinates are performed using cubic splines.

2.2. Linear analysis

We assume that the potential V is constant and we want to study the linearized Madelung system about the stationary state $n_0 = 1$ and $q_0 = 0$:

$$\partial_t n + \nabla \cdot q = 0, \qquad \partial_t q - \frac{\varepsilon^2}{4}\nabla\Delta n = 0.$$

Notice that by linearizing the Madelung system in Lagrangian coordinates with a null potential about $\tau_0 = 1$, the first three equations of (5) have the same linearization as the system in Eulerian coordinates, with the substitution $n \to \tau$, $q \to -v$ and $x \to m$.

We first start by studying a time discretization of the linearized system. Note that the density is solution of a wave equation for the bilaplacian operator $\partial_t^2 n + \frac{\varepsilon^2}{4}\Delta^2 n = 0$. Let us consider the following semi-implicit discretization in time of the system, where Δt is the time step:

$$\frac{n^{k+1} - n^k}{\Delta t} + \nabla \cdot q^{k+1} = 0, \qquad \frac{q^{k+1} - q^k}{\Delta t} - \frac{\varepsilon^2}{4}\nabla\Delta n^k = 0, \tag{6}$$

which corresponds to the explicit discretization of the wave equation form. By a partial Fourier transform on the variable x, and denoting $\hat{n}$ the transform of n, we obtain

$$\frac{\hat{n}^{k+1} - 2\hat{n}^k + \hat{n}^{k-1}}{\Delta t^2} + \frac{\varepsilon^2}{4}\xi^4\hat{n}^k = 0.$$

The necessary condition for this scheme to be stable is $\frac{\varepsilon\xi^2\Delta t}{4} < 1$. In view of the space discretization of mesh size Δx, we assume that the range of admissible wave-number ξ is $[0, \xi^* = 2\pi/\Delta x]$. This gives the following stability criterion:

$$\Delta t < \frac{\Delta x^2}{\varepsilon\pi^2}. \tag{7}$$

Note that this semi-implicit treatment does not require more computational effort than the explicit scheme. Knowing q^k and n^k for a given time step, it suffices to solve the second equation of (6) to get q^{k+1} first, and then the first equation of (6) to get n^{k+1}.

In order to mimic the influence of a decentered space discretization, we have considered a viscous perturbation of the linearized Madelung system. It appears that even if the numerical viscosity stabilizes the scheme, the viscosity must be smaller than ε in order not to destroy the dispersive behavior of the Schrödinger equation and provide a correct discretization of the semi-classical limit. For this reason, we favoured a centered space discretization with centered finite-differences.

3. Numerical results

We are going to test both schemes in Eulerian and Lagrangian coordinates on a bounded domain [0, 1] with periodic boundary conditions and a constant potential $V(x) = 100$. The first test case is taken from [6,7,1]. The initial density is given by $n^0 = e^{-50(x-0.5)^2}$ and the initial current is given by $q^0 = 0.2(2x - 1)n^0$. Fig. 1 shows the results for the scheme in Eulerian coordinates (2)–(4). We plot the density, current and Bohm potential at $t = 0.54$ for different ε. As ε tends to zero, the density and the current tend to smooth limits as already noted in [6,7,1]. In our simulations, the mesh size is fixed and equal to $\Delta x = 0.01$. The time step Δt is taken proportional to $1/\varepsilon$: for $\varepsilon = 0.0256$, $\Delta t =$
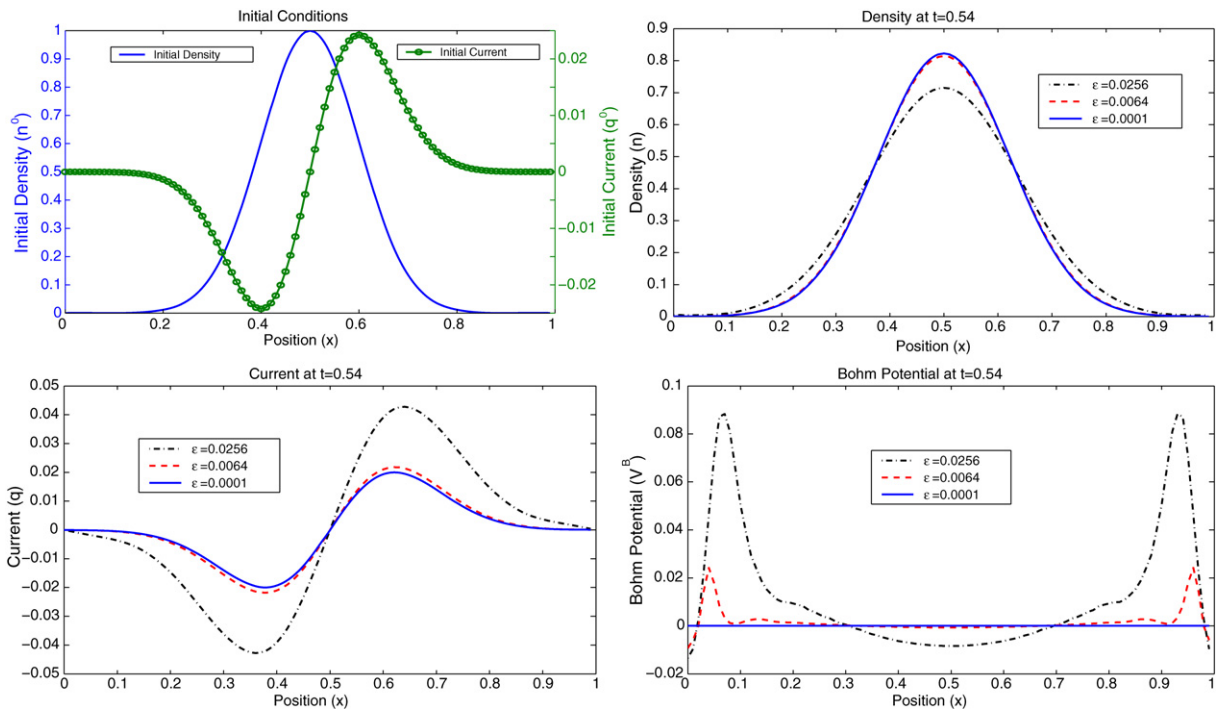

