

Kinetic theory study on non-equilibrium dense fluids

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Chapter 1

General introduction

In general, there are three states (or phases) of matter: gas, liquid, and solid. Both gas and liquid are called fluids because they can freely change their form. Fluids are not necessarily composed of only one gas or liquid phase but can be a mixture of different phases. In particular, a fluid flow that is a mixture of gas and liquid is called a gas-liquid two-phase flow. This type of flow is seen in daily life, such as a river flowing with the inclusion of air and the atmosphere containing fog or mist. Gas-liquid two-phase flows are often encountered in engineering situations such as combustion caused by fuel atomization or cavitation caused by screw rotation. Therefore, it is also important to understand the details of gas-liquid two-phase flows in engineering.

Gas-liquid two-phase flows have been classified into various types according to their flow pattern. In particular, a flow in which many bubbles are dispersed in a liquid is called a bubble flow, while a flow in which droplets are dispersed in a gas is called a droplet flow. Since the properties of bubble and droplet flows are strongly influenced by the behavior of droplets and bubbles, simulations of these flows have to accurately capture the processes of droplet and bubble shape change, growth, and collapse. With this background in mind, methods such as the Marker and Cell (MAC) method and the Volume of Fluid (VOF) method have been developed in conventional fluid dynamics to track the shape changes of bubbles and droplets in detail. These methods treat the interface between the gas and liquid phases (hereafter referred to as the interface) as a free surface advected by the fluid motion. Accordingly, these methods basically track shape changes based on the assumption of phase equilibrium. However, in order to capture the dynamics of bubbles and droplets not only during deformation but also during growth and collapse, it is desirable to treat fluid transport across the interface by incorporating phase changes such as evaporation and condensation. Since evaporation and condensation are non-equilibrium phenomena caused by the breakdown of phase equilibrium, a different methodology that does not assume thermal or phase equilibrium should be used when incorporating these effects. That is why microscopic

approaches like molecular gas dynamics come into play.

In molecular gas dynamics, a fluid is considered to be a collection of many molecules, and the distribution of molecular positions and velocities (velocity distribution function) is used as a fundamental quantity to understand fluid motion. The velocity distribution function changes according to the Boltzmann equation, and macroscopic physical quantities in conventional fluid mechanics, such as fluid density, flow velocity, and temperature, are expressed as moments of the velocity distribution function. Following the development of asymptotic and numerical methods for the Boltzmann equation, methodologies have also been developed to incorporate the results obtained by these methods into a fluid dynamics framework that considers the effects of evaporation and condensation at the interface. Thus, the application of molecular gas dynamics has provided new knowledge fundamental to the fluid dynamic treatment of gas-liquid two-phase flows. The knowledge gained is, however, essentially dedicated to describing the gas phase side. This might be seen as a limitation of the Boltzmann equation, which deals with ideal gases. In fact, in molecular gas dynamics, the macroscopic state of the liquid phase side is usually assumed to be given, and the interface is treated as a boundary to the gas phase, reflecting the given state of the liquid phase.

In order to advance from such microscopic treatment in molecular gas dynamics, it is desirable to introduce a method for simultaneous treatment of gas-liquid two-phase. In this dissertation, we propose a new kinetic equation that can describe the gas-liquid two-phase simultaneously and show a promising way for analyzing both phases simultaneously. Such a method will not lose effectiveness even when changes in the two phases occur on the same scale, such as in the collapse processes of droplets and bubbles, where both the gas and liquid phases cannot be kept in equilibrium.

The study of incorporating real gas effects, such as molecular volume exclusion and intermolecular attraction, into the Boltzmann equation dates back to the Enskog and Enskog-Vlasov equations. These equations are useful in studying dense gases (or even liquids) but much more complicated than the Boltzmann equation, mainly due to the finite size effect of the molecules and the non-negligible correlations. Although numerical methods such as the Fourier spectral and stochastic particle simulation methods have also been developed, they are still computationally demanding and challenging compared to the Boltzmann equation. It is then natural to introduce simplified models of the Enskog and Enskog-Vlasov equations,

expecting them to play a useful role like the Bhatnagar–Gross–Krook (BGK) model for the Boltzmann equation. Indeed, a model called the Shakhov–Enskog model has recently been proposed and applied to some simple flows, showing reasonable agreement with the numerical results of the Enskog equation.

Despite the above advantages, the original Enskog equation, the Enskog–Vlasov equation, and their models do not guarantee the H theorem, one of the fundamental properties of molecular gas dynamics. Since the H theorem corresponds to the second law of thermodynamics, it should play an important role in understanding two-phase phenomena such as interface formation and deformation. In order to recover this fundamental property, a new kinetic model equation for van der Waals fluids has been developed in [1]. In this dissertation, we will further develop this kinetic model.

Although the kinetic model in [1] has the advantage mentioned above, it does not recover the realistic Prandtl number inherited from its BGK-type collision term. Therefore, the extension of the model is to be discussed aiming at the remedy of this shortcoming and, at the same time, the recovery of proper transport coefficients. A preliminary study of the entropic property of the Ellipsoidal-Statistical (ES)-type collision model is first done in Chapter 2 along this line. Gained knowledge is used in Chapters 3 and 4, which propose two types of extension based on the ES-type collision model. The newly proposed model in Chapter 4 is then further applied to the study of a single droplet or bubble in Chapter 5. The analyses in Chapter 5 provide new aspects of the two- and three-dimensional nature of the interface for the formation of droplets and/or bubbles and their stability, which have been lacking in the studies under the one-dimensional and periodic setting as in [3], and advance our understanding of multi-dimensional two-phase flows.

Chapter 2 is a preparation for adopting the ES-type model as the collision term. The ES model is an extension of the BGK model that provides an additional degree of freedom for properly adjusting the Prandtl number. The H theorem is proved for the ES model provided that the Prandtl number is not less than $2/3$, and it is expected to hold only conditionally when the Prandtl number is below $2/3$. The relation between the degree of the non-equilibrium state and the condition that the H theorem still holds even below $2/3$ is clarified.

Chapter 3 discusses the first attempt to extend the kinetic model in [1] to recover the

proper transport coefficients. Based on the study in Chapter 2, the BGK-type term in [1] is replaced by the ES-type with supplemental modifications. Although the proposed model guarantees the H theorem only conditionally, it is shown to hold in the one-dimensional periodic phase transition problem.

Chapter 4 begins with a brief review of the kinetic models developed in [2] and Chapter 3 and proposes another new ES-type model that guarantees the H theorem unconditionally. The same test simulation as in Chapter 3 is also provided, and the quantitative comparisons between the two ES-type models are presented and discussed.

Chapter 5 studies the single droplet or bubble based on the model proposed in Chapter 4. In the thermal equilibrium state, the model is reduced to the same density equation as that obtained by van Kampen. Assuming that the density field is isotropic, the equation is solved to provide a useful classification of the solution of the steady droplet and/or bubble in terms of the dynamical system arguments. The stability of the solutions thus classified is studied numerically by direct simulation of the kinetic model. The obtained results are also discussed in the light of the H theorem and related free energy arguments, which are the advantages of the proposed kinetic model.

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Chapter 2

On the entropic property of the Ellipsoidal-Statistical model with the Prandtl number below $2/3$

2.1 Introduction

The Ellipsoidal-Statistical (ES) model is a relaxation-type kinetic equation proposed by Holway [1], which involves the celebrated Bhatnagar–Gross–Krook (BGK) model [2] as a special case. It has a simple structure as the other kinetic models but still satisfies the H theorem and reproduces a realistic value of the Prandtl number. Since the proof of its H theorem in [3], it has been attracting many researchers as an alternative to the BGK model, e.g., [4,5,6,7,8].

In the case of monatomic gases, that proof was made for the Prandtl number not less than $2/3$. In some practical applications, however, such a restriction might affect our choice of the Prandtl number. Indeed, for the hard-sphere gas (one of the most representative models in the kinetic theory) the Prandtl number is known to be 0.660694 [9], which is slightly lower than $2/3$.¹ In [10,11], we were also in such an embarrassing situation that the Prandtl number of nitrogen gas is slightly below the corresponding bound for polyatomic gases and made a compromise (by around 10 %) in setting the value of the Prandtl number in numerical computations.

The above lower bound $2/3$ is, however, the condition that the H theorem holds unconditionally. There is still a room for that the H theorem holds even for the Prandtl number below that bound under some restriction. In the present paper, we are going to study this issue and provide a critical condition for the H theorem to be valid for the Prandtl number below $2/3$. The paper is organized as follows. First, the ES model is briefly reviewed in Sec. 2.2. Then, the derivation of the concerned condition is delivered in Sec. 2.3, which is

¹In the case of the dense gas, the deviation from $2/3$ can be enhanced to be down to about 86% of the value at the dilute gas limit, according to the Enskog theory; see, e.g., J. O. Hirschfelder, C. F. Curtiss and R. B. Bird, *Molecular Theory of Gases and Liquids*, John Wiley & Sons, New York, 1964, Sec. 9.3.

followed by some numerical tests in Sec. 2.4. The paper is concluded in Sec. 2.5.

2.2 ES model and H theorem

Let us denote by f the velocity distribution function (VDF) of gas molecules, which is a function of time t , space position X_i , and molecular velocity ξ_i . Then, the collision term of the ES model $Q_{\text{ES}}(f)$ for monatomic gases reads [3]

$$Q_{\text{ES}}(f) = A_c(T)\rho(\mathcal{G}[f] - f), \quad (2.1a)$$

$$\mathcal{G}[f] = \frac{\rho}{\sqrt{\det(2\pi\mathcal{T})}} \exp\left(-\frac{1}{2}(\mathcal{T}^{-1})_{ij}(\xi_i - v_i)(\xi_j - v_j)\right), \quad (2.1b)$$

$$\rho = \int f d\xi, \quad v_i = \frac{1}{\rho} \int \xi_i f d\xi, \quad \mathcal{T}_{ij} = (1 - \nu)RT\delta_{ij} + \nu\Theta_{ij}, \quad (2.1c)$$

$$\Theta_{ij} = \frac{1}{\rho} \int (\xi_i - v_i)(\xi_j - v_j) f d\xi, \quad T = \frac{1}{3R}\Theta_{ii}, \quad (2.1d)$$

where ρ , v_i , and T are respectively the density, flow velocity, and temperature of the gas; R is the specific gas constant (the Boltzmann constant divided by the mass of a molecule); δ_{ij} is the Kronecker delta; $A_c(T)(> 0)$ is a positive function of T such that $A_c(T)\rho$ is the collision frequency of the gas molecules. Note that $\mathcal{T}$ (or $\mathcal{T}_{ij}$) is a 3×3 matrix, that Θ_{ij} (or Θ) is the stress tensor divided by the density, and that the summation convention applies in the definitions of $\mathcal{G}$ and T and throughout the present paper. The ν is an adjustable parameter to make the Prandtl number Pr a realistic value, and the H theorem is proved to hold unconditionally in the range $-1/2 \leq \nu < 1$ [3]. Because of the relation $\text{Pr} = 1/(1 - \nu)$ (or $\nu = 1 - 1/\text{Pr}$), this range is identical to $2/3 \leq \text{Pr} < \infty$.

For our purpose, the relevant steps in the proof in [3] are to show that (i) $\mathcal{T}$ is positive definite and that (ii) the inequality $\det \mathcal{T} \geq \det \Theta$ holds, where the equality holds only when Θ is a scalar multiple of the identity matrix (see Sec. 2.A). If (i) and (ii) remain valid even for $\nu < -1/2$ (or $\text{Pr} < 2/3$) under some condition, the H theorem remains valid as well under that condition. In the present paper, we are concerned with the case $-1 \leq \nu < -1/2$, which corresponds to the case $1/2 \leq \text{Pr} < 2/3$.

2.3 Derivation of condition

Thanks to its definition, Θ is a symmetric positive definite matrix and thus has positive real eigenvalues λ_1 , λ_2 , and λ_3 , as far as the VDF is non-negative. Hence, without loss of

generality, we may assume that $0 < \lambda_1 \leq \lambda_2 \leq \lambda_3$ and accordingly may put $\lambda_1 = (1 - \epsilon)\lambda$, $\lambda_2 = (1 - \theta\epsilon)\lambda$, and $\lambda_3 = \lambda$, where $0 \leq \epsilon < 1$, $0 \leq \theta \leq 1$, and $\lambda > 0$. Since by definition $3RT$ is nothing else than the trace of Θ , it is related to the eigenvalues as $3RT = \lambda_1 + \lambda_2 + \lambda_3$ [or $3RT = (3 - \epsilon(1 + \theta))\lambda$]. Note that ϵ indicates the degree of deviation of the minimum from the maximum eigenvalue and that θ is the ratio of the difference between the largest two eigenvalues to that between the minimum and the maximum eigenvalue.

2.3.1 On the condition for $\mathcal{T}$ to be positive definite

In the frame of the mutually orthogonal eigenvectors of Θ , the $\mathcal{T}$ as well as Θ is diagonalized:

$$\begin{aligned} \mathcal{T} &= \nu\Theta + (1 - \nu)RT\text{Id} \\ &= \lambda \begin{pmatrix} 1 - \epsilon\nu - \frac{\epsilon(1-\nu)(1+\theta)}{3} & 0 & 0 \\ 0 & 1 - \epsilon\theta\nu - \frac{\epsilon(1-\nu)(1+\theta)}{3} & 0 \\ 0 & 0 & 1 - \frac{\epsilon(1-\nu)(1+\theta)}{3} \end{pmatrix}, \end{aligned}$$

where Id is the 3×3 identity matrix. Since the three diagonal components multiplied by λ are eigenvalues of $\mathcal{T}$, the condition for $\mathcal{T}$ to be positive definite is simply reduced to

$$1 - (\epsilon/3)(1 - \nu)(1 + \theta) > 0, \quad \text{i.e.,} \quad 0 \leq \epsilon < \frac{3}{1 - \nu} \frac{1}{1 + \theta}, \quad (2.2)$$

in the present parameter range $-1 \leq \nu < -1/2$. Note that, since $0 \leq \epsilon < 1$ by construction, the constraint (2.2) is effective only when the right-hand side of the last inequality is less than unity, namely

$$\theta > \frac{3}{1 - \nu} - 1 = \frac{2 + \nu}{1 - \nu} \equiv \theta_{\mathcal{T}}(\nu), \quad (2.3)$$

is fulfilled. The above $\theta_{\mathcal{T}}$ varies monotonically from $1/2$ to 1 when ν varies from -1 to $-1/2$.

2.3.2 On the condition for $\det \mathcal{T} \geq \det \Theta$ to hold and the restriction on the equality

After straightforward manipulations, the difference D of $\det \mathcal{T}$ with $\det \Theta$ is written as

$$\begin{aligned} D &\equiv \det \mathcal{T} - \det \Theta \\ &= \frac{1}{3} \lambda^3 \epsilon^2 (1 - \nu) \left\{ (1 + \nu)(\theta^2 - \theta + 1) \right. \\ &\quad \left. - \frac{1}{9} \epsilon (1 + \theta) [2\nu + 1 + (1 - \nu)\theta] [(2\nu + 1)\theta + 1 - \nu] \right\}. \end{aligned} \quad (2.4)$$

Here, we need to care the restriction in (ii) of the last paragraph of Sec. 2.2 that $D = 0$ holds only when Θ is a scalar multiple of the identity matrix, which is identical to $\epsilon = 0$ in

the present notation. Hence the condition for $D \geq 0$ with this restriction is reduced to that the inside of the curly brackets is positive, i.e.,

$$(1 + \nu)(\theta^2 - \theta + 1) > \frac{1}{9}\epsilon(1 + \theta)[2\nu + 1 + (1 - \nu)\theta][(2\nu + 1)\theta + 1 - \nu], \quad (2.5)$$

for $\epsilon \neq 0$ in the range $-1 \leq \nu < -1/2$. The left-hand side is non-negative because $0 \leq \theta \leq 1$, while the sign of the right-hand side depends on that of the factor $F(\theta; \nu) \equiv [2\nu + 1 + (1 - \nu)\theta][(2\nu + 1)\theta + 1 - \nu]$. Let the smaller and larger zeros of F with fixed ν be θ_a and θ_b , i.e., $\theta_a = -(2\nu + 1)/(1 - \nu)$ and $\theta_b = -(1 - \nu)/(2\nu + 1)$. Then, it is readily seen that $0 < \theta_a < 1 < \theta_b$ and that $F \geq 0$ for $\theta_a \leq \theta \leq \theta_b$ and $F < 0$ elsewhere. Hence, we have the following condition:

$$\begin{cases} 0 \leq \epsilon < 1, & \text{for } 0 \leq \theta \leq \theta_a, \\ 0 \leq \epsilon < \frac{9(1 + \nu)(\theta^2 - \theta + 1)}{(1 + \theta)F(\theta; \nu)} \equiv \mathcal{F}(\theta; \nu), & \text{for } \theta_a < \theta \leq 1. \end{cases} \quad (2.6)$$

2.3.3 Combined condition

We shall merge the conditions (2.2) and (2.6) by taking account of the original range of ϵ , i.e., $0 \leq \epsilon < 1$.

Let us start with the observation that $\theta_{\mathcal{T}} - \theta_a = 3(\nu + 1)/(1 - \nu) \geq 0$, so that $\theta_a \leq \theta_{\mathcal{T}} < 1$ for $-1 \leq \nu < -1/2$. As described before, the condition (2.2) becomes effective only when $\theta > \theta_{\mathcal{T}}$. Our first concern is the size relation between $3/[(1 - \nu)(1 + \theta)]$ in (2.2) and $\mathcal{F}(\theta; \nu)$ in (2.6) in the range $\theta_{\mathcal{T}} < \theta \leq 1$. Then, checking the size relation is reduced to checking the sign of the following quantity

$$\Delta \equiv F(\theta; \nu) - 3(1 - \nu)(1 + \nu)(\theta^2 - \theta + 1),$$

because all of $(1 + \theta)$, $(1 - \nu)$, and F are positive. Here, $\Delta \geq 0$ implies $3/[(1 - \nu)(1 + \theta)] \geq \mathcal{F}$.

The simple substitution of F shows, after some manipulations, that

$$\begin{aligned} \Delta &= (1 - \nu)(-\nu - 2)\theta^2 + (2\nu^2 + 2\nu + 5)\theta + (1 - \nu)(-\nu - 2) \\ &= [(1 - \nu)\theta - (\nu + 2)][-(\nu + 2)\theta + (1 - \nu)] \\ &= -(1 - \nu)(\nu + 2)(\theta - \theta_{\mathcal{T}})(\theta - \frac{1}{\theta_{\mathcal{T}}}). \end{aligned} \quad (2.7)$$

Remind that $\theta_{\mathcal{T}} < 1$ for $-1 \leq \nu < -1/2$. Thus $\Delta > 0$, i.e., $\mathcal{F} < 3/[(1 - \nu)(1 + \theta)]$ for $\theta_{\mathcal{T}} < \theta \leq 1$. Our next concern is the size relation between $\mathcal{F}$ and unity in the range

$\theta_a < \theta \leq \theta_T$, because $3/[(1-\nu)(1+\theta)]$ is over or equal to unity in this range. Then, because $\Delta \leq 0$ for $\theta_a < \theta \leq \theta_T$, we have $1 \leq 3/[(1-\nu)(1+\theta)] \leq \mathcal{F}$, so that there is no restriction on ϵ in the concerned range of θ .

To summarize, we have arrived at the following statement of criterion.

Let $\lambda_1 \leq \lambda_2 \leq \lambda_3$ be positive real eigenvalues of the symmetric positive definite matrix Θ defined by (2.1d). Let $\epsilon = 1 - \lambda_1/\lambda_3$ and $\theta = (1 - \lambda_2/\lambda_3)/(1 - \lambda_1/\lambda_3)$, where $0 \leq \epsilon < 1$ and $0 \leq \theta \leq 1$ by construction. Then, for $-1 \leq \nu < -1/2$, which corresponds to $1/2 \leq \text{Pr} < 2/3$, the following criterion must be fulfilled in order for the H theorem to remain valid:

$$\begin{cases} 0 \leq \epsilon < 1, & \text{for } 0 \leq \theta \leq \frac{2+\nu}{1-\nu}, \\ 0 \leq \epsilon < \mathcal{F}(\theta; \nu), & \text{for } \frac{2+\nu}{1-\nu} < \theta \leq 1, \end{cases} \quad (2.8)$$

where $\mathcal{F}$ is the one defined by (2.6).

2.4 Simple test problems

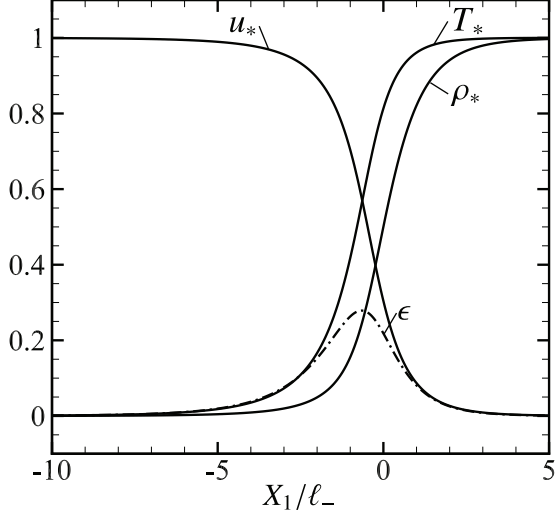
In order to see how much the derived condition (2.8) is practically restrictive, we shall carry out a couple of numerical tests such that the strong anisotropic behavior of the gas be expected. One is the strong shock wave problem, the other is the time-dependent Couette flow problem. A couple of additional tests, which are simple but severe, motivated by the result of the Couette flow will be conducted as well.

2.4.1 Shock wave test

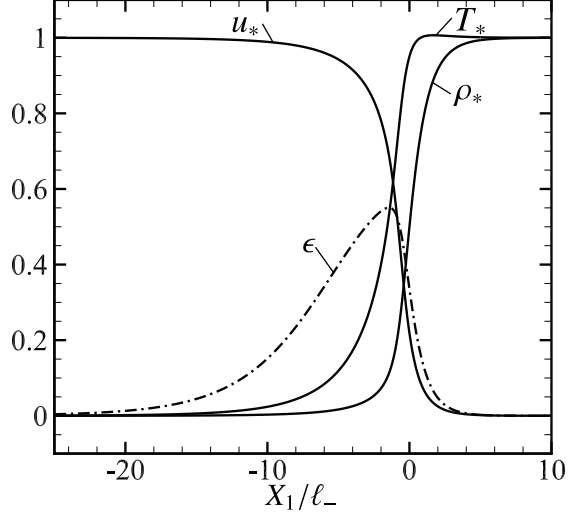
Consider a normal shock wave standing at rest against a uniform flow of a monatomic gas. Let X_1 be the spatial coordinate along the flow direction whose origin is located at the center of the shock.² Let ρ_- , T_- , and $(u_-, 0, 0)$ be the density, temperature, and flow velocity of the uniform equilibrium state at upstream infinity, while ρ_+ , T_+ , and $(u_+, 0, 0)$ be those at downstream infinity. Then, under the spatially uniform and the null flow-velocity assumption in the X_2 - and X_3 -directions, the problem is formulated as

$$\xi_1 \frac{\partial f}{\partial X_1} = Q_{\text{ES}}(f), \quad -\infty < X_1 < \infty, \quad (2.9a)$$

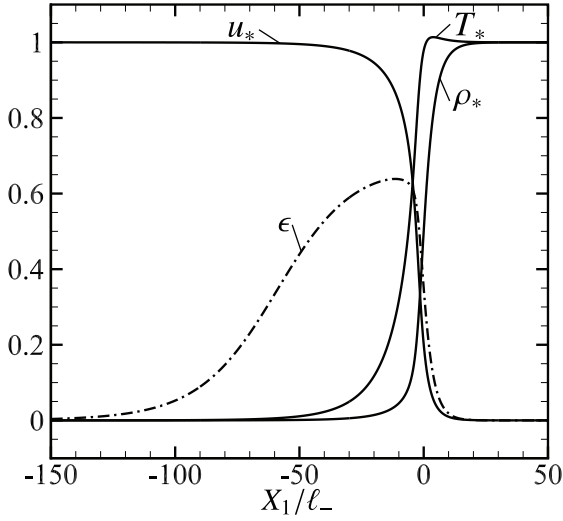
²The center of the shock is defined by the position where the density ρ takes the average of the densities at the upstream and downstream infinities.



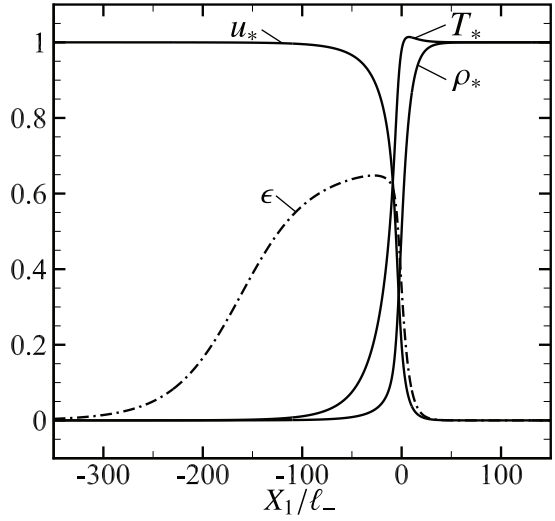
(a) $M_- = 2$



(b) $M_- = 5$



(c) $M_- = 20$



(d) $M_- = 40$

Figure 2.1: Structure of the shock wave for typical Mach numbers M_- in the case of $\text{Pr} = 2/3$. (a) $M_- = 2$, (b) $M_- = 5$, (c) $M_- = 20$, and (d) $M_- = 40$. Here, ℓ_- is the mean free path of molecules in the equilibrium state at rest with density ρ_- and temperature T_- . In each panel, solid lines indicate $\rho_* = (\rho - \rho_-)/(\rho_+ - \rho_-)$, $u_* = (v_1 - u_+)/ (u_- - u_+)$, and $T_* = (T - T_-)/(T_+ - T_-)$ respectively, while a dash-dotted line indicates ϵ .

under the upstream and the downstream condition

$$f(X_1, \boldsymbol{\xi}) \rightarrow \frac{\rho_{\pm}}{(2\pi RT_{\pm})^{3/2}} \exp\left(-\frac{(\xi_1 - u_{\pm})^2 + \xi_2^2 + \xi_3^2}{2RT_{\pm}}\right), \quad \text{as } X_1 \rightarrow \pm\infty, \quad (2.9b)$$

where the upstream and the downstream quantities are related by the Rankine–Hugoniot conditions [12]:

$$\frac{\rho_-}{\rho_+} = \frac{u_+}{u_-} = 1 - \frac{2}{\gamma + 1} \frac{M_-^2 - 1}{M_-^2}, \quad \frac{T_+}{T_-} = 1 + \frac{2(\gamma - 1)}{(\gamma + 1)^2} \frac{(\gamma M_-^2 + 1)(M_-^2 - 1)}{M_-^2}. \quad (2.10)$$

Here $\gamma = 5/3$ and $M_- (\geq 1)$ is the Mach number of the flow at upstream infinity, i.e., $M_- = u_- / \sqrt{\gamma RT_-}$.

The problem can be reduced to that of the marginal VDFs [13]. After the reduction, it is solved numerically by the standard iterative finite-difference method. The numerical accuracy is carefully checked enough to assure the main conclusions drawn from the present computations. Here we omit the details of the numerical method itself, grid resolution, etc. and simply present the obtained results.

It is readily seen that Θ is diagonal³ in the present coordinates system, and its diagonal components are nothing else than the eigenvalues λ_1 , λ_2 , and λ_3 [or $(1 - \epsilon)\lambda$, $(1 - \epsilon\theta)\lambda$, and λ]. Firstly, the computations have been performed for $M_- = 2, 5, 10, 20, 40$, and 60 under the setting $\text{Pr} = 2/3$. Figure 2.1 shows the structure of the shock wave in some typical cases. In all the cases, Θ_{11} is found to be the largest among the diagonal components. Because the problem is isotropic in the directions normal to X_1 -direction, $\Theta_{22} = \Theta_{33}$ and thus $\theta \equiv 1$. Then, the condition (2.8) is simplified as

$$0 \leq \epsilon < \mathcal{F}(1; \nu) = \frac{9}{2} \frac{1 + \nu}{(\nu + 2)^2}, \quad (2.11)$$

or equivalently

$$0 \leq \epsilon < \frac{(\text{Pr} - 1/2)}{(\text{Pr} - 1/3)^2} \text{Pr} \equiv \mathcal{S}(\text{Pr}), \quad (2.12)$$

using the relation $\nu = 1 - 1/\text{Pr}$. Note that $\mathcal{S}(\text{Pr})$ monotonically increases from 0 to 1 as Pr increases from $1/2$ to $2/3$. The obtained profiles of ϵ , which is given by $1 - \Theta_{33}/\Theta_{11}$ here, inside the shock are also shown by dash-dotted lines in Fig. 2.1. With the aid of (2.12), the lower bound of the acceptable Prandtl number for each Mach number is suggested from the figure, the result of which is shown in Table 2.1. With these results in mind, further

Table 2.1: The maximum ϵ for various Mach numbers M_- in the case of $\text{Pr} = 2/3$. Pr_* is the lower bound of acceptable Prandtl number suggested by $\max \epsilon = \mathcal{S}(\text{Pr}_*)$; see (2.12).

