# Pressure tensor calculation in a class of nonideal gas lattice Boltzmann models

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In nonideal gas lattice Boltzmann (LB) models, obtaining the correct form of the pressure tensor is essential in determining many of the statistical mechanical properties such as the surface tension and the density profile. Here we outline a general approach for calculating the pressure tensor in LB models with interactions beyond nearest neighbors. The statistical mechanical properties calculated from such a pressure tensor are shown to agree very well with those measured from numerical experiments. Comparisons with alternative theories are also made.

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## I. INTRODUCTION

In recent years the lattice Boltzmann (LB) method has evolved into a promising method of computational fluid dynamics (CFD) [1,2]. It is particularly promising in simulating complex fluid flows as its kinetic nature allows direct modeling of the microscopic physics responsible for the macroscopic complexity. For example, to simulate multiphase flows using the LB method, one models the underlying physics that is responsible for the formation of multiple phases in a fluid system instead of the dynamics of the interfaces. In one of the approaches this was done by introducing an interaction among the constituent particles [3,4]. The application of this class of nonideal gas LB models has been particularly fruitful [5–9].

In fluid simulations using the LB method, the macroscopic behavior of the fluid system, such as the dynamics of the density, velocity, and temperature fields, the equation of state, and the surface tension coefficient, are all consequences of the microscopic or mesoscopic dynamics of the distribution function. To be able to simulate a fluid system with a given set of parameters, it is necessary to derive the macroscopic properties from the microscopic ones that the "input parameters" in LB models. Therefore, accurately solving the mesoscopic kinetic model to obtain the macroscopic properties has been critical in the development of the LB methods. This is particularly true for the models of complex fluids as their macroscopic behaviors are more complex and more difficult to obtain than those of an ideal gas.

In a nonideal gas system exhibiting multiple phases, many of the macroscopic properties can be obtained through knowledge of the part of the pressure tensor due to interactions. In a continuum, calculating the pressure tensor from the interaction potential is at the center of studies of capillary phenomena [10]. Correspondingly, in the LB system, determination of the pressure tensor in the presence of intermolecular interactions is also critical in the development of LB models and methodology. For the nonideal gas LB model in Refs. [3,4], the pressure tensor was obtained for the simplest case of nearest-neighbor interactions. Much of the macroscopic behavior was also derived. Recently it was found necessary to extend the interaction beyond the range of the nearest neighbors to improve the isotropy of the interface [11,12] and to better control the surface tension [12]. Moreover, the form of the pressure tensor has been debated and some of the end results have rather significant consequences at the macroscopic level [5,12,13]. In this paper, we reexamine this issue and provide a general methodology for calculating the pressure tensor for interactions over an arbitrary range. As an example, we obtain the pressure tensor for the interaction defined over two layers of neighbors in a two-dimensional LB model. In agreement with [12], we also found that while the equation of state is determined essentially by the second-order terms in the pressure tensor, the surface tension coefficient is directly proportional to the fourth-order tensor constructed using the distance vectors of the interacting neighbors.

The paper is organized as the following. In Sec. II, we briefly review the nonideal gas LB models. The calculation of the pressure tensor is carried out in Sec. III. The macroscopic properties of the pressure tensor is summarized in Sec. IV. Finally in Sec. V, a comparison between our results and an alternatively obtained pressure tensor is given.

## II. LB MODEL FOR NONIDEAL GASES

We follow previously outlined notation [14]. The motion of a fluid is described by a set of discrete single-particle distribution function values $\{f_a : a = 1, \ldots, d\}$ obeying the following dimensionless, velocity-discretized Boltzmann equation with a Bhatnagar-Gross-Krook (BGK) [15] collision model:

$$\frac{\partial f_a}{\partial t} + \boldsymbol{\xi}_a \cdot \boldsymbol{\nabla} f_a + \boldsymbol{g} \cdot \boldsymbol{\nabla}_\xi f_a = -\frac{1}{\tau}[f_a(\boldsymbol{x}, t) - f_a^{eq}],$$

$$a = 1, \ldots, d, \tag{1}$$

where $\boldsymbol{x}$ and $t$ are spatial coordinates and time, $\tau$ the relaxation time, $\boldsymbol{g}$ the acceleration of the body force, and $\{\boldsymbol{\xi}_a : a = 1, \ldots, d\}$ the set of discrete velocities that coincide with the abscissas of a Gauss-Hermite quadrature in velocity space. $f_a$ is essentially the single-particle distribution function evaluated at $\boldsymbol{\xi}_a$. The equilibrium distribution $f_a^{eq}$ is a truncated Hermite expansion of the Maxwellian. At second order and assuming constant temperature, it is

