Kinetic theory for a simple modeling of phase transition: Dynamics out of local equilibrium

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(Dated: September 27, 2018)

Abstract

This is a continuation of the previous work (Takata & Noguchi, J. Stat. Phys., 2018) that introduces the presumably simplest model of kinetic theory for phase transition. Here, main concern is to clarify the stability of uniform equilibrium states in the kinetic regime, rather than that in the continuum limit. It is found by the linear stability analysis that the linear neutral curve is invariant with respect to the Knudsen number, though the transition process is dependent on the Knudsen number. Numerical computations of the (nonlinear) kinetic model demonstrate the transition processes in detail.

PACS numbers: 51.10.+y, 64.60.A-, 64.70.F-, 51.30.+i
I. INTRODUCTION

Recently, the first author has proposed a simple kinetic model for the description of phase transition in Ref. [1]. In this reference, the model is proposed as presumably the simplest kinetic theory model that enables us to reproduce the phase transition phenomena. A functional that decreases monotonically in time is also found for this model. In the continuum limit (or the local equilibrium), it recovers the Cahn–Hilliard type equation; based on this limiting equation, the linear stability of uniform states is studied to find a neutral curve and numerical computations of the Cahn–Hilliard type equation are carried out as well. The details of the phase transition in the continuum limit have been clarified.

The model is, however, not limited to the dynamics in the continuum limit in contrast to the lattice Boltzmann models (e.g. Refs. [2, 3]), but rather aims at the dynamics in the kinetic regime (or out of local equilibrium) as Refs. [4–7]. In the present paper, we take a further step to study the stability of uniform equilibrium states in the kinetic regime. To be more specific, we are going to study the stability problem by our kinetic theory model directly, not through the Cahn–Hilliard type equation, and try to understand the influence of the Knudsen number. The paper is organized as follows. After summarizing our model in Sec. II, the dimensionless formulation is given in Sec. III for the clarity of similarity rule in the problem to be studied. Then, a linear stability of uniform equilibrium states is investigated in Sec. IV in a way similar to Ref. [8], but in more comprehensive way. The invariance of the neutral curve with respect to the Knudsen number is shown as well. Results of numerical computations, together with supplemental discussions, are presented in Sec. V. The paper is concluded in Sec. VI.

II. PROBLEM AND ITS FORMULATION

Consider a system (or a fluid) composed of innumerable molecules in a periodic spatial domain $D$:

$$\frac{\partial f}{\partial t} + \xi_i \frac{\partial f}{\partial X_i} + F_i \frac{\partial f}{\partial \xi_i} = C_*(f),$$ (1a)

$$C_*(f) = A(\rho)(\rho M_s - f), \quad \rho = \int f d\xi,$$ (1b)

$$F_i = -\frac{\partial \Phi}{\partial X_i}, \quad \phi = \Phi_S + \Phi_L,$$ (1c)
$\Phi_S = -RT_s \ln(1 - b\rho) + \frac{b\rho RT_s}{1 - b\rho} - 2a\rho, \ (a, b > 0), \quad (1d)$

$\Phi_L = -\kappa \frac{\partial^2 \rho}{\partial X^2}, \ (\kappa > 0), \quad (1e)$

$M_* = \frac{1}{(2\pi RT_*)^{3/2}} \exp\left(-\frac{\xi^2}{2RT_*}\right), \quad (1f)$

where $t$ is a time, $X = (X_1, X_2, X_3)$ a spatial position, $\xi = (\xi_1, \xi_2, \xi_3)$ a molecular velocity, $f(t, X, \xi)$ a velocity distribution function (VDF), $mF = m(F_1, F_2, F_3)$ a force acting on a single molecule, with $m$ being its mass, and $\phi$ a corresponding potential. $C_*[f]$ is the so-called collision term and plays a role of a thermal bath, driving the system toward a thermal equilibrium at a specified temperature $T_*$ which is fixed and given. Note that the present collision term conserves neither momentum nor energy, in contrast to the usual intermolecular collision term. $A$ is a positive function of local density $\rho$ and $R = k_B/m$ with $k_B$ being the Boltzmann constant. $\kappa$, $a$, and $b$ are positive constants, the latter two of which are the ones occurring in the van der Waals equation of state [see (4) below]. Hence, $\Phi_S$ is a potential purely related to the van der Waals equation of state. In the meantime, $\Phi_L$ is a potential which comes from a collection of nonlocal attractive interaction of molecules. In the present paper, we exclusively consider the case where it can be reduced to be local and of Laplacian form by the isotropic and rapid decay assumptions in $X$ (see Ref. [1] for details). We will investigate the time evolution of the system from an initial distribution

$$f(0, X, \xi) = f_{in}(X, \xi), \quad (2)$$

a perturbed state from a uniform one $f = \rho_0 M_*$ with $\rho_0$ being the initial average density of the fluid, aiming at studying the stability of the uniform state. It is readily checked that the mass is conserved in the present system. Accordingly, the average density is constant in time.

