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A lattice Boltzmann model for the nonlinear Schrödinger equation

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Abstract
The lattice Boltzmann model for the nonlinear Schrödinger equation is proposed. The new model is based on the technique of the higher order moment of equilibrium distribution functions and a series of lattice Boltzmann equations in different time scales. The Euler equations are derived from the nonlinear Schrödinger equation by removing non-physical pressure. We have simulated two irrotational flows. These numerical results agree well with classical ones.

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1. Introduction

The lattice Boltzmann method (LBM) originated from a Boolean fluid model known as the lattice gas automata (LGA) [1] for modeling fluid flows has been developed as a new alternative method for computational fluid dynamics (CFD). During the past few years much progress has been made that extends the LBM as a tool for simulating many complex problems, such as multi-phase flow, suspensions flow and flow in porous media: flows which are quite difficult to simulate by the conventional method [2–5]. On the other hand, the lattice Boltzmann model has undergone a number of further refinements. A recent study by Yan *et al* showed that the lattice Bhatnagar–Gross–Krook (LBGK) model could be used to simulate wave motion [6], the soliton wave [7] and Lorenz attractor [8]. All of these models can be derived by using a higher order moment method with a multi-scale technique and the famous LBGK model. The LBGK model is one of the simple models in the LBM. It is often used to simulate fluid flows [2].

The LBGK model starts from mesoscopic kinetic equations, i.e. the lattice Boltzmann equation, to determine macroscopic fluid flows. The kinetic nature brings certain advantages over conventional numerical methods, such as their algorithmic simplicity, parallel computation, easy handling of complex boundary conditions and efficient hydrodynamics simulations [2–5].

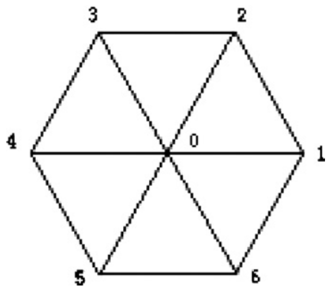


Figure 1. A two-dimensional FHP lattice.

Now, we focus on the lattice Boltzmann model for the nonlinear Schrödinger equation [9–11]. The nonlinear Schrödinger equation (NLSE) governs the complex quantity $A(\mathbf{x}, t)$. It is used to describe many complex physical phenomena. The NLSE reads

$$\frac{\partial A}{\partial t} = \frac{1}{2} i \nabla^2 A + iA + iB, \tag{1}$$

where A, B are complex variables, i is the unit of the imaginary number. We denote $A = A_1 + iA_2$, $B = B_1 + iB_2$, that is to say, $u_1 = A_1$, $u_2 = A_2$, $b_1 = B_1$, $b_2 = B_2$. By introducing $K_{\sigma\beta}$ as

$$[K] = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \equiv K_{\sigma\beta},$$

the nonlinear Schrödinger equation can be written as

$$\frac{\partial u_\sigma}{\partial t} = \frac{1}{2} K_{\sigma\beta} \nabla^2 u_\beta + K_{\sigma\beta} u_\beta + K_{\sigma\beta} b_\beta, \qquad \sigma = 1, 2; \quad \beta = 1, 2, \tag{2}$$

where $\sigma = 1$ and 2 refers to the real and imaginary parts, $\beta = 1$ and 2 denotes the dimensions.

We have much interest in its lattice Boltzmann model and relations between fluid flows and the nonlinear Schrödinger equation. The lattice Boltzmann scheme has recently begun to receive considerable attention as an alternative numerical scheme for simulation of fluid flows and nonlinear systems. The conventional lattice Boltzmann method, however, requires a real one-particle distribution function. Because the nonlinear Schrödinger equation is scripted by the complex quantity, the strategy we select to build the lattice Boltzmann scheme is to separate the nonlinear Schrödinger equation into real and imaginary parts to obtain a two-species reaction–diffusion system [12]. This paper consists of three parts: (1) a lattice Boltzmann model for the nonlinear Schrödinger equation is proposed; (2) the Euler equations are obtained from the nonlinear Schrödinger equation by eliminating the non-physical pressure term, and (3) two numerical simulation examples are given.

In the following section, the lattice Boltzmann model is described. In section 3, we contribute the Euler equations by adjusting the complex variable B in equation (1). In section 4, we give a numerical example, and section 5 gives concluding remarks.

2. The lattice Boltzmann model for the nonlinear Schrödinger equation

2.1. Lattice Boltzmann equation

Let us consider a two-dimensional lattice (see figure 1) with b links that connect the center site to b neighboring nodes. The velocity of particles moving along the link is $\boldsymbol{e}_\alpha$, the speed is $|e_\alpha| = c$. The distribution function $F_\alpha^\sigma(\mathbf{x}, t)$ is defined as the particles density of the component $\boldsymbol{\sigma}$ at position $\mathbf{x}$, time t, with velocity $\boldsymbol{e}_\alpha$.

The macroscopic quantity $u_\sigma(\mathbf{x}, t)$ is defined as follows:

$$u_\sigma(\mathbf{x}, t) = \sum_\alpha F_\alpha^\sigma(\mathbf{x}, t). \tag{3}$$

In order to obtain an available macroscopic quantity $u_\sigma(\mathbf{x}, t)$, we assume that the distribution $F_\alpha^\sigma(\mathbf{x}, t)$ has the local equilibrium distribution function $F_\alpha^{\sigma,\mathrm{eq}}(\mathbf{x}, t)$, and

$$\sum_\alpha F_\alpha^{\sigma,\mathrm{eq}}(\mathbf{x}, t) = u_\sigma(\mathbf{x}, t). \tag{4}$$

