The solution of the nonlinear Schrödinger equation using Lattice- Boltzmann

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Abstract. We present the solution of the nonlinear Schrödinger equation using the lattice Boltzmann method. We show results for two dimensions using a **d2q9** lattice velocity scheme. To implement the expansion B.G.K. (Bhatnagar-Gross-Krook), we assume the distribution function as a complex valued function, whose real and complex components satisfy the Boltzmann equation. The strategy followed to obtain the motion equation is to define adequately the second moment of the distribution as a symmetric tensor. We obtain stable structures for given values of the nonlinear coupling constant.

1. Introduction

Nonlinear terms in Physics laws provide an amazing range of new dynamic effects. This is the case of the nonlinear Schrödinger equation (NLSEq), which plays a key role in describing the dynamics of Bose-Einstein condensation [1,2] In the past Lattice-Boltzmann has been successfully applied to the solution of the Schrödinger equation [3], and the Dirac equation its relativistic version of the problem [4]. Moreover, the NLSEq has brought a massive investigation into soliton behavior [5,6].
This paper proposes, using the lattice Boltzmann method a solution to the NLSEq. In section 2, we begin with a review of the lattice-Boltzmann technique and the moment relations of the equilibrium distribution functions applied to derivation of the NLSEq. In section 3, we obtain the NLSE equation, using a hypothesis in the Π^0 tensor. In section 4, we obtain the equilibrium distribution functions that we use on a **d2q9** lattice velocity scheme for the computational scheme. In section 5, we present results and at last, in section 6, we give conclusions.

2. The lattice-Boltzmann model

It is considered a bi-dimensional model where the velocities of particles are discretized on the grid into ***d*** direction. The lattice-Boltzmann equation is:

$$f_{i,j}(\vec{x}+\vec{e}_x\delta t, t+\delta t) - f_{i,j}(\vec{x},t) = -\frac{1}{\tau}(f_{i,j}(\vec{x},t) - f^{eq}{}_{i,j}(\vec{x},t)) \tag{1}$$

Where f_i is the probability density function of finding the group particle ***i***, of the ***j*** species, in the spatial point $\vec{x}$ and time ***t*** and δt is the time step. The left hand side of equation (1) is the B.G.K. approximation [7], where τ is the non-dimensional relaxation time that measures the approaching rated to the statistical equilibrium. Expanding the left-hand side of equation (1) up to second order, in a Taylor series, we have:

$$f_{i,j}(\vec{x}+\vec{e}_\alpha\delta t, t+\delta t)-f_{i,j}(\vec{x},t)=\delta t\left(\frac{\partial}{\partial t}+e_x\frac{\partial}{\partial x_1}+e_y\frac{\partial}{\partial y_1}\right)f_{i,j}+\frac{\delta t^2}{2}\left(\frac{\partial}{\partial t}+e_x\frac{\partial}{\partial x_1}+e_y\frac{\partial}{\partial y_1}\right)^2 f_{i,j} \quad (2)$$

Assuming the spatial and temporal derivatives as:

$$\frac{\partial}{\partial x}=\mathcal{E}\frac{\partial}{\partial x_1};\ \frac{\partial}{\partial y}=\mathcal{E}\frac{\partial}{\partial y_1};\ \frac{\partial}{\partial t}=\mathcal{E}\frac{\partial}{\partial t_1}+\mathcal{E}^2\frac{\partial}{\partial t_2} \quad (3)$$

The parameter $\mathcal{E}=\Delta\mathrm{x}/\mathrm{L}$, where Δx is the spatial size grid and L the spatial system size. Expanding the distribution function $f_{i,j}$ in a perturbative series:

$$f_{i,j}=f^0{}_{i,j}+\mathcal{E}f^1{}_{i,j}+\mathcal{E}^2 f^2{}_{i,j} \quad (4)$$

We obtain at first order in $\mathcal{E}$:

$$-\frac{1}{\tau}\left(\mathcal{E}f^1{}_{i,j}\right)=\delta t(\mathcal{E}\frac{\partial}{\partial t_1}+\mathcal{E}e_x\frac{\partial}{\partial x_1}+\mathcal{E}e_y\frac{\partial}{\partial y_1})f^0{}_{i,j} \quad (5)$$