The flow velocity $v = (v_1, v_2, v_3)$, stress tensor $p_{ij}$, pressure $p$, and temperature $T$ are defined as

$$\rho v_i = \int \xi_i f d\xi, \quad p_{ij} = \int c_i c_j f d\xi + \int \rho \Phi'_S(\rho) d\rho \delta_{ij}, \quad (3a)$$

$$p = \frac{1}{3} p_{ii}, \quad T = \frac{1}{3\rho R} \int c^2 f d\xi, \quad (3b)$$

where $c_i = \xi_i - v_i$ and the above definition of $p$ is consistent with the van der Waals equation
of state
\[ p = \frac{\rho RT}{1 - b\rho} - \rho^2a, \]  
within the isothermal approximation \( T \simeq T_* \). The non-isothermal case is excluded in the present simple model, as discussed in detail in Ref. [1]. For the present system, it is shown in Ref. [1] that the following functional \( \mathcal{M} \) monotonically decreases in time:

\[
\mathcal{M}(t) = \int_D \{ \int f \ln \frac{f}{\rho_0 M_s} d\xi + \int \frac{\Phi_S}{RT_*} d\rho + \frac{\rho \Phi_L}{2RT_*} \} dX
\]

Note that, because \( \Phi_S \) is supposed to vanish in the low density limit \( \rho \to 0 \), the second term of the above integrand is reduced to

\[
\int \Phi_S d\rho = -\rho RT_* \ln(1 - b\rho) - a\rho^2.
\]

To summarize, the above model describes a non-ideal gas that interacts with thermal bath through the simple collision term. Our concern is the stability of uniform equilibrium states in such a closed non-isolated system. Incidentally, we recently become aware of Ref. [9] which studies the stability of uniform equilibrium states by the kinetic theory. However, considered there is an ideal gas under a collective attractive interaction in an isolated system, and accordingly the studied phenomenon is qualitatively different. Indeed, the details such as the linear stability analysis and its results, the derived H theorem, etc. are all different from ours.

III. DIMENSIONLESS NOTATION

For the later convenience and for the clarity of similarity law for the present system, we introduce the following dimensionless notation:

\[
t = \frac{L}{(2RT_*)^{1/2}} \tilde{t}, \quad X_i = L x_i, \quad \xi_i = (2RT_*)^{1/2} \tilde{\xi}_i, \]

\[
\rho = \rho_0 \tilde{\rho}, \quad f = \frac{\rho_0}{(2RT_*)^{3/2}} \tilde{f}, \quad A(\rho) = A(\rho_0) \tilde{A}(\tilde{\rho}), \]

\[
\phi = 2RT_* \tilde{\phi}, \quad \Phi_S = 2RT_* \tilde{\Phi}_S, \quad \Phi_L = 2RT_* \tilde{\Phi}_L, \]

\[
\kappa = (2RT_* L^2 / \rho_0) \tilde{\kappa}, \quad a = \tilde{a}RT_*/\rho_0, \quad b = \tilde{b}/\rho_0.
\]
where $\mathbf{x} = (x_1, x_2, x_3)$, $\mathbf{\zeta} = (\zeta_1, \zeta_2, \zeta_3)$, $\zeta = |\mathbf{\zeta}|$, and $L$ is the characteristic length of the system, typically its period. Then the original equation and the initial condition are recast as

$$\frac{\partial \tilde{f}}{\partial t} + \zeta_i \frac{\partial \tilde{f}}{\partial x_i} - \frac{\partial \tilde{\phi}}{\partial x_i} \frac{\partial \tilde{f}}{\partial \zeta_i} = \frac{2}{\sqrt{\pi}} \frac{\tilde{A}(\tilde{\rho})}{\text{Kn}} (\tilde{\rho} E - \tilde{f}),$$  \hspace{1cm} (6a)

$$\tilde{f}(0, \mathbf{x}, \mathbf{\zeta}) = \tilde{f}_\text{in}(\mathbf{x}, \mathbf{\zeta}),$$  \hspace{1cm} (6b)

where

$$\tilde{\rho} = \int \tilde{f} d\zeta, \hspace{0.5cm} E = \pi^{-3/2} \exp(-\zeta^2), \hspace{0.5cm} \tilde{\phi} = \tilde{\Phi}_S + \tilde{\Phi}_L,$$  \hspace{1cm} (7a)

$$\tilde{\Phi}_S(\tilde{\rho}) = -\frac{1}{2} \ln(1 - \tilde{b} \tilde{\rho}) - \tilde{\alpha} \tilde{\rho} + \frac{\tilde{b} \tilde{\rho}}{2(1 - \tilde{b} \tilde{\rho})}, \hspace{0.5cm} (\tilde{\alpha}, \tilde{b} > 0),$$  \hspace{1cm} (7b)

$$\tilde{\Phi}_L = -\tilde{\kappa} \frac{\partial^2 \tilde{\rho}}{\partial x_i^2}, \hspace{0.5cm} (\tilde{\kappa} > 0), \hspace{0.5cm} \tilde{A}(\tilde{\rho}) > 0,$$  \hspace{1cm} (7c)

and Kn is the Knudsen number defined as

$$\text{Kn} = \frac{(8RT_*/\pi)^{1/2}}{A(\rho_0)L}.$$  \hspace{1cm} (7d)

In the above, the Strouhal number is set to be unity by the specific choice of reference time $L/(2RT_*)^{1/2}$ in (5a).