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$$f_a^{eq} = w_a n \left[ 1 + \boldsymbol{\xi}_a \cdot \boldsymbol{u} + \frac{(\boldsymbol{\xi}_a \cdot \boldsymbol{u})^2 - u^2}{2} \right], \qquad (2)$$

where $w_a$ is the Hermite quadrature weight corresponding to the abscissa $\boldsymbol{\xi}_a$, and $n$ and $\boldsymbol{u}$ are the number density and velocity of the fluid given by

$$n = \sum_{a=1}^{d} f_a, \quad n\boldsymbol{u} = \sum_{a=1}^{d} f_a \boldsymbol{\xi}_a. \qquad (3)$$

Hereinafter, all velocities are scaled with respect to the sound speed. Sufficient quadrature accuracy and truncation level ensure that $n$ and $\boldsymbol{u}$ obey the correct hydrodynamic equations [14].

In the nonideal gas LB model [3], the force experienced by the particles at $\boldsymbol{x}$ from the particles at $\boldsymbol{x}'$ is assumed to be in the following form:

$$\boldsymbol{F}(\boldsymbol{x}, \boldsymbol{x}') = -G(|\boldsymbol{x} - \boldsymbol{x}'|)\psi(\boldsymbol{x})\psi(\boldsymbol{x}')(\boldsymbol{x}' - \boldsymbol{x}), \qquad (4)$$

where $\psi(\boldsymbol{x})$ is a function of the local properties at $\boldsymbol{x}$ only. Within the constraints that the interaction has to (a) satisfy Newton's third law and conserve momentum globally and (b) be along the vector between the two interacting lattice sites, the above form of interaction is perhaps the most general one.

To model the van der Waals force, the function $\psi(\boldsymbol{x})$ was made to only depend on the density [3]—i.e., $\psi(\boldsymbol{x}) = \psi(n(\boldsymbol{x}))$. Contrary to the case in continuum where the detail of the interaction is given by a pairwise potential as a function of the distance between two interacting particles, in the mesoscopic LB description, where the space is discretized with a minimum interparticle distance, the interaction detail is given by the function $\psi(n)$ which plays the role of an "effective mass." The effect of the function $\psi(n)$ can be heuristically explained by the fact that the density is implicitly a measure of the averaged distance between two particles.

For fast-decaying forces, if the sites that interact with the particles on $\boldsymbol{x}$ are limited to their $N$ neighbors, not necessarily the nearest ones, the total force exerted on particles at $\boldsymbol{x}$ is given by summing Eq. (4) over all $\boldsymbol{x}'$. Requiring that the interaction be isotropic—i.e., that $G(\boldsymbol{x} - \boldsymbol{x}')$ be a function of $|\boldsymbol{e}_a|$ only—we can define the normalizing factor $w(|\boldsymbol{e}_a|^2)$ and write

$$\boldsymbol{F} = -G\psi(\boldsymbol{x}) \sum_{a=1}^{N} w(|\boldsymbol{e}_a|^2)\psi(\boldsymbol{x} + \boldsymbol{e}_a)\boldsymbol{e}_a, \qquad (5)$$

where $G$ is the overall interaction strength. The force is repulsive when $G > 0$ and attractive when $G < 0$.