M_-	2	5	10	20	40	60
$\max \epsilon$	0.2786	0.5506	0.6137	0.6387	0.6478	0.6499
Pr_*	0.5184	0.5454	0.5539	0.5576	0.5590	0.5593
$(3/2)\text{Pr}_*$	0.7776	0.8181	0.8309	0.8364	0.8385	0.8390

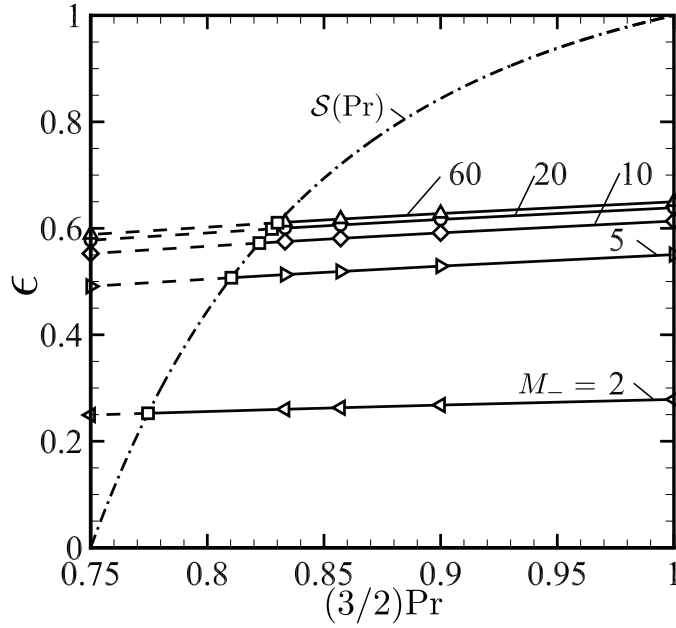


Figure 2.2: The maximum value of ϵ vs. $(3/2)\text{Pr}$ for various upstream Mach numbers M_- . Symbols indicates the results of computations. The results of common M_- are connected by solid lines in the acceptable range of Pr and by dashed lines in the range where condition (2.8) is violated.

computations have been carried out for different Prandtl numbers as well. The maximum values of ϵ in individual computations are plotted against Pr for each Mach number in Fig. 2.2. It is seen that they depend only weakly on Pr for every fixed value of M_- . The intersections of solid lines and the curve $\epsilon = \mathcal{S}(\text{Pr})$ are indicated by the symbol $\square$. Their abscissas indicate the actual lower bounds of acceptable Prandtl number for the individual M_- . They are all slightly smaller than the values of Pr_* in Table 2.1 for those M_- . It is seen that in the present test the condition (2.8) [or (2.12)] is tolerant; even for $M_- = 60$, $(3/2)\text{Pr}$ can be down to $\simeq 0.83$, i.e., a reduction of Pr by around 17% from $2/3$ is acceptable.

Incidentally, even for $\text{Pr} = 1/2$ (or $\nu = -1$), where the condition (2.12) is violated, stable numerical computations have been carried out. It would be partially explained by that the condition (2.2) for $\mathcal{T}$ to be positive definite is reduced to $0 \leq \epsilon < 3/4$ and is never violated in those computations (see Fig. 2.2).

2.4.2 Couette flow and sliding plate test

Consider a monatomic rarefied gas in the gap between two parallel plates which are kept at a common uniform temperature T_0 . The confined gas is in the equilibrium state at rest with the temperature T_0 and the density ρ_0 . Set the X_1 -direction to be normal to the plates, with its origin at the middle of the gap. Let the gap width be L . At the instance $t = 0$, the two plates suddenly start sliding with a constant speed V in the directions opposite to each other: the plate at $X_1 = L/2$ moves in the X_2 -direction, while that at $X_1 = -L/2$ in the $-X_2$ -direction. Assuming the diffuse reflection boundary condition on the plates, the problem is formulated as

$$\frac{\partial f}{\partial t} + \xi_1 \frac{\partial f}{\partial X_1} = Q_{\text{ES}}(f), \quad -L/2 < X_1 < L/2, \quad (2.13a)$$

under the initial and the boundary condition

$$f(0, X_1, \boldsymbol{\xi}) = \frac{\rho_0}{(2\pi RT_0)^{3/2}} \exp\left(-\frac{\xi_1^2 + \xi_2^2 + \xi_3^2}{2RT_0}\right), \quad (2.13b)$$

$$f(t, \pm L/2, \boldsymbol{\xi}) = \frac{\sigma_{\pm}}{(2\pi RT_0)^{3/2}} \exp\left(-\frac{\xi_1^2 + (\xi_2 \mp V)^2 + \xi_3^2}{2RT_0}\right), \quad \xi_1 \gtrless 0, \quad (2.13c)$$

³Thanks to the assumption made just before (2.9a), the problem is rotationally invariant around the X_1 -axis. The off-diagonal components are thus null.

where

$$\sigma_{\pm} = \sqrt{\frac{2\pi}{RT_0}} \int_{\xi_1 \geq 0} |\xi_1| f(t, \pm L/2, \boldsymbol{\xi}) d\boldsymbol{\xi}. \quad (2.13d)$$

This is the time-dependent Couette flow problem.

As the previous test case, the problem can be reduced to that of the marginal VDFs [13]. After the reduction, it is solved numerically by the standard finite-difference method implicit in time. The numerical accuracy is carefully checked enough to assure the main conclusions drawn from the present computations. We again omit all the details of the numerical computations. In the present test, Θ is not diagonal in the specified Cartesian coordinates, and the three eigenvalues are given by Θ_{33} and $\lambda_{\pm} \equiv [\Theta_{11} + \Theta_{22} \pm \sqrt{(\Theta_{11} - \Theta_{22})^2 + 4\Theta_{12}^2}]/2$.

The computations have been carried out for various values of V , the reference Knudsen number, and the Prandtl number. In the present test, ϵ is found to be always $1 - \lambda_-/\lambda_+$ and to take its maximum value on the plates at the initial stage of the time evolution. Consequently, that value is found to depend only on the plate speed, neither on the Knudsen number nor the Prandtl number, because at the initial stage the collision integral is not effective. These observations imply that the most severe situation is identical to the initial stage of the Rayleigh problem [14,15] and is represented by the combination of the initial data for incident molecules and the boundary condition for reflected molecules on the plates. That is, the most severe test can be conducted by the following VDF:

$$f(\boldsymbol{\xi}) = \begin{cases} \frac{\rho_0}{(2\pi RT_0)^{3/2}} \exp\left(-\frac{\xi_1^2 + (\xi_2 - V)^2 + \xi_3^2}{2RT_0}\right), & \xi_1 < 0, \\ \frac{\rho_0}{(2\pi RT_0)^{3/2}} \exp\left(-\frac{\xi_1^2 + \xi_2^2 + \xi_3^2}{2RT_0}\right), & \xi_1 > 0. \end{cases} \quad (2.14)$$

Note that this is identical to the steady free molecular solution of the Couette flow with one plate sliding with speed V and the other plate at rest. The above reduction of test, which we call a sliding plate test, allows us to assess the condition of our interest in detail.

For the above VDF (2.14), ϵ and θ are readily obtained as

$$\epsilon = \epsilon_S(\hat{V}) \equiv \frac{\frac{\hat{V}^2}{2} \sqrt{1 + \frac{16}{\pi \hat{V}^2}}}{1 + \frac{\hat{V}^2}{4} \left(\sqrt{1 + \frac{16}{\pi \hat{V}^2}} + 1 \right)}, \quad \theta = \theta_S(\hat{V}) \equiv \frac{1}{2} \left(1 + \frac{1}{\sqrt{1 + \frac{16}{\pi \hat{V}^2}}} \right), \quad (2.15)$$

where $\hat{V} = V/\sqrt{2RT_0}$. Note that (a) $\theta > 1/2$ from the above, while $0 < \theta_a \leq 1/2$ in the range $-1 \leq \nu < -1/2$ or $1/2 \leq \text{Pr} < 2/3$. It is also found that $0 \leq \epsilon_S(\hat{V}) < 1$. Hence,

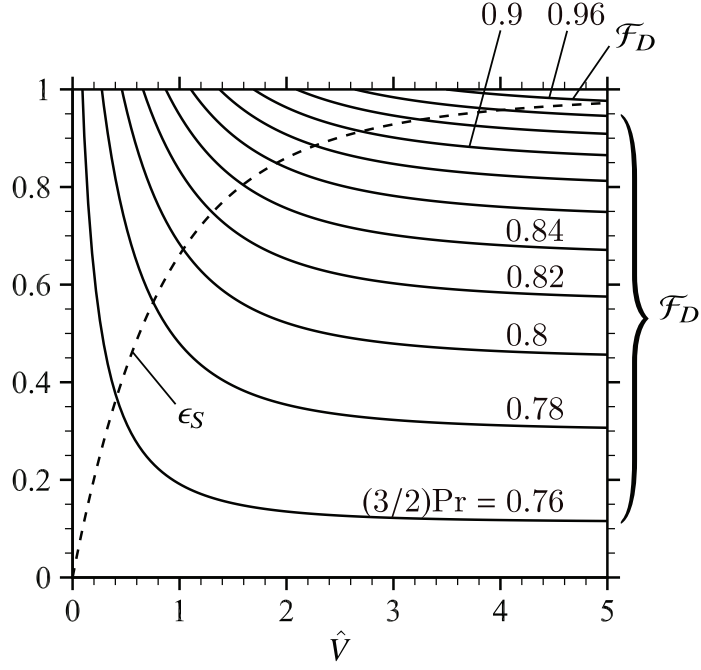


Figure 2.3: The functions $\mathcal{F}_D$ and ϵ_S in the criterion (2.16). The solid lines indicate $\mathcal{F}_D$ for $(3/2)\text{Pr} = 0.76, 0.78, 0.8, \dots, 0.96$, while the dashed line indicates ϵ_S .

plugging (2.15) into (2.8) yields the following criterion for the H theorem to remain valid in the present test:

$$0 \leq \epsilon_S(\hat{V}) < \frac{9(2 - 1/\text{Pr})[\theta_S(\hat{V})^2 - \theta_S(\hat{V}) + 1]}{[1 + \theta_S(\hat{V})]F(\theta_S(\hat{V}); 1 - 1/\text{Pr})} \equiv \mathcal{F}_D(\hat{V}; \text{Pr}), \quad (2.16)$$

where the relation $\nu = 1 - 1/\text{Pr}$ has been used to convert ν to Pr . The function $\mathcal{F}_D$ is plotted by solid lines for various values of Pr in Fig. 2.3, together with ϵ_S by a dashed line. It is seen from the figure that, by the 20 % (resp. 16 %) reduction of Prandtl number from $2/3$, the condition (2.16) is satisfied for the sliding speed $\hat{V} \lesssim 1.03$ (resp. 1.59).

Incidentally, in the time-dependent Couette flow test, even when the condition (2.8) is violated, numerical computations have been carried out stably and consistently, as far as the condition (2.2) is satisfied. This observation agrees with the shock wave test for $\text{Pr} = 1/2$.

2.4.3 Pushing or pulling plate test

Motivated by the sliding plate test, we consider another severe test by the following VDF:

$$f(\boldsymbol{\xi}) = \begin{cases} \frac{\rho_0 \hat{\sigma}}{(2\pi RT_0)^{3/2}} \exp\left(-\frac{(\xi_1 - U)^2 + \xi_2^2 + \xi_3^2}{2RT_0}\right), & \xi_1 > U, \\ \frac{\rho_0}{(2\pi RT_0)^{3/2}} \exp\left(-\frac{\xi_1^2 + \xi_2^2 + \xi_3^2}{2RT_0}\right), & \xi_1 < U, \end{cases} \quad (2.17)$$

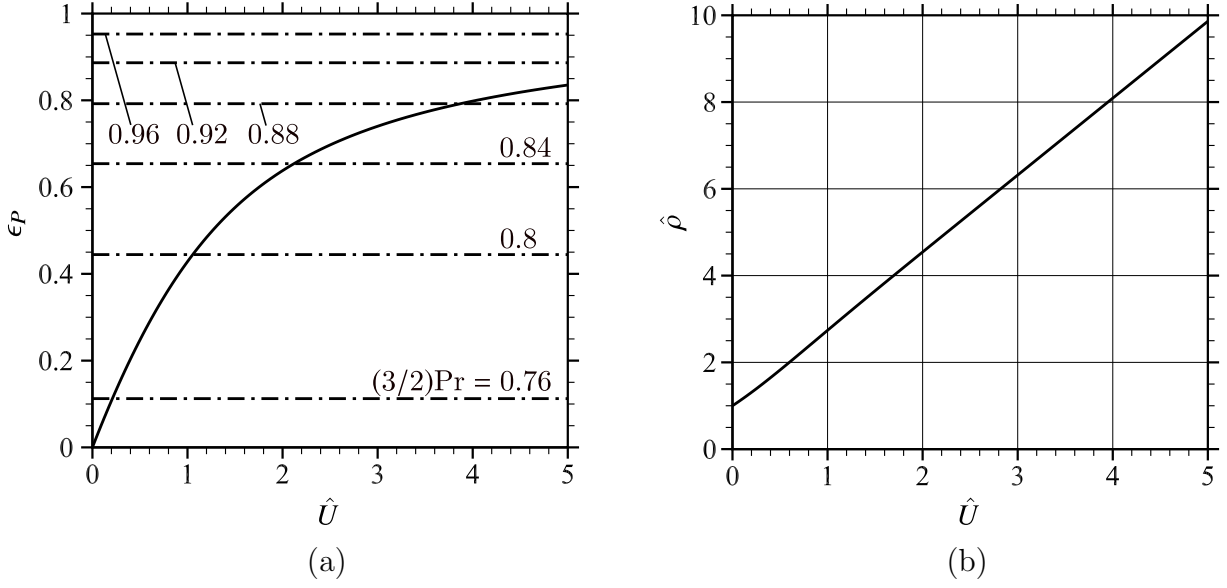


Figure 2.4: The function ϵ_P and the dimensionless density $\hat{\rho}$ in the range $0 < \hat{U} < 5$. (a) ϵ_P , (b) $\hat{\rho}$. In (a), the values of $\mathcal{S}(Pr)$ for $(3/2)Pr = 0.76, 0.8, 0.84, \dots, 0.96$ are also indicated by dash-dotted lines for reference.

where

$$\hat{\sigma}(\hat{U}) = \frac{1}{\rho_0} \sqrt{\frac{2\pi}{RT_0}} \int_{\xi_1 < U} |\xi_1 - U| f d\xi = \exp(-\hat{U}^2) + \sqrt{\pi} \hat{U} [1 + \text{erf}(\hat{U})],$$

$$\hat{U} = U / \sqrt{2RT_0}.$$

The above VDF mimics the gas on the plate at the initial instance of a sudden plate motion in the normal direction with a constant speed $|U|$, by supposing that, before starting the plate motion, the gas is in the equilibrium state at rest with density ρ_0 and temperature T_0 . Here, $U > 0$ implies the pushing plate while $U < 0$ implies the pulling plate.

In this case, Θ is diagonal with $\Theta_{22} = \Theta_{33}$ as in the shock wave test, and the diagonal components are given by

$$\Theta_{11}/(RT_0) = 1 + (\hat{U}/\sqrt{\pi})\hat{\sigma}(\hat{U})/\hat{\rho}(\hat{U}), \quad \Theta_{22} = \Theta_{33} = RT_0, \quad (2.18)$$

where $\hat{U} = U/\sqrt{2RT_0}$ and $\hat{\rho}(\hat{U}) = (1/2)[\hat{\sigma}(\hat{U}) + 1 + \text{erf}(\hat{U})]$ is the gas density divided by ρ_0 . Note that $\hat{\sigma} > 0$ because of its definition. Accordingly, $\Theta_{11} \geq RT_0$ for $\hat{U} \geq 0$ and ϵ is written as

$$\epsilon = 1 - (RT_0/\Theta_{11})^{\pm 1}, \quad \hat{U} \gtrless 0, \quad (2.19)$$

in the present test. In the pushing plate case ($\hat{U} > 0$), θ is equal to 1, and the condition (2.8) takes the same form as (2.12). Substitution of (2.19) into (2.12) eventually leads to

the following condition:

$$0 \leq \epsilon_P(\hat{U}) < \mathcal{S}(\text{Pr}), \quad (2.20)$$

where

$$\epsilon_P(\hat{U}) = 1 - \left(1 + (\hat{U}/\sqrt{\pi})\hat{\sigma}(\hat{U})/\hat{\rho}(\hat{U})\right)^{-1}, \quad \hat{U} > 0. \quad (2.21)$$

Figure 2.4 shows the functions ϵ_P and $\hat{\rho}$ respectively in (a) and (b), where the values of $\mathcal{S}(\text{Pr})$ are also shown for reference in (a). In contrast, in the pulling plate case ($\hat{U} < 0$), θ is equal to 0, and no restriction on the range of ϵ arises (see (2.6)). That is, the ES model with $\text{Pr} < 2/3$ keeps a good entropic property unconditionally in the pulling plate test. The present test assesses the robustness of the desired entropic property for small Prandtl numbers against the anisotropy caused by strong compression (or expansion). In this sense, the type of test is similar to that in the shock wave case. Nevertheless, the observed robustness looks quite different. One possible explanation is the compression rate measured by the density. In the shock wave test, the ratio of density ρ_+/ρ_- between the upstream and the downstream infinity is at most four even in the limit $M_- \rightarrow \infty$, see (2.10). But here, the ratio of the density to its initial value $\hat{\rho}$ or its inverse is beyond this value already around $\hat{U} = 1.70$ (or -0.73). The present test is thus much harder than the shock wave test.

2.5 Concluding remarks

In the present paper, we have investigated the criterion for the H theorem to hold even for the ES model with the Prandtl number below $2/3$. The derived condition that covers the range $1/2 \leq \text{Pr} < 2/3$ shows that indeed there is a room for the H theorem to remain valid. The practical tolerance of the condition is assessed numerically by a couple of tests, i.e., the strong shock wave and the time-dependent Couette flow problem, and then further assessed by the sliding and the pushing/pulling plate problem. The condition is tolerant in the shock wave test enough to accept about 18% reduction of Pr below $2/3$ even for the strong shock wave with $M_- = 5$, while it is rather restrictive in the Couette flow, the sliding plate, and the pushing plate test in the sense that the acceptable reduction of Pr of the same level is achieved only within 1.4 for both $\hat{U}$ and $\hat{V}$. The latter three tests show that the collisionless gas state caused by the sudden motion of boundary can be a practical source of restriction on the entropic property of the ES model for small Prandtl numbers below $2/3$. However,

in the pulling plate test, there is no restriction on the entropic property, and the Prandtl number below $2/3$ is acceptable despite such a sudden motion of the boundary.

2.A A brief review of the H theorem in P. Andries et al. (2000)

Proposition 2.1 (the H theorem) of [3], together with the outline of its proof, is shown here in terms of the notation in the present paper.

Let

$$S(\rho, \mathbf{v}, \mathcal{T}) = \min_{g \in \mathcal{X}} \langle H(g) \rangle, \quad (2.22)$$

where $H(f) = f \ln f$, $\langle \bullet \rangle = \int \bullet d\boldsymbol{\xi}$, and $\mathcal{X}(\rho, \mathbf{v}, \mathcal{T})$ is the set defined by $\mathcal{X} = \{g \geq 0, (1 + \xi_i^2)g \in L^1(\mathbb{R}^3), \langle g \rangle = \rho, \langle \xi_i g \rangle = \rho v_i, \langle \xi_i \xi_j g \rangle = \rho v_i v_j + \rho \mathcal{T}_{ij}\}$. Then, the following proposition is proved in [3].

Proposition: For symmetric positive definite tensor Θ and $-1/2 \leq \nu < 1$ we have

- (a) the tensor $\mathcal{T}$ defined in (2.1c) is symmetric positive definite and the set $\mathcal{X}(\rho, \mathbf{v}, \mathcal{T})$ is not empty,
- (b) the unique minimizer in (2.22) is the Gaussian $\mathcal{G}[f]$ defined in (2.1b),
- (c) the entropy of the Gaussian $\mathcal{G}[f]$ satisfies $\langle H(\mathcal{G}) \rangle = S(\rho, \mathbf{v}, \mathcal{T}) \leq S(\rho, \mathbf{v}, \Theta) \leq \langle H(f) \rangle$,
- (d) consequently the entropy inequalities

$$\int Q_{\text{ES}}(f) \ln f d\boldsymbol{\xi} \leq 0, \quad (2.23)$$

$$\frac{\partial}{\partial t} \int H(f) d\boldsymbol{\xi} + \frac{\partial}{\partial X_i} \int \xi_i H(f) d\boldsymbol{\xi} \leq 0, \quad (2.24)$$

hold.

- (e) the equality $\langle H(\mathcal{G}) \rangle = \langle H(f) \rangle$ implies $f = \frac{\rho}{(2\pi RT)^{3/2}} \exp(-\frac{(\boldsymbol{\xi} - \mathbf{v})^2}{2RT})$.

The outline of proof of (a)–(e) given in [3] is as follows.

On (a): The first part is assured by straightforward manipulations in terms of the eigenvalues of Θ (i.e., λ_1 , λ_2 , and λ_3) for $-1/2 \leq \nu \leq 1$. Then second part is valid for such $\mathcal{T}$, because $\mathcal{G}[f]$ belongs to that set.

On (b): The proof relies on the definition of H and its convexity.

On (c): The equality $\langle H(\mathcal{G}) \rangle = S(\rho, \mathbf{v}, \mathcal{T})$ is nothing else than (b). The inequality $S(\rho, \mathbf{v}, \mathcal{T}) \leq S(\rho, \mathbf{v}, \Theta)$ is first reduced to $\det \mathcal{T} \geq \det \Theta$ by using (b). Then, the reduced inequality is validated by an extension of the Brunn–Minkowsky inequality in the range $-1/2 \leq \nu \leq 1$. The inequality $S(\rho, \mathbf{v}, \Theta) \leq \langle H(f) \rangle$ is a consequence of the definition of S .

On (d): This is an immediate consequence of (c) and the convexity of H .

On (e): Because of (d), the equality $\langle H(\mathcal{G}) \rangle = \langle H(f) \rangle$ implies $S(\rho, \mathbf{v}, \Theta) = \langle H(f) \rangle$, which in turn implies that f is the Gaussian with $\mathcal{T}$ being replaced by Θ . It also implies $S(\rho, \mathbf{v}, \mathcal{T}) = S(\rho, \mathbf{v}, \Theta)$, which leads to $\det \mathcal{T} = \det \Theta$. Then, direct calculations of this equality show that Θ is a scalar multiple of the identity matrix and thus f is the Maxwellian given in (e).

As is clear from the above outline, the clue steps for the extension of the validity range of the H theorem are to show that (i) $\mathcal{T}$ is positive definite and (ii) $\det \mathcal{T} \geq \det \Theta$, including that the equality in (ii) holds only when f is the Maxwellian. The discussions in Sec. 2.3 of the present paper focus on the above (i) and (ii).

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Chapter 3

An attempt on an ES-model-based construction of a kinetic equation for a dense gas

3.1 Introduction

Phase transition is a common phenomenon that has been investigated variously from a microscopic to a macroscopic point of view. In the kinetic theory, gas flows caused by the phase transition have been studied so far, e.g., [1,2,3,4,5,6,7], mostly assuming that the state of its condensed phase is given. In the last two decades, a new trend that takes account of the real gas effects emerges, relying on the Enskog or the Enskog–Vlasov equation, thanks to the developments of a stochastic [8] and a deterministic [9] numerical algorithm. However, the studies based on those equations are still computationally demanding, even compared with the Boltzmann equation. A construction of a simpler kinetic equation is worthwhile studying toward a further understanding of the non-equilibrium aspect of dense gas flows. It is also expected to advance our understanding of the kinetic theory for dense gases through close observations of the influence of the simplification procedure.

Based on the above points of view, we have been attempting to construct a simpler kinetic equation. The first construction was made under the isothermal assumption [10,11] and then its extension [12] was made for removing the isothermal assumption. These simple kinetic equations were successfully applied to the study of phase separations from a uniform equilibrium state. They are equipped with a monotonically decreasing function, in contrast to the original Enskog and the Enskog–Vlasov equation, that makes it possible to give thermodynamic interpretations of the numerical simulation results. In spite of these benefits, the previous models still have a potential weakness that they do not have transport properties consistent with the existing Enskog theory, since the Bhatnagar–Gross–Krook (BGK)-type [13,14] collision term is adopted. In the present study, we will report an attempt to fix the weakness mainly by using the Ellipsoidal-Statistical (ES)-type [15,16] collision term. A merit and a demerit of the attempt will be discussed based on the results of [17], and some results

of numerical simulations of the phase separation from a uniform equilibrium state will be presented.

3.2 Previous model

3.2.1 Previous BGK-based model

The model constructed in [10,11] under the isothermal assumption is presumably the simplest kinetic model that reproduces phase change phenomena and is characterized by two features: first, by its relaxation collision term that drives the system towards a resting Maxwellian of a given uniform temperature and, second, by treating the long-range and the short-range collective interaction in the force term. The collective short-range one is determined in a heuristic phenomenological way to be treated as a local internal force. The model conserves only the mass; the momentum and energy are not conserved because the relaxation term is intended to represent interactions with a heat bath. Even with the simplest model, we were able to study a linear stability of a given uniform equilibrium state, to observe numerically the occurrence of phase change from a single-phase to a two-phase state, and also to establish a minimization problem in spatially periodic systems for the van der Waals fluids.

Motivated by satisfactory results in [10,11], an attempt [12] was also made to remove the isothermal assumption with the aid of a BGK-type collision term. This section briefly summarizes the model in [12] and serves as a starting point for the discussion that follows.

Let $f(t, \mathbf{X}, \boldsymbol{\xi})$ be the velocity distribution function (VDF) of molecules, where t , $\mathbf{X}$, and $\boldsymbol{\xi}$ are a time, a position, and a molecular velocity, respectively. The previous BGK-based model [12] developed from the simplest isothermal model [10,11] is written as

$$\frac{\partial f}{\partial t} + \xi_i \frac{\partial f}{\partial X_i} + F_i \frac{\partial f}{\partial \xi_i} = A(\rho, T)(f_e - f) + Q_d[f], \quad A(\rho, T) = \frac{A_c(T)\rho}{1 - b\rho} > 0, \quad (3.1a)$$

$$F_i = -\frac{\partial}{\partial X_i}(\Phi_S(\rho, T) + \Phi_L[\rho]), \quad f_e = \frac{\rho}{(2\pi RT)^{3/2}} \exp\left(-\frac{\mathbf{c}^2}{2RT}\right), \quad \mathbf{c} = \boldsymbol{\xi} - \mathbf{v}, \quad (3.1b)$$

$$Q_d[f] = -\frac{\partial}{\partial \xi_i}[(\alpha_i + \beta c_i)f], \quad (3.1c)$$

$$\alpha_i = \frac{1}{\rho} \int \frac{\partial \Phi_S}{\partial T} d\rho \frac{\partial T}{\partial X_i}, \quad \beta = \frac{1}{3R\rho} \left\{ \frac{\partial}{\partial t} \int \frac{\partial \Phi_S}{\partial T} d\rho + \frac{\partial}{\partial X_i} (v_i \int \frac{\partial \Phi_S}{\partial T} d\rho) \right\}, \quad (3.1d)$$

where ρ , $\mathbf{v}$, and T are the density, the flow velocity, and the temperature of the gas defined

as moments of f over the whole range of $\boldsymbol{\xi}$:

$$\rho = \int f d\boldsymbol{\xi}, \quad v_i = \frac{1}{\rho} \int \xi_i f d\boldsymbol{\xi}, \quad T = \frac{1}{3R\rho} \int \mathbf{c}^2 f d\boldsymbol{\xi}, \quad (3.1e)$$

$A_c(T) > 0$ (see the Appendix A of [12]), and R is the specific gas constant. In (3.1c) and hereafter, unless otherwise stated, the integrations with respect to ρ are indefinite integrals along the isothermal process. For the van der Waals fluids, the pressure p is given by the following equation of state

$$p = \frac{\rho RT}{1 - b\rho} - a\rho^2, \quad (a, b : \text{positive constants}). \quad (3.1f)$$

The terms containing Φ_S or its derivatives represent short-range interactions of collective nature and are treated as local internal forces in fluid. With the aid of the momentum balance, the pressure p is seen to be related to f and Φ_S as

$$p = \frac{1}{3} \int \mathbf{c}^2 f d\boldsymbol{\xi} + \int \rho \frac{\partial \Phi_S}{\partial \rho} d\rho. \quad (3.1g)$$

The form of Φ_S is thus determined by comparison with (3.1f) as

$$\Phi_S = -RT \ln(1 - b\rho) + \frac{b\rho RT}{1 - b\rho} - 2a\rho. \quad (3.1h)$$

Hence it holds as well that

$$\int \frac{\partial \Phi_S}{\partial T} d\rho = -\rho R \ln(1 - b\rho). \quad (3.1i)$$

In the meantime, within the diffusive approximation, the form of Φ_L in the term F_i is reduced to

$$\Phi_L = -\kappa \Delta \rho, \quad (3.1j)$$

where $\Delta \equiv \partial^2 / \partial X_i^2$ is the Laplacian and κ is a given positive constant.¹ Further details can be found in [12].