The moments of $f$, i.e., $v_i = (2RT_*)^{1/2} \bar{v}_i$, $p_{ij} = \rho_0 RT_* \bar{p}_{ij}$, $p = \rho_0 RT_* \bar{p}$, and $T = T_* \bar{T}$ are recast as moments of $\tilde{f}$:

$$\tilde{\rho} \bar{v}_i = \int \zeta_i \tilde{f} d\zeta, \hspace{0.5cm} \tilde{p}_{ij} = 2 \int \bar{c}_i \bar{c}_j \tilde{f} d\zeta + 2 \int \tilde{\rho} \tilde{\Phi}'_S d\tilde{\rho} \delta_{ij},$$  \hspace{1cm} (8a)

$$\tilde{\rho} = \frac{1}{3} \bar{\rho}_i, \hspace{0.5cm} \bar{T} = \frac{2}{3 \rho} \int \bar{c}^2 \tilde{f} d\zeta,$$  \hspace{1cm} (8b)

where $\bar{c} = \zeta - \bar{\zeta}$. Furthermore, the equation of state (4) and the monotonically decreasing functional $\mathcal{M} = \rho_0 L^3 \tilde{\mathcal{M}}$ are rewritten as

$$\tilde{\rho} = \frac{\tilde{\rho} \bar{T}}{1 - \tilde{b} \tilde{\rho}},$$  \hspace{1cm} (9)

$$\tilde{\mathcal{M}}(\bar{t}) = \int_D \left\{ \int \tilde{f} \ln \frac{\tilde{f}}{E} d\zeta + 2 \int \tilde{\Phi}_S d\tilde{\rho} + \tilde{\rho} \tilde{\Phi}_L \right\} d\mathbf{x}$$

$$= \int_D \left\{ \int \tilde{f} \ln \frac{\tilde{f}}{E} d\zeta + 2 \int \tilde{\Phi}_S d\tilde{\rho} - \tilde{\kappa} \tilde{\rho} \frac{\partial^2 \tilde{\rho}}{\partial x_i^2} \right\} d\mathbf{x}$$

$$= \int_D \left\{ \int \tilde{f} \ln \frac{\tilde{f}}{E} d\zeta + 2 \int \tilde{\Phi}_S d\tilde{\rho} + \tilde{\kappa} \left( \frac{\partial \tilde{\rho}}{\partial x_i} \right)^2 \right\} d\mathbf{x},$$  \hspace{1cm} (10)
where $\tilde{D}$ is the counterpart of $D$ and

$$2 \int \tilde{\Phi}_S d\tilde{\rho} = -\tilde{a}\tilde{\rho}^2 - \tilde{\rho}\ln(1 - \tilde{b}\tilde{\rho}).$$

Note that the dimensionless mass in the domain $\tilde{D}$ is invariant in time and is unity, i.e.,

$$\int_{\tilde{D}} \tilde{\rho} d\tilde{x} = 1.$$

### IV. LINEAR STABILITY OF UNIFORM EQUILIBRIUM STATES

In the present section, we will study the linear stability of the uniform equilibrium state $\tilde{f} = E$. To this end, we first substitute $\tilde{f} = E + g$ into (6a) and then retain only the linear terms in $g$, assuming $|g| \ll E$, to have

$$\alpha \frac{\partial g}{\partial t} + \alpha \zeta_i \frac{\partial g}{\partial x_i} - 2\alpha(\tilde{\kappa} \frac{\partial^2}{\partial x_j^2} - \tilde{\Phi}_S'(1))\zeta_i \frac{\partial \tilde{\rho}}{\partial x_i} E = \tilde{\rho}_g E - g,$$

where $\alpha = \sqrt{\frac{\pi}{2}} \text{Kn}(>0)$, $\tilde{\rho}_g = \int g \, d\zeta$.

Now we are going to study whether the perturbation of the form $g = \exp(\sigma t + i\lambda \cdot x)h(\zeta)$, where $\lambda = (\lambda_1, \lambda_2, \lambda_3)$ with $\lambda_i$ being a positive number and $\sigma \in \mathbb{C}$, grows (i.e., $\Re \sigma > 0$) or decays (i.e., $\Re \sigma < 0$) in time, thereby finding the stability condition of the linearized system (11). Substituting it into (11) eventually yields the following identity for $h$:

$$h = \frac{1}{\alpha\lambda} \left( \frac{S - P(\zeta \cdot e)\alpha\lambda[Q + (\zeta \cdot e)]}{S^2 + |Q + (\zeta \cdot e)|^2} + \frac{i\{P(\zeta \cdot e)S\alpha\lambda + |Q + (\zeta \cdot e)|\}}{S^2 + |Q + (\zeta \cdot e)|^2} \right) \tilde{\rho}_h E,$$

where $\tilde{\rho}_h = \int h d\zeta$, $\sigma = \sigma_1 + i\sigma_2$ ($\sigma_1, \sigma_2 \in \mathbb{R}$), $e = \lambda/\lambda$, $\lambda = |\lambda|$, and

$$S = \frac{1 + \alpha\sigma_1}{\alpha\lambda}, \quad P = 2[\tilde{\kappa}\lambda^2 + \tilde{\Phi}_S'(1)], \quad Q = \frac{\sigma_2}{\lambda}.$$