The lattice Boltzmann equation is expressed as

$$F_\alpha^\sigma(\mathbf{x} + \boldsymbol{e}_\alpha, t + 1) = F_\alpha^\sigma(\mathbf{x}, t) - \frac{1}{\tau}\left[F_\alpha^\sigma(\mathbf{x}, t) - F_\alpha^{\sigma,\mathrm{eq}}(\mathbf{x}, t)\right] + \omega_\alpha^\sigma(\mathbf{x}, t), \tag{5}$$

where τ is the single relaxation time factor. $\omega_\alpha^\sigma(\mathbf{x}, t)$ is a non-collision term. It expresses the change of the particle σ by the chemical reaction [8]. We assume that $F_\alpha^{\sigma,\mathrm{eq}}(\mathbf{x}, t)$ meets these higher order moments

$$\sum_\alpha F_\alpha^{\sigma,\mathrm{eq}}(\mathbf{x}, t) e_{\alpha j} = 0, \tag{6}$$

$$\sum_\alpha F_\alpha^{\sigma,\mathrm{eq}}(\mathbf{x}, t) e_{\alpha i} e_{\alpha j} = \lambda K_{\sigma\beta} u_\beta(\mathbf{x}, t) \delta_{ij}, \tag{7}$$

where δ_{ij} is the Kronecker delta, λ is a parameter to be determined. Based on equations (4), (6), (7), we obtain the solution of the equilibrium distribution functions

$$F_\alpha^{\sigma,\mathrm{eq}}(\mathbf{x}, t) = \frac{\lambda D}{bc^2} K_{\sigma\beta} u_\beta(\mathbf{x}, t), \qquad \alpha = 1, 2, \ldots, b, \tag{8}$$

$$F_0^{\sigma,\mathrm{eq}}(\mathbf{x}, t) = u_\sigma(\mathbf{x}, t) - \frac{\lambda D}{c^2} K_{\sigma\beta} u_\beta(\mathbf{x}, t), \tag{9}$$

where $\sigma = 1$ and 2 refers to the real and imaginary parts, $\beta = 1$ and 2 denotes the dimensions, D (=2) is the number of the spatial dimensions, c is the speed of particles and α is the direction of the particle moving along.

2.2. *The macroscopic equation*

Using a small parameter k as the time step in numerical simulation, we take that it is equal to the Knudsen number [6]. The lattice Boltzmann equation in physical unit is

$$F_\alpha^\sigma(\mathbf{x} + k\boldsymbol{e}_\alpha, t + k) - F_\alpha^\sigma(\mathbf{x}, t) = -\frac{1}{\tau}\left[F_\alpha^\sigma(\mathbf{x}, t) - F_\alpha^{\sigma,\mathrm{eq}}(\mathbf{x}, t)\right] + \omega_\alpha^\sigma(\mathbf{x}, t). \tag{10}$$

In equation (10), we also assume that $\omega_\alpha^\sigma(\mathbf{x}, t)$ is the second-order term [6] written as

$$\omega_\alpha^\sigma(\mathbf{x}, t) = k^2 \theta_\alpha^\sigma(\mathbf{x}, t). \tag{11}$$

The Chapman–Enskog expansion [13] is applied to $F_\alpha^\sigma(\mathbf{x}, t)$ under the assumption that the small Knudsen number k,

$$F_\alpha^\sigma = \sum_{n=0}^{\infty} k^n F_\alpha^{\sigma,n} = F_\alpha^{\sigma,0} + kF_\alpha^{\sigma,1} + k^2 F_\alpha^{\sigma,2} + \cdots. \tag{12}$$

In equation (12), $F_\alpha^{\sigma,0}$ denotes $F_\alpha^{\sigma,\mathrm{eq}}$. We discuss changes in different time scales, introduced as $t_0, t_1, \ldots,$ thus,

$$t_0 = t, \quad t_1 = kt, \quad t_2 = k^2 t, \quad t_3 = k^3 t, \ldots,$$

therefore

$$\frac{\partial}{\partial t} = \frac{\partial}{\partial t_0} + k\frac{\partial}{\partial t_1} + k^2\frac{\partial}{\partial t_2} + k^3\frac{\partial}{\partial t_3} + k^4\frac{\partial}{\partial t_4} + O(k^5). \tag{13}$$

Performing the Taylor expansion upon equation (10), and retaining terms up to $O(k^5)$, we obtain a series of the lattice Boltzmann equations in different time t_0, t_1, t_2 scales

$$\Delta F_\alpha^{\sigma,\mathrm{eq}} = -\frac{1}{\tau}F_\alpha^{\sigma,1}, \tag{14}$$

$$\frac{\partial}{\partial t_1}F_\alpha^{\sigma,\mathrm{eq}} + \left(\frac{1}{2} - \tau\right)\Delta^2 F_\alpha^{\sigma,\mathrm{eq}} = -\frac{1}{\tau}F_\alpha^{\sigma,2} + \theta_\alpha^\sigma, \tag{15}$$

$$\left(\tau^2 - \tau + \frac{1}{6}\right)\Delta^3 F_\alpha^{\sigma,\mathrm{eq}} + 2\left(\frac{1}{2} - \tau\right)\Delta\frac{\partial}{\partial t_1}F_\alpha^{\sigma,\mathrm{eq}} + \frac{\partial}{\partial t_2}F_\alpha^{\sigma,\mathrm{eq}} + \Delta\tau\theta_\alpha^\sigma = -\frac{1}{\tau}F_\alpha^{\sigma,3}, \tag{16}$$

$$\begin{aligned}\left(-\tau^3 + \frac{3}{2}\tau^2 - \frac{7}{12}\tau + \frac{1}{24}\right)\Delta^4 F_\alpha^{\sigma,\mathrm{eq}} + 3\left(\tau^2 - \tau + \frac{1}{6}\right)\Delta^2\frac{\partial}{\partial t_1}F_\alpha^{\sigma,\mathrm{eq}} \\ + 2\left(\frac{1}{2} - \tau\right)\Delta\frac{\partial}{\partial t_2}F_\alpha^{\sigma,\mathrm{eq}} + \frac{\partial}{\partial t_3}F_\alpha^{\sigma,\mathrm{eq}} + \left(\frac{1}{2} - \tau\right)\frac{\partial^2}{\partial t_1^2}F_\alpha^{\sigma,\mathrm{eq}} \\ + \frac{\partial}{\partial t_1}\tau\theta_\alpha^\sigma + \left(\frac{1}{2} - \tau\right)\Delta^2\tau\theta_\alpha^\sigma = -\frac{1}{\tau}F_\alpha^{\sigma,4},\end{aligned} \tag{17}$$

where $\Delta \equiv \frac{\partial}{\partial t_0} + e_\alpha\frac{\partial}{\partial x}$.