Once the form of A_c and the other constant parameters are specified, the system (3.1) is closed. The system conserves the mass, momentum, and energy and was used to study the dynamics of phase separation from a uniform equilibrium state in a periodic domain in [12]. Comparisons with simulation results for the isothermal model [11] and related discussions

¹The parameter κ can be related to a in the equation of state, once the long-range attractive potential is specified. Nevertheless, κ and a are regarded as independent parameters here. This reflects a degree of freedom on the choice of attractive potential.

can be found in the Appendix D of [12]. Moreover, for the above system (3.1) in a periodic domain, a minimization problem can be established. Indeed, the following function

$$H(t) = \int_D \left(\int f \ln \frac{f}{c_0} d\boldsymbol{\xi} + \frac{1}{R} \int \frac{\partial \Phi_S}{\partial T} d\rho \right) d\mathbf{X}, \quad (3.2)$$

is found to decrease monotonically in time, where c_0 is a positive constant with the same physical dimension as f and D is a unit region of a periodic domain in $\mathbf{X}$. The monotone change of H drives the fluid (or dense gas) to an equilibrium state with a uniform temperature and uniform flow velocity. These uniform values are determined under the constraints of the total mass, momentum, and energy. However, the density is not necessarily uniform, due to the second term on the right-hand side of (3.2), i.e., a contribution of the dense gas effect that is absent in the dilute gas limit. Equipped with the monotone function H , the previous model allows us to develop thermodynamic discussions and interpretations for the phenomenon observed in numerical simulations. It is a benefit in addition to its simple structure.

3.2.2 Fluid-dynamic limit and transport properties

By taking the 1-, the ξ_j -, and the $(1/2)\boldsymbol{\xi}^2$ -moment of (3.1a), the following set of balance laws of the mass, momentum, and energy is obtained:

$$\frac{\partial}{\partial t} \rho + \frac{\partial}{\partial X_i} (\rho v_i) = 0, \quad (3.3a)$$

$$\frac{\partial}{\partial t} \rho v_j + \frac{\partial}{\partial X_i} (\rho v_i v_j + p_{ij}) + \rho \frac{\partial \Phi_L}{\partial X_j} = 0, \quad (3.3b)$$

$$\frac{\partial}{\partial t} \left[\rho \left(e + \frac{1}{2} \mathbf{v}^2 \right) \right] + \frac{\partial}{\partial X_i} \left[\rho v_i \left(e + \frac{1}{2} \mathbf{v}^2 \right) + p_{ij} v_j + q_i \right] + \rho v_i \frac{\partial \Phi_L}{\partial X_i} = 0, \quad (3.3c)$$

where p_{ij} , q_i , and e are the stress tensor, the heat-flow vector, and the specific energy defined by

$$p_{ij} = p \delta_{ij} + \int \left(c_i c_j - \frac{1}{3} \mathbf{c}^2 \delta_{ij} \right) f d\boldsymbol{\xi}, \quad q_i = \frac{1}{2} \int c_i \mathbf{c}^2 f d\boldsymbol{\xi}, \quad (3.4a)$$

$$\rho e = \frac{3}{2} \rho R T + \int \left(\Phi_S - T \frac{\partial \Phi_S}{\partial T} \right) d\rho. \quad (3.4b)$$

In the fluid-dynamic limit, the stress tensor and heat-flow vector are reduced to

$$p_{ij} = p \delta_{ij} - \frac{\rho R T}{A(\rho, T)} \left(\frac{\partial v_i}{\partial X_j} + \frac{\partial v_j}{\partial X_i} - \frac{2}{3} \frac{\partial v_k}{\partial X_k} \delta_{ij} \right), \quad q_i = -\frac{5}{2} R \frac{\rho R T}{A(\rho, T)} \frac{\partial T}{\partial X_i}, \quad (3.5)$$

by the standard procedure for the limit, which is omitted here. Accordingly the set of balance laws (3.3) is reduced to the Navier–Stokes set of equations with higher order derivative terms of density through $\nabla\Phi_L$.

We now address main issues to be discussed in the rest of the present paper. The ratio of the viscosity $\rho RT/A$ and the thermal conductivity $(5/2)R\rho RT/A$ in (3.5) implies that the Prandtl number is unity, irrespective of a specific form of A , inheriting a weakness of the BGK-type collision integral. Another weakness is that the bulk viscosity predicted by the Enskog theory [18] is absent. The next section is devoted to a modification of the model to fix these potential weaknesses.

3.3 A modified model with an ES-model-type collision term

3.3.1 Modified model and its transport properties

Key elements in the modified model are, first, to use an ES-model-type collision term [15,16] instead of the BGK-type term and, second, to put additional terms to Q_d . The modified model is written as

$$\frac{\partial f}{\partial t} + \xi_i \frac{\partial f}{\partial X_i} + F_i \frac{\partial f}{\partial \xi_i} = Q_c^\sharp[f] + Q_d^\sharp[f], \quad (3.6a)$$

$$Q_c^\sharp[f] = A^\sharp(\rho, T)(\mathfrak{G} - f), \quad \mathfrak{G} = \frac{\rho}{\sqrt{\det(2\pi\mathfrak{T})}} \exp\left(-\frac{1}{2}(\mathfrak{T}^{-1})_{ij}c_i c_j\right), \quad (3.6b)$$

$$\mathfrak{T}_{ij} = (1 - \nu(\rho))RT\delta_{ij} + \nu(\rho)\Theta_{ij}, \quad \Theta_{ij} = \frac{1}{\rho} \int c_i c_j f d\boldsymbol{\xi}, \quad (3.6c)$$

$$Q_d^\sharp[f] = -\frac{\partial}{\partial \xi_i}[(\alpha_i^\sharp + \beta^\sharp c_i)f], \quad (3.6d)$$

$$\alpha_i^\sharp = \alpha_i + \frac{1}{\rho} \frac{\partial}{\partial X_i} \left(\mu_B \frac{\partial v_k}{\partial X_k} \right), \quad \beta^\sharp = \beta + \frac{\mu_B}{3R\rho T} \left(\frac{\partial v_k}{\partial X_k} \right)^2, \quad (3.6e)$$

where F_i is the same as that in the previous model, $\mathfrak{T}^{-1}$ is the inverse of the tensor $\mathfrak{T}$, μ_B and $A^\sharp$ are positive functions of ρ and T to be determined in accordance with the Enskog theory for the transport coefficients, and $\nu(\rho)$ is an adjusting parameter function of ρ .² The modified model keeps the set of balance equations (3.3) unchanged by the following change of the stress tensor:

$$p_{ij} = p\delta_{ij} + \int \left(c_i c_j - \frac{1}{3} \mathbf{c}^2 \delta_{ij} \right) f d\boldsymbol{\xi} - \mu_B \frac{\partial v_k}{\partial X_k} \delta_{ij}. \quad (3.7)$$

²Originally in [15,16], ν is not a function but a constant for adjusting the value of the Prandtl number.

Then, in the fluid-dynamic limit, the stress tensor and heat-flow vector are reduced to

$$p_{ij} = p\delta_{ij} - \frac{1}{1 - \nu(\rho)} \frac{\rho RT}{A^\sharp(\rho, T)} \left(\frac{\partial v_i}{\partial X_j} + \frac{\partial v_j}{\partial X_i} - \frac{2}{3} \frac{\partial v_k}{\partial X_k} \delta_{ij} \right) - \mu_B \frac{\partial v_k}{\partial X_k} \delta_{ij}, \quad (3.8a)$$

$$q_i = -\frac{5}{2} R \frac{\rho RT}{A^\sharp(\rho, T)} \frac{\partial T}{\partial X_i}, \quad (3.8b)$$

by the standard procedure for the limit. Thus, in the modified model, the bulk viscosity is recovered and identified as μ_B , and the viscosity μ and the thermal conductivity λ are expressed in the form $\rho RT/((1 - \nu)A^\sharp)$ and $(5/2)R(\rho RT/A^\sharp)$, respectively. It is also seen that the Prandtl number is expressed as $\text{Pr}(\equiv (5/2)(R\mu/\lambda)) = 1/[1 - \nu(\rho)]$.

In the meantime, according to the Enskog theory, the viscosity μ , bulk viscosity μ_B , and the thermal conductivity λ are expressed as [18,19]

$$\mu = \frac{\mu_0}{\chi} \left[1 + \frac{16}{5} \phi \chi + 12.2(\phi \chi)^2 \right], \quad \mu_B = \frac{\mu_0}{\chi} (4\phi \chi)^2, \quad (3.9a)$$

$$\lambda = \frac{\lambda_0}{\chi} \left[1 + \frac{24}{5} \phi \chi + 12.1(\phi \chi)^2 \right], \quad (3.9b)$$

where μ_0 and λ_0 are respectively the viscosity and thermal conductivity in the dilute gas limit, while ϕ and χ are dense gas factors that can be related to the exclusion parameter b in the equation of state for the van der Waals fluids as

$$\phi = \frac{1}{4} b\rho, \quad \chi = \frac{1}{1 - b\rho}, \quad (3.10)$$

see the discussions in the Appendix A of [12] for details. Hence, substituting (3.10) into (3.9), $A^\sharp$ and $\nu(\rho)$ in the system (3.6) as well as the transport coefficients are all expressed in terms of ρ , T , and the exclusion parameter b :

$$A^\sharp(\rho, T) = \frac{5}{2} \frac{\rho RT}{1 - b\rho} \frac{R/\lambda_0(T)}{g_2(\frac{b\rho}{1-b\rho})}, \quad \nu(\rho) = 1 - \frac{2}{5} \frac{1}{R} \frac{\lambda_0(T)}{\mu_0(T)} \frac{g_2(\frac{b\rho}{1-b\rho})}{g_1(\frac{b\rho}{1-b\rho})} = 1 - \frac{1}{\text{Pr}_0} \frac{g_2(\frac{b\rho}{1-b\rho})}{g_1(\frac{b\rho}{1-b\rho})}, \quad (3.11a)$$

$$\mu(\rho, T) = (1 - b\rho) g_1 \left(\frac{b\rho}{1 - b\rho} \right) \mu_0(T), \quad \mu_B(\rho, T) = (1 - b\rho) \left(\frac{b\rho}{1 - b\rho} \right)^2 \mu_0(T), \quad (3.11b)$$

$$\lambda(\rho, T) = (1 - b\rho) g_2 \left(\frac{b\rho}{1 - b\rho} \right) \lambda_0(T), \quad (3.11c)$$

where

$$g_1(x) = 1 + \frac{4}{5}x + \frac{6.1}{8}x^2, \quad g_2(x) = 1 + \frac{6}{5}x + \frac{12.1}{16}x^2, \quad (3.11d)$$

and Pr_0 is the Prandtl number in the dilute gas limit, usually set as $\text{Pr}_0 = 2/3$ for monatomic gases. The system (3.6) with (3.11) thus forms a closed kinetic model with appropriate transport coefficients.

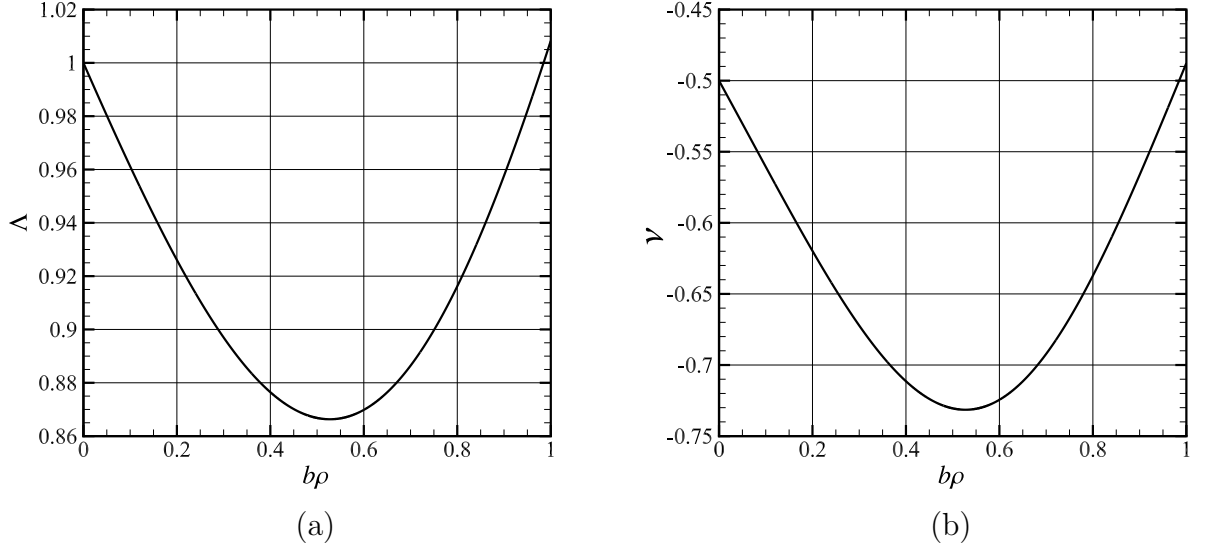


Figure 3.1: Dependence of Λ and ν on the density. (a) $\Lambda(\frac{b\rho}{1-b\rho})$ vs. $b\rho$, (b) $\nu(\rho)$ vs. $b\rho$ for $\text{Pr}_0 = 2/3$.

Before closing this small section, it should be noted that the BGK-based model (3.1) is readily recovered by putting $A^\sharp = A$, $\nu(\rho) = 0$, and $\mu_B = 0$ in the proposed model (3.6).

3.3.2 Monotonic property and related discussions

We shall discuss the monotone property of the new model (3.6) with (3.11) in a periodic domain. Let D denote a unit region of the periodic domain. Multiplying (3.6a) by $1 + \ln(f/c_0)$ and integrating the result over the whole range of ξ and over the unit region D yield

$$\begin{aligned} \frac{d}{dt} \int_D \int f \ln \frac{f}{c_0} d\xi d\mathbf{X} &= \int_D \int Q_c^\sharp[f] \ln \frac{f}{c_0} d\xi d\mathbf{X} + \int_D \int Q_d^\sharp[f] \ln \frac{f}{c_0} d\xi d\mathbf{X} \\ &= \int_D \int Q_c^\sharp[f] \ln \frac{f}{c_0} d\xi d\mathbf{X} - 3 \int_D \beta^\sharp \rho d\mathbf{X}. \end{aligned} \quad (3.12)$$

Note that the second and the third term of (3.6a) do not contribute because of the periodic condition in space and the rapid decay of VDF in molecular speed. After a few manipulations making use of the definition of β and of the periodic condition again, we have

$$\frac{d}{dt} H(t) = \int_D \int Q_c^\sharp[f] \ln \frac{f}{c_0} d\xi d\mathbf{X} - \int_D \frac{\mu_B}{RT} \left(\frac{\partial v_k}{\partial X_k} \right)^2 d\mathbf{X} \leq \int_D \int Q_c^\sharp[f] \ln \frac{f}{c_0} d\xi d\mathbf{X}, \quad (3.13)$$

see the definition (3.2). Therefore, provided that $\int Q_c^\sharp[f] \ln(f/c_0) d\xi \leq 0$, the monotonic property is retained as well in the modified model.

Although $\int Q_c^\sharp[f] \ln(f/c_0) d\xi \leq 0$ is one of the merits to use the ES-model, it should be reminded that it holds unconditionally only when the adjusting parameter function $\nu(\rho)$ is

in the range $[-1/2, 1)$, i.e., the Prandtl number $\text{Pr}(\equiv \frac{5}{2} \frac{R\mu}{\lambda}) = 1/(1 - \nu(\rho))$ should be in the range $[2/3, \infty)$. [16] In the present case, it is written from (3.11) as

$$\text{Pr} = \text{Pr}_0 \Lambda \left(\frac{b\rho}{1 - b\rho} \right), \quad \Lambda(x) = \frac{g_1(x)}{g_2(x)} = 1 - \frac{\frac{2}{5}x(1 - \frac{x}{64})}{g_2(x)}. \quad (3.14)$$

If $\Lambda \geq 1$, the monotonicity is assured unconditionally, but actually it decreases from unity as $b\rho$ increases, reaches its minimum 0.8663 at $b\rho = 0.5274$, and then increases, as shown in Fig. 3.1(a). When Λ takes its minimum, both Pr and ν for $\text{Pr}_0 = 2/3$ take their minima 0.5775 and -0.7315 , see Fig. 3.1(b) for the latter. Therefore, the monotonicity of H [or $\int Q_c^\sharp[f] \ln(f/c_0) d\boldsymbol{\xi} \leq 0$] is not fully guaranteed. Nevertheless, $\int Q_c^\sharp[f] \ln(f/c_0) d\boldsymbol{\xi} \leq 0$ still holds, provided that (i) $\mathfrak{T}$ is positive definite and (ii) $\det \mathfrak{T} \geq \det \Theta$, see [17]. This is a consequence of a close observation of the original proof [16] of the H theorem for $\nu \geq -1/2$. A similar discussion on a Fokker–Planck model can be found in [20]. Below is the quantitative criterion for $\int Q_c^\sharp[f] \ln(f/c_0) d\boldsymbol{\xi} \leq 0$ to hold obtained in [17]:

Keeping in mind that Θ is a symmetric positive definite tensor by definition, let $\lambda_1 \leq \lambda_2 \leq \lambda_3$ be its positive real eigenvalues, and introduce the notation $\epsilon \equiv 1 - \lambda_1/\lambda_3$. If three eigenvalues are the same, $\mathfrak{T}$ and Θ are identical and are reduced to $\mathfrak{T} = \Theta = RT\mathbb{I}$, where $\mathbb{I}$ is the identity tensor. Then, the conditions (i) and (ii) are automatically satisfied, i.e., there is no restriction when $\epsilon = 0$. If $\lambda_1 \neq \lambda_3$ (or $\epsilon \neq 0$), introduce another notation $\theta = (1 - \lambda_2/\lambda_3)/(1 - \lambda_1/\lambda_3)$. Note that $0 < \epsilon < 1$ and $0 \leq \theta \leq 1$ by construction. Then, for $-1 \leq \nu < -1/2$, which corresponds to $1/2 \leq \text{Pr} < 2/3$, the following criterion must be fulfilled to assure that $\int Q_c^\sharp[f] \ln(f/c_0) d\boldsymbol{\xi} \leq 0$:

$$\begin{cases} 0 < \epsilon < 1, & \text{for } 0 \leq \theta \leq \frac{2+\nu}{1-\nu}, \\ 0 < \epsilon < \frac{9(1+\nu)(\theta^2 - \theta + 1)}{(1+\theta)(1-\nu)^2(\frac{2\nu+1}{1-\nu} + \theta)(\frac{2\nu+1}{1-\nu}\theta + 1)}, & \text{for } \frac{2+\nu}{1-\nu} < \theta \leq 1. \end{cases} \quad (3.15)$$

This criterion implies that the monotonicity of $H(t)$ is assured except for highly anisotropic non-equilibrium state. Numerical assessments of the criterion can be found in [17]. Although ν in [17] is not dependent on the density, it does not affect the criterion (3.15).

3.4 Numerical simulations of phase separation

Numerical simulations have been conducted to test a capability of the proposed model for a modeling of phase separation. In each simulation, a dense gas is confined in a spatially

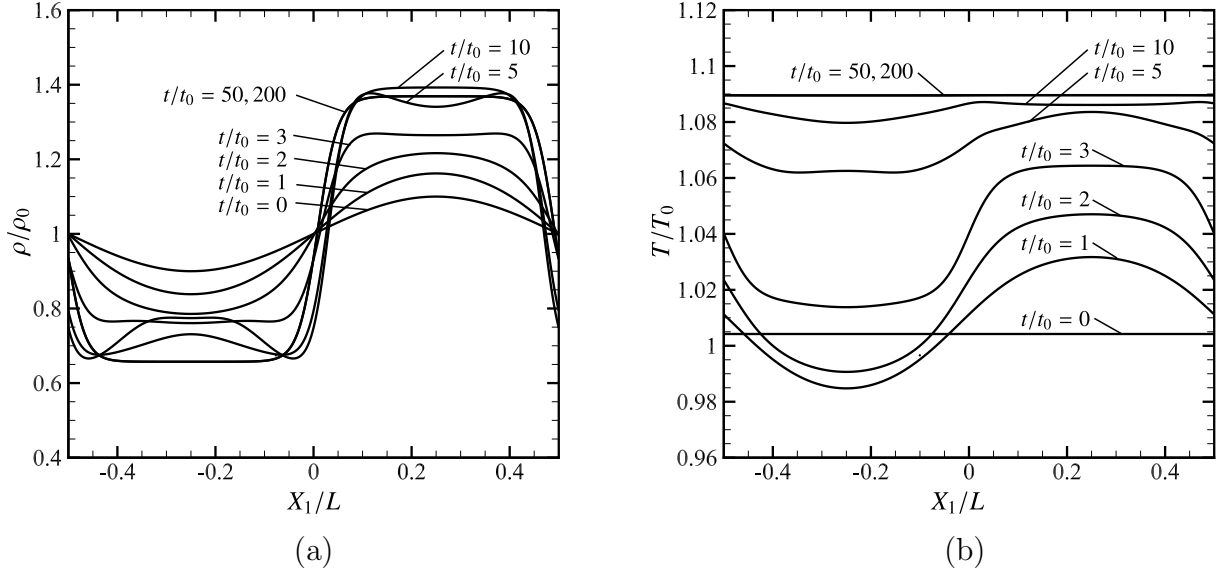


Figure 3.2: Time evolutions of the density and temperature in the case $\omega = 0.1$, $b\rho_0 = 1/3$, $c = 3.8$, $K = 1.0 \times 10^{-4}$, and $k^\# = 0.1$. (a) density, (b) temperature. In both panels, $t_0 = L/\sqrt{2RT_0}$.

one-dimensional periodic domain with D being its unit region, and a time evolution from a uniform equilibrium state at rest by an initial sinusoidal perturbation

$$\rho(0, X_1) = \rho_0[1 + \omega \sin(2\pi X_1/L)], \quad (3.16)$$

is studied, where ρ_0 is the average density of the gas, L is the length of the unit region, and ω is a factor of the initial perturbation size. Because of the total mass, momentum, energy constraints [see (3.3)], the initial disturbance of density causes the initial uniform temperature different from the temperature T_0 of the undisturbed uniform equilibrium state. The flow velocity in the initial Maxwellian is set zero.

In the present target of simulations, the tensor Θ is diagonal and isotropic in the directions perpendicular to X_1 . Hence, the criterion (3.15) is reduced to

$$\eta(t, X_1) \equiv 1 - \frac{\Theta_{22}}{\Theta_{11}} < \frac{9}{2} \frac{\nu(\rho) + 1}{[\nu(\rho) + 2]^2}, \quad (3.17)$$

if $\Theta_{11} > \Theta_{22}$ [put $\theta = 1$ in (3.15)]. If $\Theta_{11} \leq \Theta_{22}$, the monotonicity of H is automatically satisfied, since θ in the condition (3.15) is zero. Note that the most right-hand side is a monotonically increasing function of ν in the range $\nu \in (-1, -1/2]$ and never becomes below 0.7509 at the minimum $\nu \approx -0.7315$, see Fig. 3.1(b).

Figure 3.2 shows time evolutions of the density and temperature from the perturbed uniform state to a *two-phase* state in the case $\omega = 0.1$, $b\rho_0 = 1/3$, $c \equiv a/(bRT_0) = 3.8$,

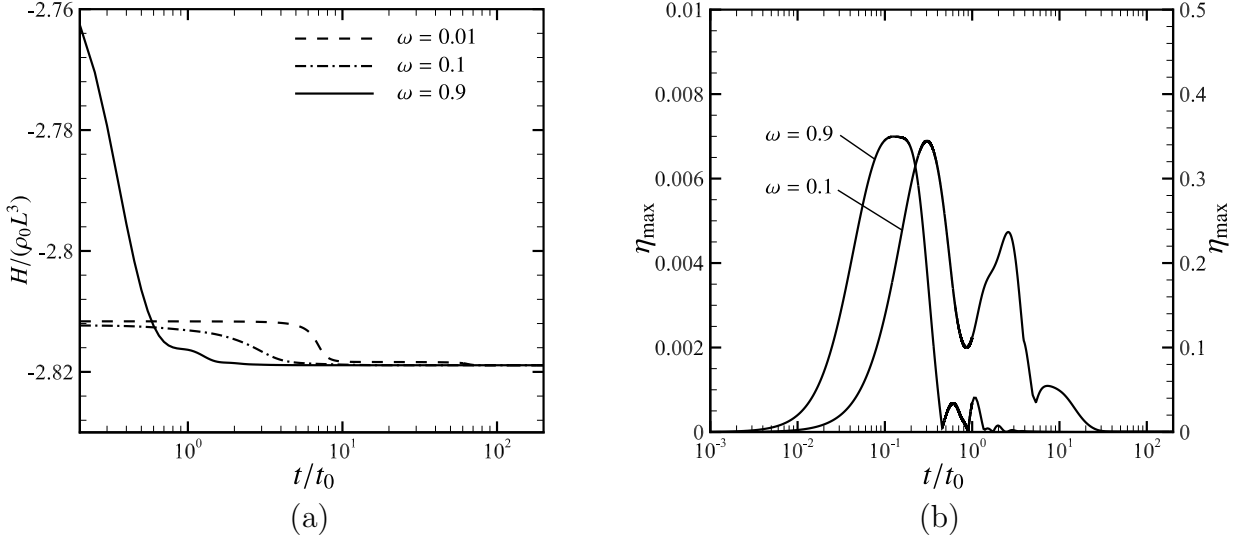


Figure 3.3: Time evolution of $H(t)$ and the anisotropy $\eta_{\max}(t)$ in the same case as Fig. 3.2. (a) $H(t)$, (b) $\eta_{\max}(t)$. In (b), the left-hand axis is for $\omega = 0.1$, while the right-hand axis is for $\omega = 0.9$. The sizes ω of the initial disturbances are shown in each panel. See also the caption of Fig. 3.2.

$K \equiv \kappa/(2bRT_0L^2) = 1.0 \times 10^{-4}$, and $k^\sharp = (\sqrt{\pi}/2)\text{Kn}^\sharp \equiv \sqrt{2RT_0}/(A^\sharp(\rho_0, T_0)L) = 0.1$, where $\text{Pr}_0 = 2/3$ and $\lambda_0(T)$ is chosen as the one for hard-sphere molecules in the dilute gas limit. Among the above parameters, the parameter set of $b\rho_0$ and $a/(bRT_0)$ controls a thermodynamic stability of the uniform equilibrium state [12]. The present choice of values falls into the thermodynamically unstable regime; accordingly, even starting with much smaller disturbance, say $\omega = 0.01$, the phase separation to the same two-phase state occurs, though the figure of results is omitted here. Thermodynamically stable, metastable, and unstable regimes are not influenced by the change of the kinetic model from (3.1) to (3.6).

Figure 3.3(a) shows time evolutions of the function $H(t)$ for three initial disturbances $\omega = 0.01, 0.1$, and 0.9 in (3.16), the other parameters being the same as Fig. 3.2. The perturbed initial state is a local Maxwellian, but is not a solution of (3.6). Hence, the H changes more largely for larger ω . It monotonically decreases in time in each case as desired. Intuitively, the degree of anisotropy of VDF is expected to be small. Indeed, as shown in Fig. 3.3(b), $\eta_{\max}(t) \equiv \max_{X_1 \in D} \eta(t, X_1)$ is by far below the lower bound of the criteria 0.7509 .

