Lattice Boltzmann simulation of a single charged particle in a Newtonian fluid

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The lattice Boltzmann method is used to study the sedimentaion of a single charged circular cylinder in a two-dimensional channel in a Newtonian fluid. When the dielectric constant of the liquid is smaller than that of the walls, there are attractive forces between the particle and the walls. The hydrodynamic force pushes the particle towards the centerline at low Reynolds numbers. Due to the competition between the Coulomb force and the hydrodynamic force in opposite directions, there is a critical linear charge density q_c at which the particle will fall vertically off centerline, which is a metastable state in addition to the stable state on centerline, for any initial position of the particle sufficiently far from the proximal wall. It is found that the rotation of the particle plays an important role in the stability of such metastable states. The particle hits on the wall or falls on the centerline when the linear charge density on the particle is greater or less than q_c. The simulation method and the new phenomena are also helpful in the study of charged multiparticle suspensions.

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The study of the interaction and dynamics in charged colloidal suspensions is of great interest in physics, chemistry, biology, and medical science. It is well known that the red cells in blood carry negative charge, and without that the behavior of aggregation of the red cells will change significantly [1]. The charge plays a very important role in the dynamics of the suspensions. On the other hand, the existence of wall may develop unexpected phenomena. For example, a strong and long-range attraction force is observed between isolated pair of like-charged spheres [2]. Although there is an extensive literature of empirical correlations describing the dynamics of charged particle suspensions [3], a fundamental understanding is limited to simple models due to the difficulty in numerically simulating each particle in liquid accurately.

It is relatively simple to study one-particle suspension in liquid. The study of the dynamics of a single charged particle in liquid will not only help develop simulation methods and understand the dynamics of multiparticle suspensions, it can also provide new phenomena. Up to now, there is little literature on the experimental and numerical study on a single charged particle in liquid. The dynamics of a single uncharged particle sedimentation, however, has attracted much attention. Early in 1981, Miyamura *et al.* [4] studied the ratio of the sphere velocities in the bounded and unbounded cases, which is called the wall correction factor. Joseph, Hu, and their co-workers studied the sedimentation of two-dimensional circular and elliptical particles in Newtonian and non-Newtonian fluid in a wide range of Reynolds number with finite-element method [5,6]. Stabilizing in centerline, oscillation and chaotic motion around the centerline and far from the centerline were observed for different Reynolds numbers. Recently, two- and three-dimensional particles in Newtonian fluid were simulated with the lattice Boltzmann method [7,8] and the simulation results were favorable to the experimental results and finite-element simulation results. In this paper, we will apply the lattice Boltzmann method to study the behavior of sedimentation of a single charged circular particle in vertical tube. Due to the competition of the hydrodynamic and electrostatic forces, there is a critical value q_c of the charge at which the particle will fall vertically off centerline, which is called a metastable state in addition to the stable state on centerline, for any initial position of the particle sufficiently far from the proximal wall. We further find that the rotation of the particle plays an important role in the stability of such metastable states. The relationship between the charged particle and the initial position of the particle to obtain a metastable state is studied.

We choose to work on a square lattice in two dimensions [9]. Let $f_i(\mathbf{x},t)$ be a non-negative real number describing the distribution function of the fluid density at site $\mathbf{x}$ at time t moving in direction $\mathbf{e}_i$. Here $\mathbf{e}_0=(0,0)$, $\mathbf{e}_i=(\cos \pi(i-1)/2,\sin \pi(i-1)/2)$, $i=1,2,3,4$, and $\mathbf{e}_i=(\cos \pi(2i-1)/4,\sin \pi(2i-1)/4)$, for $i=5,6,7,8$ are the nine possible velocity vectors. The distribution functions evolve according to a Boltzmann equation that is discrete in both space and time [9],

$$f_i(\mathbf{x}+\mathbf{e}_i,t+1)-f_i(\mathbf{x},t)=-\frac{1}{\tau}(f_i-f_i^{eq}), \tag{1}$$

where τ is the relaxation time. The density ρ and macroscopic velocity $\mathbf{u}$ are defined by

$$\rho=\sum_i f_i, \quad \rho\mathbf{u}=\sum_i f_i\mathbf{e}_i, \tag{2}$$

and the equilibrium distribution functions f_i^{eq} are usually supposed to be dependent only on the local density ρ and flow velocity $\mathbf{u}$. A suitable choice reads [9]

$$f_i^{eq}=\rho\alpha_i[1+3\mathbf{e}_i\cdot\mathbf{u}+\tfrac{9}{2}(\mathbf{e}_i\cdot\mathbf{u})^2-\tfrac{3}{2}u^2], \tag{3}$$