Due to the consistency, integrating both sides of (12) in $\zeta$ leads to the following set of identities:

$$2\pi \int_0^\infty \int_0^\pi \frac{1}{\alpha\lambda} \frac{S - (\zeta \cos \theta)P\alpha\lambda}{S^2 + Q^2} E \zeta^2 \sin \theta \, d\theta d\zeta = 1,$$
\[
\int_0^\infty \int_0^\pi \frac{P \alpha \zeta \cos \theta + \bar{Q}}{S^2 + \bar{Q}^2} E \zeta^2 \sin \theta d\theta d\zeta = 0,
\]
where \( \bar{Q} \equiv Q + \zeta \cos \theta \) and \( \theta \) is the angle between \( \zeta \) and \( e \), i.e., \( \zeta \cdot e = \zeta \cos \theta \). After some manipulations, (14) is transformed into

\[
(1 + P \alpha \lambda)SI + P \alpha \lambda Q^2 (I - 4J) = \frac{\alpha \lambda}{\pi} (1 + P),
\]
while (15) is transformed into

\[
Q \{(1 + P \alpha \lambda)(I - 4J) - P \alpha \lambda I\} = 0,
\]
where both \( I \) and \( J \) are positive functions of \( Q \) and \( S \) defined by

\[
I(Q, S) = \int_0^\infty \frac{1}{S^2 + (Q + \zeta)^2} + \frac{1}{S^2 + (Q - \zeta)^2} Ed\zeta,
\]
\[
J(Q, S) = \int_0^\infty \frac{\zeta^2 E}{(S^2 + (Q + \zeta)^2)(S^2 + (Q - \zeta)^2)} d\zeta.
\]
Note that both \( I \) and \( J \) are even in \( Q \).

Case A  When \( Q = 0 \), (17) is automatically satisfied. Then, (16) with \( Q = 0 \) takes the form

\[
2S(1 + P \alpha \lambda) \int_0^\infty \frac{E}{S^2 + \zeta^2} d\zeta = \frac{\alpha \lambda}{\pi} (1 + P),
\]
which is solved for \( P \) and is reduced to

\[
P = \frac{\alpha \lambda - \sqrt{\pi} F(S)}{\sqrt{\pi} \alpha \lambda SF(S) - \alpha \lambda},
\]
\[
F(S) \equiv 2\sqrt{\pi} S \int_0^\infty \frac{E}{S^2 + \zeta^2} d\zeta = \exp(S^2)\{1 - \text{erf}(S)\},
\]
where \( \text{erf}(x) = (2/\sqrt{\pi}) \int_0^x \exp(-s^2) ds \). Using the definitions of \( P \) and \( \tilde{\Phi}_S \) [see (13) and (7b)], we obtain

\[
\tilde{a} = \tilde{\alpha} \lambda^2 + \frac{1}{2} \frac{b(2 - \bar{b})}{(1 - \bar{b})^2} + \frac{1}{2} X,
\]
\[
X(S, \alpha \lambda) = \frac{\alpha \lambda - \sqrt{\pi} F(S)}{\alpha \lambda \{1 - \sqrt{\pi} SF(S)\}}.
\]
As seen from its definition, \( F(S) \) is monotonically decreasing in \( S \) from unity to zero and \( x > \sqrt{\pi} F(1/x) \) for \( x > 0 \), while \( SF(S) \) is monotonically increasing from zero to \( 1/\sqrt{\pi} \) in the range \( 0 \leq S < \infty \) \([10]\). Hence, for \( S \alpha \lambda > 1 \), which is equivalent to \( \sigma_1 > 0 \), \( X \) is monotonically increasing in \( S \) and approaches its infimum when \( S \to 1/(\alpha \lambda) \):

\[
X(S, \alpha \lambda) > X(\frac{1}{\alpha \lambda}, \alpha \lambda) = \frac{\alpha \lambda - \sqrt{\pi} F(1/(\alpha \lambda))}{\alpha \lambda - \sqrt{\pi} F(1/(\alpha \lambda))} = 1.
\]
Figure 1. Diagrams of phase transition. (a) Neutral curve of the linear stability. Markers with L, C, R, D, and A in the region U indicate the cases \((c, \tilde{b}) = (3.8, 4/15), (3.8, 1/3), (3.8, 2/5), (3.6, 2/5),\) and \((3.45, 1/3),\) respectively. In the shaded region U above the neutral curve \(c = 1/\{2\tilde{b}(1 - \tilde{b})^2\},\) uniform equilibrium states are linearly unstable. Markers with B1, B2, and B3 indicate the case \((c, \tilde{b}) = (3.4, 4/15), (3.3, 1/3),\) and \((3.4, 2/5),\) respectively. \(\bigcirc (\times)\) indicates that phase transition is observed (not observed) in numerical computations. Note that \(\tilde{b}\) is a measure of the volume fraction of molecules to the total volume. (b) Equiarea rule for determining two densities in stationary states after phase transition. The curve is the one for case C in (a), i.e., \((c, \tilde{b}) = (3.8, 1/3).\)

Therefore, when \(Q = 0,\) the uniform equilibrium state is unstable if

\[
\tilde{a} > \frac{1}{2} \tilde{b}(2 - \tilde{b}) + \frac{1}{2} - \frac{1}{2(1 - \tilde{b})^2}.
\]

Case B When \(Q \neq 0,\) the following two conditions must be satisfied simultaneously:

\[
(1 + PS\alpha\lambda)SI + P\alpha\lambda Q^2(I - 4J) = \frac{\alpha\lambda}{\pi}(1 + P), \tag{19a}
\]

\[
(1 + PS\alpha\lambda)(I - 4J) - PS\alpha\lambda I = 0. \tag{19b}
\]