And at second order in ε:

$$-\frac{1}{\tau}\mathcal{E}^2 f^2{}_{i,j}=\mathcal{E}^2\delta t(\frac{\partial}{\partial t_2}f^0{}_{i,j}+\frac{\delta t}{2}\left(\frac{\partial}{\partial t_1}+e_x\frac{\partial}{\partial x_1}+\mathcal{E}e_y\frac{\partial}{\partial y_1}\right)^2 f^0{}_{i,j}+\left(\frac{\partial}{\partial t_1}+e_x\frac{\partial}{\partial x_1}+e_y\frac{\partial}{\partial y_1}\right)f^1{}_{i,j}) \quad (6)$$

Also it is assumed

$$f^0{}_{i,j}=f^{eq}{}_{i,j} \quad (7)$$

Inserting equation (5) in equation (6), we obtain:

$$-\frac{1}{\tau}\left(f^2{}_{i,j}\right)=\delta t\left(\frac{\partial}{\partial t_1}+e_x\frac{\partial}{\partial x_1}+e_y\frac{\partial}{\partial y_1}\right)f^1{}_{i,j}\left(1-\frac{1}{2\tau}\right)+\delta t\left(\frac{\partial f^0{}_{i,j}}{\partial t_2}\right) \quad (8)$$

The moments of the distribution function are defined as:

$$\rho_j=\sum_i f^0{}_{i,j};\ \vec{u}_j=\sum_i\vec{e}_i f^0{}_{i,j};\ \Pi^0{}_j=\sum_i\vec{e}_i\cdot\vec{e}_i f^0{}_{i,j} \quad (9)$$

Also we assume the distribution functions $f_{i,j}$ satisfy the probability conservation condition with the equilibrium distribution $f^{eq}{}_i$ such that:

$$\sum_{i=0}^N f^{eq}{}_i=\sum_{i=0}^N f^0{}_i \quad (10)$$

3. The Schrödinger Equation

Doing algebra in equations (5) and (8) with the help of equations (10), we get:

$$\frac{\partial\rho_j}{\partial t}+\nabla\cdot\vec{u}_j=0 \quad (11)$$

And

$$\frac{\partial\vec{u}_j}{\partial t}+\nabla\cdot\Pi^0{}_j=0 \quad (12)$$

We assume $\Pi^0{}_j$ as a symmetric tensor given by:

$$\Pi^0{}_{1,\mu\nu} = \delta_{\mu\nu}\frac{\partial \rho_2}{\partial t} + (1-\delta_{\mu\nu})\lambda(\rho_1^2+\rho_2^2)\rho_2 \tag{13}$$

$$\Pi^0{}_{2,\mu\nu} = \delta_{\mu\nu}\frac{\partial \rho_1}{\partial t} + (1-\delta_{\mu\nu})\lambda(\rho_1^2+\rho_2^2)\rho_1 \tag{14}$$

Defining the complex function

$$\rho = \rho_1 + i\rho_2 \tag{15}$$

Where i is the complex number, and assuming zero the off diagonal components of $\Pi^0{}_j$, and doing some algebra, we have the NLSEq:

$$i\frac{\partial \rho}{\partial t} + \nabla^2\rho + \lambda|\rho|^2\rho = 0 \tag{16}$$

4. The equilibrium distribution function

We use the **d2q9** velocity scheme. For the directions $\vec{e}_i$ and weights w_i on each cell, we have:

$$w_i = \left\{\frac{4}{9} \to i=0;\ \frac{1}{9} \to i = 1,2,3,4;\ \frac{1}{36} \to i = 5,6,7,8\right\} \tag{17}$$

$$\textstyle\sum_i w_i\, e_{i,\alpha} = 0;\ \sum_i w_i\, e_{i,\alpha}e_{i,\beta} = \frac{1}{3}\delta_{\alpha,\beta};\quad \sum_i w_i\, e_{i,\alpha}e_{i,\beta}e_{i,\gamma} = 0 \tag{18}$$

We use the equilibrium function as:

$$f^{eq}{}_{i,j} = \begin{Bmatrix} w_i(A + B\vec{e}_i\cdot\vec{u}) & i>0 \\ w_0 C & i=0 \end{Bmatrix} \tag{19}$$