The hydrodynamic consequences of the interaction at the continuum limit can be obtained by letting the lattice scale approach zero. On expanding $\psi(\boldsymbol{x} + \boldsymbol{e}_a)$ around $\boldsymbol{x}$ and defining

$$E_{i_1 \cdots i_n}^{(n)} \equiv \sum_{a=1}^{N} w(|\boldsymbol{e}_a|^2)(\boldsymbol{e}_a)_{i_1} \cdots (\boldsymbol{e}_a)_{i_n}, \qquad (6)$$

the interaction force has the following Taylor expansion:

$$\boldsymbol{F} = -G\psi(\boldsymbol{x}) \sum_{n=0}^{\infty} \frac{1}{n!} \boldsymbol{\nabla}^{(n)} \psi : \boldsymbol{E}^{(n+1)}, \qquad (7)$$

where $\boldsymbol{\nabla}^{(n)}\psi$ is the rank-$n$ tensor obtained by applying the gradient operator $\boldsymbol{\nabla}$ to $\psi$ $n$ times and the colon (":") stands for full tensor contraction. The leading terms are

$$\boldsymbol{F} = -Gc^2 \left[ \psi \boldsymbol{\nabla} \psi + \frac{e_2 c^2}{2} \psi \boldsymbol{\nabla} (\nabla^2 \psi) + \cdots \right]. \qquad (8)$$

It can be seen that the interaction force is essentially a function of the gradient and higher derivatives of the density field. For $\boldsymbol{F}$ to be perfectly aligned with the density gradient, the tensors $\boldsymbol{E}^{(n)}$ must be fully isotropic:

$$\boldsymbol{E}^{(n)} = \begin{cases} 0, & n \text{ odd} \\ e_n c^n \Delta^{(n)}, & n \text{ even,} \end{cases} \qquad (9)$$

where $e_n$ are arbitrary scalar constants, $c$ the lattice constant, and $\Delta^{(n)}$ the rank-$n$ fully symmetric tensor [16]. Given a finite set of $\{e_a\}$, it is impossible to have all $\boldsymbol{E}^{(n)}$ isotropic. However, the weight function $w(|e_a|^2)$ can be optimized to maximize the isotropy of $\boldsymbol{E}^{(n)}$ [11,12]. For instance, with the nearest neighbors on a two-dimensional (2D) square lattice, only the tensors up to fourth order can be made isotropic. If the next level of neighbors are included, tensors up to eighth order can be made isotropic. In both cases, the coefficients $e_2$ and $e_4$ are given by the weights as

$$e_2 = 2w(1) + 4w(2) + 8w(4) + 20w(5) + 16w(8),$$

$$e_4 = \frac{1}{2}w(1) + 2w(2) + 8w(4) + 25w(5) + 32w(8).$$

Without losing generality, it is convenient to normalize the weights $w(|e_a|^2)$ so that $e_2 = 1$. In the case of nearest-neighbor interactions—i.e., $w(|e_a|^2) = 0$ for $|e_a|^2 > 2$—the isotropic conditions determines the two weights as

$$w(1) = \frac{1}{3}, \quad w(2) = \frac{1}{12}, \quad e_4 = \frac{1}{3}. \qquad (10)$$

### III. PRESSURE TENSOR CALCULATION

The intermolecular force of Eq. (5) induces an extra momentum transfer in addition to that caused by the free-streaming of the molecules. In a continuum, the pressure tensor contribution due to intermolecular force is by definition related to the force by

$$\boldsymbol{\nabla} \cdot \boldsymbol{P} = \boldsymbol{F}. \qquad (11)$$

Apparently, knowing the force is insufficient to determine the pressure tensor [10] due to the arbitrary gauge. The situation is further complicated in the discrete form by the fact that the force field given by Eq. (8) is only an approximation to Eq. (5). Even after the gauge is somehow fixed, the pressure tensor obtained by integrating an approximated force does not guarantee exact mechanical balance.