Because \(I\) and \(I - 4J\) can be converted into the Voigt functions \(U\) and \(V\) as

\[
\pi S^2 I(Q, S) = U\left(\frac{Q}{S}, \frac{1}{4S^2}\right), \tag{20a}
\]

\[
\pi SQ[I(Q, S) - 4J(Q, S)] = V\left(\frac{Q}{S}, \frac{1}{4S^2}\right), \tag{20b}
\]

the above conditions are recast as

\[
(1 + PS\alpha\lambda)U + P\alpha\lambda QV = S\alpha\lambda(1 + P), \tag{21}
\]

\[
(1 + PS\alpha\lambda)V - P\alpha\lambda QU = 0, \tag{22}
\]
where the Voigt functions $U$ and $V$ are defined for $x \in \mathbb{R}$ and $t > 0$ as [11]

\[
U(x, t) \equiv \frac{1}{\sqrt{4\pi t}} \int_{-\infty}^{\infty} \frac{1}{1 + y^2} \exp\left(-\frac{(x - y)^2}{4t}\right) dy,
\]

\[
V(x, t) \equiv \frac{1}{\sqrt{4\pi t}} \int_{-\infty}^{\infty} \frac{y}{1 + y^2} \exp\left(-\frac{(x - y)^2}{4t}\right) dy.
\]

Obviously both $U$ and $V$ are positive. Moreover $xU(x, \cdot) - V(x, \cdot)$ is positive for $x > 0$, thanks to (20). Solving the both conditions for $P$ tells that

\[
\frac{S\alpha \lambda - U}{S\alpha \lambda (U + QV/S - 1)} = -\frac{V}{S\alpha \lambda (V - UQ/S)},
\]

which is solved to give

\[
S\alpha \lambda = 0_+, \quad \frac{qU^2 + qV^2 - V}{qU - V},
\]

where $q \equiv Q/S$ and the arguments of $U$ and $V$ are $q$ and $1/(4S^2)$. In order for the uniform equilibrium state to be unstable, the second solution in the above should be larger than unity, namely

\[
\frac{qU^2 + qV^2 - V}{qU - V} > 1.
\] (24)

We will show that this is impossible.

Because the condition (19) is even in $Q$, we may assume $Q > 0$ (or $q > 0$) without loss of generality. Because $qU - V > 0$, the condition (24) is reduced to

\[
qU^2 + qV^2 - V > qU - V, \quad \text{i.e.,} \quad U^2 + V^2 - U > 0.
\]

Now let us consider the function

\[
H(q, S) \equiv U(q, \frac{1}{4S^2})^2 + V(q, \frac{1}{4S^2})^2 - U(q, \frac{1}{4S^2}).
\]

On one hand, we have

\[
\lim_{q \to 0} H(q, S) = \sqrt{\pi}SF(S)\{\sqrt{\pi}SF(S) - 1\} < 0,
\]

because \(\lim_{q \to 0} V(q, \frac{1}{4S^2}) = 0\) and \(\lim_{q \to 0} U(q, \frac{1}{4S^2}) = \frac{S}{\sqrt{\pi}} \int_{-\infty}^{\infty} \frac{1}{1+y^2} \exp(-S^2y^2) dy = \sqrt{\pi}S\exp(S^2)\{1 - \text{erf}(S)\} = \sqrt{\pi}SF(S)\). On the other hand, because the Voigt functions are known to satisfy the following equations:

\[
V(x, t) = xU(x, t) + 2t \frac{\partial U(x, t)}{\partial x},
\]

\[
U(x, t) = 1 - xV(x, t) - 2t \frac{\partial V(x, t)}{\partial x},
\]
we have

\[
\frac{\partial H}{\partial q} = 2U \frac{\partial U}{\partial q} + 2V \frac{\partial V}{\partial q} - \frac{\partial U}{\partial q}
\]

\[
= 4US^2(V - qU) + 4V S^2(1 - qV - U) - (V - qU)2S^2
\]

\[
= 2S^2\{-2q(U^2 + V^2) + V + qU\}
\]

\[
= 2S^2\{-2q - qU + V\},
\]

which is solved to yield

\[
H(q, S) = H(0, S)e^{-2S^2q^2}
\]

\[
+ \int_0^q 2S^2\{V(r, \frac{1}{4S^2}) - rU(r, \frac{1}{4S^2})\}e^{-2S^2(q^2 - r^2)}dr
\]

\[
< H(0, S)e^{-2S^2q^2} < 0,
\]

because of \(rU(r, \cdot) - V(r, \cdot) > 0\) and (25). Hence, any mode with \(Q \neq 0\) is shown not to grow exponentially, and accordingly the uniform equilibrium state is linear stable.

In the long run, we conclude that there is a mode that grows exponentially in time if the following condition is satisfied [see Fig. 1(a)]:

\[
c \equiv \frac{\bar{a}}{\bar{b}} > \frac{1}{2b(1 - \bar{b})^2}. \tag{26}
\]

Note that this coincides with that obtained from the linear stability analysis based on the Cahn–Hilliard type equation (see Ref. 1; \(\chi_{av}\) in this reference is identical to the present \(\bar{b}\)). The linear instability condition is, thus, invariant with respect to the Knudsen number, including the continuum limit.