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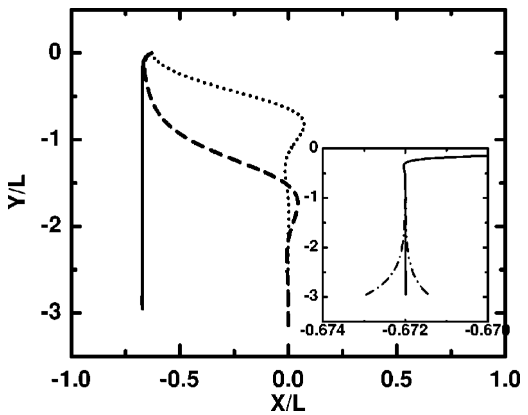

FIG. 1. The trajectories of a circular particle for $q=9.60936\times10^{-11}$ C/cm (dash), $q=q_c=1.009364\times10^{-10}$ C/cm (solid), and $q=0$ (dot), respectively. The inset is an enlarged part of the figure showing the discrepancy of the trajectories for $q=q_c$ and $q=q_c\pm\delta q$ (dash-dotted and dash-dot-dotted), where $\delta q=2.0\times10^{-16}$ C/cm.

where $\alpha_0=4/9$, $\alpha_1=\alpha_2=\alpha_3=\alpha_4=1/9$, and $\alpha_5=\alpha_6=\alpha_7=\alpha_8=1/36$. The macroscopic equations can be obtained by a Chapman-Enskog procedure [9]. The pressure p and the viscosity ν are defined by the equations $p=c_s^2\rho$ with $c_s^2=1/3$ and $\nu=(2\tau-1)/6$, respectively,

The boundary condition proposed by Filippova and Hanel [10] is used for the stationary complex geometry. Hydrodynamic forces on the particles are evaluated based on the momentum exchange of the fluid and the solid boundaries [7,8]. The translation of the center of mass of a particle is updated at each Newtonian dynamics time step by using a so-called half-step "leap-frog" scheme [11]. The accuracy and robustness of this technique had been demonstrated by simulating sedimentation of a circular cylinder in a two-dimensional channel and comparing the simulation results with those obtained from a second-order finite-element method [8].

In two dimensions the Coulomb force on a point charge located in front of an infinite plane wall can be obtained by the method of images [12]:

$$F=\frac{qq_1^{(1)}}{4\pi\epsilon_0 z},\tag{4}$$

where $q_1^{(1)}=[(\epsilon_1-\epsilon_2)/(\epsilon_1+\epsilon_2)]q$ is the charge of the image, ϵ_1 and ϵ_2 are the dielectric constants of the media around the charge and the wall, respectively. z is the distance between the charge and the infinite plane wall. The Coulomb force on a point charge between two infinite plane walls can be obtained from a series of images,

$$F=\sum_{i=1}^{\infty}\left(\frac{qq_1^{(i)}}{4\pi\epsilon_0 z_1^{(i)}}-\frac{qq_2^{(i)}}{4\pi\epsilon_0 z_2^{(i)}}\right).\tag{5}$$