Fig. 1. Numerical solutions for the first test case (Eulerian scheme). Top left: Initial conditions as function of the position x; top right, bottom left and bottom right: density, current and Bohm potential at time $t = 0.54$ as functions of x for $\varepsilon = 0.0256$ (dash-dot line), $\varepsilon = 0.0064$ (dashed line) and $\varepsilon = 0.0001$ (solid line).

Fig. 1. Solutions numériques du premier cas test (schéma eulérien). En haut à gauche : conditions initiales comme fonctions de la position x, en haut à droite, en bas à gauche et en bas à droite : densité, courant et potentiel de Bohm au temps $t = 0,54$ comme fonctions de x pour $\varepsilon = 0,0256$ (pointillés mixtes), $\varepsilon = 0,0064$ (pointillés longs) et $\varepsilon = 0,0001$ (trait plein).
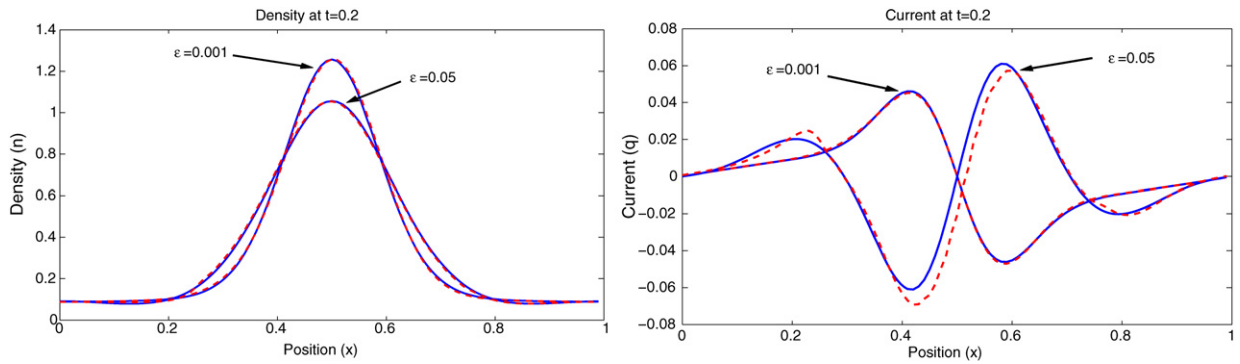
Fig. 2. Numerical solutions for the second test case (Eulerian and Lagrangian schemes). Density and current at time $t = 0.2$ as functions of x for $\varepsilon = 0.05$ and $\varepsilon = 0.001$ using the Eulerian scheme (solid line) and the Lagrangian scheme (dashed line).