V. NUMERICAL RESULTS AND DISCUSSIONS

In the present section, we demonstrate some results of numerical computations of the dimensionless system (6a) for spatially one-dimensional case in the domain \(\tilde{D} = \{x_1 | 0 \leq x_1 < 1\}\) with the initial condition

\[
\tilde{f}_{in}(x_1, \zeta) = \{1 + \epsilon \sin(2\pi x_1)\} E,
\]
Figure 2. Time evolution of density profile for cases C and B2 with $\tilde{\kappa}/\tilde{b} = 5 \times 10^{-4}$. (a) $(\sqrt{\pi}/2)Kn = 0.1$, (b) $(\sqrt{\pi}/2)Kn = 1$, (c) $(\sqrt{\pi}/2)Kn = 10$ for case C and (d) $(\sqrt{\pi}/2)Kn = 1$ for case B2. Top and bottom dashed lines in each panel indicate $\tilde{\rho}_H$ and $\tilde{\rho}_L$ predicted by the equiarea rule in Fig. 1(b).

where $\epsilon = 0.1$. Because the form of $\tilde{f} = \Psi(\tilde{t}, x_1, \zeta_1)\pi^{-1} \exp(-\zeta_2^2 - \zeta_3^2)$ is compatible to the above system and $\tilde{\rho}$ can be computed from $\Psi$, the problem can be reduced to that of $\Psi$, meaning a great reduction of computational cost. Once $\Psi$ is known, the functional $\mathcal{M}$ can be recovered as well, because $\int \tilde{f} \ln(\tilde{f}/E) d\zeta_1 = \int \Psi \ln(\Psi/E_1) d\zeta_1$ with $E_1 = \pi^{-1/2} \exp(-\zeta_2^2)$. In the actual computation, we adopt a semi-Lagrangian method (see, e.g., Refs. [12–14]) based on the Strang’s splitting [15] with uniform grids both in $x_1$ and $\zeta_1$, where the infinite domain of $\zeta_1$ is truncated into $|\zeta_1| \leq 6$. In each transport processes, the 2nd–3rd WENO interpolation has been used. The 2nd-order central finite-difference is repeatedly applied to approximate the third order derivative of $\tilde{\rho}$ occurring in the gradient of $\tilde{\Phi}_L$. We have also developed a finite-difference scheme and a Strang’s scheme with third order polynomial spline interpolation in place of the WENO interpolation. Different methods gave consistent results as increasing grid points. We omit further details on the numerical method itself and
Figure 3. Time evolution of density profile for case C \((c = 3.8 \text{ and } \tilde{b} = 1/3)\) for \((\sqrt{\pi}/2)Kn = 1\). (a) \(\tilde{\kappa}/\tilde{b} = 1 \times 10^{-3}\) and (b) \(\tilde{\kappa}/\tilde{b} = 1 \times 10^{-4}\). See also Fig. 2(b) for comparison. Top and bottom dashed lines in each panel indicate \(\tilde{\rho}_H\) and \(\tilde{\rho}_L\) predicted by the equiarea rule in Fig. 1(b).

Figure 4. Time evolution of density profile for cases L \((c = 3.8, \tilde{b} = 4/15)\) and R \((c = 3.8, \tilde{b} = 2/5)\) for \((\sqrt{\pi}/2)Kn = 1\) and \(\tilde{\kappa}/\tilde{b} = 5 \times 10^{-4}\). (a) case L and (b) case R. Top and bottom dashed lines in each panel indicate \(\tilde{\rho}_H\) and \(\tilde{\rho}_L\) predicted by the equiarea rule in Fig. 1(b). See also Fig. 2(b) (case C) for comparison.

proceed to the presentation of results.

Numerical computations have been performed mainly for cases C, L, and R indicated in Fig. 1(a) by setting \(\tilde{A}(\tilde{\rho}) = 1\). Figure 2 shows the time evolution of the density profile for case C for \((\sqrt{\pi}/2)Kn = 0.1, 1, \text{ and } 10\) and for case B2 for \((\sqrt{\pi}/2)Kn = 1\), where \(\tilde{\kappa}/\tilde{b} = 5 \times 10^{-4}\) is common among the cases. Roughly speaking, the profile in the evolution process was observed to be a little more complicated at lower density region for smaller \(\tilde{\kappa}/\tilde{b}\) and for larger Knudsen number. Figure 3 shows the evolution for \((\sqrt{\pi}/2)Kn = 1\) with different values of \(\tilde{\kappa}/\tilde{b}\). It is clear from the figure, together with Fig. 2(b), that the smaller
\(\tilde{\kappa}/\tilde{b}\) is, the thinner the interface is. Figure 4 shows the evolution in the cases L and R for \((\sqrt{\pi}/2)Kn = 1\). It is seen that the dense region is thinner for case L, while it is fatter for case R. Furthermore, the values of density plateaux after a long time are different among the cases L, C, and R. Further comparisons with Fig. 2 and Fig. 6(b) suggest that they are dependent on \(\tilde{b}\) and \(c\), neither on \(Kn\) nor on \(\tilde{\kappa}\). Indeed, the values of plateaux, say \(\tilde{\rho}_L\) and \(\tilde{\rho}_H\), can be predicted by the equiarea rule for the potential \(\Phi\) (see Fig. 1(b) and Ref. [1]), which is dependent only on \(\tilde{b}\) and \(c\).