Here $q_1^{(i)}=q_2^{(i)}=[(\epsilon_1-\epsilon_2)/(\epsilon_1+\epsilon_2)]^i q$ and

$$z_1^{(1)}=2r_1,$$

$$z_2^{(1)}=2r_2,$$

$$z_1^{(i)}=z_1^{(i-1)}+2r_2\quad(i=2n),$$

$$z_2^{(i)}=z_2^{(i-1)}+2r_1\quad(i=2n),$$

$$z_1^{(i)}=z_1^{(i-1)}+2r_1\quad(i=2n+1),$$

$$z_2^{(i)}=z_2^{(i-1)}+2r_2\quad(i=2n+1),$$

$n=1,2,3,\ldots$, r_1 and r_2 are the distances from the particle to the left wall and the right wall, respectively. In numerical simulation, only the first ten images are used to obtain sufficiently accurate results. Actually, since the factor $(\epsilon_1-\epsilon_2)/(\epsilon_1+\epsilon_2)$ in the image charge $q^{(i)}$ is smaller than 1 in absolute value, series (5) for the Coulomb force converges rapidly. For example, the Coulomb force on the particle with linear charge density $q=1.009364\times10^{-10}$ C/cm and located at $x_i=-0.62783L$ in the tube, which will be described in detail in the following section, is $f=-2.1636159\times10^{-9}$ N for the first ten images, while $f=-2.1636168\times10^{-9}$ N for the first 100 000 images.

The system is a vertical channel of width $2L=4d$, where $d=0.1$ cm is the diameter of the cylinder. The x axis is horizontal to the right and $x=0$ corresponds to the symmetric

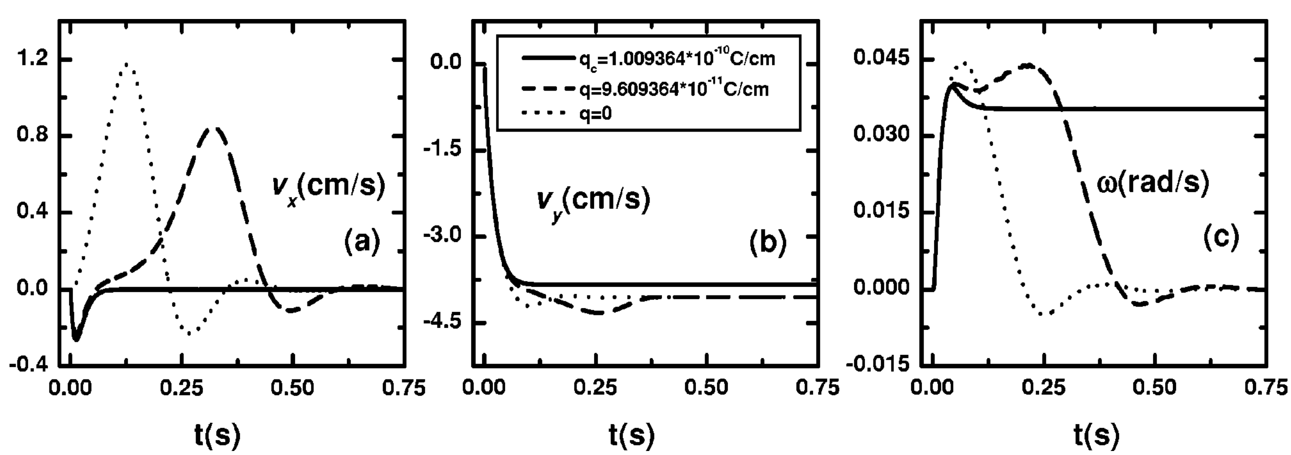

FIG. 2. The vertical velocities, the horizontal velocities, and the angular velocities of the charged circular particle for linear charge densities $q=9.60936\times10^{-11}$ C/cm (dash), $q=q_c$ (solid), and $q=0$ (dot), respectively.

axis of the channel. The cylinder is released at $x_i/L = -0.62783$ with zero initial velocity and settles under gravity. The density of the solid is 1.6 g/cm^3, while the density and the kinematic viscosity of the fluid flow are 0.8 g/cm^3 and 0.1 cm^2/s, respectively. The linear charge density on the cylinder is q and distributed uniformly on the cylinder. The liquid in the tube is lubricating oil with a dielectric constant 2.24, while the walls are made of glass with a dielectric constant 7.00. Since the dielectric constant of the liquid is less than that of the walls, there are attractive forces between the charged particle and the walls. In our simulation, the inlet of the domain is always 10d from the moving particles, whereas the downstream boundary is 15d from the boundary. Zero velocities are applied uniformly for the inlet and the normal derivative of the velocity is set to zero at the outlet.