Fig. 2. Solutions numériques du second cas test (schémas eulerien et lagrangien). Densité et courant au temps $t = 0,2$ comme fonctions de x pour $\varepsilon = 0,05$ et $\varepsilon = 0,001$ en utilisant le schéma eulérien (trait plein) et le schéma lagrangien (pointillés longs).
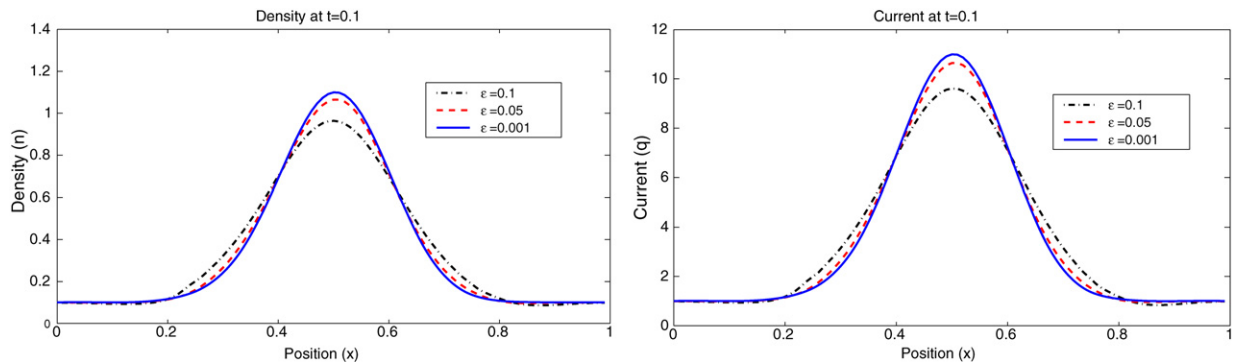

Fig. 3. Numerical solutions for the third test case (Lagrangian scheme). Density and current at time $t = 0.1$ as functions of x for $\varepsilon = 0.1$ (dash-dot line), $\varepsilon = 0.05$ (dashed line) and $\varepsilon = 0.001$ (solid line). Note that the scheme in Eulerian coordinates is unstable on this test case due to the high current.

Fig. 3. Solutions numériques pour le troisième cas test (schéma lagrangien). Densité et courant au temps $t = 0,1$ comme fonctions de x pour $\varepsilon = 0,1$ (pointillés mixtes), $\varepsilon = 0,05$ (pointillés longs) et $\varepsilon = 0,001$ (trait plein). Notons que le schéma en coordonnées euleriennes est instable sur ce cas test à cause du courant élevé.

2×10^{-4}, for $\varepsilon = 0.0064$, $\Delta t = 8 \times 10^{-4}$ and for $\varepsilon = 0.0001$, $\Delta t = 6 \times 10^{-2}$ so that the stability criterion (7) is respected. We see clearly here the advantage of using our scheme based on the Madelung formulation compared to any scheme using the Schrödinger formulation. We would like to point out that other test cases exhibiting densities near vacuum can create instabilities. This has already been noted in the literature for the pressureless Euler system [3] and the addition of the Bohm potential makes things harder (see the square root of the density at the denominator of the expression giving the Bohm potential in (1)). The scheme in the Lagrangian coordinates is even more unstable since vacuum corresponds to a singularity of the specific volume τ.

The second test case allows to compare the schemes in Lagrangian and Eulerian coordinates. We choose an initial density which is uniformly bounded from below by a positive constant $n^0 = 0.1 + e^{-50(x-0.5)^2}$ and we choose for initial current $q^0 = 0.1 \sin(2\pi x) n^0$. We plot on Fig. 2 the density and current at time $t = 0.2$ for $\varepsilon = 0.05$ and $\varepsilon = 0.001$, using the Eulerian scheme (solid line) and the Lagrangian scheme (dashed line). We take again for the Eulerian scheme $\Delta x = 0.01$. Concerning the Lagrangian scheme, the total mass is equal to 0.3507 and we take for mass discretization $\Delta m = 0.003507$. Again the time step can be taken proportional to $1/\varepsilon$ and both schemes are stable.

The third test case shows the advantage of using the scheme in Lagrangian coordinates since it allows us to consider higher currents. We choose the same initial $n^0 = 0.1 + e^{-50(x-0.5)^2}$, but we take now a higher initial current $q^0 = 10 n^0$. For $\varepsilon = 0$, it is easy to check that the soliton $n(x) = n^0(x - 10t)$, $q(x) = q^0(x - 10t)$ is the solution of the problem so that for $t = 0.1$, we have $n(x) = n^0(x)$ and $q(x) = q^0(x)$ (due to the periodic boundary conditions). Fig. 3 shows

the density and current at time $t = 0.1$ for different ε. The time step can again be taken proportional to $1/\varepsilon$. Results obtained with the scheme in Eulerian coordinates on this test case are not presented because they are unstable.

4. Conclusion

We have presented two asymptotic preserving schemes for the Schrödinger equations in the semiclassical limit, based on the Madelung formulation of Schrödinger's equation in terms of the density and flux. Both Eulerian and Lagrangian coordinate systems have been considered. A stability analysis of the linearized Madelung system shows that these schemes are asymptotically stable. The numerical results confirm this analysis and demonstrate that, for a fixed Δx, the time step can scale like $1/\varepsilon$, while the best meshing strategy for any scheme using the Schrödinger formulation is $\Delta t = \mathrm{O}(\varepsilon)$ and $\Delta x = \mathrm{o}(\varepsilon)$. These schemes however develop an instability near vacuum. More tests are under progress, in particular to evaluate the ability of the scheme to cross the caustics.

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