To derive the equations for $u_\sigma(\mathbf{x}, t)$ to first order in k, we take a summation of equation (14) with respect to α to give the first-order macroscopic equation. This equation is named as the conversation law in the first time scale t_0:

$$\frac{\partial}{\partial t_0}u_\sigma(\mathbf{x}, t) = 0. \tag{18}$$

The second-order macroscopic equation is obtained by taking (14) + (15) $\times$ k and summation over α. Thus, we have

$$\frac{\partial u_\sigma}{\partial t} = k\left(\tau - \frac{1}{2}\right)\frac{\partial^2}{\partial x_j\partial x_k}(\lambda K_{\sigma\beta}u_\beta\delta_{jk}) + k\sum_\alpha\theta_\alpha^\sigma + O(k^2). \tag{19}$$

Equation (19) is the nonlinear Schrödinger equation (2) with truncation error $O(k^2)$ when $\lambda k\left(\tau - \frac{1}{2}\right) = \frac{1}{2}$ and $k\sum_\alpha\theta_\alpha^\sigma = K_{\alpha\beta}u_\beta + K_{\alpha\beta}b_\beta$. If we assume θ_α^σ is independent of α [8], thus

$$\theta_\alpha^\sigma(\mathbf{x}, t) = \frac{1}{(b+1)k}(K_{\sigma\beta}u_\beta + K_{\sigma\beta}b_\beta), \tag{20}$$

$$\omega_\alpha^\sigma(\mathbf{x}, t) = \frac{k}{(b+1)}(K_{\sigma\beta}u_\beta + K_{\sigma\beta}b_\beta). \tag{21}$$

Equation (19) is the nonlinear Schrödinger equation with the second-order accuracy of truncation error.

2.3. The truncation error of the model

Taking (14) + (15) × k + (16) × k^2 + (17) × k^3 and summation over α, we have

$$\frac{\partial u_\sigma}{\partial t} = k\left(\tau - \frac{1}{2}\right)\frac{\partial^2}{\partial x_j \partial x_k}(\lambda K_{\sigma\beta} u_\beta \delta_{jk}) + K_{\sigma\beta} u_\beta + K_{\sigma\beta} b_\beta + E_3 + E_4 + O(k^4). \tag{22}$$

In equation (22), E_3 is the third-order error term, E_4 is the fourth-order error term

$$E_3 = 0, \tag{23}$$

$$\begin{aligned} E_4 = &-k^3\left(C_4 - 3C_2C_3 + C_2^3\right)\lambda K_{\sigma\beta}\frac{3c^2}{D+2}\nabla^4 u_\beta \\ &- k^3\left(3C_3 + \tau C_2 - C_3^3\right)\frac{bc^2}{(b+1)kD}K_{\sigma\beta}(\nabla^2 u_\beta + \nabla^2 b_\beta) \\ &- k^3(C_2+\tau)\frac{\lambda}{k}\left(K_{\sigma\beta}K_{\beta\eta} + K_{\sigma\beta}K_{\gamma\xi}\frac{\partial b_\beta}{\partial u_\gamma}\delta_{\eta\xi}\right)\left[-C_2\nabla^2 u_\eta + \frac{1}{k}(u_\eta + b_\eta)\right], \end{aligned} \tag{24}$$

in which $C_2 = \frac{1}{2} - \tau$, $C_3 = \tau^2 - \tau + \frac{1}{6}$, $C_4 = -\tau^3 + \frac{3}{2}\tau^2 - \frac{7}{12}\tau + \frac{1}{24}$. The detail derivation of the error terms is given in the appendix.

In equation (24), the main term is $\nabla^4 u_\beta$. Its coefficient is

$$\mu_4 = -k^3\left(C_4 - 3C_2C_3 + C_2^3\right)\lambda K_{\sigma\beta}\frac{3c^2}{D+2}. \tag{25}$$

The stability of the lattice Boltzmann scheme equation (5) is controlled by this coefficient of the term $\nabla^4 u_\beta$, whether negative or not [14]. If the lattice Boltzmann scheme is stable, μ_4 has to be negative, say, $C_4 - 3C_2C_3 + C_2^3 > 0$. In this paper, $\tau = 1.51$, $C_4 - 3C_2C_3 + C_2^3 = 0.946\,134$.

3. The nonlinear Schrödinger equation for the potential flows

The nonlinear Schrödinger equation can be transformed into the Euler equations of the potential flows by using the transformation [11]

$$A(\mathbf{x}, t) = R(\mathbf{x}, t)\,\mathrm{e}^{\mathrm{i}\phi(\mathbf{x},t)}. \tag{26}$$

Putting equation (26) into the nonlinear Schrödinger equation, and setting

$$\mathrm{i}B = \mathrm{i}\xi\,\mathrm{e}^{\mathrm{i}\phi}, \tag{27}$$

where ξ is a real variable, we have

$$\begin{aligned} \frac{\partial R}{\partial t}\mathrm{e}^{\mathrm{i}\phi} + \mathrm{i}\,\mathrm{e}^{\mathrm{i}\phi}R\frac{\partial \phi}{\partial t} = &\ \mathrm{i}\,\mathrm{e}^{\mathrm{i}\phi}R + \frac{1}{2}\mathrm{i}\,\mathrm{e}^{\mathrm{i}\phi}\frac{\partial^2 R}{\partial x_j^2} \\ &+ (-1)\left[\frac{1}{2}\mathrm{i}\left(\frac{\partial \phi}{\partial x_j}\right)^2 \mathrm{e}^{\mathrm{i}\phi}R + \mathrm{e}^{\mathrm{i}\phi}\frac{\partial \phi}{\partial x_j}\frac{\partial R}{\partial x_j} + \frac{1}{2}\mathrm{e}^{\mathrm{i}\phi}R\frac{\partial^2\phi}{\partial x_j^2}\right] + \mathrm{i}\xi\,\mathrm{e}^{\mathrm{i}\phi}. \end{aligned} \tag{28}$$