Feng *et al.* simulated the sedimentation of a single uncharged cylinder with finite-element method [6]. It was found that the cylinder stayed at the centerline finally for the terminal Reynolds number Re$<$8.5, where Re is defined by Re$=u_p d/\nu$, with u_p the terminal velocity and ν the viscosity. To study the effect due to charge, we have performed a systematic simulation for cases with $0.5<\mathrm{Re}<8.5$. No qualitative difference was found for the sedimentary behavior of the charged particle from our numerical simulation. As a result, we show in this paper only the typical case with Re ≈ 4. In the simulation, the radius of the cylinder is 13 lattice units and $\tau = 0.6$.

Figure 1 displays the trajectory of the cylinder with a linear charge density $q = 9.60936\times 10^{-11}$ C/cm together with the case for $q=0$. Unlike that of the neutral particle, the cylinder moves towards the wall first and then approaches the centerline with overshoot due to the electrostatic interaction between the charged particle and the wall. When the charged particle is close to the centerline, its trajectory is quite similar to that of the neutral particle, since the electrostatic force vanishes at the centerline. The time-dependent velocity and angular velocity are shown as dashed lines in Fig. 2. The x component of the velocity decreases first and then increases. There are two peaks on the angular velocity, while only one peak without charge. The angular velocity falls to 0 finally for both cases. It is interesting to find that when the linear charge density q is a bit larger, at $q = q_c = 1.009364\times 10^{-10}$ C/cm, there is a metastable state shown as the solid line in Fig. 1. The particle moves towards the proximal wall first and then falls down vertically. The velocity is shown in Fig. 2. After transient the x component of the velocity vanishes very quickly, while the y component keeps as a constant. The y component of the velocity for the charged particle is smaller than that of the neutral particle, since it is close to the boundary so that the wall correction factor [4] is larger. It it noted from Fig. 2 that the angular velocity does not approach 0. In Fig. 3 we show the streamlines around the cylinder for the metastable state. The velocity distribution is also asymmetric.

Now we discuss the stability of the metastable state. Numerically we cannot determine whether the metastable state is really a ‘‘metastable state’’ or only a transient state with lifetime dependent on charge q, since we have no idea on whether the particle will stay at the off-centered trajectory or not (even for $q=q_c$) if we simulate for extremely long time. The unavoidable numerical error makes the problem more difficult. However, we can obtain a domain of attraction for the metastable state by defining some constraint for $|y/L|$ or time t and a tolerable error. For instance, if there is a constraint for $|y/L|$ as $|y/L|<3$ and x_i/L has a tolerance of 0.001, the domain of attraction for the linear charge density is $\delta q = 2.0\times 10^{-16}$ C/cm. In Fig. 1, we also show the trajectory of the particle for $q = q_c \pm \delta q$. The discrepancy is small and apparent in the inset, which is an enlarged part of the figure. We emphasize that the ‘‘metastable state’’ we have defined in this paper may not be a real metastable state.