Finally, comparisons are made among the BGK-based model (3.1) with $A_c = (5/2)R^2T/[\lambda_0(T)g_2(\frac{b\rho}{1-b\rho})]$ (model **I**), the proposed model [(3.6) and (3.11) with $\text{Pr}_0 = 2/3$] (model **II**), and the proposed model with $\mu_B = 0$ (model **III**), where $\lambda_0(T)$ is chosen as the one for

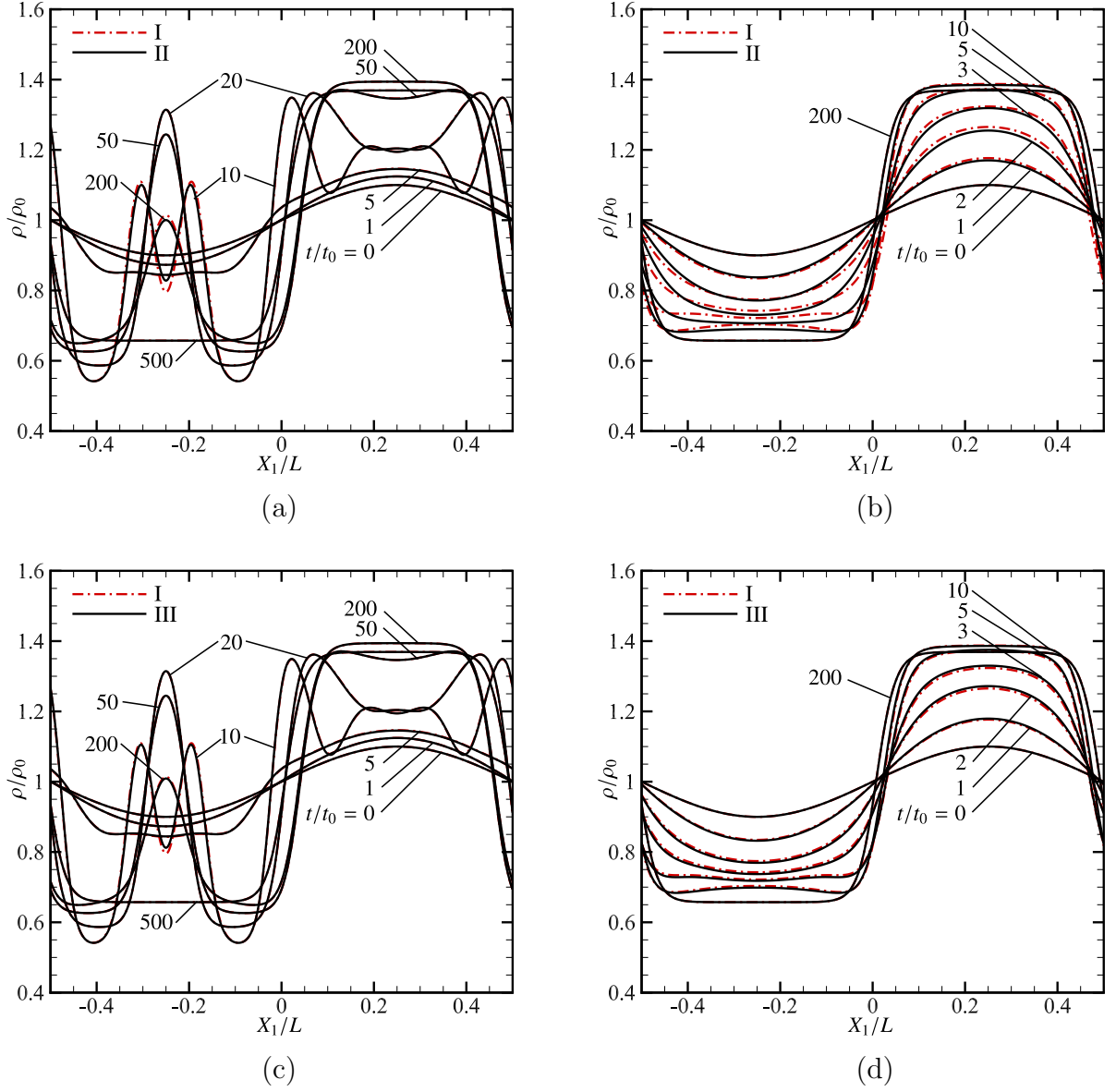


Figure 3.4: Comparisons of time evolutions of density profiles among different models **I**, **II**, and **III** in the case $\omega = 0.1$, $b\rho_0 = 1/3$, $c = 3.8$, and $K = 1.0 \times 10^{-4}$. (a) **I** vs. **II** for $k = 0.01$, (b) **I** vs. **II** for $k = 0.5$, (c) **I** vs. **III** $k = 0.01$, and (d) **I** vs. **III** for $k = 0.5$. See the caption of Fig. 3.2.

hard-sphere molecules. The specific choice of A_c in the model **I** makes $A(\rho, T)$ the same as $A^\sharp(\rho, T)$, and accordingly makes k defined by $k = \sqrt{2RT_0}/[A(\rho_0, T_0)L]$ the same as $k^\sharp$. This choice may be interpreted as that the thermal conductivity λ is taken to be common among the different models in comparisons. Figures. 3.4(a) and 3.4(b) show that the transient process from a single-phase to a two-phase state is close to each other between the models **I** and **II**, especially for $k = 0.01$. However, the results of the models **I** and **III** are much closer to each other, even for $k = 0.5$, as observed in Figs. 3.4(c) and 3.4(d). This means that the difference between the models **I** and **II** is mainly attributed to the effect of the bulk viscosity of the model **II** in the present comparisons.

3.5 Concluding remarks

In the present work, an ES-model-based kinetic equation for a dense gas has been proposed. The model recovers the viscosity, the thermal conductivity, and the bulk viscosity properly. In these aspects, the proposed model has preferable features for the modeling of a dense gas. It has, however, a potential limitation on a monotonicity of the H function; that is, a monotonic property in time is not assured for highly anisotropic non-equilibrium situations as discussed in [17]. Numerical simulations of the phase separation from a uniform equilibrium state are also performed and show the enough ability of the model in such phase separation studies. The two-phase state shows a reasonable agreement with that obtained by the previous model in [12]. Improvement of the monotonic property is left for future works.

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Chapter 4

Constructions of simple kinetic equations for a dense gas

4.1 Introduction

Phase transition is a common phenomenon and has been studied variously from a microscopic to a macroscopic point of view. In the kinetic theory, gas flows caused by the phase transition have been investigated, mostly assuming that the state of its condensed phase is specified, e.g., [1,2,3,4,5,6,7]. In the meantime, a new research direction that employs the real gas effect by the Enskog or the Enskog–Vlasov equation becomes common recently in the literature, thanks to the developments of a stochastic [8] and a deterministic [9] numerical algorithm for them. However, the studies based on those equations are still computationally demanding, even compared to the Boltzmann equation.

A construction of a simpler kinetic equation is thus worth exploring for accelerating that new direction of researches on non-ideal gas flows. It is also expected to advance our understanding of the kinetic theory approach for dense gases through close observations of the influence of the simplification procedure. Motivated by the research background described above, we have been trying to find a simple promising framework of a kinetic model for non-ideal gas phenomena. So far, the models making use of a simple relaxation term and the BGK-type collision term [10,11] worked as desired in [12,13,14]. Nevertheless, they have a potential demerit in transport properties due to the specific choice of the collision model. In order to fix the demerit, a couple of models based on the Ellipsoidal-Statistical (ES)-type collision term [15,16] will be introduced in the present paper.

The paper is organized as follows. Our previous models are briefly reviewed in Sec. 4.2. Then, a couple of new proposals based on the ES-model are presented in Sec. 4.3, where the first ES-based model is described in Sec. 4.3.1 and its potential limitation on the H theorem is explained in Sec. 4.3.2. Then, the second ES-based model is described in Sec. 4.3.3, where the H theorem for the second model is presented. The fluid dynamic limit of the proposed

models is also discussed on the basis of the Chapman–Enskog method in the Appendix. Preliminary numerical tests are presented in Sec. 4.4. The paper is concluded in Sec. 4.5.

4.2 Previous models

4.2.1 Outline of previous models

Our attempts for the construction of a simple kinetic model started from the following simplest one under the isothermal assumption:

$$\frac{\partial f}{\partial t} + \xi_i \frac{\partial f}{\partial X_i} + F_i^* \frac{\partial f}{\partial \xi_i} = C_*[f], \quad C_*[f] = A_*(\rho)(\rho M_* - f), \quad (4.1a)$$

$$F_i^* = -\frac{\partial}{\partial X_i}(\Phi_S^*(\rho) + \Phi_L[\rho]), \quad M_* = \frac{1}{(2\pi RT_*)^{3/2}} \exp\left(-\frac{\xi^2}{2RT_*}\right), \quad (4.1b)$$

where $f(t, \mathbf{X}, \boldsymbol{\xi})$ is the velocity distribution function (VDF) of molecules, with t , $\mathbf{X}$, and $\boldsymbol{\xi}$ being a time, a position, and a molecular velocity respectively; $m\mathbf{F}^*$ is a potential force acting on a molecule with a mass m , R is the specific gas constant, and $A_*(\rho)$ is a positive function of the gas density ρ defined by

$$\rho = \int f d\boldsymbol{\xi}. \quad (4.1c)$$

Here and in what follows, the integral with respect to $\boldsymbol{\xi}$ represents the definite one over its whole space, unless otherwise stated. With the density ρ , a uniform given temperature T_* , and two parameters a and b , the equation of state for the van der Waals fluids is written as

$$p = \frac{\rho RT_*}{1 - b\rho} - a\rho^2, \quad (4.1d)$$

under the isothermal assumption. The form of Φ_S^* is then determined as

$$\Phi_S^*(\rho) = \Phi_S(\rho, T_*) \equiv -RT_* \ln(1 - b\rho) + \frac{b\rho RT_*}{1 - b\rho} - 2a\rho, \quad (4.1e)$$

in order to recover the non-ideal gas effect in the equation of state (4.1d) through the relation

$$p = \rho RT_* + \int \rho \frac{d\Phi_S^*(\rho)}{d\rho} d\rho. \quad (4.1f)$$

Within the diffusive approximation, the form of Φ_L is reduced to

$$\Phi_L = -\kappa \Delta \rho, \quad (4.1g)$$

where $\Delta \equiv \partial^2/\partial X_i^2$ is the Laplacian and κ is a given positive constant.¹ Once the collision frequency A_* is specified, the above system is closed. In what follows, let us call this system (4.1) the isothermal model. The isothermal model was considered to identify the key or minimum mechanism in the transition dynamics from a uniform equilibrium state to a phase separated equilibrium state, see [12,13].

Main features of the isothermal model are as follows. Firstly, a non-local effect of interaction is treated in $\Phi_L[\rho]$ as a long-range attractive term. It is localized only after applying a diffusive approximation. In contrast, short-range interactions of molecules are treated to be local from the beginning by the terms of $\Phi_S^*(\rho)$ and $C_*[f]$ in (4.1).² Secondly, the resting Maxwellian ρM_* with a given uniform temperature T_* is used in place of the local Maxwellian in $C_*[f]$. This feature implies that the system does not conserve the momentum nor energy. Thus, in the isothermal model, the main driving mechanism toward the equilibrium state is the interaction of molecules with a heat bath, not within themselves.

The next model developed from the system (4.1) adopts the BGK-type collision integral in place of $C_*[f]$ in (4.1a) and takes the following form:

$$\frac{\partial f}{\partial t} + \xi_i \frac{\partial f}{\partial X_i} + F_i \frac{\partial f}{\partial \xi_i} = Q_c[f] + Q_d[f], \quad (4.2a)$$

$$F_i = -\frac{\partial}{\partial X_i}(\Phi_S(\rho, T) + \Phi_L[\rho]), \quad (4.2b)$$

$$Q_c[f] = A(\rho, T)(f_e - f), \quad A(\rho, T) = \frac{A_c(T)\rho}{1 - b\rho} > 0, \quad (4.2c)$$

$$f_e = \frac{\rho}{(2\pi RT)^{3/2}} \exp\left(-\frac{\mathbf{c}^2}{2RT}\right), \quad \mathbf{c} = \boldsymbol{\xi} - \mathbf{v}, \quad (4.2d)$$

$$Q_d[f] = -\frac{\partial}{\partial \xi_i}[(\alpha_i + \beta c_i)f], \quad \alpha_i = \frac{1}{\rho} \int \frac{\partial \Phi_S}{\partial T} d\rho \frac{\partial T}{\partial X_i}, \quad (4.2e)$$

$$\beta = \frac{1}{3R\rho} \left\{ \frac{\partial}{\partial t} \int \frac{\partial \Phi_S}{\partial T} d\rho + \frac{\partial}{\partial X_i} \left(v_i \int \frac{\partial \Phi_S}{\partial T} d\rho \right) \right\}, \quad (4.2f)$$

where $A_c(T) > 0$ (see the Appendix A of [14]), $\mathbf{v}$ and T are the gas flow velocity and temperature defined as

$$\mathbf{v} = \frac{1}{\rho} \int \boldsymbol{\xi} f d\boldsymbol{\xi}, \quad T = \frac{1}{3R\rho} \int \mathbf{c}^2 f d\boldsymbol{\xi}. \quad (4.2g)$$

¹ κ can be related to a in the equation of state, once the long-range attractive potential is specified. Here κ and a are regarded as independent parameters. This reflects a degree of freedom on the choice of attractive potential.

²Both Φ_S^* and C_* are nonlinear with respect to f . C_* becomes linear only when $A_*(\rho)$ is independent of ρ . In contrast, Q terms in (4.2), (4.9), and (4.20) that appear later are all nonlinear with respect to f .

The indefinite integral with respect to ρ in (4.2) is taken along the isothermal process to get

$$\int \frac{\partial \Phi_S}{\partial T} d\rho = -\rho R \ln(1 - b\rho), \quad (4.3)$$

for the van der Waals fluids. Note that the equation of state takes the original form

$$p = \frac{\rho RT}{1 - b\rho} - a\rho^2 \left(= \rho RT + \int \rho \frac{\partial \Phi_S}{\partial \rho} d\rho \right), \quad (4.4)$$

in place of (4.1d), since the gas is no longer assumed to be isothermal. Hereafter, the system (4.2) – (4.4) is referred to as the BGK-based model.

Due to the temperature dependence of Φ_S , a new term Q_d is added on the right-hand side of (4.2a) for a well-balanced construction of the model. The BGK-based model conserves the mass, the momentum, and the energy and was used as well to study the dynamics of phase separation from a uniform equilibrium state in a periodic and an isolated system in [14]. Comparisons with simulation results for the isothermal model and related discussions can be found in the Appendix D of [14].

Besides their simplicity, both the isothermal and the BGK-based model have an advantage that there is a monotonically decreasing functional:

$$H^*(t) = \int_D \left(\int f \ln \frac{f}{\rho_0 M_*} d\boldsymbol{\xi} + \frac{1}{RT_*} \left[\int \Phi_S^* d\rho + \frac{\kappa}{2} (\nabla \rho)^2 \right] \right) d\mathbf{X}, \quad (4.5a)$$

for the isothermal model [12,13] and

$$H(t) = \int_D \left(\int f \ln \frac{f}{c_0} d\boldsymbol{\xi} + \frac{1}{R} \int \frac{\partial \Phi_S}{\partial T} d\rho \right) d\mathbf{X}, \quad (4.5b)$$

for the BGK-based model [14], where D is a unit region of a periodic domain, ρ_0 is a reference density, and c_0 is a positive constant with the same physical dimension as f . Occurrence of M_* and $\kappa(\nabla \rho)^2$ in (4.5a) is due to that the isothermal model is for the systems in contact with the heat bath, while the BGK-based model is for periodic (or isolated) systems. In other words, H^* corresponds to the free energy, while H corresponds to the (negative) entropy in the thermodynamics. Note that the second term on the right-hand side of (4.5b) is a contribution of the dense gas effect. Equipped with the monotone functional, these models provided thermodynamically consistent discussions and interpretations to numerical simulation results for the phase change, e.g., [14]. It is a benefit in addition to their simple structures.

4.2.2 Fluid-dynamic limits and transport properties

The isothermal model leads to a Cahn–Hilliard-type equation:

$$\frac{\partial \rho}{\partial t} - \frac{\partial}{\partial X_j} \left[\frac{\rho}{A_*(\rho)} \frac{\partial}{\partial X_j} \left(\Phi - \kappa \frac{\partial^2 \rho}{\partial X_i^2} \right) \right] = 0, \quad (4.6a)$$

$$\Phi = -2a\rho + RT_* \left(\frac{1}{1-b\rho} + \ln \frac{b\rho}{1-b\rho} \right), \quad (4.6b)$$

in the fluid-dynamic limit, owing to a strong momentum-dissipation property of the collision term $C_*[f]$, see [12] for details. A derivation of the Cahn–Hilliard equation from the kinetic theory has been recently discussed as well in [17].

The BGK-based model yields the following balance laws of the mass, momentum, and energy:

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial X_i} (\rho v_i) = 0, \quad (4.7a)$$

$$\frac{\partial}{\partial t} (\rho v_j) + \frac{\partial}{\partial X_i} (\rho v_i v_j + p_{ij}) + \rho \frac{\partial \Phi_L}{\partial X_j} = 0, \quad (4.7b)$$

$$\frac{\partial}{\partial t} \left[\rho \left(e + \frac{1}{2} \mathbf{v}^2 \right) \right] + \frac{\partial}{\partial X_i} \left[\rho v_i \left(e + \frac{1}{2} \mathbf{v}^2 \right) + p_{ij} v_j + q_i \right] + \rho v_i \frac{\partial \Phi_L}{\partial X_i} = 0, \quad (4.7c)$$

where p_{ij} , q_i , and e are, respectively, the stress tensor, the heat-flow vector, and the specific internal energy defined by

$$p_{ij} = p\delta_{ij} + \int \left(c_i c_j - \frac{1}{3} \mathbf{c}^2 \delta_{ij} \right) f d\boldsymbol{\xi}, \quad q_i = \frac{1}{2} \int c_i \mathbf{c}^2 f d\boldsymbol{\xi}, \quad (4.7d)$$

$$\rho e = \frac{3}{2} \rho RT + \int \left(\Phi_S - T \frac{\partial \Phi_S}{\partial T} \right) d\rho, \quad (4.7e)$$

and p is the pressure defined in (4.4). The derivation of (4.7) can be found in [14]. In the fluid-dynamic limit, the stress tensor and heat-flow vector are reduced to

$$p_{ij} = p\delta_{ij} - \frac{\rho RT}{A(\rho, T)} \left(\frac{\partial v_i}{\partial X_j} + \frac{\partial v_j}{\partial X_i} - \frac{2}{3} \frac{\partial v_k}{\partial X_k} \delta_{ij} \right), \quad q_i = -\frac{5}{2} R \frac{\rho RT}{A(\rho, T)} \frac{\partial T}{\partial X_i}, \quad (4.8)$$

and accordingly the balance law of equation (4.7) is reduced to the Navier–Stokes set of equations with a self-consistent force term, see the Appendix. Here, as is seen from (4.8), the viscosity μ and the thermal conductivity λ are given respectively by $\mu = \rho RT/A(\rho, T)$ and $\lambda = (5/2) R \rho RT/A(\rho, T)$. These expressions imply that the Prandtl number $\text{Pr} \equiv (5R/2)(\mu/\lambda)$ is unity, inheriting a weakness of the BGK-type collision integral in the transport property. Another weakness is that the bulk viscosity predicted by the Enskog theory [18] is absent. In the next section, we propose a modification of the BGK-based model to fix its demerit in transport properties.

4.3 Modified models in terms of the Ellipsoidal-Statistical (ES)-type collision term

The key elements in the modification of the BGK-based model are, first, to use an ES-type collision term [15,16] instead of the BGK-type term and, second, to add additional terms to Q_d . Here, two different ways of modification are presented.

4.3.1 The first ES-based model

The main idea of the first modified model proposed recently in [19] is to make the adjusting parameter ν in the ES-type collision integral dependent on ρ . The model is hereafter referred to as the first ES-based model and reads

$$\frac{\partial f}{\partial t} + \xi_i \frac{\partial f}{\partial X_i} + F_i \frac{\partial f}{\partial \xi_i} = Q_c^\sharp[f] + Q_d^\sharp[f], \quad (4.9a)$$

$$Q_c^\sharp[f] = A^\sharp(\rho, T)(\mathcal{G} - f), \quad \mathcal{G} = \frac{\rho}{\sqrt{\det(2\pi\mathcal{T})}} \exp\left(-\frac{1}{2}(\mathcal{T}^{-1})_{ij}c_i c_j\right), \quad (4.9b)$$

$$\mathcal{T}_{ij} = [1 - \nu(\rho)] RT \delta_{ij} + \nu(\rho) \Theta_{ij}, \quad \Theta_{ij} = \frac{1}{\rho} \int c_i c_j f d\boldsymbol{\xi}, \quad (4.9c)$$

$$Q_d^\sharp[f] = -\frac{\partial}{\partial \xi_i}[(\alpha_i^\sharp + \beta^\sharp c_i)f], \quad (4.9d)$$

$$\alpha_i^\sharp = \alpha_i + \frac{1}{\rho} \frac{\partial}{\partial X_i} \left(\mu_B \frac{\partial v_k}{\partial X_k} \right), \quad \beta^\sharp = \beta + \frac{\mu_B}{3R\rho T} \left(\frac{\partial v_k}{\partial X_k} \right)^2, \quad (4.9e)$$

where F_i is the same as that in the BGK-based model, $\mathcal{T}^{-1}$ is the inverse of the tensor $\mathcal{T}$, μ_B and $A^\sharp$ are positive functions of ρ and T to be determined in accordance with the Enskog theory for the transport coefficients, and $\nu(\rho)$ is an adjusting parameter function of ρ also to be determined later in (4.15b).

The modified model keeps the set of balance equations (4.7) as it stands by the following change of definition of the stress tensor:

$$p_{ij} = p\delta_{ij} + \int \left(c_i c_j - \frac{1}{3} \mathbf{c}^2 \delta_{ij} \right) f d\boldsymbol{\xi} - \mu_B \frac{\partial v_k}{\partial X_k} \delta_{ij}. \quad (4.10)$$

In the fluid-dynamic limit, the stress tensor and heat-flow vector are reduced to

$$p_{ij} = p\delta_{ij} - \frac{1}{1 - \nu(\rho)} \frac{\rho RT}{A^\sharp(\rho, T)} \left(\frac{\partial v_i}{\partial X_j} + \frac{\partial v_j}{\partial X_i} - \frac{2}{3} \frac{\partial v_k}{\partial X_k} \delta_{ij} \right) - \mu_B \frac{\partial v_k}{\partial X_k} \delta_{ij}, \quad (4.11)$$

$$q_i = -\frac{5}{2} R \frac{\rho RT}{A^\sharp(\rho, T)} \frac{\partial T}{\partial X_i}. \quad (4.12)$$

See the Appendix for the derivation of (4.11) and (4.12). Thus, μ_B introduced in (4.10) is the bulk viscosity, $\rho RT/((1-\nu)A^\sharp)$ the viscosity μ , and $(5/2)R(\rho RT/A^\sharp)$ the thermal conductivity λ . Hence, the Prandtl number is expressed in terms of ν as $\text{Pr}(\equiv (5/2)(R\mu/\lambda)) = 1/(1-\nu)$.

In order to make the model equipped with the desired transport properties, it is necessary to determine $\nu(\rho)$ in accordance with the Enskog theory for transport properties. In the Enskog theory, the viscosity μ , bulk viscosity μ_B , and the thermal conductivity λ are expressed as [18,20]

$$\mu = \frac{\mu_0}{\chi} \left[1 + \frac{16}{5}\phi\chi + 12.2(\phi\chi)^2 \right], \quad \mu_B = \frac{\mu_0}{\chi} (4\phi\chi)^2, \quad (4.13a)$$

$$\lambda = \frac{\lambda_0}{\chi} \left[1 + \frac{24}{5}\phi\chi + 12.1(\phi\chi)^2 \right], \quad (4.13b)$$

where μ_0 and λ_0 are respectively the viscosity and thermal conductivity of the gas in the dilute gas limit, while ϕ and χ are dense gas factors that can be related to the exclusion parameter b in the equation of state for the van der Waals fluids, i.e.,

$$\phi = \frac{1}{4}b\rho, \quad \chi = \frac{1}{1-b\rho}; \quad (4.14)$$

see the discussions in the Appendix A of [14] for details. Hence, substituting (4.14) into (4.13), $A^\sharp$ and ν in the system (4.9) as well as the transport coefficients are all expressed in terms of the exclusion parameter b , ρ , and T :

$$A^\sharp(\rho, T) = \frac{5}{2} \frac{\rho RT}{1-b\rho} \frac{R/\lambda_0(T)}{g_2(\frac{b\rho}{1-b\rho})}, \quad (4.15a)$$

$$\nu(\rho) = 1 - \frac{2}{5} \frac{1}{R} \frac{\lambda_0(T)}{\mu_0(T)} \frac{g_2(\frac{b\rho}{1-b\rho})}{g_1(\frac{b\rho}{1-b\rho})} = 1 - \frac{1}{\text{Pr}_0} \frac{g_2(\frac{b\rho}{1-b\rho})}{g_1(\frac{b\rho}{1-b\rho})}, \quad (4.15b)$$

$$\mu(\rho, T) = (1-b\rho)g_1\left(\frac{b\rho}{1-b\rho}\right)\mu_0(T), \quad (4.15c)$$

$$\mu_B(\rho, T) = (1-b\rho)\left(\frac{b\rho}{1-b\rho}\right)^2\mu_0(T), \quad (4.15d)$$

$$\lambda(\rho, T) = (1-b\rho)g_2\left(\frac{b\rho}{1-b\rho}\right)\lambda_0(T), \quad (4.15e)$$

where

$$g_1(x) = 1 + \frac{4}{5}x + \frac{6.1}{8}x^2, \quad g_2(x) = 1 + \frac{6}{5}x + \frac{12.1}{16}x^2, \quad (4.15f)$$

and Pr_0 is the Prandtl number in the dilute gas limit, which is usually set as $\text{Pr}_0 = 2/3$ for monatomic gases. The system (4.9) with (4.15) thus forms a closed kinetic model with

appropriate transport coefficients. Note that the model recovers the BGK-based model with $A_c = (5/2)R^2T/\lambda_0(T)$ as a special case by discarding (4.15d) and (4.15f) and putting $g_1 = g_2 = 1$, $\mu_B = 0$, and $\text{Pr}_0 = 1$ (see Sec. 4.2.1).

4.3.2 A slight limitation on the monotonicity of the first ES-based model

We shall discuss the monotone property of the model (4.9) with (4.15) in a periodic domain. Let D denote a unit region of the periodic domain. Multiplying (4.9a) by $1 + \ln(f/c_0)$ and integrating the result over the whole range of $\boldsymbol{\xi}$ and over the unit region D yields

$$\begin{aligned} \frac{d}{dt} \int_D \int f \ln \frac{f}{c_0} d\boldsymbol{\xi} d\mathbf{X} &= \int_D \int (Q_c^\# [f] + Q_d^\# [f]) \ln \frac{f}{c_0} d\boldsymbol{\xi} d\mathbf{X} \\ &= \int_D \int Q_c^\# [f] \ln \frac{f}{c_0} d\boldsymbol{\xi} d\mathbf{X} - 3 \int_D \beta^\# \rho d\mathbf{X}, \end{aligned} \quad (4.16)$$

where the second and the third term of (4.9a) do not contribute because of the periodic condition in space and the rapid decay of VDF in molecular speed. Then, after a few manipulations making use of (4.2f) and the periodic condition,

$$\begin{aligned} \frac{d}{dt} H(t) &= \int_D \int Q_c^\# [f] \ln \frac{f}{c_0} d\boldsymbol{\xi} d\mathbf{X} - \int_D \frac{\mu_B}{RT} \left(\frac{\partial v_k}{\partial X_k} \right)^2 d\mathbf{X} \\ &\leq \int_D \int Q_c^\# [f] \ln \frac{f}{c_0} d\boldsymbol{\xi} d\mathbf{X}, \end{aligned}$$

is obtained. Therefore, if

$$\int Q_c^\# [f] \ln \frac{f}{c_0} d\boldsymbol{\xi} \leq 0, \quad (4.17)$$

holds, the monotonic property is retained as well in the first ES-based model.