By removing $\mathrm{e}^{\mathrm{i}\phi}$ from two sides of equation (28), and separating real and imaginary parts, we have

$$\frac{\partial R}{\partial t} = -\frac{\partial R}{\partial x_j}\frac{\partial \phi}{\partial x_j} - \frac{1}{2}R\frac{\partial^2 \phi}{\partial x_j^2}, \tag{29}$$

$$R\frac{\partial\phi}{\partial t} = R + \frac{1}{2}\frac{\partial^2 R}{\partial x_j^2} - \frac{1}{2}R\left(\frac{\partial\phi}{\partial x_j}\right)^2 + \xi. \tag{30}$$

Multiplying equation (29) by $2R$ gives

$$\frac{\partial R^2}{\partial t} = -\frac{\partial}{\partial x_j}\left(R^2\frac{\partial\phi}{\partial x_j}\right). \tag{31}$$

Multiplying equation (30) by $\frac{1}{R}$ gives

$$\frac{\partial\phi}{\partial t} = 1 + \frac{1}{2R}\frac{\partial^2 R}{\partial x_j^2} - \frac{1}{2}\left(\frac{\partial\phi}{\partial x_j}\right)^2 + \frac{\xi}{R}. \tag{32}$$

Multiplying equation (32) by operator $\frac{\partial}{\partial x_k}$ gives

$$\frac{\partial^2\phi}{\partial t\partial x_k} = -\frac{\partial\phi}{\partial x_j}\frac{\partial^2\phi}{\partial x_k\partial x_j} + \frac{\partial}{\partial x_k}\left(\frac{1}{2R}\frac{\partial^2 R}{\partial x_j^2} + \frac{\xi}{R}\right). \tag{33}$$

Equations (31), (33) can be considered as the Euler equations of the potential flows if we define the density ρ and velocity v_j as follows:

$$\rho(\mathbf{x}, t) \equiv R^2(\mathbf{x}, t), \tag{34}$$

$$v_j(\mathbf{x}, t) \equiv \frac{\partial}{\partial x_j}\phi(\mathbf{x}, t). \tag{35}$$

Equations (31), (33) become

$$\frac{\partial\rho}{\partial t} = -\frac{\partial\rho v_j}{\partial x_j}, \tag{36}$$

$$\frac{\partial v_k}{\partial t} = -v_j\frac{\partial v_k}{\partial x_j} + \frac{\partial}{\partial x_k}\left(\frac{1}{2R}\frac{\partial^2 R}{\partial x_j^2} + \frac{\xi}{R}\right). \tag{37}$$

The non-physical pressure term contained in equation (37) is $\frac{1}{\rho}\frac{\partial p}{\partial x_k} = -\frac{\partial}{\partial x_k}\left(\frac{1}{2R}\frac{\partial^2 R}{\partial x_j^2} + \frac{\xi}{R}\right)$. Now, we are to remove this term.

In the incompressible flows, for the sake of convenience, we select that $\rho = \text{const}$. Thus, $R = \sqrt{\rho} = \text{const}$. Equation (31) becomes

$$\nabla^2\phi = 0. \tag{38}$$

In equation (37), the pressure is written as

$$p = -\rho\left(\frac{1}{2R}\frac{\partial^2 R}{\partial x_j^2} + \frac{\xi}{R}\right). \tag{39}$$

According to $\rho(\mathbf{x}, t) \equiv R^2(\mathbf{x}, t)$, the pressure becomes

$$p = -\rho\frac{\xi}{R} = -R\xi.$$

Therefore,

$$\xi = -\frac{p}{R}, \tag{40}$$

$$B = -\frac{p}{R}\,\mathrm{e}^{\mathrm{i}\phi}. \tag{41}$$

In the case $R = \text{const}$, equation (37) describes an incompressible flow.

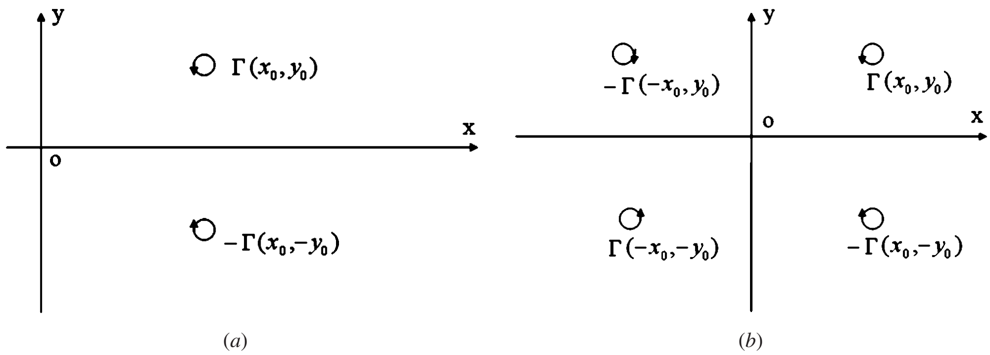


Figure 2. Point vortices and their image point vortices. (*a*) A point vortex above the *x*-axis, (*b*) a point in the corner of the *x*- and *y*-axes.

4. Numerical examples

In this section we apply the lattice Boltzmann model to two irrotational flows: (1) a point vortex flow above the *x*-axis, (2) a point vortex in the corner of the *x*- and *y*-axes.