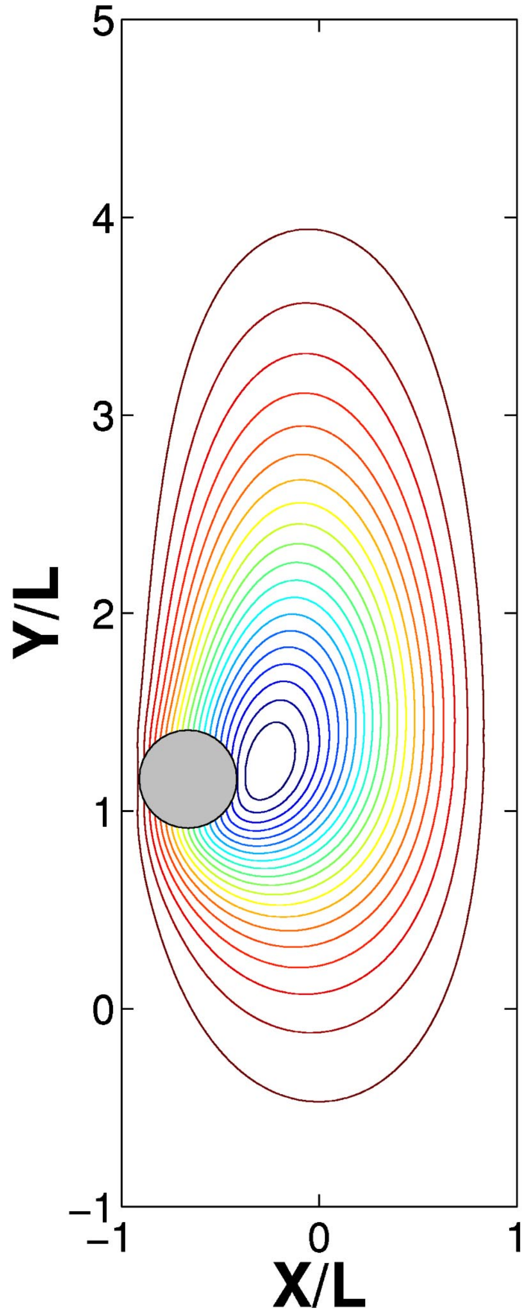

FIG. 3. The streamlines around the cylinder for the metastable state.

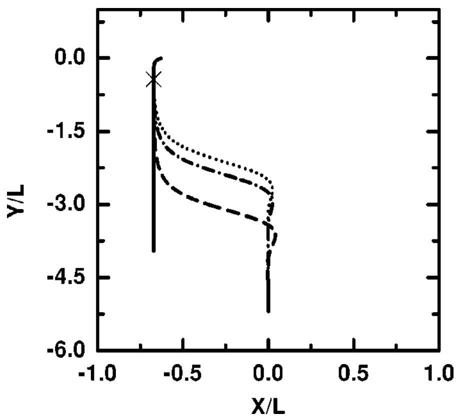

FIG. 4. The trajectories of the circular particle for $q = q_c$ while the angular velocity decreases gradually according to $\omega = \omega_0 \exp[-\beta(t-t_0)]$ for $\beta = 10$ (dash-dot) and $\beta = 400$ (dot), respectively. The solid line is the original trajectory without perturbation. The cross is the position of the particle at $t = t_0 = 0.13$ s. The dashed line corresponds to the case with the exponential decay for ω only existing in the small time period $t_0 < t < t_0 + \delta t$, where $\delta t = 0.0052$ s and $\beta = 400$.

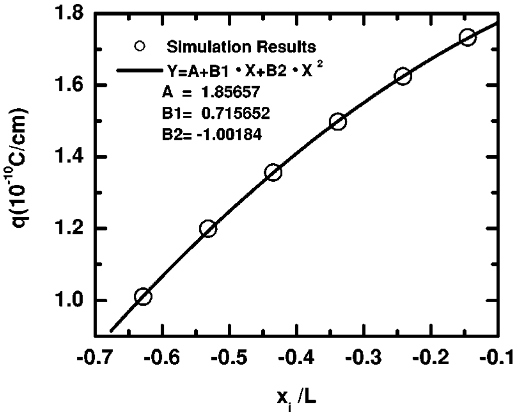

FIG. 6. The critical linear charge density q_c for different initial position x_i.

However, if we simulate only for a limit time with a tolerable error, we cannot say whether the trajectory leaves the critical trajectory at $q = q_c$ or not; this trajectory at $q = q_c$ behaves like a metastable state and we still call it as a metastable state in this paper.

The rotation plays an important role in the stability of the metastable states. To illustrate the effect, we introduce an exponential decay for the angular velocity $\omega = \omega_0 \exp[-\beta(t-t_0)]$, which may be caused by an additional friction, where ω_0 is the angular velocity for the original metastable state and β is a parameter. The metastable state loses its stability, as shown in the trajectories and velocities in Figs. 4 and 5 for $t_0 = 0.13$ s, $\beta = 10$ and 400, respectively. The x component of the velocity increases gradually from 0 and the particle moves towards the centerline. It is found that the faster the decreasing of the angular velocity, the larger the speed of the particle returning to the centerline. In the figures we also display the case with the exponential decay for ω only existing in the small time period $t_0 < t < t_0 + \delta t$, where $\delta t = 0.0052$ s and $\beta = 400$. It is interesting to find that the stability of the metastable state is lost although the angular velocity restores very quickly from $t > t_0 + \delta t$. Comparing the previous case with the same $\beta = 400$, the particle returns to the centerline more slowly.