Although the property (4.17) is one of merits to use the ES-type collision model, it should be reminded that (4.17) holds unconditionally only when the adjusting parameter ν is in the range $[-1/2, 1)$, i.e., the Prandtl number $\text{Pr}(\equiv \frac{5}{2} \frac{R\mu}{\lambda}) = 1/(1 - \nu)$ should be in the range $[2/3, \infty)$ [16]. In the present case, it is seen from (4.15) that

$$\text{Pr} = \text{Pr}_0 \Lambda \left(\frac{b\rho}{1 - b\rho} \right), \quad \Lambda(x) = \frac{g_1(x)}{g_2(x)} = 1 - \frac{\frac{2}{5}x(1 - \frac{x}{64})}{g_2(x)}. \quad (4.18)$$

Since $\text{Pr}_0 = 2/3$ is the usual setting for monatomic gases, $\Lambda \geq 1$ is required for (4.17) to hold unconditionally. However, Λ decreases from unity as $b\rho$ increases, reaches its minimum 0.8663 at $b\rho = 0.5274$, and then increases, as shown in Fig. 4.1. When Λ takes its minimum,

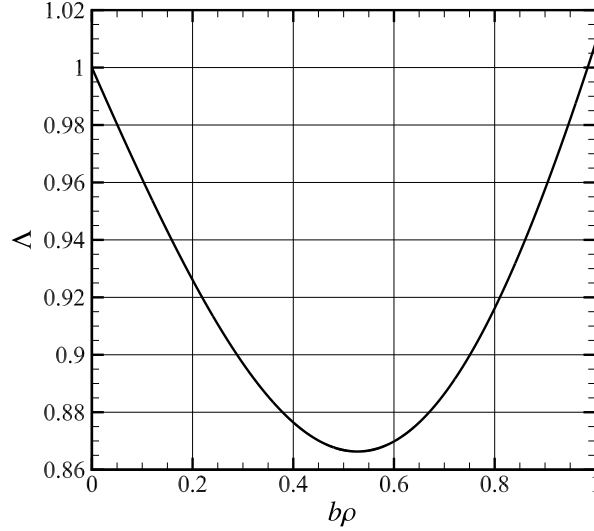


Figure 4.1: $\Lambda(\frac{b\rho}{1-b\rho})$ versus a rescaled density $b\rho$. See (4.18).

the corresponding values of Pr and ν are respectively 0.5775 and -0.7315 . Therefore, the monotonicity of H is not guaranteed in the first ES-based model. Nevertheless, by a close examination of the original proof of the H theorem for $\nu \geq -1/2$ in [16], it was made clear in [21] that (4.17) still holds, provided that (i) $\mathcal{T}$ is positive definite and (ii) $\det \mathcal{T} \geq \det \Theta$. A similar discussion on a Fokker–Planck model can be found in [22]. Below is the quantitative criterion obtained in [21] for $\int \ln(f/c_0) Q_c^\sharp[f] d\xi \leq 0$ to hold:

Proposition 4.1. *Let $\lambda_1 \leq \lambda_2 \leq \lambda_3$ be the positive real eigenvalues of Θ that is a symmetric positive definite tensor by definition. If three eigenvalues are the same, $\mathcal{T}$ and Θ are identical, so that $\mathcal{T} = \Theta = RT\mathbb{I}$, where $\mathbb{I}$ is the identity tensor. The two conditions (i) and (ii) are then automatically satisfied. Next suppose that $\lambda_1 \neq \lambda_3$, and introduce additional notation $\epsilon \equiv 1 - \lambda_1/\lambda_3$ and $\theta = (1 - \lambda_2/\lambda_3)/(1 - \lambda_1/\lambda_3)$. Note that $0 < \epsilon < 1$ and $0 \leq \theta \leq 1$ by construction. Then, for $-1 \leq \nu < -1/2$, which corresponds to $1/2 \leq \text{Pr} < 2/3$, the following criterion must be fulfilled for (4.17) to hold $\int \ln(f/c_0) Q_c^\sharp[f] d\xi \leq 0$:*

$$\begin{cases} 0 < \epsilon < 1, & \text{for } 0 \leq \theta \leq \frac{2+\nu}{1-\nu}, \\ 0 < \epsilon < \frac{9(1+\nu)(\theta^2 - \theta + 1)}{(1+\theta)(1-\nu)^2(\frac{2\nu+1}{1-\nu} + \theta)(\frac{2\nu+1}{1-\nu}\theta + 1)}, & \text{for } \frac{2+\nu}{1-\nu} < \theta \leq 1. \end{cases} \quad (4.19)$$

The criterion (4.19) is a posteriori condition, and its practical restriction should be checked carefully. Numerical assessment of the criterion can be found in [21], where (4.17) is shown to hold except for highly anisotropic non-equilibrium states.

4.3.3 The second ES-based model

The second ES-based model is motivated by the slight limitation of the first ES-based model on the monotonicity described in Sec. 4.3.2. The main idea is to keep the adjusting parameter ν in the range $[-1/2, 1)$,³ thereby keeping the monotonic property of $H(t)$ by modifying $Q_d^\sharp$ term. The second ES-based model reads

$$\frac{\partial f}{\partial t} + \xi_i \frac{\partial f}{\partial X_i} + F_i \frac{\partial f}{\partial \xi_i} = Q_c^b[f] + Q_d^b[f], \quad (4.20a)$$

$$Q_c^b[f] = A^b(\rho, T)(\mathcal{G} - f), \quad \mathcal{G} = \frac{\rho}{\sqrt{\det(2\pi\mathcal{T})}} \exp\left(-\frac{1}{2}(\mathcal{T}^{-1})_{ij}c_i c_j\right), \quad (4.20b)$$

$$\mathcal{T}_{ij} = (1 - \nu)RT\delta_{ij} + \nu\Theta_{ij}, \quad \Theta_{ij} = \frac{1}{\rho} \int c_i c_j f d\xi, \quad (4.20c)$$

$$Q_d^b[f] = -\frac{\partial}{\partial \xi_i}[(\alpha_i^b + \beta^b c_i)f], \quad (4.20d)$$

$$\begin{aligned} \alpha_i^b &= \alpha_i + \frac{1}{\rho} \frac{\partial}{\partial X_j} \left[\mu_P \left(\frac{\partial v_i}{\partial X_j} + \frac{\partial v_j}{\partial X_i} - \frac{2}{3} \frac{\partial v_k}{\partial X_k} \delta_{ij} \right) + \mu_B \frac{\partial v_k}{\partial X_k} \delta_{ij} \right] \\ &= \alpha_i^\sharp + \frac{1}{\rho} \frac{\partial}{\partial X_j} \left[\mu_P \left(\frac{\partial v_i}{\partial X_j} + \frac{\partial v_j}{\partial X_i} - \frac{2}{3} \frac{\partial v_k}{\partial X_k} \delta_{ij} \right) \right], \end{aligned} \quad (4.20e)$$

$$\begin{aligned} \beta^b &= \beta + \frac{1}{3R\rho T} \left\{ \frac{\partial}{\partial X_k} \left(\lambda_P \frac{\partial T}{\partial X_k} \right) \right. \\ &\quad \left. + \frac{\partial v_i}{\partial X_j} \left[\mu_P \left(\frac{\partial v_i}{\partial X_j} + \frac{\partial v_j}{\partial X_i} - \frac{2}{3} \frac{\partial v_k}{\partial X_k} \delta_{ij} \right) + \mu_B \frac{\partial v_k}{\partial X_k} \delta_{ij} \right] \right\} \\ &= \beta^\sharp + \frac{1}{3R\rho T} \left\{ \frac{\partial}{\partial X_k} \left(\lambda_P \frac{\partial T}{\partial X_k} \right) + \mu_P \frac{\partial v_i}{\partial X_j} \left(\frac{\partial v_i}{\partial X_j} + \frac{\partial v_j}{\partial X_i} - \frac{2}{3} \frac{\partial v_k}{\partial X_k} \delta_{ij} \right) \right\}, \end{aligned} \quad (4.20f)$$

where μ_B is the same as before [see (4.15d)] and

$$A^b(\rho, T) = \frac{5}{2} \frac{\rho RT}{1 - b\rho} \frac{R}{\lambda_0(T)} \left(= g_2 \left(\frac{b\rho}{1 - b\rho} \right) A^\sharp(\rho, T) \right), \quad (4.21a)$$

$$\nu = 1 - \frac{2}{5} \frac{1}{R} \frac{\lambda_0(T)}{\mu_0(T)} = 1 - \frac{1}{\text{Pr}_0}, \quad (4.21b)$$

$$\mu_P(\rho, T) = (1 - b\rho) g_1^b \left(\frac{b\rho}{1 - b\rho} \right) \mu_0(T), \quad (4.21c)$$

$$\lambda_P(\rho, T) = (1 - b\rho) g_2^b \left(\frac{b\rho}{1 - b\rho} \right) \lambda_0(T), \quad (4.21d)$$

$$g_1^b(x) = g_1(x) - 1, \quad g_2^b(x) = g_2(x) - 1. \quad (4.21e)$$

³With this choice of ν , Q_c^b introduced soon below is reduced to the original ES collision term for dilute gases except for the density dependence of the factor A^b , see (4.21a). Comparing (4.21a) with (4.15a) and (4.15b), it is seen that the factors g_1 and g_2 are excluded from Q_c^b . Accordingly, the differences of these factors from 1, i.e., g_1^b and g_2^b , are included in $Q_d^\sharp$ and give rise to the so-called potential contribution to the momentum and the energy transport.

Comparing (4.21e) with (4.15f), it is seen that $g_1^b(x) > 0$ and $g_2^b(x) > 0$ for $x > 0$; thus $\mu_P > 0$ and $\lambda_P > 0$ for $0 \leq b\rho < 1$. Then, by the following change of the definitions of p_{ij} and q_i :

$$p_{ij} = p\delta_{ij} + \int \left(c_i c_j - \frac{1}{3} \mathbf{c}^2 \delta_{ij} \right) f d\mathbf{\xi} - \mu_P \left(\frac{\partial v_i}{\partial X_j} + \frac{\partial v_j}{\partial X_i} - \frac{2}{3} \frac{\partial v_k}{\partial X_k} \delta_{ij} \right) - \mu_B \frac{\partial v_k}{\partial X_k} \delta_{ij}, \quad (4.22)$$

$$q_i = \frac{1}{2} \int c_i \mathbf{c}^2 f d\mathbf{\xi} - \lambda_P \frac{\partial T}{\partial X_i}, \quad (4.23)$$

the second ES-based model retains the set of conservation laws (4.7) as it stands. Furthermore, in the fluid dynamic limit, the stress tensor and heat-flow vector are reduced to

$$p_{ij} = p\delta_{ij} - \mu \left(\frac{\partial v_i}{\partial X_j} + \frac{\partial v_j}{\partial X_i} - \frac{2}{3} \frac{\partial v_k}{\partial X_k} \delta_{ij} \right) - \mu_B \frac{\partial v_k}{\partial X_k} \delta_{ij}, \quad (4.24a)$$

$$q_i = -\lambda \frac{\partial T}{\partial X_i}, \quad (4.24b)$$

where μ and λ are the same as those in (4.15); see the Appendix for the derivation. Substitution of (4.24) to (4.7) gives the Navier–Stokes set of equations with a self-consistent force term.

In contrast to the first ES-based model, ν is a constant parameter in the second ES-based model and it can be set as $\nu = -1/2$. Thus,

$$\int Q_c^b[f] \ln \frac{f}{c_0} d\mathbf{\xi} \leq 0, \quad (4.25)$$

holds unconditionally. This is an advantage over the first ES-based model, because with this property, $H(t)$ can be shown monotonically decreasing.

Proposition 4.2. *For the system (4.20) with (4.21), $H(t)$ defined by (4.5b) in a spatially periodic domain monotonically decreases in time t . Furthermore, $H(t)$ reaches a stationary state if and only if f is a Maxwellian with a uniform temperature and a uniform flow velocity.*

Proof. By following the calculations in (4.16),

$$\begin{aligned} \frac{d}{dt} \int_D \int f \ln \frac{f}{c_0} d\mathbf{\xi} d\mathbf{X} &= \int_D \int (Q_c^b[f] + Q_d^b[f]) \ln \frac{f}{c_0} d\mathbf{\xi} d\mathbf{X} \\ &= \int_D \int Q_c^b[f] \ln \frac{f}{c_0} d\mathbf{\xi} d\mathbf{X} - 3 \int_D \beta^b \rho d\mathbf{X}. \end{aligned} \quad (4.26)$$

Since the β -part in β^b gives rise the second term of (4.5b), the above is reduced to

$$\frac{d}{dt} H(t) = \int_D \int Q_c^b[f] \ln \frac{f}{c_0} d\mathbf{\xi} d\mathbf{X} - 3 \int_D (\beta^b - \beta) \rho d\mathbf{X}. \quad (4.27)$$

Note that the first term in (4.27) is designed to be nonpositive as far as $\nu \in [-1/2, 1)$, which is a marked contrast to the case of the first ES-based model. As to the second term of (4.27), the following transformation from the definition of β^b is possible:

$$\begin{aligned}
(\beta^b - \beta)\rho &= \frac{1}{3RT} \left\{ \frac{\partial}{\partial X_k} \left(\lambda_P \frac{\partial T}{\partial X_k} \right) \right. \\
&\quad \left. + \frac{\partial v_i}{\partial X_j} \left[\mu_P \left(\frac{\partial v_i}{\partial X_j} + \frac{\partial v_j}{\partial X_i} - \frac{2}{3} \frac{\partial v_k}{\partial X_k} \delta_{ij} \right) + \mu_B \frac{\partial v_k}{\partial X_k} \delta_{ij} \right] \right\} \\
&= \frac{1}{3R} \left\{ \frac{\partial}{\partial X_k} \left(\frac{\lambda_P}{T} \frac{\partial T}{\partial X_k} \right) + \frac{\lambda_P}{T^2} \left(\frac{\partial T}{\partial X_k} \right)^2 \right. \\
&\quad \left. + \frac{1}{2} \frac{\mu_P}{T} \left(\frac{\partial v_i}{\partial X_j} + \frac{\partial v_j}{\partial X_i} - \frac{2}{3} \frac{\partial v_k}{\partial X_k} \delta_{ij} \right)^2 + \frac{\mu_B}{T} \left(\frac{\partial v_k}{\partial X_k} \right)^2 \right\}. \tag{4.28}
\end{aligned}$$

Here, the following identities have been used:

$$\left(\frac{\partial v_i}{\partial X_j} + \frac{\partial v_j}{\partial X_i} - \frac{2}{3} \frac{\partial v_k}{\partial X_k} \delta_{ij} \right) \delta_{ij} = 0, \tag{4.29a}$$

$$\frac{\partial v_i}{\partial X_j} \left(\frac{\partial v_i}{\partial X_j} + \frac{\partial v_j}{\partial X_i} - \frac{2}{3} \frac{\partial v_k}{\partial X_k} \delta_{ij} \right) = \frac{1}{2} \left(\frac{\partial v_i}{\partial X_j} + \frac{\partial v_j}{\partial X_i} - \frac{2}{3} \frac{\partial v_k}{\partial X_k} \delta_{ij} \right)^2. \tag{4.29b}$$

Note that the first term on the most right hand side of (4.28) is a divergence form and vanishes once the integration over the spatial domain D is taken, thanks to the periodic condition and the divergence theorem. Since the other terms of (4.28) are all non-negative, $\int_D (\beta^b - \beta) \rho d\mathbf{X} \geq 0$ holds, and

$$\frac{d}{dt} H(t) = \int_D \int Q_c^b[f] \ln \frac{f}{c_0} d\boldsymbol{\xi} d\mathbf{X} - 3 \int_D (\beta^b - \beta) \rho d\mathbf{X} \leq 0. \tag{4.30}$$

The last equality holds if and only if $\int_D \int Q_c^b[f] \ln(f/c_0) d\boldsymbol{\xi} d\mathbf{X} = 0$ and $\int_D (\beta^b - \beta) \rho d\mathbf{X} = 0$. The former condition requires that f is a Maxwellian, while the latter condition requires a uniform temperature and $\partial v_i / \partial X_j + \partial v_j / \partial X_i = 0$. Then, the last condition on the velocity gradients admits a flow field that is a superposition of a uniform flow and a rigid body rotation. However, the rigid body rotation conflicts with the periodic condition, and the flow velocity is uniform in the present case. $\square$

Remark 4.1. The density is not necessarily uniform in a stationary state. The uniform temperature and flow velocity at the stationary state are determined in accordance with the initial state.

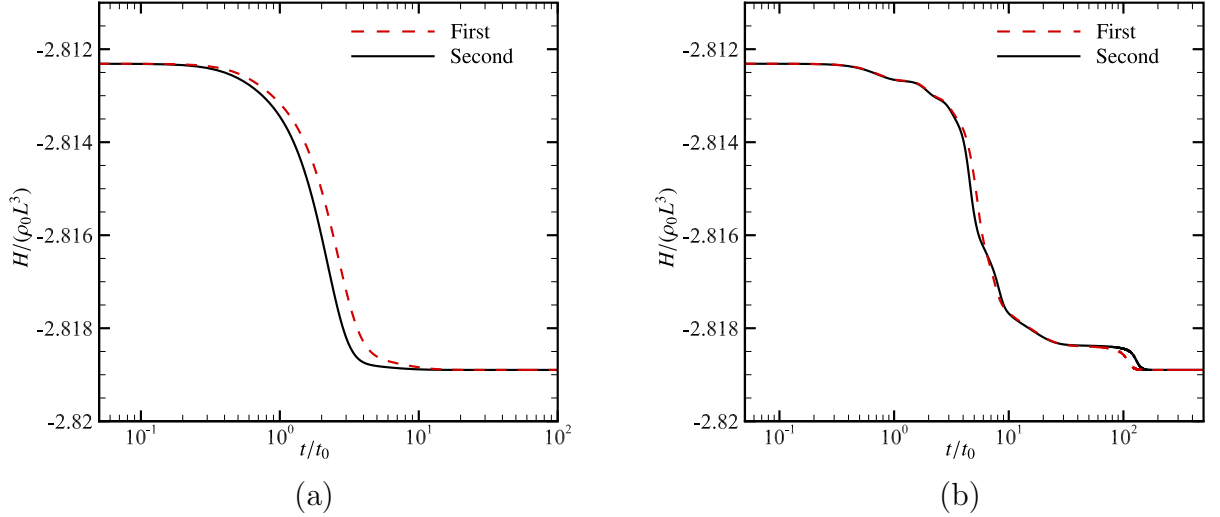


Figure 4.2: Time evolution of $H(t)$ from the perturbed uniform state with $\omega = 0.1$ in the case $b\rho_0 = 1/3$, $c \equiv a/(bRT_0) = 3.8$, and $K \equiv \kappa/(2bRT_0L^2) = 1.0 \times 10^{-4}$. (a) $k^b = 0.1$ and (b) $k^b = 0.01$. The solid line indicates the result of the second ES-based model, while the dashed red line indicates the result of the first ES-based model. $t_0 = L/\sqrt{2RT_0}$.

4.4 Preliminary tests

Numerical simulations have been conducted to check quantitative differences between two ES-based models. In each simulation, a dense gas is confined in a spatially one-dimensional periodic domain with D being its unit region, and a time evolution from a uniform equilibrium state at rest by an initial sinusoidal perturbation

$$\rho(0, X_1) = \rho_0[1 + \omega \sin(2\pi X_1/L)], \quad (4.31)$$

is studied, where ρ_0 is the average density of the gas, L is the length of the unit region, and ω is a factor of the initial perturbation size. Because of the total mass, momentum, and energy constraints [see (4.7)], the initial disturbance of density is given in such a way that the initial uniform temperature is different from the temperature T_0 of the undisturbed uniform equilibrium state, while the initial flow velocity is zero. Since comparisons between the BGK-based and the first ES-based model can be found in [19], we report preliminary results of comparisons between the first and the second ES-based model. In the numerical results to be presented below, the first ES-based model is well inside the valid range of the H theorem.

Figure 4.2 shows time evolutions of the function $H(t)$ from the initial disturbed state with $\omega = 0.1$ for the case $b\rho_0 = 1/3$, $c \equiv a/(bRT_0) = 3.8$, $K \equiv \kappa/(2bRT_0L^2) = 1.0 \times 10^{-4}$, and

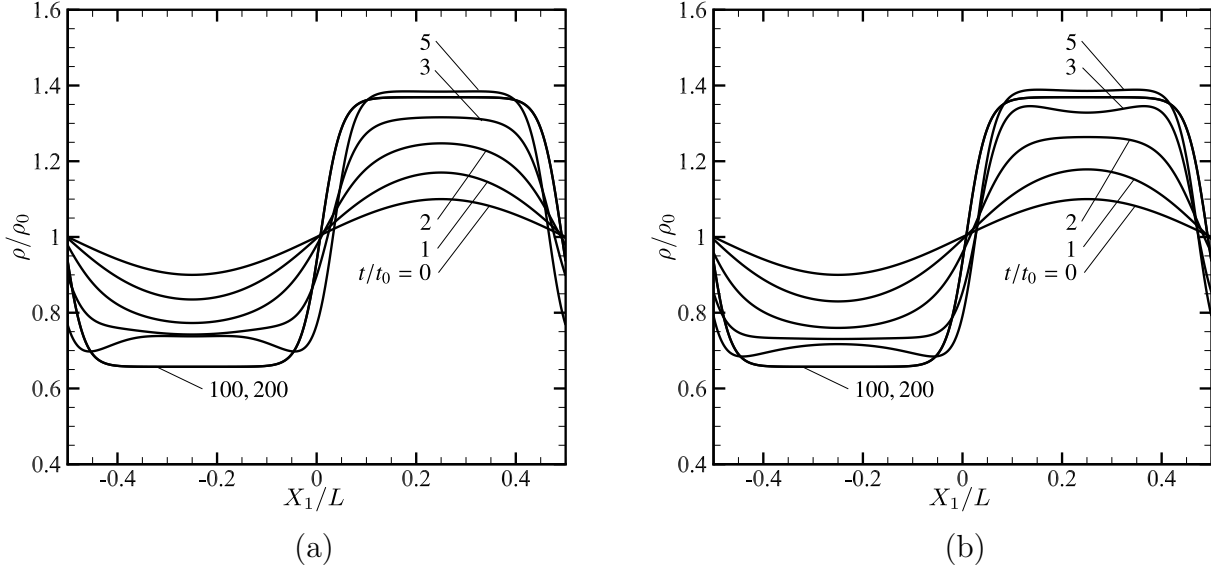


Figure 4.3: Time evolution of the density profile from the initial disturbed state with $\omega = 0.1$ for the case $b\rho_0 = 1/3$, $c = 3.8$, $K = 1.0 \times 10^{-4}$, and $k^b = 0.1$. (a) the first ES-based model, (b) the second ES-based model. See also the caption of Fig. 4.2.

$k^b \equiv \sqrt{2RT_0}/(A^b(\rho_0, T_0)L) = 0.1$ and 0.01 , where $\text{Pr}_0 = 2/3$ and $\lambda_0(T)$ is chosen as the one for hard-sphere molecules in the dilute gas limit. In both ES-based model, the function $H(t)$ monotonically decreases as the time increases. However, the evolution in the first model is delayed for $k^b = 0.1$. Indeed, instantaneous density profiles do not necessarily agree between the two models during the time evolution, though the time evolution of density profile is similar as a whole irrespective of $k^b = 0.1$ or 0.01 ; see Figs. 4.3 and 4.4. The final stationary states are not influenced by the difference of models, which also applies to the BGK-based model [19].

4.5 Concluding remarks

In the present paper, our constructions of simple kinetic models are presented, including a couple of new proposals based on the ES-type collision integral. The ES-based models have an advantage over our previous models in that they reproduce transport properties appropriately. The two models have a difference in the monotone property that is also desired as a kinetic model. The first ES-based model does not fully satisfy the H theorem, while the second ES-based model satisfies it unconditionally. In this sense, the latter has a better property qualitatively. In order to assess the quantitative difference between them, numerical simulations of the one-dimensional phase separation problem have been conducted

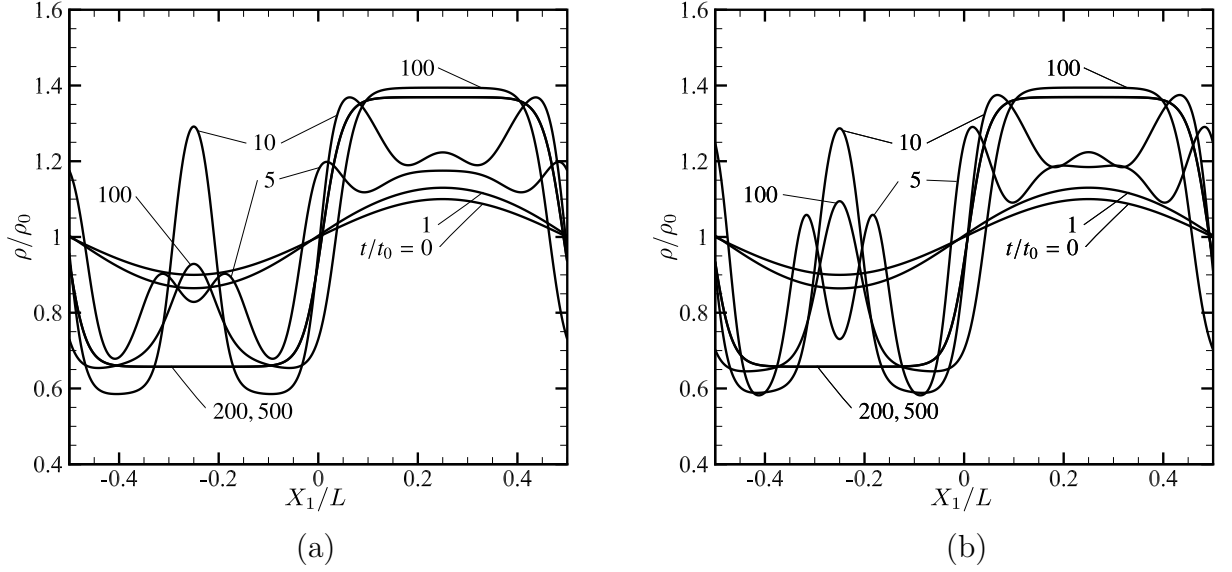


Figure 4.4: Time evolution of the density profile from the initial disturbed state with $\omega = 0.1$ for the case $b\rho_0 = 1/3$, $c = 3.8$, $K = 1.0 \times 10^{-4}$, and $k^b = 0.01$. (a) the first ES-based model, (b) the second ES-based model. See also the caption of Fig. 4.2.

for the parameter setting that falls into the thermodynamically unstable regime. Thermodynamically stable, metastable, and unstable regimes were not influenced by the change of the kinetic model presented in this paper. As a whole, the two ES-based models behave similarly, but do not necessarily agree to each other in the time evolution of density profile. Further numerical assessment is needed. Although computationally demanding, simulations of higher dimensions are also within our scope and will be treated in forthcoming papers.

4.A The fluid-dynamic limit of the second ES-based model

In this Appendix, the fluid-dynamic limit of the second ES-based model will be studied based on the Chapman–Enskog (CE) method along the lines of Harold Grad [23,24]. The case of the first ES-based model is similar, and the case of the BGK-based model is much simpler.

In order to avoid unnecessary increase of notations and to indicate the scaling, we shall artificially multiply μ_P , λ_P , and μ_B by a small parameter ε and Q_c^b by $1/\varepsilon$ instead of making (4.20) dimensionless. After the analysis, the artificial parameter ε is removed or set as unity.

Since μ_P , λ_P , and μ_B are all confined in the difference between Q_d^b and Q_d , we denote it

by $\varepsilon\tilde{Q}_d^b$, i.e., $Q_d^b = Q_d + \varepsilon\tilde{Q}_d^b$, rewrite (4.20) as

$$\frac{\partial f}{\partial t} + \xi_i \frac{\partial f}{\partial X_i} + F_i \frac{\partial f}{\partial \xi_i} = \frac{1}{\varepsilon} Q_c^b[f] + Q_d[f] + \varepsilon\tilde{Q}_d^b[f], \quad (4.32)$$

and consider a solution of this equation in the form $f = f(\rho_r, \nabla\rho_r, \boldsymbol{\xi})$, where and hereafter $\rho_r = \int \psi_r f d\boldsymbol{\xi}$ ($r = 0, 1, \dots, 4$) with $\psi_0 = 1$, $\psi_i = \xi_i$ ($i = 1, 2, 3$), $\psi_4 = \boldsymbol{\xi}^2/2$, and, unlike the usual notation, $\nabla\rho_r$ represents a spatial derivative of ρ_r of arbitrary order. Note that $\{\rho_0, \rho_i, \rho_4\} = \{\rho, \rho v_i, (3/2)\rho RT + (1/2)\rho \mathbf{v}^2\}$ ($i = 1, 2, 3$) and that the present form of f depends on t and $\mathbf{X}$ only through ρ_r and $\nabla\rho_r$. By multiplying (4.32) with ψ_r and integrating the result with respect to $\boldsymbol{\xi}$, the time derivative of ρ_r can be expressed in the form

$$\frac{\partial \rho_r}{\partial t} + \mathcal{F}_r(\rho_r, \nabla\rho_r, \varepsilon) = 0, \quad (r = 0, 1, \dots, 4). \quad (4.33)$$

From now on, we seek the solution f in a series of ε :

$$f = \sum_{n=0}^{\infty} \varepsilon^n f^{(n)}(\rho_r, \nabla\rho_r, \boldsymbol{\xi}). \quad (4.34)$$

Accordingly, (4.33) is rewritten as

$$\frac{\partial \rho_r}{\partial t} + \sum_{n=0}^{\infty} \varepsilon^n \mathcal{F}_r^{(n)}(\rho_r, \nabla\rho_r) = 0, \quad (r = 0, 1, \dots, 4), \quad (4.35)$$

and thus the time derivative of f is expressed as

$$\frac{\partial f}{\partial t} = \frac{\partial f}{\partial \rho_r} \frac{\partial \rho_r}{\partial t} + \frac{\partial f}{\partial \nabla\rho_r} \frac{\partial \nabla\rho_r}{\partial t} = - \sum_{n=0}^{\infty} \varepsilon^n \left(\frac{\partial f}{\partial \rho_r} \mathcal{F}_r^{(n)} + \frac{\partial f}{\partial \nabla\rho_r} \nabla \mathcal{F}_r^{(n)} \right). \quad (4.36)$$

Here and hereafter the summation convention rule is applied to the repeated r and ∇ . The form of $\mathcal{F}_r^{(n)}$ will be determined in the course of analysis that follows.