Here we obtain the pressure tensor using its basic definition—i.e., the momentum transfer rate through an area
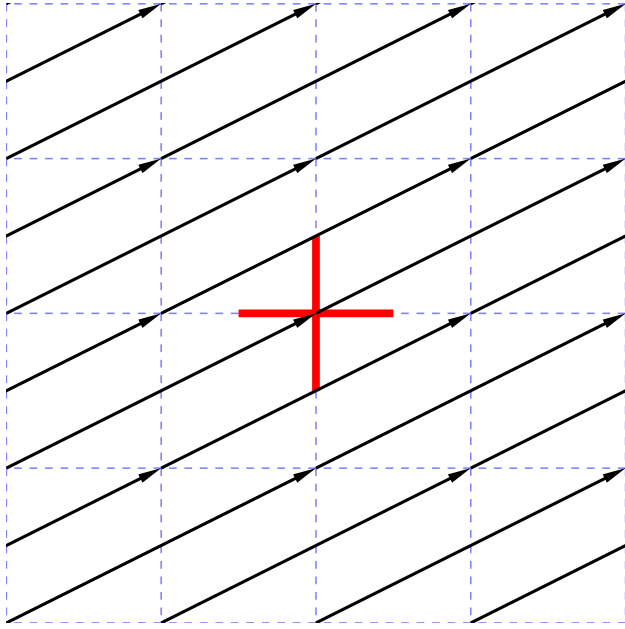
FIG. 1. (Color online) Force flux through surface elements. Numbers of force vectors along $e_a = \{2, 1\}$ through a vertical and a horizontal area element are proportional to $(e_a)_x (= 2)$ and $(e_a)_y (= 1)$, respectively.

of surface. Given an infinitesimal area element $dA$ and letting $dF$ be the interaction force through $dA$, the pressure tensor $P$ is defined as

$$dF = dA \cdot P. \qquad (12)$$

By integrating over a closed volume, the physical essence of the above is that the surface integral of the pressure tensor over a closed volume has to equal to the total force acting on the volume, namely:

$$\oint P \cdot dA = \int F \, dv. \qquad (13)$$

Using the Gauss integration theorem, we realize that Eq. (12) is essentially the integral form of Eq. (11). In discrete form, the equation above becomes

$$\sum_x P \cdot A = \sum F, \qquad (14)$$

which will be our basis for deriving the pressure tensor.

Consider all interaction forces along a single force vector—i.e., one of the $e_a$ in Eq. (5). For simplicity, we plot all the forces on a two-dimensional Cartesian lattice in Fig. 1. It can be seen that the number of force vectors across a unit vertical surface element $dA = e_x$ is $(e_a)_x$ and that across a unit horizontal surface element is $(e_a)_y$. Therefore, if all forces along $e_a$ are of the same magnitude—say, $F$—the pressure tensor contribution by this class of forces is simply $f e_a e_a$. To determine the pressure tensor contribution from a force field where each force element has different magnitude, we simply replace $F$ by an averaged force strength, where the average is over all force vectors across the surface area.
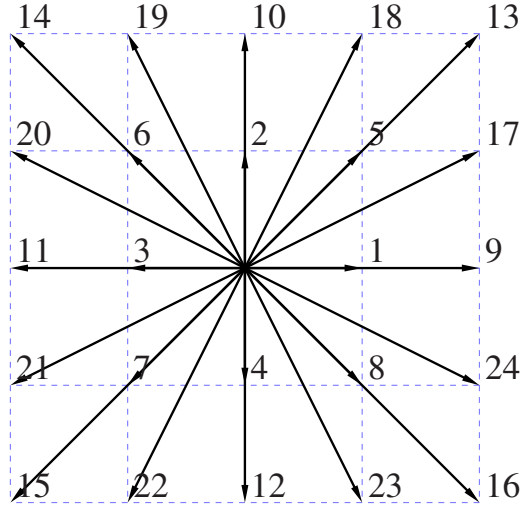


FIG. 2. (Color online) Interaction neighbors. Shown are all forces acting on the site at the center. The interaction range is limited to the square of two layers for the convenience of computation.

To illustrate, we first consider the case of the nearest-neighbor interaction where all force vectors across any surface element centered at $x$ either start or end at $x$. The averaged force magnitude for the forces going across $x$ along the vector $e_a$ is simply

$$-\frac{Gw(|e_a|^2)}{2} [\psi(x)\psi(x + e_a) + \psi(x - e_a)\psi(x)]. \qquad (15)$$

The pressure tensor at location $x$ due to the interaction force (5) is therefore

$$P = -\frac{G}{2}\psi(x)\sum_{a=1}^{N} w(|e_a|^2)\psi(x + e_a)e_a e_a. \qquad (16)$$

The above expression was previously given for the hexagonal lattice where $w(|e_a|^2) = 1$ [4].