4.1. The point vortex above the x-axis

A point vortex of strength Γ at $z_0 = x_0 + \mathrm{i}y_0$, the complex potential is

$$w(z) = \frac{\Gamma}{2\pi \mathrm{i}} \log(z - z_0), \tag{42}$$

where $z = x + \mathrm{i}y$. Putting the point vortex above the *x*-axis, see figure 2(*a*), we could write the complex potential as

$$w(z) = \frac{\Gamma}{2\pi \mathrm{i}} \log \frac{z - z_0}{z - \bar{z}_0}. \tag{43}$$

The potential function is the real part of $w(z)$:

$$\phi(x, y) = \frac{\Gamma}{2\pi} \Theta, \tag{44}$$

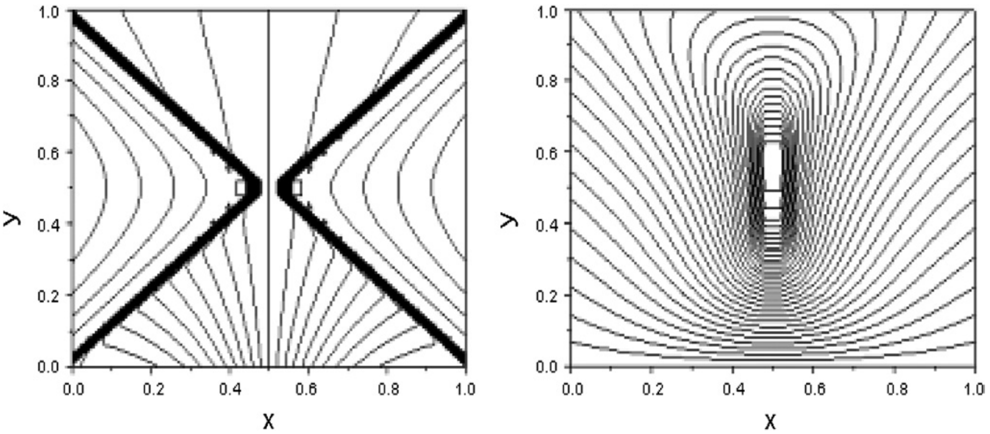
$$\psi(x, y) = -\frac{\Gamma}{2\pi} \log \eta. \tag{45}$$

In equations (44), (45),

$$\Theta = \mathrm{Arc}\tan\left(\frac{b}{a}\right), \qquad \eta = \sqrt{\left(\frac{a}{c}\right)^2 + \left(\frac{b}{c}\right)^2}.$$

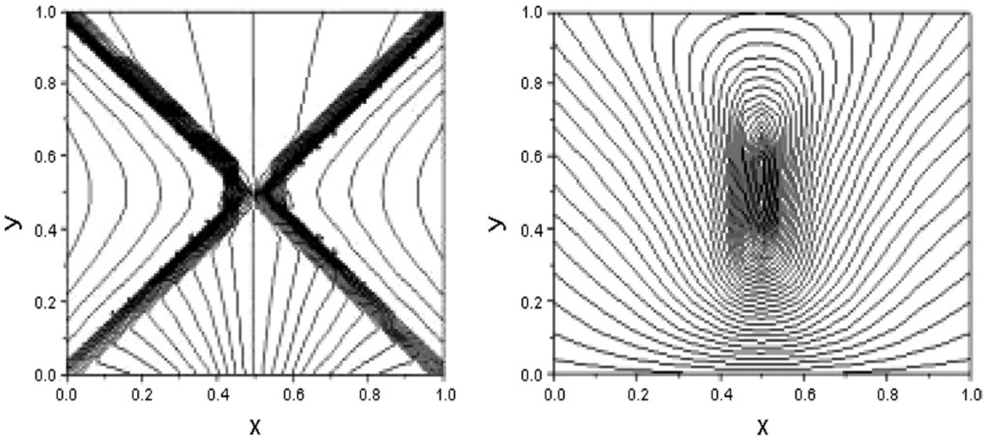
Here $a = (x - x_0)^2 + (y - y_0)^2$, $b = -2y_0(x - x_0)$, $c = (x - x_0)^2 + (y + y_0)^2$.

A point vortex follows with strength Γ at $z_0 = \frac{1}{2} + \mathrm{i}\frac{1}{2}$. Suppose first that in the absence of the *x*-axis, see figure 2(*a*), according to the mapping theorem, we obtain the velocity potential (44) and the stream function (45), contours of the potential function ϕ and the stream function ψ are plotted in figure 3.



(*a*) (*b*)

Figure 3. Contours of the theoretical result. (*a*) Potential function ϕ, (*b*) stream function ψ. $z_0 = \frac{1}{2} + \mathrm{i}\frac{1}{2}$. Contours number is 40.



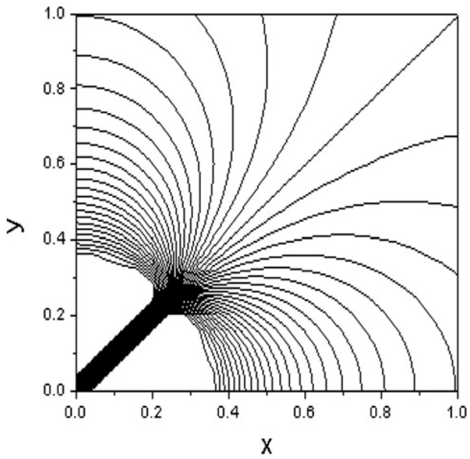
(*a*) (*b*)

Figure 4. Contours of the numerical result by using the lattice Boltzmann model to FHP lattice. (*a*) Potential function ϕ, (*b*) stream function ψ. $z_0 = \frac{1}{2} + \mathrm{i}\frac{1}{2}$. Parameters are $c = 3.0$, $\tau = 1.51$, lattice size $= 100 \times 100$, time $t = 10\,000\Delta t$, $R = 1$. Contours number is 40.