Substitution of (4.34) and (4.36) into (4.32) gives the following series of equations:

$$A^{b(0)}(f^{(0)} - \mathcal{G}[f]^{(0)}) = 0, \quad (4.37a)$$

$$\begin{aligned} A^{b(0)}(f^{(1)} - \mathcal{G}[f]^{(1)}) = & \left(\frac{\partial f^{(0)}}{\partial \rho_r} \mathcal{F}_r^{(0)} + \frac{\partial f^{(0)}}{\partial \nabla\rho_r} \nabla \mathcal{F}_r^{(0)} \right) \\ & - \xi_i \frac{\partial f^{(0)}}{\partial X_i} - F_i^{(0)} \frac{\partial f^{(0)}}{\partial \xi_i} + Q_d[f]^{(0)}, \end{aligned} \quad (4.37b)$$

$$\begin{aligned} A^{b(0)}(f^{(2)} - \mathcal{G}[f]^{(2)}) \\ = A^{b(1)}(\mathcal{G}[f]^{(1)} - f^{(1)}) + \sum_{\ell=0}^1 \left(\frac{\partial f^{(\ell)}}{\partial \rho_r} \mathcal{F}_r^{(1-\ell)} + \frac{\partial f^{(\ell)}}{\partial \nabla\rho_r} \nabla \mathcal{F}_r^{(1-\ell)} \right) \\ - \xi_i \frac{\partial f^{(1)}}{\partial X_i} - F_i^{(0)} \frac{\partial f^{(1)}}{\partial \xi_i} - F_i^{(1)} \frac{\partial f^{(0)}}{\partial \xi_i} + Q_d[f]^{(1)} + \tilde{Q}_d^b[f]^{(0)}, \end{aligned} \quad (4.37c)$$

and so on, where

$$\mathcal{G}[f] = \sum_{n=0}^{\infty} \mathcal{G}[f]^{(n)} \varepsilon^n, \quad F_i = \sum_{n=0}^{\infty} F_i^{(n)} \varepsilon^n, \quad (4.38a)$$

$$A^b(\rho, T) = \sum_{n=0}^{\infty} A^{b(n)} \varepsilon^n, \quad Q_d^b[f] = \sum_{n=0}^{\infty} (Q_d[f]^{(n)} + \varepsilon \tilde{Q}_d^b[f]^{(n)}) \varepsilon^n. \quad (4.38b)$$

Under the conventional condition

$$\int \psi_r f d\boldsymbol{\xi} = \int \psi_r f^{(0)} d\boldsymbol{\xi}, \quad (4.39)$$

we solve (4.37) from the lowest order. Before going into details, it should be noted that, by (4.39) and the property of the ES collision integral [16]:

$$\int \psi_r \mathcal{G}[f] d\boldsymbol{\xi} = \int \psi_r f d\boldsymbol{\xi}, \quad (r = 0, 1, \dots, 4), \quad (4.40a)$$

$$\int c_i c_j \mathcal{G}[f] d\boldsymbol{\xi} = \rho \mathcal{T}_{ij} = (1 - \nu) \rho RT \delta_{ij} + \nu \rho \Theta_{ij}, \quad (4.40b)$$

it holds that

$$\int \psi_r \mathcal{G}[f]^{(0)} d\boldsymbol{\xi} = \int \psi_r f^{(0)} d\boldsymbol{\xi}, \quad (4.41a)$$

$$\int \psi_r f^{(n+1)} d\boldsymbol{\xi} = 0, \quad \int \psi_r \mathcal{G}[f]^{(n+1)} d\boldsymbol{\xi} = 0, \quad (4.41b)$$

where $r = 0, 1, \dots, 4$ and $n = 0, 1, 2, \dots$.

Let us now start with the solution of (4.37a). Since $\mathcal{G}[f]^{(0)} = \lim_{\varepsilon \rightarrow 0} \mathcal{G}[f] = \mathcal{G}[f^{(0)}]$, (4.37a) is reduced to

$$f^{(0)} = \mathcal{G}[f^{(0)}],$$

and thus $f^{(0)}$ is a local Maxwellian:

$$f^{(0)} = \frac{\rho}{(2\pi RT)^{3/2}} \exp\left(-\frac{|\boldsymbol{\xi} - \mathbf{v}|^2}{2RT}\right),$$

where the condition (4.39) has been used. By the same condition, it is also seen that

$$F_i^{(0)} = F_i, \quad A^{b(0)} = A^b, \quad Q_d^b[f]^{(0)} = Q_d[f^{(0)}], \quad (4.42a)$$

$$F_i^{(n+1)} = 0, \quad A^{b(n+1)} = 0, \quad Q_d^b[f]^{(n+1)} = Q_d[f^{(n+1)}] + \tilde{Q}_d^b[f^{(n)}], \quad (4.42b)$$

where $n = 0, 1, \dots$, since F_i , A^b , Q_d , and $\tilde{Q}_d^b$ are all expressed in terms of ρ_r and $\nabla \rho_r$ and thus Q_d and $\tilde{Q}_d^b$ can be treated as linear operators acting on the expanded VDF $f^{(n)}$.

Furthermore, (4.37b) is reduced to

$$f^{(1)} = \mathcal{G}[f]^{(1)} + \frac{1}{A^b} \left(\frac{\partial f^{(0)}}{\partial \rho_r} \mathcal{F}_r^{(0)} - \xi_i \frac{\partial f^{(0)}}{\partial X_i} - F_i \frac{\partial f^{(0)}}{\partial \xi_i} + Q_d[f^{(0)}] \right), \quad (4.43)$$

since $f^{(0)}$ is independent of $\nabla\rho_r$. From (4.41b) with $n = 0$, the ψ_s -moment of (4.43) ($s = 0, 1, \dots, 4$) gives the following constraint for (4.37b) to be solvable:

$$\mathcal{F}_s^{(0)} = \int \xi_i \psi_s \frac{\partial f^{(0)}}{\partial \rho_r} d\boldsymbol{\xi} \frac{\partial \rho_r}{\partial X_i} - F_i \int \frac{\partial \psi_s}{\partial \xi_i} f^{(0)} d\boldsymbol{\xi} - \int \psi_s Q_d[f^{(0)}] d\boldsymbol{\xi}. \quad (4.44)$$

The above constraint is consistent with the definition of $\mathcal{F}_s$ at the leading order ($n = 0$) [see (4.33) or (4.35)] and eventually leads to the following expressions of $\mathcal{F}_s^{(0)}$:

$$\mathcal{F}_0^{(0)} = \int \xi_i \frac{\partial f^{(0)}}{\partial \rho_r} d\boldsymbol{\xi} \frac{\partial \rho_r}{\partial X_i} = \frac{\partial \rho_i}{\partial X_i} = \frac{\partial \rho v_i}{\partial X_i}, \quad (4.45a)$$

$$\begin{aligned} \mathcal{F}_j^{(0)} &= \int \xi_i \xi_j \frac{\partial f^{(0)}}{\partial \rho_r} d\boldsymbol{\xi} \frac{\partial \rho_r}{\partial X_i} - F_j \rho - \alpha_j \rho \\ &= \frac{\partial}{\partial X_i} \left[\rho v_i v_j + \left(\rho RT + \int \rho \frac{\partial \Phi_S}{\partial \rho} d\rho \right) \delta_{ij} \right] + \rho \frac{\partial \Phi_L}{\partial X_j} \\ &= \frac{\partial}{\partial X_i} (\rho v_i v_j + p \delta_{ij}) + \rho \frac{\partial \Phi_L}{\partial X_j}, \quad (j = 1, 2, 3), \end{aligned} \quad (4.45b)$$

$$\begin{aligned} \mathcal{F}_4^{(0)} &= \frac{1}{2} \int \xi_i \xi^2 \frac{\partial f^{(0)}}{\partial \rho_r} d\boldsymbol{\xi} \frac{\partial \rho_r}{\partial X_i} - F_i \rho v_i - (\alpha_i \rho v_i + 3\beta \rho RT) \\ &= \frac{\partial}{\partial X_i} \left[\left(\frac{5}{2} RT + \frac{1}{2} \mathbf{v}^2 \right) \rho v_i \right] + \frac{\partial}{\partial t} \int \left(\Phi_S - T \frac{\partial \Phi_S}{\partial T} \right) d\rho \\ &\quad + \frac{\partial}{\partial X_i} \left[v_i \int \left(\Phi_S - T \frac{\partial \Phi_S}{\partial T} \right) d\rho + v_i \int \rho \frac{\partial \Phi_S}{\partial \rho} d\rho \right] + \rho v_i \frac{\partial \Phi_L}{\partial X_i} \\ &= \frac{\partial}{\partial X_i} \left[\left(e + \frac{1}{2} \mathbf{v}^2 \right) \rho v_i + p v_i \right] + \frac{\partial}{\partial t} \int \left(\Phi_S - T \frac{\partial \Phi_S}{\partial T} \right) d\rho + \rho v_i \frac{\partial \Phi_L}{\partial X_i}. \end{aligned} \quad (4.45c)$$

If we stop the solution procedure at this stage and substitute (4.45) into (4.35) truncated at $n = 0$, the Euler set of equations, i.e., (4.7) with $p_{ij} = p \delta_{ij}$ and $q_i = 0$, is obtained.

In order to complete the solution of $f^{(1)}$, it is necessary to evaluate $\mathcal{G}[f]^{(1)}$. The evaluation needs some direct calculations to conclude

$$\mathcal{G}[f]^{(1)} = \frac{2\nu}{(2RT)^2} \Theta_{kl}^{(1)} c_k c_l f^{(0)}, \quad (4.46a)$$

where

$$\rho \Theta_{ij}^{(1)} = \int c_i c_j f^{(1)} d\boldsymbol{\xi}. \quad (4.46b)$$

Then, taking the $c_i c_j$ -moment of (4.43) eventually lead to

$$\int c_i c_j f^{(1)} d\boldsymbol{\xi} (= \rho \Theta_{ij}^{(1)}) = -\frac{\rho RT}{(1-\nu)A^b} \left(\frac{\partial v_i}{\partial X_j} + \frac{\partial v_j}{\partial X_i} - \frac{2}{3} \frac{\partial v_k}{\partial X_k} \delta_{ij} \right), \quad (4.47)$$

with the aid of (4.46a). Substitution of (4.46a) and (4.47) into (4.43) completes the solution of $f^{(1)}$. With thus obtained $f^{(1)}$, it is also seen that

$$\frac{1}{2} \int c_i c^2 f^{(1)} d\boldsymbol{\xi} = -\frac{5}{2} \frac{R}{A^b} \rho RT \frac{\partial T}{\partial X_i}. \quad (4.48)$$

Finally, let us consider (4.37c), which is slightly simplified as

$$f^{(2)} = \mathcal{G}[f]^{(2)} + \frac{1}{A^b} \left(\frac{\partial f^{(0)}}{\partial \rho_r} \mathcal{F}_r^{(1)} + \frac{\partial f^{(1)}}{\partial \rho_r} \mathcal{F}_r^{(0)} + \frac{\partial f^{(1)}}{\partial \nabla \rho_r} \nabla \mathcal{F}_r^{(0)} - \xi_i \frac{\partial f^{(1)}}{\partial X_i} - F_i \frac{\partial f^{(1)}}{\partial \xi_i} + Q_d[f^{(1)}] + \tilde{Q}_d^b[f^{(0)}] \right), \quad (4.49)$$

by using the results obtained so far in the Appendix. Because of (4.41b) with $n = 1$, the ψ_s -moment of (4.49) gives the following constraint for (4.37c) to be solvable:

$$\mathcal{F}_s^{(1)} = \frac{\partial}{\partial X_i} \int \xi_i \psi_s f^{(1)} d\boldsymbol{\xi} - \int \psi_s Q_d[f^{(1)}] d\boldsymbol{\xi} - \int \psi_s \tilde{Q}_d^b[f^{(0)}] d\boldsymbol{\xi}, \quad (4.50)$$

which is again consistent with the definition of $\mathcal{F}_s$ at the order $n = 1$. (4.50) is further reduced to

$$\mathcal{F}_0^{(1)} = 0, \quad (4.51a)$$

$$\mathcal{F}_j^{(1)} = \frac{\partial}{\partial X_i} \int c_i c_j f^{(1)} d\boldsymbol{\xi} - \rho(\alpha_j^b - \alpha_j), \quad (j = 1, 2, 3), \quad (4.51b)$$

$$\begin{aligned} \mathcal{F}_4^{(1)} = & \frac{\partial}{\partial X_i} \left(\frac{1}{2} \int c_i \mathbf{c}^2 f^{(1)} d\boldsymbol{\xi} + v_j \int c_i c_j f^{(1)} d\boldsymbol{\xi} \right) \\ & - \rho(\alpha_i^b - \alpha_i) v_i - 3(\beta^b - \beta) \rho R T. \end{aligned} \quad (4.51c)$$

Noting that

$$\rho(\alpha_i^b - \alpha_i) = \frac{\partial}{\partial X_j} \left[\mu_P \left(\frac{\partial v_i}{\partial X_j} + \frac{\partial v_j}{\partial X_i} - \frac{2}{3} \frac{\partial v_k}{\partial X_k} \delta_{ij} \right) + \mu_B \frac{\partial v_k}{\partial X_k} \delta_{ij} \right], \quad (4.52a)$$

$$\begin{aligned} 3(\beta^b - \beta) \rho R T + \rho(\alpha_j^b - \alpha_j) v_j = & \frac{\partial}{\partial X_k} \left(\lambda_P \frac{\partial T}{\partial X_k} \right) \\ & + \frac{\partial}{\partial X_j} \left[\mu_P \left(\frac{\partial v_i}{\partial X_j} + \frac{\partial v_j}{\partial X_i} - \frac{2}{3} \frac{\partial v_k}{\partial X_k} \delta_{ij} \right) v_i + \mu_B \frac{\partial v_k}{\partial X_k} v_j \right], \end{aligned} \quad (4.52b)$$

(4.51b) and (4.51c) are finally expressed as

$$\mathcal{F}_j^{(1)} = - \frac{\partial}{\partial X_i} \left[\mu \left(\frac{\partial v_i}{\partial X_j} + \frac{\partial v_j}{\partial X_i} - \frac{2}{3} \frac{\partial v_k}{\partial X_k} \delta_{ij} \right) + \mu_B \frac{\partial v_k}{\partial X_k} \delta_{ij} \right], \quad (4.53)$$

$$\mathcal{F}_4^{(1)} = - \frac{\partial}{\partial X_i} \left[\lambda \frac{\partial T}{\partial X_i} + \mu v_j \left(\frac{\partial v_i}{\partial X_j} + \frac{\partial v_j}{\partial X_i} - \frac{2}{3} \frac{\partial v_k}{\partial X_k} \delta_{ij} \right) + \mu_B v_i \frac{\partial v_k}{\partial X_k} \right], \quad (4.54)$$

where

$$\mu = \mu_P + \frac{\rho R T}{(1 - \nu) A^b}, \quad \lambda = \lambda_P + \frac{5}{2} \frac{R}{A^b} \rho R T. \quad (4.55)$$

Thus, (4.35) truncated at $n = 1$ gives the Navier–Stokes set of equations, i.e., (4.7) with

$$p_{ij} = p \delta_{ij} - \mu \left(\frac{\partial v_i}{\partial X_j} + \frac{\partial v_j}{\partial X_i} - \frac{2}{3} \frac{\partial v_k}{\partial X_k} \delta_{ij} \right) - \mu_B \frac{\partial v_k}{\partial X_k} \delta_{ij}, \quad (4.56)$$

$$q_i = - \lambda \frac{\partial T}{\partial X_i}. \quad (4.57)$$

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Chapter 5

Single droplet/bubble and its stability: Kinetic theory and dynamical system approaches

5.1 Introduction

Two-phase systems with/without the phase change have been variously studied so far by the thermal-fluid-dynamic way from the physics, chemical physics, mathematical physics, and engineering point of view. When the dynamic aspects are of interest, the Cahn–Hilliard equation [1] or its variants have been widely used in the thermodynamic discussions, while the Navier–Stokes equation for two-phase fluids has been used in the fluid dynamic discussions (e.g., [2,3]). However, the dynamic process does not necessarily occur under the phase equilibrium. This is the point that has motivated studies using microscopic approaches that are free from the phase equilibrium constraint in recent decades. Molecular dynamics (MD) [4,5,6] and kinetic theory [7,8,9,10,11,12] are typical approaches taken in such studies.

Probably the most fundamental setting for understanding the elementary process of the phase change from a single to a two-phase state would be the problem of a single droplet/bubble in the infinite expanse of the fluid. Such a setting is the simplest, at least conceptually, but is not necessarily well understood. For instance, though some MD simulations can be found in the literature, they are usually conducted under a periodic condition. Therefore, in drawing conclusions about single droplet/bubble formation from those simulations, we need to examine carefully whether there are still interactions with other droplets/bubbles, whether the simulation is for an energy conservative or isothermal system, and so on. Our previous 1D simulations using a kinetic model equation [8,11] are not exception as well, and they do not provide direct information about the single droplet/bubble formation.

With this background, Busuioc *et al.* [12] recently conducted numerical simulations of a single bubble on the basis of the Enskog–Vlasov equation [13]. However, their main goal is to develop a stochastic particle simulation method for the Enskog–Vlasov equation. In

the present paper, we more focus on the analysis of a steady single droplet/bubble and its stability, thereby deepening our understanding of the elementary process in phase change. The dynamics-like interpretation of the phase change in the context of van der Waals fluids can be traced back to, for example, the work by van Kampen [14,15] based on the equilibrium statistical thermodynamics. He clearly explained the two-phase equilibrium in terms of the thermodynamical potential by the resemblance with a classical point mass dynamics, especially for one-dimensional case. Indeed, we have made use of his interpretation in our previous work [16] for the discussion of one-dimensional case. In the present work, we shall step forward to multidimensional cases that require more detailed study of the dynamical system, thereby showing peculiar features that is absent from one-dimensional case.

The main ingredients of the present study are the low-dimensional dynamical system analysis [17,18] on the steady solution and simple numerical simulations for the instability assessment of the steady solution via the kinetic model developed in [19]. Our approach is thus distinctive to the order-parameter models with fluctuations [20] in the literature. In the simulations in Sec. 5.5, physical (thermal) fluctuations are not added to the single droplet/bubble solution obtained in the study of dynamical system to be discussed in Sec. 5.4.4. Instead, the numerical errors coming from discretization and numerical approximations play the role of fluctuations there. Hence, the collapse of the single droplet/bubble to be observed in Sec. 5.4.4 simply suggests that such a droplet/bubble is linearly unstable.

The paper is organized as follows. First, the kinetic model that our analysis is based on is presented in Sec. 5.2. The model was proposed in [19] as an extension of our previous models [16,11]. The H-theorem and the reproducibility of appropriate transport properties were established for the model. Next in Sec. 5.3, steady solutions of a single droplet/bubble that is isotropic to the origin of the coordinates are investigated within the uniform resting Maxwellians and the problem is reduced to the one for the radial density field. The reduced problem is treated and studied as a low-dimensional dynamical system in Sec. 5.4 by using the concepts of the phase space vector field, fixed point, and *flow*¹ that are familiar in the field of nonlinear dynamical system [17,18]. In particular, it will be clarified in Sec. 5.4.3 that the *flow* changes qualitatively whether the set of parameters of the far-field uniform state falls into the unstable region or the metastable region [11,21]. The structure of the

¹To discriminate from the fluid flow, the flow in the phase space is italicized in the present paper.

single droplet/bubble will be also discussed in Sec. 5.4.4. In Sec. 5.5, the instability of the obtained steady solution is assessed by direct numerical simulations of the kinetic model. The paper is concluded in Sec. 5.6.

5.2 Kinetic model equation

We study a single droplet/bubble in an infinite expanse of the van der Waals fluid using the kinetic model proposed in [19] under the name of the second Ellipsoidal-Statistical (ES)-based model:

$$\frac{\partial f}{\partial t} + \xi_i \frac{\partial f}{\partial X_i} + F_i \frac{\partial f}{\partial \xi_i} = Q_c^b[f] + Q_d^b[f], \quad (5.1a)$$

$$f \rightarrow \frac{\rho_\infty}{(2\pi RT_\infty)^{\frac{3}{2}}} \exp\left(-\frac{\xi_i^2}{2RT_\infty}\right), \quad (|\mathbf{X}| \rightarrow \infty). \quad (5.1b)$$

where t is time, $\mathbf{X}$ (or X_i) is spatial position, $\boldsymbol{\xi}$ (or ξ_i) is molecular velocity, $f(t, \mathbf{X}, \boldsymbol{\xi})$ is the velocity distribution function (VDF), R is the specific gas constant, and ρ_∞ and T_∞ are positive constants for the far-field density and temperature, respectively. Q_c^b is the ES-type collision model [22,23] given by

$$Q_c^b[f] = A^b(\rho, T)(\mathcal{G} - f), \quad (5.2)$$

$$\mathcal{G} = \frac{\rho}{\sqrt{\det(2\pi\mathcal{T})}} \exp\left(-\frac{1}{2}(\mathcal{T}^{-1})_{ij}c_i c_j\right), \quad (5.3)$$

$$c_i = \xi_i - v_i, \quad \mathcal{T}_{ij} = (1 - \nu)RT\delta_{ij} + \nu\Theta_{ij}, \quad (5.4)$$

$$\rho = \int f d\boldsymbol{\xi}, \quad v_i = \frac{1}{\rho} \int \xi_i f d\boldsymbol{\xi}, \quad (5.5)$$

$$T = \frac{1}{3\rho R} \int c_k^2 f d\boldsymbol{\xi}, \quad \Theta_{ij} = \frac{1}{\rho} \int c_i c_j f d\boldsymbol{\xi}. \quad (5.6)$$

Here, ν is an adjusting parameter for the Prandtl number in the range $-1/2 \leq \nu < 1$. $\mathcal{T}^{-1}$ is the inverse of the tensor $\mathcal{T}$. ρ , $\mathbf{v}$ (or v_i), and T are, respectively, the density, flow velocity, and temperature. Q_d^b is a correction term to Q_c^b for exclusive effects of molecules and $\mathbf{F}$ (or F_i) is a force acting on a molecule per unit mass. They are assumed to take the form:

$$Q_d^b[f] = -\frac{\partial}{\partial \xi_i}[(\alpha_i^b + \beta^b c_i)f], \quad (5.7)$$

$$F_i = -\frac{\partial}{\partial X_i}(\Phi_S + \Phi_L). \quad (5.8)$$

There are still some quantities that should be specified. In the above, F_i is composed of two potential forces: the long-range Φ_L and short-range Φ_S . Φ_L is purely attractive and can be

expressed within the diffusion approximation [16,11] as

$$\Phi_L = -\kappa \frac{\partial^2 \rho}{\partial X_i^2}, \quad (5.9)$$

where κ is a positive constant. Φ_S is a combined potential of repulsion and attraction and, by applying a local approximation due to the short-range nature, its form can be specified, together with A^b , in accordance with the equation of state for the van der Waals fluid [16,11]:

$$p = \frac{\rho RT}{1 - b\rho} - a\rho^2, \quad (0 < b\rho < 1), \quad (5.10)$$

as follows:

$$\Phi_S = -RT \ln(1 - b\rho) + \frac{b\rho RT}{1 - b\rho} - 2a\rho, \quad (5.11)$$

$$A^b = \frac{5}{2} \frac{\rho RT}{1 - b\rho} \frac{R}{\lambda_0(T)}. \quad (5.12)$$

Here p is the pressure, a and b are positive constant, and λ_0 is the thermal conductivity in the dilute gas limit. Moreover, by setting the viscosity and thermal conductivity to those of the Enskog equation [24,25], all the remaining quantities can be specified as

$$\alpha_i^b = \alpha_i + \frac{1}{\rho} \left[\mu_P \frac{\partial v_i}{\partial X_j} + \mu_B \frac{\partial v_k}{\partial X_k} \delta_{ij} \right], \quad (5.13)$$

$$\beta^b = \beta + \frac{1}{3\rho RT} \left\{ \frac{\partial}{\partial X_k} \left(\lambda_P \frac{\partial T}{\partial X_k} \right) + \frac{\partial v_i}{\partial X_j} \left[\mu_P \frac{\partial v_i}{\partial X_j} + \mu_B \frac{\partial v_k}{\partial X_k} \delta_{ij} \right] \right\}, \quad (5.14)$$

$$\alpha_i = \frac{1}{\rho} \int \frac{\partial \Phi_S}{\partial T} d\rho \frac{\partial T}{\partial X_i}, \quad \beta = \frac{1}{3\rho R} \left\{ \frac{\partial}{\partial t} \int \frac{\partial \Phi_S}{\partial T} d\rho + \frac{\partial}{\partial X_i} \left(v_i \int \frac{\partial \Phi_S}{\partial T} d\rho \right) \right\}, \quad (5.15)$$

$$\frac{\partial v_i}{\partial X_j} = \frac{\partial v_i}{\partial X_j} + \frac{\partial v_j}{\partial X_i} - \frac{2}{3} \frac{\partial v_k}{\partial X_k} \delta_{ij}, \quad (5.16)$$

$$\mu_P = (1 - b\rho) g_1^b \left(\frac{b\rho}{1 - b\rho} \right) \mu_0(T), \quad \mu_B = (1 - b\rho) \left(\frac{b\rho}{1 - b\rho} \right)^2 \mu_0(T), \quad (5.17)$$

$$\lambda_P = (1 - b\rho) g_2^b \left(\frac{b\rho}{1 - b\rho} \right) \lambda_0(T), \quad (5.18)$$

$$\text{Pr}_0 = \frac{5}{2} R \frac{\mu_0}{\lambda_0} = \frac{2}{3}, \quad \nu = 1 - \frac{1}{\text{Pr}_0} = -\frac{1}{2}, \quad (5.19)$$

$$g_1^b(x) = \frac{4}{5}x + \frac{6.1}{8}x^2, \quad g_2^b(x) = \frac{6}{5}x + \frac{12.1}{16}x^2. \quad (5.20)$$

Here, additional comments would be in order. μ_P , μ_B , and λ_P represent the exclusion effect of molecules on the viscosity, bulk viscosity, and thermal conductivity, respectively. μ_0 and Pr_0 represent the viscosity and the Prandtl number in the dilute gas limit. For the above kinetic model equation with the quantities so specified, the H-theorem has been shown to

hold for periodic systems in [19]. This completes the presentation of the kinetic model used in the remainder of the paper.

5.3 Steady single droplet/bubble isotropic to the origin

In the present section, a steady single droplet/bubble in an infinite expanse of the van der Waals fluid will be considered. Since such a single droplet/bubble is in the thermal equilibrium state, the solution is sought within the resting Maxwellian with uniform temperature T_∞ (see Sec. 5.A):

$$f(\mathbf{X}, \boldsymbol{\xi}) = \frac{\rho(\mathbf{X})}{(2\pi RT_\infty)^{3/2}} \exp\left(-\frac{\boldsymbol{\xi}^2}{2RT_\infty}\right). \quad (5.21)$$

By substitution of (5.21), (5.1a) is reduced to

$$\frac{\partial}{\partial X_i} (RT_\infty \ln \rho + \Phi_S + \Phi_L) = 0. \quad (5.22)$$

Integrating (5.22) once with respect to $\mathbf{X}$ and substituting (5.9) and (5.11) reduces the original problem (5.1) to a much simpler form:

$$\kappa \frac{\partial^2 \rho}{\partial X_i^2} = RT_\infty \left(\ln \frac{b\rho}{1-b\rho} + \frac{1}{1-b\rho} - \lambda_* \right) - 2a\rho, \quad (5.23a)$$

$$\rho \rightarrow \rho_\infty, \quad (|\mathbf{X}| \rightarrow \infty). \quad (5.23b)$$

Here λ_* is a dimensionless constant that is related to ρ_∞ and T_∞ . Indeed, since $\rho \rightarrow \rho_\infty$ as $\mathbf{X} \rightarrow \infty$ by (5.23b), $\partial^2 \rho / \partial X_i^2 \rightarrow 0$ in the same limit, leading to the relation

$$RT_\infty \left(\ln \frac{b\rho_\infty}{1-b\rho_\infty} + \frac{1}{1-b\rho_\infty} - \lambda_* \right) = 2a\rho_\infty. \quad (5.24)$$

In the meantime, the critical density ρ_c and temperature T_c are related to the van der Waals constants a and b as

$$3\rho_c = \frac{1}{b}, \quad T_c = \frac{8a}{27Rb}. \quad (5.25)$$

Hence, the dimensionless quantities

$$\eta = b\rho \left(= \frac{\rho}{3\rho_c} \right), \quad \tilde{T} = \frac{T}{T_c}, \quad x_i = \frac{X_i}{L}, \quad (5.26)$$

are naturally introduced with $3\rho_c$, T_c , and

$$L = \sqrt{\frac{\kappa}{bRT_c}}, \quad (5.27)$$

being the reference density, temperature, and length, respectively. Then, (5.23) is recast as

$$\frac{\partial^2 \eta}{\partial x_i^2} = \Pi(\eta; \eta_\infty, \tilde{T}_\infty), \quad (5.28a)$$

$$\eta \rightarrow \eta_\infty, \quad (|\mathbf{x}| \rightarrow \infty), \quad (5.28b)$$

where $\eta_\infty = b\rho_\infty$, $\tilde{T}_\infty = T_\infty/T_c$, and

$$\Pi(\eta; \eta_\infty, \tilde{T}_\infty) \equiv \tilde{T}_\infty [\Lambda(\eta, \tilde{T}_\infty) - \Lambda(\eta_\infty, \tilde{T}_\infty)], \quad (5.28c)$$

$$\Lambda(X, Y) \equiv \ln \left(\frac{X}{1-X} \right) + \frac{1}{1-X} - \frac{27}{4} \frac{X}{Y}, \quad (5.28d)$$

$$\lambda_* = \Lambda(\eta_\infty, \tilde{T}_\infty). \quad (5.28e)$$

Note that Π has two parameters, η_∞ and $\tilde{T}_\infty$, but its variation with respect to η is characterized only by $\tilde{T}_\infty$. Π has two extrema below the critical temperature ($\tilde{T}_\infty < 1$), but above the critical temperature ($\tilde{T}_\infty \geq 1$) it increases monotonically with respect to η ; see Fig. 5.1. In fact, Π is a dimensionless version of the specific Gibbs free energy [11], and thus appears later in the thermodynamic discussion of phase equilibrium. In the sequel, η_∞ and $\tilde{T}_\infty$ will be suppressed in the argument of Π , unless confusion is anticipated.