Equation (16) is accurate in the case of nearest-neighbor interactions where all forces acting on a lattice node either start or end at that node. When the force range is extended beyond the nearest neighbors so that force vectors through an area element do not always pass through the lattice node at the center or they stride across the lattice node, Eq. (16) needs to be modified to take into account the variable force magnitudes, although the number of force vectors along the vector $e_a$ and going across a unit area element $e_a$ is still $e_a e_a$. As an example, we consider the interaction forces defined over two layers of neighbors, as illustrated in Fig. 2 [12,17,18]. The 24 neighbors fall into five symmetry groups which can be uniquely labeled by the square of the length of the vectors. For instance, the group of vectors 9–12 have a length of 2. For convenience, hereinafter we shall refer to this group as group 4. The pressure tensor is the sum of the contributions from each of the five groups which we will consider one by one.

Groups 1 and 2 are the nearest neighbors. The contributions to the pressure tensor are given by Eq. (16): i.e.,
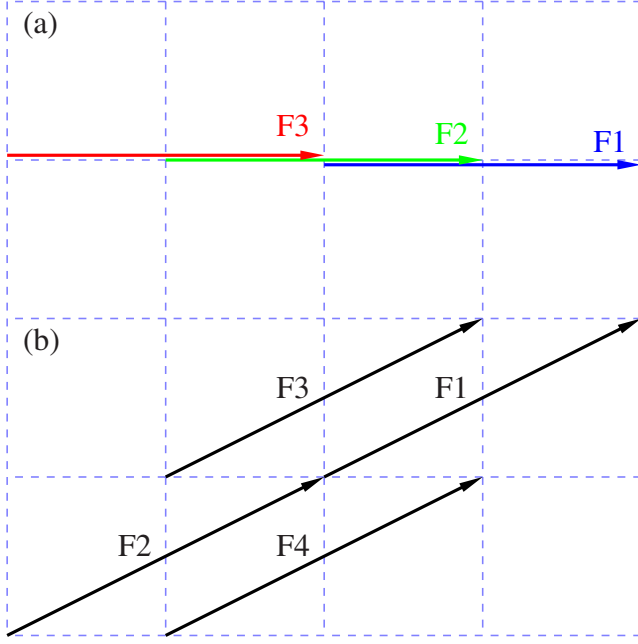
FIG. 3. (Color online) Force vectors that contribute to the pressure tensor. (a) Group-4 vectors and (b) group-5 vectors.

$$P_1 = -\frac{G}{2}\psi(x)\sum_{a=1}^{8} w(|e_a|^2)\psi(x+e_a)e_a e_a. \quad (17)$$

To calculate the contributions of groups 4 and 8—i.e., the speed-2 counterparts of groups 1 and 2—let us consider the force vectors of $e_9$ as an example. Shown in Fig. 3(a) are such vectors near a lattice site. The total numbers of interaction pairs across a vertical and a horizontal area elements are 2 and 0, respectively, consistent with the previous analysis. Taking into account the magnitudes of the three pairs of interactions, the pressure tensor contribution of groups 4 and 8 can be written as

$$P_2 = -\frac{G}{4}\psi(x)\sum_{a=9}^{16} w(|e_a|^2)\psi(x+e_a)e_a e_a$$

$$-\frac{G}{4}\sum_{a=9}^{16} w(|e_a|^2)\psi\left(x-\frac{e_a}{2}\right)\psi\left(x+\frac{e_a}{2}\right)e_a e_a. \quad (18)$$

Note here that the interactions in the second terms have been double counted for both $e_a$ and $-e_a$, and therefore the additional factor of 1/2.