Time evolutions of the functional \(\tilde{M}\) are shown in Fig. 5 for various parameters. Here, the integration in space occurring in \(\tilde{M}\) should be understood as
\[
\int_{\tilde{D}} \tilde{D} \cdot \ldots \cdot d \tilde{x} = \int_{0}^{1} \ldots dx_1.
\]
As expected, \(\tilde{M}\) is always monotonic and decreasing in time, while individual parts of it, say
\[
\tilde{M}_{ln} \equiv \int_{\tilde{D}} \int \tilde{f} \ln \frac{\tilde{f}}{E} d \zeta dx,
\]
\[
\tilde{M}_A \equiv \tilde{M}_{ln} + 2 \int_{\tilde{D}} \int \tilde{\Phi}_S d \tilde{\rho} dx,
\]
\[
\tilde{M}_L \equiv \int_{\tilde{D}} \tilde{\rho} \tilde{\Phi}_L dx = \bar{\kappa} \int_{\tilde{D}} \left( \frac{\partial \tilde{\rho}}{\partial x_i^2} \right)^2 dx = \tilde{M} - \tilde{M}_A,
\]
are not necessarily monotonic. It is clear from Figs. 5(a)–(c) that the transition is slower for larger Knudsen number.

Going back to the density profiles, and let us now discuss how the values of density plateaux after a long time are determined. Since \(\tilde{M}\) is monotonically decreasing, the system approaches to its stationary state, which motivates us to consider the variational problem of \(\tilde{M}\) with respect to \(\tilde{f}\). Variational problem of \(\tilde{M}\) with respect to \(\tilde{f}\) followed by van Kampen’s interpretation [16] leads to the equiarea rule in Fig. 1(b) for determining those values in one-dimensional case. Let us consider the first variation of (10) under the constraint of \(\int_{\tilde{D}} \tilde{\rho} dx \equiv \int_{\tilde{D}} \int \tilde{f} d \zeta dx = 1:\)

\[
\delta \tilde{M} = \int_{\tilde{D}} \int \left\{ 1 + \ln \frac{\tilde{f}}{E} + 2 \tilde{\Phi}_S(\tilde{\rho}) - \bar{\kappa} \frac{\partial^2 \tilde{\rho}}{\partial x_i^2} - \tilde{\rho} \frac{\partial}{\partial x_i^2} - \lambda \right\} \delta \tilde{f} d \zeta dx
\]
\[
= \int_{\tilde{D}} \int \left\{ 1 + \ln \frac{\tilde{f}}{E} + 2 \tilde{\Phi}_S(\tilde{\rho}) - 2 \bar{\kappa} \frac{\partial^2 \tilde{\rho}}{\partial x_i^2} - \lambda \right\} \delta \tilde{f} d \zeta dx,
\]
where \(\lambda\) is the Lagrange multiplier, which is constant in \(x\) and \(\zeta\). Thus, it holds that
\[
1 + \ln \frac{\tilde{f}}{E} + 2 \tilde{\Phi}_S(\tilde{\rho}) - 2 \bar{\kappa} \frac{\partial^2 \tilde{\rho}}{\partial x_i^2} - \lambda = 0,
\]
Figure 5. Time evolution of $\tilde{M}$, $\tilde{M}_A$, and $\tilde{M}_{\text{in}}$. Panels (a)–(c) are case C with $\tilde{\kappa}/\tilde{b} = 5 \times 10^{-4}$ for different Knudsen numbers: (a) $(\sqrt{\pi}/2)\text{Kn} = 0.1$, (b) $(\sqrt{\pi}/2)\text{Kn} = 1$, and (c) $(\sqrt{\pi}/2)\text{Kn} = 10$. Panel (d) is case C with $\tilde{\kappa}/\tilde{b} = 3 \times 10^{-4}$ and $(\sqrt{\pi}/2)\text{Kn} = 0.1$. Panel (e) is case D for $(\sqrt{\pi}/2)\text{Kn} = 10$ and $\tilde{\kappa}/\tilde{b} = 5 \times 10^{-4}$, while Panel (f) is case B2 for $(\sqrt{\pi}/2)\text{Kn} = 1$ and $\tilde{\kappa}/\tilde{b} = 5 \times 10^{-4}$.

at the stationary state. Then, taking into account the balance among the component terms, $\ln(\tilde{f}/E)$ is found to be independent of $\zeta$, leading to $\tilde{f} = \tilde{\rho}E$. Hence, the above condition is reduced to

$$1 + \ln \tilde{\rho} + 2\Phi_S(\tilde{\rho}) - 2\tilde{\kappa} \frac{\partial^2 \tilde{\rho}}{\partial x_i^2} - \lambda = 0,$$

or equivalently

$$\tilde{\kappa} \frac{\partial^2 \tilde{\rho}}{\partial x_i^2} = \Phi(\tilde{\rho}) - \frac{1}{2} \lambda,$$

$$\Phi(\tilde{\rho}) \equiv \frac{1}{2} + \frac{1}{2} \ln \tilde{\rho} + \Phi_S = -\tilde{\alpha} \tilde{\rho} + \frac{1}{2} \frac{1}{1 - \tilde{b} \tilde{\rho}} + \frac{1}{2} \ln \frac{\tilde{\rho}}{1 - \tilde{b} \tilde{\rho}}.$$