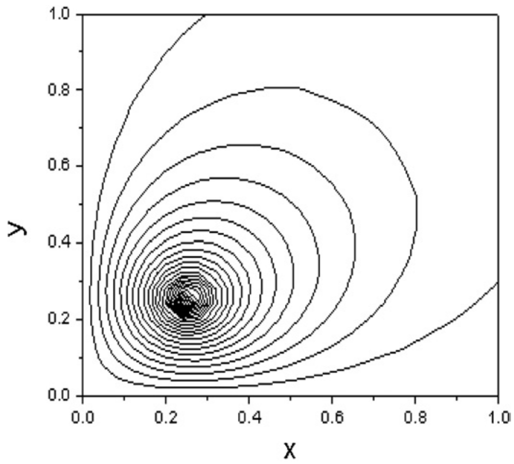
We select a region $[0, 1] \times [0, 1]$ and the x-axis is a wall. The point vortex is at the site $x_0 = \frac{1}{2}$, $y_0 = \frac{1}{2}$. Figure 4 is the contours of the potential function ϕ and the stream function ψ calculated by using the LBM at time $t = 10\,000\Delta t$ in which time step is $\Delta t = \Delta x/c = 1.667 \times 10^{-3}$. The initial condition is a point vortex flow without the x-axis. Boundary conditions are $\frac{\partial^2\phi}{\partial x^2}\big|_{x=0} = 0$, $\frac{\partial^2\phi}{\partial x^2}\big|_{x=1} = 0$, $\frac{\partial\phi}{\partial y}\big|_{y=0} = 0$, $\frac{\partial^2\phi}{\partial y^2}\big|_{y=1} = 0$. In the boundary $y = 0$, the normal component of velocity is zero; other three boundaries are Von Neumann conditions. This numerical result agrees well with the classical result [15].

4.2. The point vortex in a corner

A point vortex of strength Γ at $z_0 = x_0 + \mathrm{i}y_0$, the complex potential is equation (42), where $z = x + \mathrm{i}y$. The point vortex is put into a corner of two walls, x- and y-axes, see figure 2(*b*).



(a)



(b)

Figure 5. Contours of the theoretical result. (a) Potential function ϕ, (b) stream function ψ. $z_0 = \frac{1}{4} + \mathrm{i}\frac{1}{4}$. Contours number is 40.

According to the mapping theorem, the complex potential reads as

$$w(z) = \frac{\Gamma}{2\pi\mathrm{i}} \log \frac{z^2 - z_0^2}{z^2 - \bar{z}_0^2}. \tag{46}$$

The potential function is the real part of $w(z)$:

$$\phi(x, y) = \frac{\Gamma}{2\pi}\Theta, \tag{47}$$

$$\psi(x, y) = -\frac{\Gamma}{2\pi} \log \eta. \tag{48}$$

In equations (47), (48),

$$\Theta = \mathrm{Arc}\tan\left(\frac{b}{a}\right), \qquad \eta = \sqrt{a^2 + b^2}.$$

Here

$$a = \frac{\left[(x^2 - y^2) - \left(x_0^2 - y_0^2\right)\right]^2 + 4\left(x^2y^2 - x_0^2y_0^2\right)}{\left[(x^2 - y^2) - \left(x_0^2 - y_0^2\right)\right]^2 + 4(xy + x_0y_0)^2}, \tag{49}$$

$$b = -\frac{4x_0y_0\left[(x^2 - y^2) - \left(x_0^2 - y_0^2\right)\right]}{\left[(x^2 - y^2) - \left(x_0^2 - y_0^2\right)\right]^2 + 4(xy + x_0y_0)^2}. \tag{50}$$

These contours of the potential function ϕ and the stream function ψ are plotted in figure 5.

We select a region $[0, 1] \times [0, 1]$ and the x- and y-axes are two walls. The point vortex is at the site $x_0 = \frac{1}{4}$, $y_0 = \frac{1}{4}$. Figure 6 is the contours of the potential function ϕ and the stream function ψ calculated by using the LBM at time $t = 10\,000\Delta t$ in which the time step is $\Delta t = \Delta x/c = 1.667 \times 10^{-3}$. The initial condition is a point vortex flow without the x- and y-axes. Boundary conditions are $\frac{\partial\phi}{\partial x}\big|_{x=0} = 0$, $\frac{\partial^2\phi}{\partial x^2}\big|_{x=1} = 0$, $\frac{\partial\phi}{\partial y}\big|_{y=0} = 0$, $\frac{\partial^2\phi}{\partial y^2}\big|_{y=1} = 0$. In the two boundaries $x = 0$ and $y = 0$, the normal component of velocity is zero; other boundaries $x = 1$ and $y = 1$ are Von Neumann conditions. This numerical result also agrees well with the classical result [15].

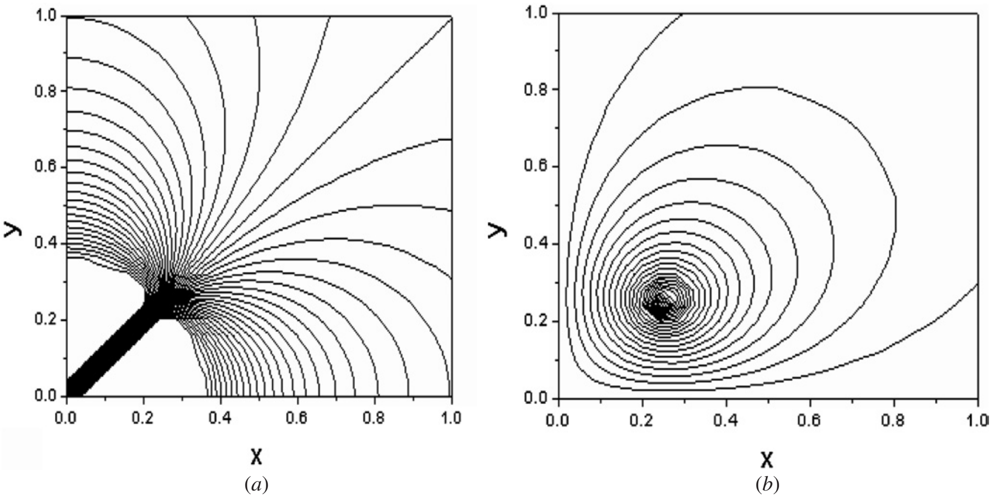


Figure 6. Contours of the numerical result by using the lattice Boltzmann model to FHP lattice. (*a*) Potential function ϕ, (*b*) stream function ψ. $z_0 = \frac{1}{4} + \mathrm{i}\frac{1}{4}$. Parameters are $c = 3.0$, $\tau = 1.51$, lattice size $= 100 \times 100$, time $t = 10\,000\Delta t$, $R = 1$. Contours number is 40.