For group 5, it is clear from Fig. 3(b) that the contribution comes equally from four classes of vectors. The contributions from $F_1$ and $F_2$ can be written as

$$P_3 = -\frac{G}{4}w(5)\psi(x)\sum_{a=17}^{24} \psi(x+e_a)e_a e_a, \quad (19)$$

whereas those from $F_3$ and $F_4$ involve pair products among the nearest neighbors. For brevity, we use two subscripts to note the location of the neighbors: e.g., $\psi_{1,1}=\psi(x+e_x+e_y)$, $\psi_{0,-1}=\psi(x-e_y)$, and so on. The pressure tensor contribution is

$$P_4 = \frac{G}{4}w(5)[(\psi_{1,1}\psi_{-1,0} + \psi_{1,0}\psi_{-1,-1})e_{17}e_{17}$$

$$+ (\psi_{1,1}\psi_{0,-1} + \psi_{0,1}\psi_{-1,-1})e_{18}e_{18}$$

$$+ (\psi_{0,1}\psi_{1,-1} + \psi_{-1,1}\psi_{0,-1})e_{19}e_{19}$$

$$+ (\psi_{-1,1}\psi_{1,0} + \psi_{-1,0}\psi_{1,-1})e_{20}e_{20}]. \quad (20)$$

Finally the pressure tensor due to the interaction force of Eq. (5) defined over the interaction range of 2 is the sum of contributions from all five groups:

$$P = P_1 + P_2 + P_3 + P_4. \quad (21)$$

Overall, we have a way of obtaining the pressure tensor based on the principle of Eq. (14). The number of interaction pairs with the interaction force going across surface elements centered at $x$ is given by Eq. (16), and the pressure tensor is obtained by multiplying each interaction pair with an appropriate force strength. Consequently, Eq. (14) is guaranteed to hold exactly, and moreover, the arbitrary gauge is removed as the physical significance of the force flux is clear at the discrete level.

## IV. CONTINUUM LIMIT

The pressure tensor in the continuum limiter can be found by substituting the Taylor expansion of $\psi(x+\delta x)$ into Eqs. (17)–(20). The results are lengthy and unnecessary for our purposes here. Thus, we choose to omit it and only consider a one-dimensional two-phase equilibrium where all gradients are in the same direction—say, the $x$ direction. Taking into account the constraints (9) and after summing all the fragments in Eqs. (17)–(20), the pressure tensor can be written as

$$P_{xx} = \frac{Gc^2}{2}\psi^2 + \frac{Gc^4}{12}\left[\alpha\left(\frac{d\psi}{dx}\right)^2 + \beta\psi\frac{d^2\psi}{dx^2}\right], \quad (22a)$$

$$P_{yy} = \frac{Gc^2}{2}\psi^2 + \frac{Gc^4}{4}\left[\gamma\left(\frac{d\psi}{dx}\right)^2 + \eta\psi\frac{d^2\psi}{dx^2}\right], \quad (22b)$$

$$P_{xy} = P_{yx} = 0, \quad (22c)$$

where $\alpha=1-3e_4$, $\beta=1+6e_4$, $\gamma=-4[w(5)+4w(8)]$, and $\eta = \gamma+e_4$.

Following the previous approach [4], at equilibrium, the normal component of the pressure tensor, $P_{xx}$, must equal to the constant static pressure in the bulk, $p_0$. Combining with the ideal gas part of the pressure, we have

$$p_0 = n\theta + \frac{Gc^2}{2}\psi^2 + \frac{Gc^4}{12}\left[\alpha\left(\frac{d\psi}{dx}\right)^2 + \beta\psi\frac{d^2\psi}{dx^2}\right]. \quad (23)$$

Using the relation

$$\frac{d^2\psi}{dz^2} = \frac{1}{2}\frac{d}{d\psi}\left(\frac{d\psi}{dz}\right)^2, \quad (24)$$

we can integrate Eq. (23) to obtain

$$\left(c\frac{dn}{dz}\right)^2 = \frac{8(1-\epsilon)\psi^\epsilon}{Gc^2\psi'^2}\int\left(p_0 - n\theta - \frac{Gc^2}{2}\psi^2\right)\frac{\psi'}{\psi^{1+\epsilon}}dn,$$

$$(25)$$

where $\epsilon = -2\alpha/\beta = (6e_4 - 2)/(6e_4 + 1)$. Since $dn/dz$ vanishes in the bulk of both phases, the densities in the gas and liquid phases, denoted by $n_g$ and $n_l$, respectively, must satisfy the following relation:

$$\int_{n_g}^{n_l}\left(p_0 - n\theta - \frac{G}{2}\psi^2\right)\frac{\psi'}{\psi^{1+\epsilon}}dn.$$

$$(26)$$

Using the equation above and the equation of state in both phases,

$$p_0 = n_g\theta + \frac{Gc^2}{2}\psi^2(n_g) = n_l\theta + \frac{Gc^2}{2}\psi^2(n_l),$$

$$(27)$$

$n_l$, $n_g$, and $p_0$ can be solved to arbitrary precision by numerical integration. The surface tension coefficient is defined as

$$\sigma \equiv \int_{-\infty}^{\infty}(p_0 - p_T)dx = \int_{-\infty}^{\infty}(P_{xx} - P_{yy})dx.$$

$$(28)$$

Using Eqs. (22a)–(22c) and the boundary condition $d\psi/dz = 0$ at $z = \pm\infty$, we have

$$\sigma = -\frac{e_4 Gc^4}{2}\int_{n_g}^{n_l}\psi'^2\frac{dn}{dz}dn.$$

$$(29)$$

The extended interaction range only modifies the previous results [4] by the constants $\epsilon$ in Eqs. (25). When the interaction range reduces to that of the nearest neighbors—i.e., $w(1)=1/3$, $w(2)=1/12$, and $w(4)=w(5)=w(8)=0$—we have $e_4=1/3$, $\alpha=\gamma=0$, $\beta=3$, $\eta=1/3$, and $\epsilon=0$, recovering the previous results. In particular, the normal component of the pressure tensor in Eq. (23) is

$$p_0 = n\theta + \frac{Gc^2}{2}\psi^2 + \frac{Gc^4}{4}\psi\frac{d^2\psi}{dx^2}.$$

$$(30)$$

It is important to note that the surface tension coefficient is proportional to the single constant $e_4$ independent of the weights of $w(5)$ and $w(8)$, while the equation of state is completely determined by the constant $e_2$. Essentially the same feature was previously noted by Sbragaglia *et al.* [12]. Given the $\psi$ function, and therefore the equation state, the surface tension can be adjusted independently by changing $e_4$, except for a small effect on the density profile through the constant $\epsilon$ in Eq. (25). Interesting macroscopic consequences are observed when the surface tension coefficient is adjusted to a negative value [17,18].

## V. DISCUSSION

In this paper, a procedure is defined to obtain the pressure tensor from a given interaction force. This procedure is based on Eq. (14) instead of its continuum differential form of Eq. (11) to ensure exact force balance in discrete form. As a consequence, the Taylor expansion of the force and pressure tensor, given by Eqs. (5) and (16), respectively, do not satisfy Eq. (11) term by term. We believe the reason is, at least partially, that, although the long-wavelength limit of Eq. (14) is Eq. (11), the differential operator and the finite-difference operator involved in the transition from Eq. (14) to Eq. (11) do not commute. For the purpose of accurately predicting the macroscopic behavior of the LB model, the accurate form of Eq. (14) should be used.