By interpreting this condition as a motion of point mass following van Kampen (see Refs. 1, 16), we can conclude that the equiarea rule

$$\int_{\tilde{\rho}_L}^{\tilde{\rho}_H} \Phi(r) dr = \frac{\lambda}{2} (\tilde{\rho}_H - \tilde{\rho}_L), \quad \text{with} \quad \Phi(\tilde{\rho}_H) = \Phi(\tilde{\rho}_L) = \frac{\lambda}{2}, \quad (27) \]
Figure 6. Time evolution of the density and functional $M$ in case A, i.e., $(c, \tilde{b}) = (3.45, 1/3)$. (a) $\tilde{\rho}$ for $\bar{\kappa}/\bar{b} = 5 \times 10^{-4}$, (b) $\tilde{\rho}$ for $\bar{\kappa}/\bar{b} = 1 \times 10^{-4}$, and (c) $M$ for both values of $\bar{\kappa}/\bar{b}$, where Kn is commonly set as $(\sqrt{\pi}/2)Kn = 1$. Top and bottom dashed lines in (a) and (b) indicate $\tilde{\rho}_H$ and $\tilde{\rho}_L$, respectively.

applies, where $\tilde{\rho}_H$ and $\tilde{\rho}_L$ respectively denote larger and smaller values of density plateaux. This rule determines $\tilde{\rho}_H$ and $\tilde{\rho}_L$ as sketched in Fig. 1(b). Note that the curve of $\Phi$ is dependent only on $\tilde{b}$, once $\tilde{a}$ (or $c$) is fixed, so are the values of $\tilde{\rho}_H$ and $\tilde{\rho}_L$.

In closing the present section, we remark that a clear separation of plateaux and interfaces might not be achieved in the above neighborhood of the neutral curve, if $\bar{\kappa}/\bar{b}$ is not sufficiently small. Figure 6(a) demonstrates such an example (case A, $\bar{\kappa}/\bar{b} = 5 \times 10^{-4}$ and $(\sqrt{\pi}/2)Kn = 1$). In the case, the phase transition is incomplete and the evolution ceases with a smooth profile as in Fig. 6(a). In the meantime, the interface ought to be thinner for smaller $\bar{\kappa}$ and the transition is more likely to be completed. Indeed, for case A with $\bar{\kappa}/\bar{b} = 1 \times 10^{-4}$ and $(\sqrt{\pi}/2)Kn = 1$, a clear separation of different plateaux and interfaces is observed, as in Fig. 6(b). Then, the equiarea rule revives for the prediction of the values of density plateaux.

VI. CONCLUSION

In the present paper, we have investigated the stability of uniform equilibrium states in the kinetic regime. The linear stability analysis shows that the linear unstable condition is the same as that of the Cahn–Hilliard type equation in Ref. [1], irrespective of the Knudsen number. The condition is not affected by $\kappa$ (or $\bar{\kappa}$) as well, the measure of the collective long-range interaction effect occurring in $\Phi_L$ (or $\bar{\Phi}_L$). By numerical computations we have indeed observed the phase transition after perturbing uniform equilibrium states that lie
above the neutral curve in the diagram of Fig. 1(a). We did not observe unstable uniform equilibrium states below this curve (cases B1, B2, and B3 in Fig. 1(a)), though the computed cases are limited. The numerical results show that \( \kappa \) (or \( \tilde{\kappa} \)) mainly affects the thickness of the interface between different phases; the smaller \( \kappa \) (or \( \tilde{\kappa} \)) is, the thinner the interface is. The Knudsen number affects the transition process but does not affect the values of density plateaux at the final states. They are determined by another diagram, i.e., the equiarea rule, in Fig. 1(b), as far as the interface is thin enough for the clear separation of different plateaux to emerge. The numerical results further show that the functional \( \mathcal{M} \) (or \( \tilde{\mathcal{M}} \)) indeed monotonically decreases as predicted in Ref. [1], though its component terms are not necessarily monotonic in the transition process.

**Acknowledgements**  The present work is supported in part by JSPS KAKENHI Grant Number 17K18840.

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In order to show that $SF(S)$ is monotonically increasing, let us consider $G(x) \equiv \sqrt{\pi \{1 - \text{erf}(x)\}} - \frac{2x}{1+2x^2} \exp(-x^2)$. Then, by direct calculations, it is seen that $G' < 0$. Since $G(0) = \sqrt{\pi}$ and $G(\infty) = 0$, $G > 0$ for $0 \leq x < \infty$. This leads to $\sqrt{\pi}F(x) > \frac{2x}{1+2x^2}$, so that $\sqrt{\pi}xF(x) - 1 > -\frac{1}{1+2x^2}$. Therefore, $(xF)' = F + xF' = F + 2x(xF - \frac{1}{\sqrt{\pi}}) > F - \frac{2}{\sqrt{\pi}}\frac{2x}{1+2x^2} > 0$, which concludes that $SF(S)$ is monotonically increasing in $0 \leq S < \infty$. The limiting value of $xF(x)$ as $x \to \infty$ can be found in the literature.

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