5. Concluding remarks

In this paper, a new lattice Boltzmann model for the nonlinear Schrödinger equation is proposed. The new model is based on the technique of the higher order moment of equilibrium distribution functions and a series of lattice Boltzmann equations in different time scales. The irrotational Euler equations are derived from this nonlinear Schrödinger equation by removing non-physical pressure.

Our target is to simulate the nonlinear Schrödinger equation, say, to propose a new numerical method. We find that this model can be used to simulate the irrotational flows. These two sample numerical examples show that numerical results agree well with classical ones.

Finally, we point out that this method and the main idea in the paper, including a series of the lattice Boltzmann equations in different time scales, conversation laws in time scales t_0, t_1, and its equilibrium distribution, can be spread into the corresponding three-dimensional irrotational flows. Nevertheless, there are many problems to be solved to develop this model as a tool of simulating the nonlinear Schrödinger equation or the Euler equations. We would discuss these problems in forthcoming papers.

Appendix

Taking (14) + (15) $\times$ k + (16) $\times$ k^2 and summation over α, we have

$$\frac{\partial u_\sigma}{\partial t} = k\left(\tau - \frac{1}{2}\right)\frac{\partial^2}{\partial x_j \partial x_k}(\lambda K_{\sigma\beta} u_\beta \delta_{jk}) + K_{\sigma\beta} u_\beta + K_{\sigma\beta} b_\beta + E_3 + O(k^3), \tag{A.1}$$

in which E_3 is the third-order error term

$$E_3 = -\sum_\alpha k^2 \left[\left(\tau^2 - \tau + \frac{1}{6}\right)\Delta^3 F_\alpha^{\sigma,\mathrm{eq}} + 2\left(\frac{1}{2} - \tau\right)\Delta \frac{\partial}{\partial t_1} F_\alpha^{\sigma,\mathrm{eq}} + \Delta\tau\theta_\alpha^\sigma\right]. \tag{A.2}$$

In order to find E_3, term $\sum_\alpha \frac{\partial F_\alpha^{\sigma,\mathrm{eq}}}{\partial t_1}$ needs to be determined. According to equation (15),

$$\frac{\partial}{\partial t_1} F_\alpha^{\sigma,\mathrm{eq}} = -\left(\frac{1}{2} - \tau\right) \Delta^2 F_\alpha^{\sigma,\mathrm{eq}} - \frac{1}{\tau} F_\alpha^{\sigma,2} + \theta_\alpha^\sigma. \tag{A.3}$$

Taking summation over α, we obtain

$$\begin{aligned}\frac{\partial u_\sigma}{\partial t_1} &= \sum_\alpha \left[-\left(\frac{1}{2} - \tau\right) \Delta^2 F_\alpha^{\sigma,\mathrm{eq}} - \frac{1}{\tau} F_\alpha^{\sigma,2} + \theta_\alpha^\sigma\right] \\ &= \left(\tau - \frac{1}{2}\right) \sum_\alpha \Delta^2 F_\alpha^{\sigma,\mathrm{eq}} + \frac{1}{k}(K_{\sigma\beta} u_\beta + K_{\sigma\beta} b_\beta) \\ &= \left(\tau - \frac{1}{2}\right)\left[\sum_\alpha \frac{\partial^2 F_\alpha^{\sigma,\mathrm{eq}}}{\partial t_0^2} + 2\sum_\alpha e_{\alpha_j} \frac{\partial^2 F_\alpha^{\sigma,\mathrm{eq}}}{\partial x_j \partial t_0} + \sum_\alpha e_{\alpha i} e_{\alpha j} \frac{\partial^2 F_\alpha^{\sigma,\mathrm{eq}}}{\partial x_i \partial x_j}\right] + \frac{K_{\sigma\beta}}{k}(u_\beta + b_\beta),\end{aligned}$$

namely,

$$\frac{\partial u_\sigma}{\partial t_1} = \left(\tau - \frac{1}{2}\right)\left[\frac{\partial^2}{\partial x_j \partial x_k} \lambda K_{\sigma\beta} u_\beta \delta_{jk}\right] + \frac{K_{\sigma\beta}}{k}(u_\beta + b_\beta). \tag{A.4}$$

Equation (A.4) is named as the conversation law in the second time scale t_1. Combining equations (8), (9), (18), we obtain

$$-\sum_\alpha k^2 \left(\tau^2 - \tau + \frac{1}{6}\right) \Delta^3 F_\alpha^{\sigma,\mathrm{eq}} = 0, \tag{A.5}$$

$$\sum_\alpha \left[\left(\frac{1}{2} - \tau\right) \Delta \frac{\partial}{\partial t_1} F_\alpha^{\sigma,\mathrm{eq}}\right] = 0, \tag{A.6}$$

$$-\sum_\alpha k^2 \tau \Delta \theta_\alpha^\sigma = 0. \tag{A.7}$$

Therefore,

$$E_3 = -\sum_\alpha k^2 \left[\left(\tau^2 - \tau + \frac{1}{6}\right) \Delta^3 F_\alpha^{\sigma,\mathrm{eq}} + 2\left(\frac{1}{2} - \tau\right) \Delta \frac{\partial}{\partial t_1} F_\alpha^{\sigma,\mathrm{eq}} + \Delta \tau \theta_\alpha^\sigma\right] = 0. \tag{A.8}$$

Taking (14) + (15) $\times\, k$ + (16) $\times\, k^2$ + (17) $\times\, k^3$ and summation over α, we have

$$\frac{\partial u_\sigma}{\partial t} = k\left(\tau - \frac{1}{2}\right) \frac{\partial^2}{\partial x_j \partial x_k}(\lambda K_{\sigma\beta} u_\beta \delta_{jk}) + K_{\sigma\beta} u_\beta + K_{\sigma\beta} b_\beta + E_3 + E_4 + O(k^4), \tag{A.9}$$

in which E_4 is the fourth-order error term

$$\begin{aligned}E_4 = -k^3 \sum_\alpha \Bigg[&\left(-\tau^3 + \frac{3}{2}\tau^2 - \frac{7}{12}\tau + \frac{1}{24}\right) \Delta^4 F_\alpha^{\sigma,\mathrm{eq}} + 3\left(\tau^2 - \tau + \frac{1}{6}\right) \Delta^2 \frac{\partial}{\partial t_1} F_\alpha^{\sigma,\mathrm{eq}} \\ &+ \left(\frac{1}{2} - \tau\right) \frac{\partial^2}{\partial t_1^2} F_\alpha^{\sigma,\mathrm{eq}} + \frac{\partial}{\partial t_1} \tau \theta_\alpha^\sigma + \left(\frac{1}{2} - \tau\right) \Delta^2 \tau \theta_\alpha^\sigma\Bigg].\end{aligned} \tag{A.10}$$