Noticing the difference in the Taylor expansions of the force and pressure tensor and with some additional argument of matching results of thermodynamic theory, He and Doolen [13] proposed that Eq. (30) should be replaced by the following expression:
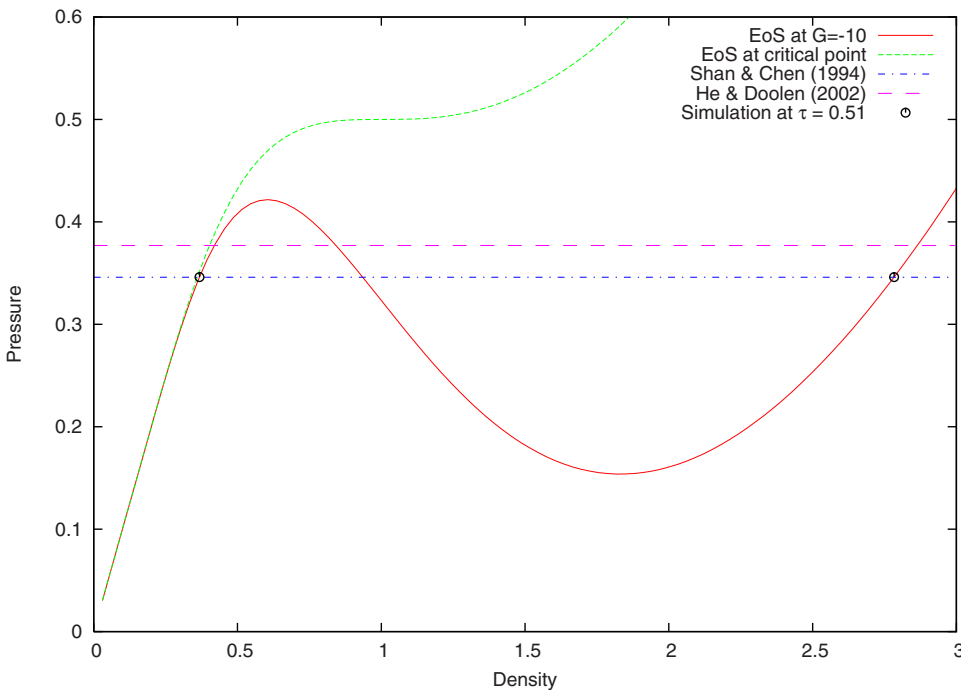


FIG. 4. (Color online) Equation of state for $\psi(n)=\exp(-1/n)$ (curves) and the equilibrium pressure (horizontal lines) predicted by the two theories outlined in Refs. [4,13]. Simulation results at $\tau=0.51$ are shown as circles.

$$P = \left[ n\theta + \frac{G}{2}\psi^2 + \frac{G}{2}\left( \psi\nabla^2\psi + \frac{1}{2}|\boldsymbol{\nabla}\psi|^2 \right) \right]\delta - \frac{G}{2}\boldsymbol{\nabla}\psi\boldsymbol{\nabla}\psi,$$

(31)

where a constant temperature and the D2Q9 [19] model is assumed. Following the same calculation outlined above, they obtained a slightly different expression corresponding to Eq. (25):

$$\left(\frac{dn}{dz}\right)^2 = \frac{4\psi}{G\psi'^2}\int\left(p_0 - n\theta - \frac{G}{2}\psi^2\right)\frac{\psi'}{\psi^2}dn.$$

(32)

The prediction of the equilibrium pressure of the two-phase system differs only in the parameter $\epsilon$. For nearest-neighbor interactions, the theory given in this paper and Ref. [4] gives $\epsilon=0$ while Ref. [13] gives $\epsilon=1$. A consequence of this difference is that according to Eq. (32), the only potential consistent with the Maxwell construction is $\psi(n)\propto n$, which does not lead to a valid liquid-vapor two-phase system, while according to Eq. (25), the potential consistent with the Maxwell construction is $\psi(n)=\exp(-1/n)$, which indeed gives the basic features of a two-phase system.

We would like to point out that combining Eq. (11) and macroscopic thermodynamic arguments which do not have any microscopic link to the discrete LB dynamics is at least inaccurate in predicting the macroscopic properties of the discrete LB model. To show the differences of the two forms of the pressure tensors, in Fig. 4 we compare the predictions of the coexistence pressure by both theories—i.e., Eqs. (25) and (32)—with result of numerical simulations. The comparison is made for the case of nearest-neighbor interactions for which the present theory reduces to Ref. [4]. The $p$-$\rho$ curves corresponding to the potential $\psi(n)=\exp(-1/n)$ are plotted at both the critical temperature and a typical subcritical temperature. With this choice of the potential, the integrals in both Eqs. (25) and (32) can be carried out analytically and $n_l$, $n_g$, $p_0$, and $\sigma$ solved. Plotted as the two horizontal lines is the pressure $p_0$ as predicted by the two theories. It is to be seen that Eq. (25) predicts coexistence densities much more closely. It should also be noted that Eq. (25) is exactly what the Maxwell construction requires for this choice of $\psi$. Agreement with numerical results also implies that the numerical results are consistent with the Maxwell construction.

## ACKNOWLEDGMENTS

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