Since our aim is to study a steady single droplet/bubble, it is enough to consider the isotropic field with respect to the origin of the coordinates. Hence, η is assumed to be a function of the radius $r \equiv |\mathbf{x}|$ ($\mathbf{x} \in \mathbb{R}^D$ with D being the spatial dimension²) only and (5.28) is further reduced to

$$\frac{1}{r^{D-1}} \frac{d}{dr} \left(r^{D-1} \frac{d\eta}{dr} \right) = \Pi(\eta), \quad (0 \leq r < \infty), \quad (5.29a)$$

$$\eta(r) \rightarrow \eta_\infty, \quad (r \rightarrow \infty). \quad (5.29b)$$

We seek nonuniform solutions of (5.29) that satisfy $\eta(0) = \eta_O (\neq \eta_\infty)$, $d\eta/dr(0) = 0$ at the origin and $\eta \rightarrow \eta_\infty$ as $r \rightarrow \infty$. Since these conditions at the origin and at a far field are too many for the second order differential equation, such solutions do not always exist. Hence, putting aside the condition (5.29b), we shall first consider (5.29a) under only the condition at the origin

$$\eta(0) = \eta_O, \quad \frac{d\eta}{dr}(0) = 0, \quad (5.30)$$

²Both the spatial and molecular velocity space are originally three-dimensional. However, depending on the spatial dependence of the problem under consideration, we may set $D = 1, 2$, or 3 . The droplet/bubble geometry is a sphere when $D = 3$, a cylinder when $D = 2$, and a slab when $D = 1$.

transform it to a system of simultaneous first-order ordinary differential equations, and then study the resulting system as *flows* in low-dimensional phase space [17,18]. Among such *flows*, the steady solution of a single droplet/bubble is chosen as a *flow* that satisfies the far-field condition (5.29b).

5.4 *Flows* in phase space

5.4.1 Preliminary analysis

In the present subsection, as a preliminary analysis, we consider the behavior of the dimensionless density η qualitatively on the basis of

$$\frac{d\eta}{dr} = \int_0^r \Pi(\eta(s)) \left(\frac{s}{r}\right)^{D-1} ds, \quad (5.31)$$

that is obtained by integrating (5.29a) multiplied with r^{D-1} and using the condition (5.30).

As is clear from (5.31), the property of $\Pi(\eta)$ determines whether η increases or decreases with respect to r . As is mentioned in Sec. 5.3 and shown in Fig. 5.1, $\Pi(\eta)$ is monotonic when $\tilde{T}_\infty \geq 1$ and has two extrema when $\tilde{T}_\infty < 1$. Thus, $\Pi(\eta)$ has only one zero [Fig. 5.1(a)] when $\tilde{T}_\infty \geq 1$. When $\tilde{T}_\infty < 1$, $\Pi(\eta)$ has at most three zeros and the number of zeros depends on the value of η_∞ [Figs. 5.1(b)–5.1(f)]. But in any case $\eta = \eta_\infty$ is always a zero of $\Pi(\eta)$.

First the following proposition holds.

Proposition. *If $\Pi(\eta)$ has one or two zeros, then there is no spatially nonuniform solution of (5.29).*

Proof. First suppose that $\Pi(\eta)$ has only one zero [Case A: Figs. 5.1(a)–5.1(c)]. Obviously, this zero is $\eta = \eta_\infty$. Hence, for $\eta_O \leq \eta_\infty$, $\Pi(\eta_O) \leq 0$ holds [Figs. 5.1(a)–5.1(c)], and furthermore $d\eta/dr \leq 0$ holds by (5.31). This means that the change of η from η_O ($\leq \eta_\infty$) to η_∞ is not possible.

Next suppose that $\Pi(\eta)$ has two zeros. Then, one of the zeros is an extremum point [Case B: Figs. 5.1(d) – 5.1(e)]. By repeating the same discussion as in the previous case, it is readily seen that both zeros cannot be reached by starting from η_O larger or smaller than both zeros. However, the extremum point might be reached if starting from η_O between two zeros (there is no way to reach the other zero). Therefore, the extremum point is a candidate of η_∞ . However, since $\Pi(\eta)$ is either positive definite or negative definite in the process of

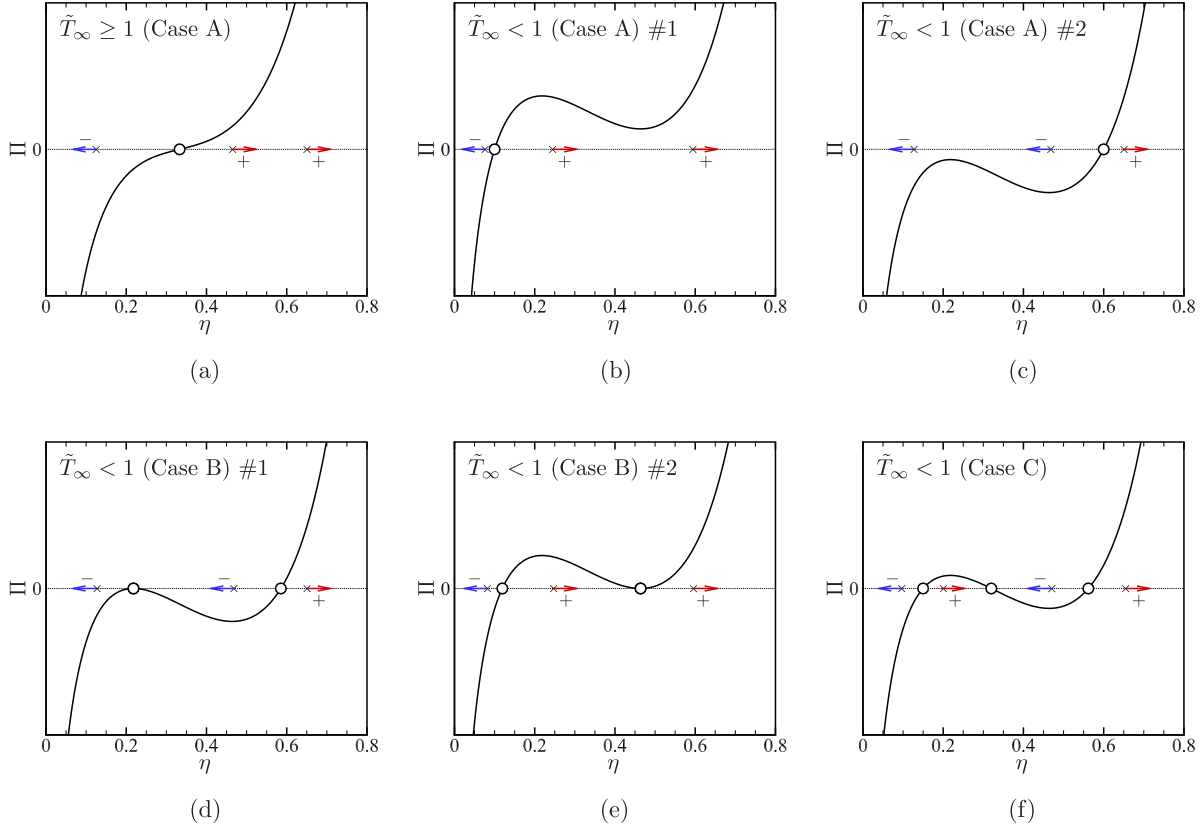


Figure 5.1: Classification of $\Pi(\eta)$ and phase-portrait-like diagram. $\Pi(\eta)$ has only one zero point in Case A, two zero points in Case B, and three zero points in Case C, respectively. (a) Case A with $\tilde{T}_\infty \geq 1$. (b) Case A with $\tilde{T}_\infty < 1$ and the extrema are positive. (c) Case A with $\tilde{T}_\infty < 1$ and the extrema are negative. (d) Case B and the local maximum is zero. (e) Case B and the local minimum is zero. (f) Case C. In each panel, the arrow indicates the change direction of η starting from η_O at the point $\times$, while $+$ and $-$ indicate the sign of the corresponding value of $\int_0^r \Pi(\eta(s))(s/r)^{D-1} ds$.

reaching the extremum point, $d\eta/dr \neq 0$ by (5.31) at the extremum point. This means that η cannot approach a certain constant as $r \rightarrow \infty$ and the extremum point cannot be η_∞ . $\square$

Thanks to the above Proposition, we can focus on the case that $\Pi(\eta)$ has three zeros [Case C: Fig. 5.1(f)]. Let η_a , η_b , and η_c be the three zeros ($\eta_a < \eta_b < \eta_c$). Then $\Pi(\eta)$ has one inflection point $\eta = 1/3$, which always lies between the two extrema. Since the inflection point lies between the two extrema and the two extrema lie between η_a and η_c , $\eta_a < 1/3 < \eta_c$ holds. In addition, it is readily seen that $\Pi'(\eta_a) > 0$, $\Pi'(\eta_b) < 0$, and $\Pi'(\eta_c) > 0$ hold as well, where $\Pi' = d\Pi/d\eta$. Again along the same lines as the one zero case in the proof, it is seen that any zeros of $\Pi(\eta)$ cannot be reached starting from η_O larger than η_c or smaller than η_a . To reach zero, $\eta_a < \eta_O < \eta_c$ is required at least. However, in the present stage, the process

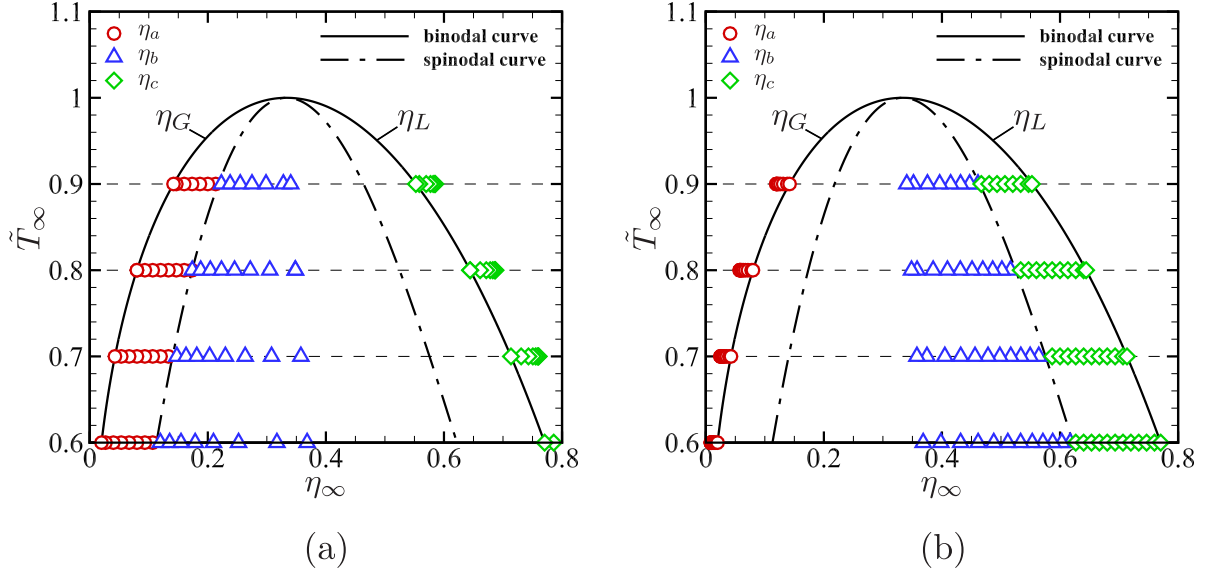


Figure 5.2: Parameter diagram in $\eta_\infty \tilde{T}_\infty$ plane. Dashed-dotted: Spinodal curve (5.33). Solid line: Binodal curve (5.34). Outside of binodal curve is the stable region, inside of spinodal curve is the unstable region, and between the spinodal and the binodal curve is the metastable region. Open circles (red), triangles (blue), and diamonds (green), respectively, indicate examples of η_a , η_b , and η_c (three zeros of Π) at $\tilde{T}_\infty = 0.6, 0.7, 0.8$, and 0.9 . (a) The case where $\eta_\infty = \eta_a$ lies in the metastable region (droplet). (b) The case where $\eta_\infty = \eta_c$ lies in the metastable region (bubble).

of approaching zero is not so obvious.³ The three zeros can be candidates of η_∞ . When η_∞ is the middle zero η_b , $\Pi'(\eta_\infty) = \Pi'(\eta_b) < 0$ holds, implying from (5.28c) and (5.28d) that

$$\tilde{T}_\infty < \frac{27}{4}\eta_\infty(1 - \eta_\infty)^2 (\leq 1) \quad \Leftrightarrow \quad a > \frac{RT_\infty}{2\rho_\infty(1 - b\rho_\infty)^2}. \quad (5.32)$$

This is identical to the parameter region where a uniform resting equilibrium state is unstable and the so-called spinodal decomposition is expected to occur (unstable region) [11]; see Fig. 5.2. Therefore, if the solution with $\eta_\infty = \eta_b$ is found, it represents a single droplet/bubble in the unstable region. When η_∞ is the minimum or maximum zero (η_a or η_c), $\Pi'(\eta_\infty) > 0$ holds and the inequality in condition (5.32) is reversed. Hence, if the solution with $\eta_\infty = \eta_a$ or $\eta_\infty = \eta_c$ is found, it represents a single droplet/bubble outside of the unstable region. The pair $(\eta_\infty, \tilde{T}_\infty)$ for such a solution is expected to fall in the metastable region. The metastable region is the one bounded by the spinodal curve

$$\tilde{T}_\infty = \frac{27}{4}\eta_\infty(1 - \eta_\infty)^2 (\leq 1), \quad (5.33)$$

³It is expected by (5.31) that η approaches the maximum and minimum zeros monotonically. However, it approaches the middle zero oscillationally, or even oscillate eternally around it. The solution that does not approach any zeros is not appropriate as a solution of the single droplet/bubble.

and the binodal curve that is obtained by eliminating η_O from the following two equalities:⁴

$$\Pi(\eta_O) = \Pi(\eta_\infty), \quad p(\eta_O, \tilde{T}_\infty) = p(\eta_\infty, \tilde{T}_\infty); \quad (5.34)$$

see Fig. 5.2. The binodal line has two branches when regarded as a function of $\tilde{T}_\infty$. For later convenience, let η_L be the branch giving the larger value of η_∞ and let η_G be the branch giving the smaller value, respectively.

5.4.2 Set up for *flow* analyses

Let us first introduce the following variables η_1, η_2, η_3 that are functions of r :

$$\eta_1(r) \equiv \eta(r), \quad \eta_2(r) \equiv \frac{d\eta}{dr}, \quad \eta_3(r) \equiv r, \quad (5.35)$$

and rewrite (5.29a) as a set of ordinary differential equations [17]:

$$\frac{d\eta_1}{dr} = \eta_2, \quad (5.36a)$$

$$\frac{d\eta_2}{dr} = -\frac{D-1}{\eta_3}\eta_2 + \Pi(\eta_1), \quad (5.36b)$$

$$\frac{d\eta_3}{dr} = 1. \quad (5.36c)$$

The right-hand side of (5.36) gives a three-dimensional constant phase vector field that is characterized by far-field parameters η_∞ and $\tilde{T}_\infty$. The projection of the trajectory in the phase space on the $\eta_1\eta_2$ plane has three fixed points $(\eta_a, 0)$, $(\eta_b, 0)$, and $(\eta_c, 0)$. Since Π does not change whether $\eta_\infty = \eta_a$, η_b , or η_c , the fixed points are common for $\eta_\infty = \eta_a$, η_b , or η_c .

The *flow* with respect to r is determined by (5.36) with the condition

$$(\eta_1, \eta_2, \eta_3) = (\eta_O, 0, 0), \quad (r = 0), \quad (5.37)$$

and the *flow* representing a single droplet/bubble is the one that further satisfies the condition

$$(\eta_1, \eta_2, \eta_3) \rightarrow (\eta_\infty, 0, \infty), \quad (r \rightarrow \infty). \quad (5.38)$$

In Sec. 5.4.3, we will study the *flows* numerically, classify them, and identify the conditions under which a steady single droplet/bubble solution can be found.

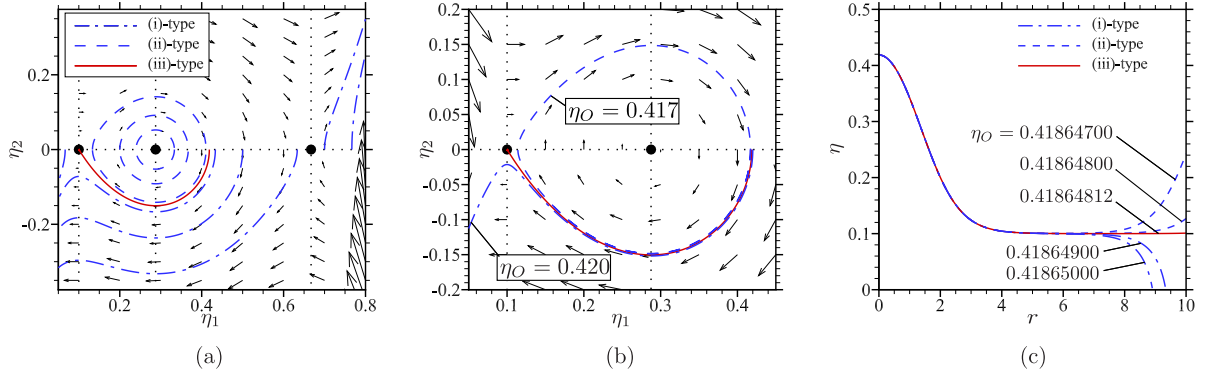


Figure 5.3: Vector field, trajectory, and corresponding radial density distribution in the case $D = 1$ for $\eta_\infty = 0.1$ and $\tilde{T}_\infty = 0.8$. (a) Vector field and some trajectory samples. (b) Close-up of critical and near-critical trajectories. (c) Radial density distributions of the trajectories. In panels (a) and (b), closed circles indicate the fixed points in the $\eta_1\eta_2$ plane, the dashed-dotted (blue), the dashed (blue), and the solid (red) line indicate the (i)-type, (ii)-type, and (iii)-type trajectory, respectively.

5.4.3 Results: Trajectory of *flow* and classification

Equation (5.36) with (5.37) is solved by the fourth order Runge-Kutta method [26] after a uniform discretization with respect to r . The step size Δr of r is uniform and set as $\Delta r = 1.0 \times 10^{-5}$. The step size was enough fine to draw firm conclusions for the discussions below about the *flow* properties.

5.4.3.1 Case $D = 1$

Let us start with the spatially one-dimensional case ($D = 1$), since it provides a clear-cut-off of main features of the present dynamical system. Since the first term on the right-hand side of (5.36b) vanishes, the vector field does not depend on η_3 . Hence, the problem is reduced to the two-dimensional dynamical system on the $\eta_1\eta_2$ plane. The three points $(\eta_\alpha, 0)$ ($\alpha = a, b, c$) on the η_1 axis are indeed fixed points of the reduced set of equations (5.36a) and (5.36b) on the $\eta_1\eta_2$ plane. Since η_∞ is a zero of Π , it must coincide with η_a , η_b , or η_c .

Figure 5.3(a) shows the vector field in the case $(\eta_\infty, \tilde{T}_\infty) = (0.1, 0.8)$. The pair of the parameters lies in the metastable region and three zeros of Π , i.e., η_a , η_b , and η_c , are 0.1, 0.287521, and 0.6767059 in this example; see Fig. 5.2(a). In Fig. 5.3(a), the trajectories

⁴Equation (5.34) is the phase equilibrium condition in the thermodynamics such that the specific Gibbs free energy and pressure are both equal between two phases. See [11].

of *flow* starting from various points $(\eta_1, \eta_2) = (\eta_O, 0)$ are also plotted. There are three categories of trajectory according to the value of η_O :

- (i) Trajectory for which $(\eta_1, \eta_2) \rightarrow (0, -\infty)$ or $(1, \infty)$ as $r \rightarrow \infty$ [dashed-dotted line in Fig. 5.3(a)],
- (ii) Periodic trajectory around the middle fixed point $(\eta_b, 0)$ on the η_1 axis [dashed line in Fig. 5.3(a)],
- (iii) Trajectory that reaches $(\eta_a, 0) = (\eta_\infty, 0)$ [solid line in Fig. 5.3(a)].

The periodic trajectory occurs because of the antisymmetric vector field with respect to η_1 axis. The trajectory that can reach the far-field state is only the (iii)-type and represents a single droplet solution [see the solid line in Fig. 5.3(c)]. The (iii)-type is the boundary between (i)-type and (ii)-type trajectory families [see Fig. 5.3(b)], and there is a one to one correspondence between η_O and η_∞ for the (iii)-type. This aspect as the boundary can be observed clearly in Fig. 5.3(c), where the density distributions for $\eta_O = 0.41865000$ and 0.41864900 are of (i)-type and those for $\eta_O = 0.41864800$ and 0.41864700 are of (ii)-type. The single droplet density distribution is of (iii)-type and the corresponding value of η_O lies between 0.418640800 and 0.41864900 ($\eta_O = 0.41864812$ up to eight decimal points).

The vector field and *flow* trajectories shown in Fig. 5.3 do not change if we set $\eta_\infty = 0.287521 (= \eta_b)$ or $\eta_\infty = 0.667059 (= \eta_c)$ in place of $\eta_\infty = 0.1 (= \eta_a)$, since Π remains unchanged (see Sec. 5.4.2). Hence, none of (i)–(iii)-type trajectories reach the far-field state if $\eta_\infty = \eta_b$ or $\eta_\infty = \eta_c$. As is seen from Fig. 5.2(a), the pair $(\eta_b, \tilde{T}_\infty)$ lies in the unstable region, while $(\eta_c, \tilde{T}_\infty)$ lies in the stable region. Therefore, steady single droplet solutions are not found when the pair of the far-field parameters $(\eta_\infty, \tilde{T}_\infty)$ lies in the unstable or stable region.

As discussed in Sec. 5.4.1, the pair of parameters $(\eta_b, \tilde{T}_\infty)$ always lies in the unstable region. In contrast, $(\eta_a, \tilde{T}_\infty)$ and $(\eta_c, \tilde{T}_\infty)$ lie either in the metastable or stable region. It is numerically verified that if the former lies in the metastable region, the latter in the stable region and vice versa (see Fig. 5.2). Therefore, if $(\eta_c, \tilde{T}_\infty)$ lies in the metastable region as in Fig. 5.2(b), then the (iii)-type trajectory flows into the fixed point $(\eta_c, 0)$ and represents a steady single bubble (not droplet) solution. Thus, irrespective of whether a droplet or a

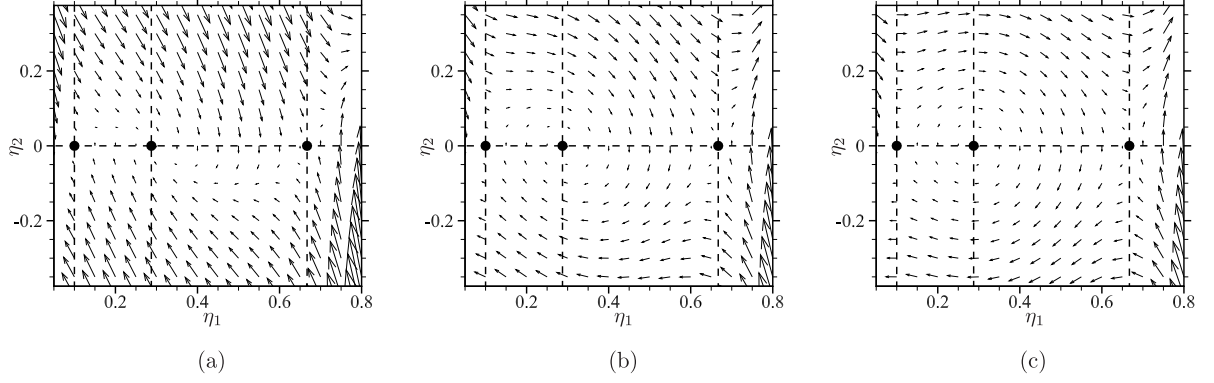


Figure 5.4: In-plane vector fields in the case $D = 2$ for $\eta_\infty = 0.1$ and $\tilde{T}_\infty = 0.8$. (a) $\eta_3 = 0.5$. (b) $\eta_3 = 2.0$. (c) $\eta_3 = 100.0$. Closed circles indicate the fixed points $(\eta_\alpha, 0)$ ($\alpha = a, b, c$) in the $\eta_1\eta_2$ plane.

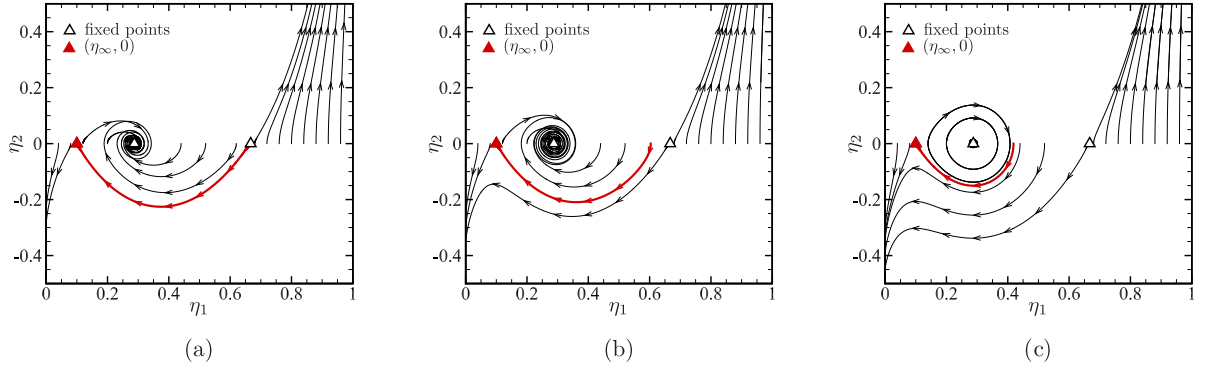


Figure 5.5: In-plane trajectories starting from various values of η_O on the η_1 axis for $\eta_\infty = 0.1$ and $\tilde{T}_\infty = 0.8$. (a) $D = 3$. (b) $D = 2$. (c) $D = 1$. Thick line (red) is the in-plane trajectory of a single droplet and ends at a point representing the far-field condition [closed triangle (red)]. Open triangle: the fixed point in the $\eta_1\eta_2$ plane. Closed triangle (red): the point $(\eta_\infty, 0)$ that represents the far-field condition.

bubble, the (iii)-type trajectory is interpreted as the one flowing into a fixed point. When this fixed point is $(\eta_a, 0)$, the trajectory represents a single droplet. When the fixed point is $(\eta_c, 0)$, the trajectory represents a single bubble. Again, when the pair of the far-field parameters lies in the unstable or stable region, single bubble solutions are not found.

Finally, it should be noted that as $(\eta_a, \tilde{T}_\infty)$ approaches $(\eta_G, \tilde{T}_\infty)$ on one branch of the binodal curve, the corresponding $(\eta_c, \tilde{T}_\infty)$ approaches $(\eta_L, \tilde{T}_\infty)$ on the other branch of the binodal curve. In this limit, the (iii)-type trajectory becomes a curve connecting $(\eta_a, 0)$ and $(\eta_c, 0)$ on the $\eta_1\eta_2$ plane.

5.4.3.2 Cases $D = 2$ and $D = 3$

Since the first term on the right-hand side remains in (5.36b), the vector field is no longer uniform with respect to η_3 . Nevertheless, since the η_3 component of the vector field is simple and uniform, we discuss the *flows* by their projection on the $\eta_1\eta_2$ plane for the sake of simplicity. The projection of the trajectory or *flow* will be called the in-plane trajectory or in-plane *flow* in the sequel. As in the case of $D = 1$, three points $(\eta_\alpha, 0)$ ($\alpha = a, b, c$) on the η_1 axis still remain the fixed points for the in-plane dynamics on the $\eta_1\eta_2$ plane. However, in contrast to the case $D = 1$, the in-plane vector field is no longer antisymmetric with respect to the η_1 axis. This is the influence of the first term on the right-hand side of (5.36b). Consequently, periodic trajectories in the case of $D = 1$ are deformed to spiral in-plane trajectories on the $\eta_1\eta_2$ plane. The influence of the first term is larger for larger D . It decreases as η_3 (or r) increases (see Fig. 5.4).