Using equations (10), (18) and (19) we can determine A, B and C. Then, the equilibrium distribution functions that satisfies the NLSEq is:

$$f^{eq}{}_{i,1} = \begin{cases} 3w_i\left(\vec{e}_i\cdot\vec{u} + \frac{\partial\rho_2}{\partial t} - \lambda(\rho_1^2+\rho_2^2)\rho_2\right) & i>0 \\ w_0\left(\frac{9}{4}\rho_1 - \frac{5}{4}\left(\frac{\partial\rho_2}{\partial t} - \lambda(\rho_1^2+\rho_2^2)\rho_2\right)\right) & i=0 \end{cases} \tag{20}$$

$$f^{eq}{}_{i,2} = \begin{cases} 3w_i\left(\vec{e}_i\cdot\vec{u} + \frac{\partial\rho_1}{\partial t} - \lambda(\rho_1^2+\rho_2^2)\rho_1\right) & i>0 \\ w_0\left(\frac{9}{4}\rho_2 - \frac{5}{4}\left(\frac{\partial\rho_1}{\partial t} - \lambda(\rho_1^2+\rho_2^2)\rho_1\right)\right) & i=0 \end{cases} \tag{21}$$

5. Results

The derivative operator of $\rho(x,t)$ used in the distribution functions is discretized as:

$$\frac{\partial\rho}{\partial t} = \frac{\rho(x,y,t+\delta t) - \rho(x,y,t)}{\delta t} \tag{22}$$

The system is initialized with the function:

$$f_{i,j}(x,y,0) = A_1 cos(D(x+2)^2 + D(y+2)^2) \tag{23}$$

The simulation starts at $t_0 = 0$, with the Equation (22) in all the points of the system, and for the two components. Figure (1) presents the simulation results using **d2q9** velocity scheme for grid size of **120x120** and **λ=0.7**. The two panels show the solution from different perspectives. In left panel, we have a top view colormap. A three-dimensional shaded surface is presented in the right panel.

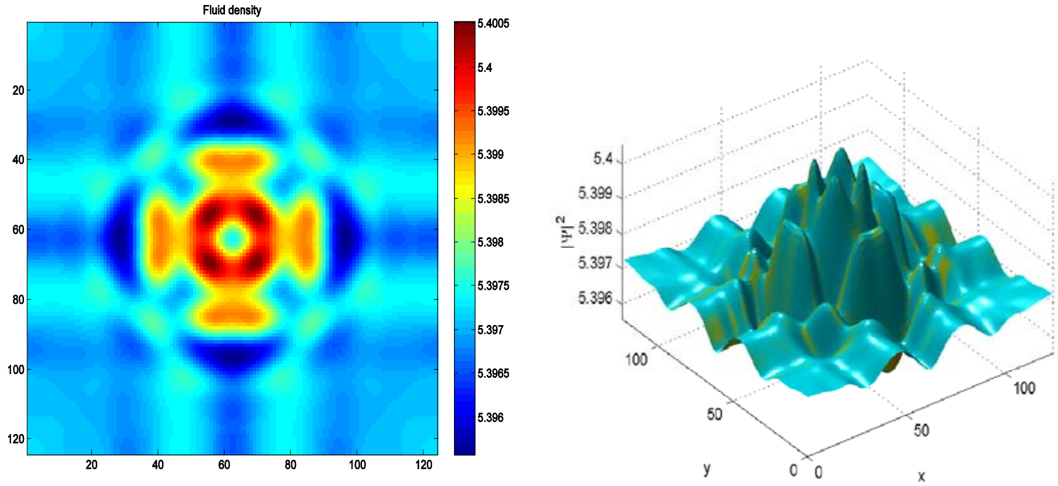

Figure 1. The numerical result of the **d2q9** lattice Boltzmann model. The two panels are the numerical results at times *t = 100*, lattice size *L=120, λ=0.7, Δx =Δy = 1/L.*

6. Conclusions

We have solved the nonlinear Schrödinger equation using a definition of the tensor $\mathbf{\Pi^0}$ defined in the Chapman-Enskog expansion. As a future work, the method can be extended to **3d,** employing **d3q15** and **d3q19** lattice schemes and using cubic-quintic nonlinear terms in the Schrödinger equation.

Acknowledgments

This work was supported by Universidad Nacional de Colombia (DIB-8003355).

7. References

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