The metastable state does not restrict to a particular initial position. Numerically we find that there is a critical linear charge density q_c corresponding to a metastable state for any initial position sufficiently far from the proximal wall. Figure 6 displays the critical linear charge density q_c for different initial positions. We remind that the radius of the particle is $0.25L$ so that $|x_i|/L$ must be less than 0.75. Moreover, since the charged particle always moves towards the proximal wall first, there is no metastable state when $|x_i| > x_c$. Numerically we find that x_c/L is about 0.67.

To conclude, we have applied the lattice Boltzmann method to study the sedimentaion of a single charged circular cylinder in a two-dimensional channel in a Newtonian fluid. The Coulomb interaction force on the charged particle is obtained by the method of images. When the dielectric constant of the liquid is smaller than that of the walls, there are attractive forces between the particle and the walls in

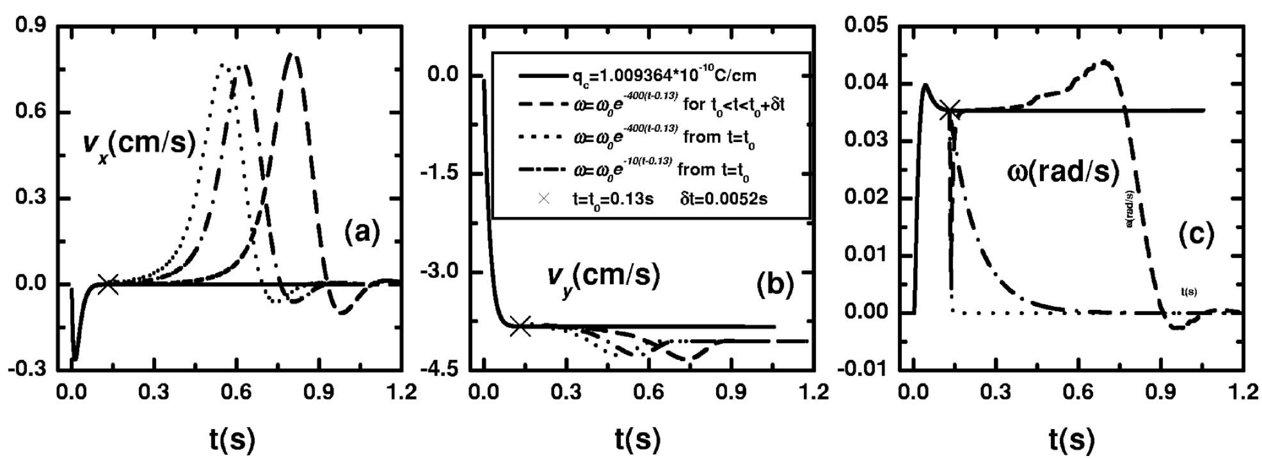

FIG. 5. The vertical velocities, the horizontal velocities, and the angular velocities of the charged circular particle corresponding to the trajectories displayed in Fig. 4.

addition to the hydrodynamic force. Since the hydrodynamic force pushes the particle towards the centerline at low Reynolds number, there are two forces in opposite directions—the Coulomb force and the hydrodynamic force. Metastable states are found in which the particles move down vertically off centerline for critical linear charge densities q_c. We further find that the rotation of the particle plays an important role for the stability of such metastable states. Any perturbation on the rotation makes the metastable state unstable and the particle return to the centerline as that of the neutral particles. When the linear charge density on the particle is greater or less than q_c, the particle hits on the wall or falls on the centerline. The simulation method and the new phenomena is also helpful in the study of charged multiparticle suspensions.

Although the numerical simulations are performed in two dimensions, similar behavior is expected in three dimensions. In three dimensions, the hydrodynamic force also pushes the particle towards the centerline at low Reynolds numbers, while the Coulomb force attracts the particle to the proximal wall. The equilibrium of these two forces at a critical charge density for any off centerline initial position results in the metastable state that the particle moves down vertically off centerline. This will be presented in our another paper.

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