In order to find E_4, term $\sum_\alpha \frac{\partial^2 F_\alpha^{\sigma,\mathrm{eq}}}{\partial t_1^2}$ needs to be determined. According to equation (A.3), we have

$$\frac{\partial F_\alpha^{\sigma,\mathrm{eq}}}{\partial t_2} = \left(\frac{1}{2} - \tau\right)^2 \Delta^4 F_\alpha^{\sigma,\mathrm{eq}} + \frac{1}{\tau}\left(\frac{1}{2} - \tau\right) \Delta^2 F_\alpha^{\sigma,2} - \left(\frac{1}{2} - \tau\right) \Delta^2 \theta_\alpha^\sigma - \frac{1}{\tau} \frac{\partial}{\partial t_1} F_\alpha^{\sigma,2} + \frac{\partial \theta_\alpha^\sigma}{\partial t_1}. \tag{A.11}$$

By putting $\frac{\partial F_\alpha^{\sigma,\mathrm{eq}}}{\partial t_1}$ and $\frac{\partial^2 F_\alpha^{\sigma,\mathrm{eq}}}{\partial t_1^2}$ into equation (A.10), E_4 is written as

$$E_4 = -k^3 \sum_\alpha \Big[\left(C_4 - 3C_2C_3 + C_2^3\right)\Delta^4 F_\alpha^{\sigma,\mathrm{eq}} - \frac{3}{\tau} C_3 \Delta^2 F_\alpha^{\sigma,2} + 3C_3\Delta^2\theta_\alpha^\sigma + \frac{1}{\tau} C_2^3 \Delta^2 F_\alpha^{\sigma,2} - C_3^3\Delta^2\theta_\alpha^\sigma - \frac{1}{\tau} C_2 \frac{\partial F_\alpha^{\sigma,2}}{\partial t_1} + C_2 \frac{\partial \theta_\alpha^\sigma}{\partial t_1} + \tau \frac{\partial \theta_\alpha^\sigma}{\partial t_1} + C_2\tau\Delta^2\theta_\alpha^\sigma \Big]. \quad \text{(A.12)}$$

In equation (A.12), $C_2 = \frac{1}{2} - \tau$, $C_3 = \tau^2 - \tau + \frac{1}{6}$, $C_4 = -\tau^3 + \frac{3}{2}\tau^2 - \frac{7}{12}\tau + \frac{1}{24}$. According to $\sum_\alpha F_\alpha^{\sigma,2} = 0$, E_4 is written as follows:

$$E_4 = -k^3 \sum_\alpha \left[\left(C_4 - 3C_2C_3 + C_2^3\right)\Delta^4 F_\alpha^{\sigma,\mathrm{eq}} + \left(3C_3 + \tau C_2 - C_3^3\right)\Delta^2\theta_\alpha^\sigma + (C_2 + \tau)\frac{\partial \theta_\alpha^\sigma}{\partial t_1} \right]. \quad \text{(A.13)}$$

In equation (A.13), $\Delta^4 F_\alpha^{\sigma,\mathrm{eq}}$, $\Delta^2\theta_\alpha^\sigma$ and $\frac{\partial \theta_\alpha^\sigma}{\partial t_1}$ need to be found

$$\sum_\alpha \Delta^4 F_\alpha^{\sigma,\mathrm{eq}} = \sum_\alpha \left(\frac{\partial}{\partial t_0} + e_{\alpha j}\frac{\partial}{\partial x_j} \right)^4 F_\alpha^{\sigma,\mathrm{eq}} = \lambda K_{\sigma\beta} \frac{3c^2}{D+2} \nabla^4 u_\beta, \quad \text{(A.14)}$$

$$\sum_\alpha \Delta^2 \theta_\alpha^{\sigma,\mathrm{eq}} = \frac{bc^2}{(b+1)kD} K_{\sigma\beta}(\nabla^2 u_\beta + \nabla^2 b_\beta), \quad \text{(A.15)}$$

$$\sum_\alpha \frac{\partial \theta_\alpha^\sigma}{\partial t_1} = \frac{\lambda}{k} \left(K_{\sigma\beta}K_{\beta\eta} + K_{\sigma\beta}K_{\gamma\xi}\frac{\partial b_\beta}{\partial u_\gamma}\delta_{\eta\xi} \right) \left[-C_2\nabla^2 u_\eta + \frac{1}{k}(u_\eta + b_\eta) \right], \quad \text{(A.16)}$$

in which $\nabla^2 = \frac{\partial^2}{\partial x_j \partial x_j}$, $\nabla^4 = \frac{\partial^4}{\partial x_j \partial x_j \partial x_j \partial x_j}$. Combining (A.14)-(A.16), we have

$$\begin{aligned} E_4 = & -k^3\left(C_4 - 3C_2C_3 + C_2^3\right)\lambda K_{\sigma\beta}\frac{3c^2}{D+2}\nabla^4 u_\beta \\ & - k^3\left(3C_3 + \tau C_2 - C_3^3\right)\frac{bc^2}{(b+1)kD} K_{\sigma\beta}(\nabla^2 u_\beta + \nabla^2 b_\beta) \\ & - k^3(C_2+\tau)\frac{\lambda}{k}\left(K_{\sigma\beta}K_{\beta\eta} + K_{\sigma\beta}K_{\gamma\xi}\frac{\partial b_\beta}{\partial u_\gamma}\delta_{\eta\xi} \right) \left[-C_2\nabla^2 u_\eta + \frac{1}{k}(u_\eta + b_\eta) \right]. \end{aligned} \quad \text{(A.17)}$$

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