Figs. 5.5(a) and 5.5(b) show the in-plane *flow* trajectories in the case $(\eta_\infty, \tilde{T}_\infty) = (0.1, 0.8)$. The case for $D = 1$ is also shown in Fig. 5.5(c) for reference. The pair of parameters for this figure lies in the metastable region [see Fig. 5.2(a)]; three zeros of Π , i.e., η_a , η_b , and η_c , are 0.1, 0.287521, and 0.667059, respectively. As is demonstrated in Figs. 5.5(a) and 5.5(b), the in-plane trajectories are classified into three, depending on the value of η_O :

- (i) In-plane trajectory for which $(\eta_1, \eta_2) \rightarrow (0, -\infty)$ or $(1, \infty)$ as $r \rightarrow \infty$,
- (ii) Spiral in-plane trajectory that flows into $(\eta_b, 0)$,⁵
- (iii) In-plane trajectory that flows into $(\eta_a, 0)$.

Since $\eta_\infty = \eta_a$ in Fig. 5.5, the (iii)-type in-plane trajectory represents a steady single droplet. When η_∞ coincides with other zeros, i.e., $\eta_\infty = 0.287521 (= \eta_b)$ or $\eta_\infty = 0.667059 (= \eta_c)$, the same vector field and trajectories are obtained, since $\Pi(\eta)$ remains unchanged (see Sec. 5.4.2). Hence, as in the case $D = 1$, the *flow* to the far-field condition cannot be found for the pair $(\eta_\infty, \tilde{T}_\infty) = (\eta_c, \tilde{T}_\infty)$ that is in the stable region. However, the *flows* to the far-field condition

⁵The in-plane trajectories may cross each other as in Figs. 5.5(a) and 5.5(b) because they are projections of the original $\eta_1\eta_2\eta_3$ phase space trajectories. As a matter of course, original trajectories do not cross. The same comments applies to Figs. 5.6(a) and 5.6(b).

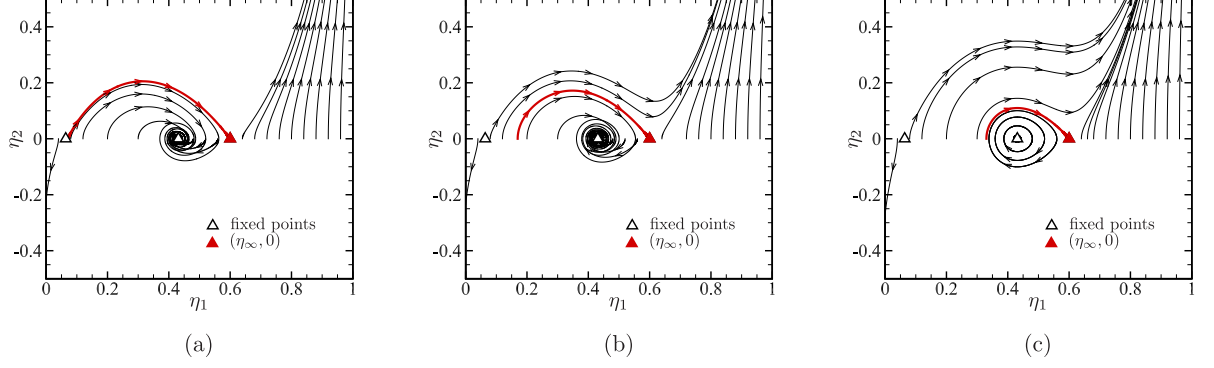


Figure 5.6: In-plane trajectories starting from various values of η_O on the η_1 axis for $\eta_\infty = 0.6$ and $\tilde{T}_\infty = 0.8$. See the caption of Fig. 5.5. (a) $D = 3$. (b) $D = 2$. (c) $D = 1$.

are possible for the pair $(\eta_\infty, \tilde{T}_\infty) = (\eta_b, \tilde{T}_\infty)$ that is in the unstable region. This is a new type of admissible solution that is not found in the case $D = 1$.

As is mentioned in Sec. 5.4.3.1, the pair $(\eta_b, \tilde{T}_\infty)$ is always in the unstable region, while $(\eta_a, \tilde{T}_\infty)$ and $(\eta_c, \tilde{T}_\infty)$ are either in the metastable and the stable region. Hence, when $(\eta_c, \tilde{T}_\infty)$ is in the metastable region [see Fig. 5.2(b)], the (iii)-type in-plane trajectory flows into the fixed point $(\eta_c, 0)$ and represents a single bubble. Figure 5.6 shows such an example. Therefore, the (iii)-type in-plane trajectory flows into a fixed point $(\eta_a, 0)$ [or $(\eta_c, 0)$] and represents a single droplet (or bubble), provided that $(\eta_a, \tilde{T}_\infty)$ [or $(\eta_c, \tilde{T}_\infty)$] lies in the metastable region.

To summarize, the (iii)-type in-plane trajectory that is consistent with the far-field condition is found for $D = 2$ and 3 , as in the case $D = 1$, provided that the pair of parameters of far-field condition lies in the metastable region. This type of trajectory represents a single droplet or bubble, depending on whether $\eta_\infty = \eta_a$ or $\eta_\infty = \eta_c$. In addition, the (ii)-type in-plane trajectory is newly found to be consistent with the far-field condition in the unstable region. The properties of these solutions for $D = 2$ and 3 will be further discussed in Sec. 5.4.4.

5.4.4 Discussions

5.4.4.1 Property of solution in the unstable region

As noted in Sec. 5.4.1, when $(\eta_\infty, \tilde{T}_\infty)$ lies in the unstable region, $\eta_b = \eta_\infty$. In this case, a single droplet/bubble solution was not found for $D = 1$. However, for $D = 2$ and 3 , the (ii)-type in-plane trajectories are found to represent a solution that satisfies the far-field condition, i.e., $\eta \rightarrow \eta_\infty$ as $r \rightarrow \infty$. Figure 5.7 shows an example of such a solution in the

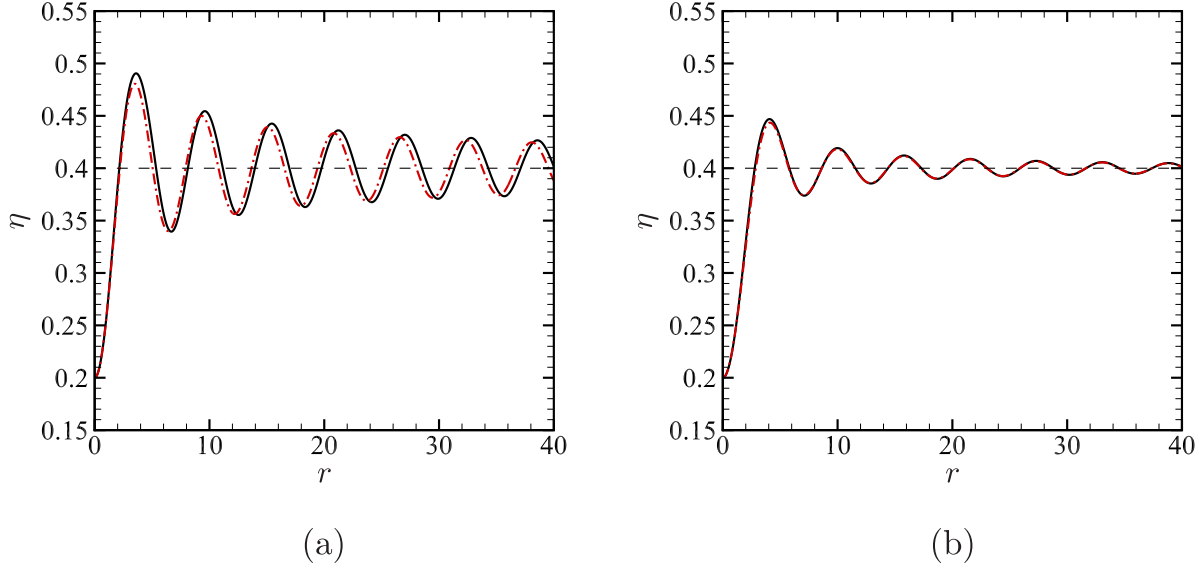


Figure 5.7: Radial density distribution for the (ii)-type in-plane trajectory in the unstable region in the case $\eta_O = 0.2$, $\eta_\infty = 0.4$, and $\tilde{T}_\infty = 0.8$. (a) $D = 2$. (b) $D = 3$. Solid line: solution of (5.36) that satisfies both conditions (5.37) and (5.38). Dashed-dotted line (red): $\bar{\eta} + \eta_\infty$ by the approximation (5.40) for the corresponding conditions. In panel (b), the deviation of lines is barely visible.

case $\eta_O = 0.2$, $\eta_\infty = 0.4$, and $\tilde{T}_\infty = 0.8$. The dimensionless density η is rippled around its far-field value η_∞ with damping the amplitude as r increases. The damping process is very slow and looks dependent on the spatial dimension D . To evaluate the damping behavior in the far field, Taylor expansion is used around η_∞ to transform (5.29a) to the equation for the perturbation part $\bar{\eta} = \eta - \eta_\infty$. Taking into account $\Pi(\eta_\infty) = 0$, (5.29a) is reduced to

$$\frac{d^2\bar{\eta}}{dr^2} + \frac{D-1}{r} \frac{d\bar{\eta}}{dr} - \Pi'(\eta_\infty)\bar{\eta} = O(\bar{\eta}^2). \quad (5.39)$$

Note that $\Pi'(\eta_\infty) < 0$ (see Sec. 5.4.1). By setting $z = [-\Pi'(\eta_\infty)]^{1/2}r$ and dropping $O(\bar{\eta}^2)$ term, an approximate equation of (5.39) is obtained and read

$$\frac{d^2\bar{\eta}}{dz^2} + \frac{D-1}{z} \frac{d\bar{\eta}}{dz} + \bar{\eta} = 0. \quad (5.40)$$

The solution of (5.40) can be expressed by the Bessel functions, $J_0(z)$ and $Y_0(z)$, of the first and the second kind of order 0 for $D = 2$ and by the spherical Bessel functions, $j_0(z)$ and $y_0(z)$, of the first and the second kind of order 0 for $D = 3$. For large z , it is well known that J_0 and Y_0 decay with the rate $z^{-1/2}$, while j_0 and y_0 decay with the rate z^{-1} (see, e.g., Sec. 9.2 of [27]). Hence, the observed ripple of density can be estimated to decay with the same rate and η approaches η_∞ as $z \rightarrow \infty$. Indeed, the solution of (5.29a) is well fitted by

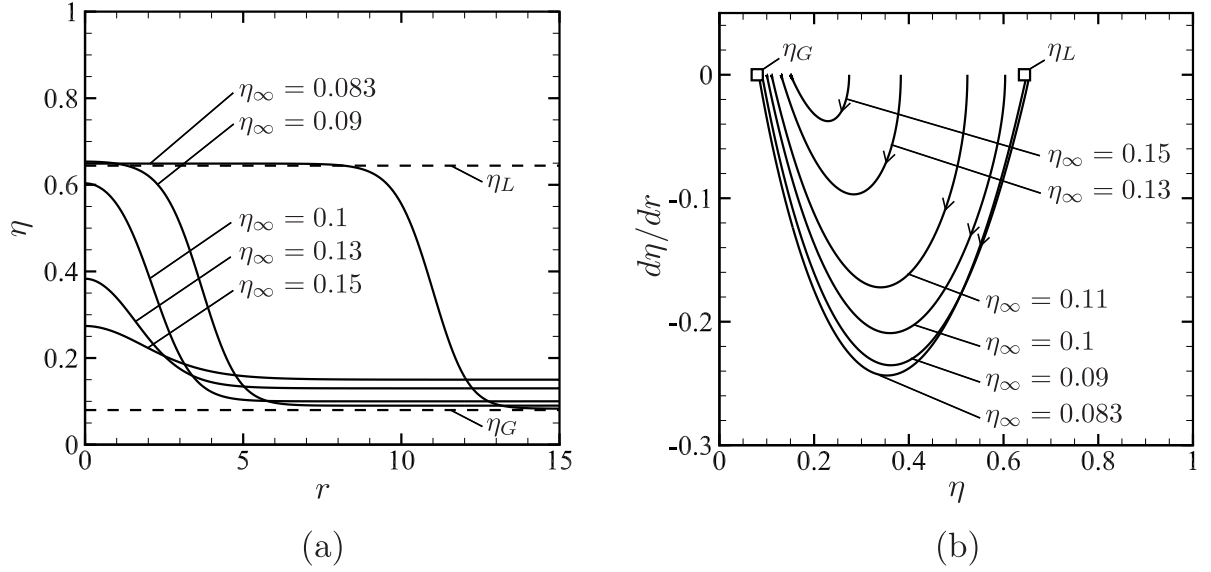


Figure 5.8: Radial density distributions and corresponding (iii)-type in-plane trajectories of single droplets for $\tilde{T}_\infty = 0.8$ in the case $D = 2$. (a) Radial density distribution. (b) In-plane trajectory. In panel (b), the arrows indicate the directions of *flow* on the individual trajectories and open squares indicate the values on the liquid-side branch η_L and the gas-side branch η_G of the binodal curve at $\tilde{T}_\infty = 0.8$.

the approximate solution $\bar{\eta} + \eta_\infty$ obtained from (5.40), see Fig. 5.7. As is clear in this figure, the influence of $O(\bar{\eta}^2)$ term is small even near the origin, and the approximation (5.40) well reproduces the solution of (5.29a) in the entire domain.

Because of the slow decay of the ripple of density, the solution above may affect the far field and might lose the physical meaning as a single droplet/bubble. Fortunately, however, it is not so. To evaluate the average deviation from η_∞ caused by the solution, consider the quantity

$$(D/Z^D) \int_0^Z z^{D-1} \bar{\eta}(z) dz, \quad (5.41)$$

replace $\bar{\eta}$ by J_0 and Y_0 for $D = 2$ (or j_0 and y_0 for $D = 3$), and take the limit as $Z \rightarrow \infty$. Then, the result is found to be zero. Namely, the solution does not affect the average density in the whole domain and thus η_∞ is not affected. In this sense, the (ii)-type in-plane trajectory for $\eta_\infty = \eta_b$ makes sense as a solution for a single droplet/bubble in the case $D = 2$ or 3. Additional side evidence is presented in Sec. 5.B.

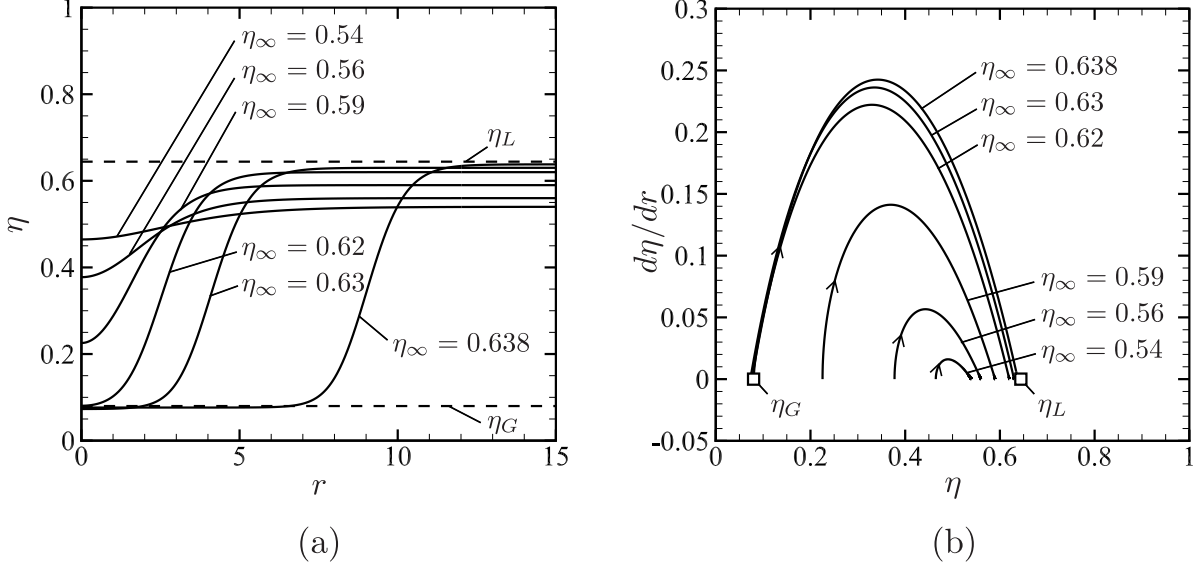


Figure 5.9: Radial density distributions and corresponding (iii)-type in-plane trajectories of single bubbles for $\tilde{T}_\infty = 0.8$ in the case $D = 2$. See the caption of Fig. 5.8.

5.4.4.2 Property of solution in the metastable region

When $\eta_\infty = \eta_a$ or η_c , the trajectories that satisfy the far-field condition were found, irrespective of the spatial dimension. Figs. 5.8 and 5.9 show various radial density distributions and corresponding in-plane trajectories when varying η_∞ within the metastable region for $\tilde{T}_\infty = 0.8$ in the case $D = 2$. The density changes monotonically with respect to r . In Fig. 5.8 the radius of droplet increases with decreasing η_∞ , while in Fig. 5.9 the radius of bubble increases with increasing η_∞ . In both cases, as the radius increases, the density ratio between two phases increases and tends to saturate in such a way that the pair of η_O and η_∞ approaches the pair of values $\eta_L(\tilde{T}_\infty)$ and $\eta_G(\tilde{T}_\infty)$ on the binodal curve. Since $\Pi(\eta_O) = \Pi(\eta_\infty) = 0$ on the binodal curve (5.34), the corresponding radial density distribution from η_O to η_∞ is the one represented by the in-plane trajectory that connects two fixed points $(\eta_a, 0)$ and $(\eta_c, 0)$. This provides an interpretation of the density distribution for the pair of parameters on the binodal curve in light of the *flow* in phase space.

In the meantime, if $\Pi(\eta_O) \neq 0$, then $d^2\eta/dr^2 \neq 0$ at the origin by (5.29a). It implies that the interior of droplet/bubble with such a η_O is not sufficiently uniform and that the Young–Laplace (YL) relation [21,28] may be broken.

The YL relation is the condition of mechanical balance on the Gibbs surface that is a discontinuous boundary model between uniform two phases with different density [21].

Denoting the radius of the Gibbs surface (Gibbs radius, for short) by $\mathcal{R}_I$, the inside uniform pressure by p_O , the outside uniform pressure by p_∞ , and the surface tension of the interface by γ , the mechanical balance condition is written as

$$\Delta p \equiv p(\eta_\infty, \tilde{T}_\infty) - p(\eta_O, \tilde{T}_\infty) = \frac{(D-1)\gamma}{\mathcal{R}_I}. \quad (5.42)$$

On the one hand, since the Gibbs surface is defined under a constraint of the total mass in the system, the Gibbs radius $\mathcal{R}_I$ is determined by the relation

$$\int (\rho - \rho_\infty) d\mathbf{X} = \frac{\pi}{2D} (2\mathcal{R}_I)^D (\rho_O - \rho_\infty). \quad (5.43)$$

On the other hand, since the surface tension is defined by the free energy associated with the interface per unit area, appropriate consideration of the free energy is necessary. Fortunately, it can be done along the same line as in [11] and the free energy $\mathcal{H}$ of the system relative to the far-field uniform state is given by

$$\mathcal{H} = \frac{1}{RT_\infty} \int \left(\rho \mathcal{F}(\rho) - \rho_\infty \mathcal{F}(\rho_\infty) + \frac{\kappa}{2} \left(\frac{\partial \rho}{\partial X_i} \right)^2 \right) d\mathbf{X}, \quad (5.44)$$

$$\begin{aligned} \mathcal{F}(\rho) &= \left(\ln \frac{b\rho}{1-b\rho} + \frac{3}{2} \right) RT_\infty - a\rho + \text{const.} \\ &= RT_c \Pi(\eta) - \frac{p}{\rho} + \text{const.}, \end{aligned} \quad (5.45)$$

in the case that the VDF is a resting Maxwellian with temperature T_∞ . Under the ansatz of the Gibbs surface, $\mathcal{H}$ is expressed with the aid of the interface free energy $\mathcal{I}$ as

$$\mathcal{H} = \frac{\pi}{2D} \frac{(2\mathcal{R}_I)^D}{RT_\infty} [\rho_O \mathcal{F}(\rho_O) - \rho_\infty \mathcal{F}(\rho_\infty)] + \frac{\mathcal{I}}{RT_\infty}. \quad (5.46)$$

Since the surface tension γ is $\mathcal{I}$ divided by the surface area $(2\mathcal{R}_I)^{D-1}\pi$, it is expressed by (5.44) and (5.46) as

$$\gamma = \frac{\mathcal{H}RT_\infty}{(2\mathcal{R}_I)^{D-1}\pi} + \frac{\mathcal{R}_I}{D} [\rho_\infty \mathcal{F}(\rho_\infty) - \rho_O \mathcal{F}(\rho_O)]. \quad (5.47)$$

Figure 5.10 plots Δp and $\gamma/\mathcal{R}_I$, obtained separately, against the Gibbs radius $\mathcal{R}_I$ in the case $D = 2$. As a reference, $\mathcal{R}_I$ versus η_∞ is also shown in the upper right corner of each panel. It is seen that, as η_∞ becomes closer to η_L or η_G (the values on the binodal curve), the Gibbs radius $\mathcal{R}_I$ becomes larger⁶ and the violation of the YL relation becomes smaller. However, if

⁶In the droplet case, the Gibbs radius increases with increasing η_∞ for $\eta_\infty \gtrsim 0.1725$, while it increases with decreasing η_∞ for $\eta_\infty \lesssim 0.5163$ in the bubble case; see the corresponding panel of Fig. 5.10. However, the results for η_∞ in these ranges are omitted in Fig. 5.10, since they represent the solutions with moderately varying density and the concept of interface loses its meaning.

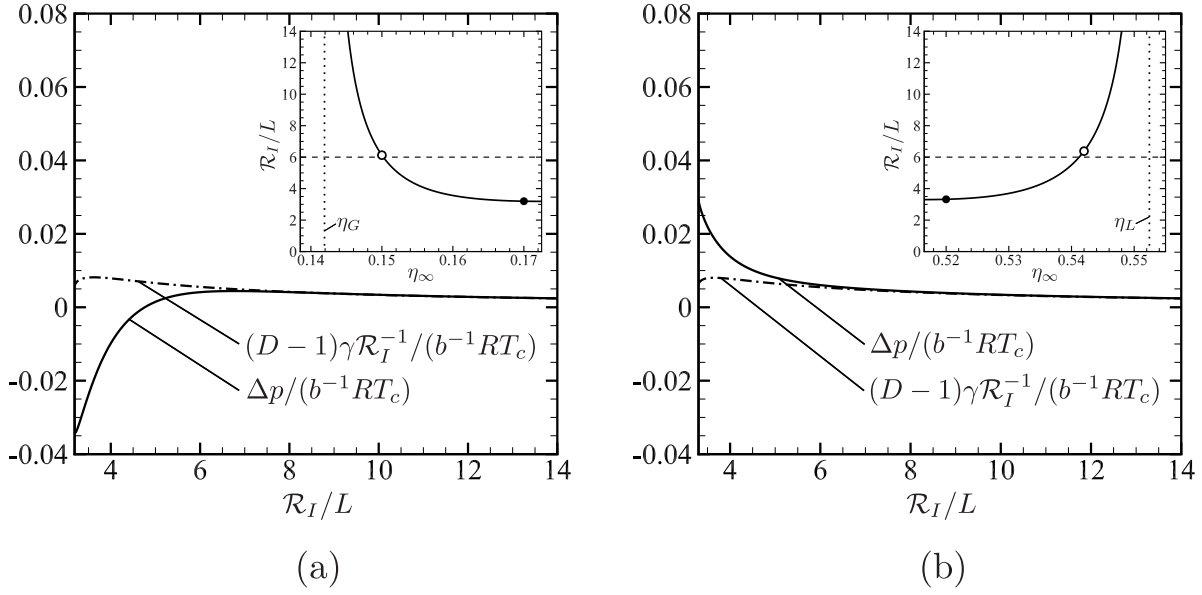


Figure 5.10: Dependence of pressure difference Δp between inside and outside of droplet/bubble and the corresponding surface tension γ on the Gibbs radius $\mathcal{R}_I$ for $\tilde{T}_\infty = 0.9$ in the case $D = 2$. (a) Droplet. (b) Bubble. Solid line: pressure difference. Dashed-dotted line: surface tension divided by $\mathcal{R}_I$. Deviation between the lines indicate the breakdown of the Young–Laplace relation (5.42). The upper-right plot in each panel is η_∞ vs $\mathcal{R}_I$. The open and closed circles indicate the cases for which the simulations to be shown in Figs. 5.12–5.15 have been conducted.

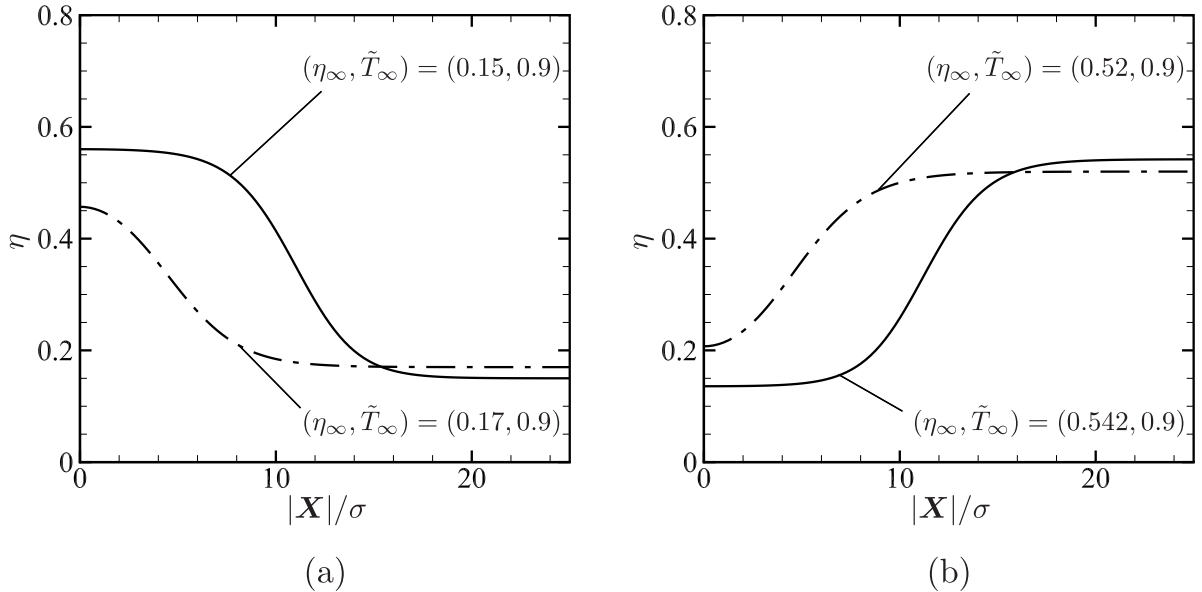


Figure 5.11: Radial density distribution of droplets and bubbles for stability assessment ($\tilde{T}_\infty = 0.9$ and $D = 2$). (a) Droplets. (b) Bubbles. Solid lines are the cases shown by open circles in Fig. 5.10, while dashed-dotted lines are those shown by closed circles in Fig. 5.10.

η_∞ is away from η_L or η_G so that $\mathcal{R}_I/L \lesssim 6$, then the YL relation is violated, which supports the expectation stated at the end of the second paragraph of Sec. 5.4.4.1. The criterion in the case $D = 3$ is almost the same, i.e., $\mathcal{R}_I/L \lesssim 6$, which is omitted here.

5.5 Stability of single droplet/bubble

To assess the stability of (ii)-type and (iii)-type steady solutions, direct numerical simulations of (5.1) have been conducted with the resting Maxwellian (5.21) being the initial condition and with $\kappa = a\sigma^{27}$ in the case $D = 2$. The density of the initial Maxwellian is the one obtained through the study in Secs. 5.3 and 5.4. The numerical computations are conducted by first eliminating the ξ_3 dependence from (5.1) by using Chu's method [29] in a finite spatial and molecular velocity domain truncated as $|X_1|, |X_2| \leq L_d$ and $|\xi_1|, |\xi_2| \leq 6\sqrt{2RT_c}$. The partial elimination of the velocity variable is the benefit of using model equation over the Enskog–Vlasov equation, which is the standard technique in the literature of rarefied gas dynamics; see, e.g., [30]. The VDF is assumed to be zero outside of the truncated domain of molecular velocity, while it is assumed to be kept at the initial Maxwellian outside of the truncated spatial domain. Only the first quadrant of space $0 \leq X_1, X_2 \leq L_d$ is treated by assuming the mirror symmetry with respect to $X_1 = 0$ and $X_2 = 0$. The numerical scheme is based on the semi-Lagrangian and Strang splitting method [31,32,33] and a uniform time step $0.02t_c$ is used, where $t_c = \sigma/\sqrt{2RT_c}$ is the reference time. The stability is assessed by observing whether the initial Maxwellian is maintained for a long time. The collapse of unstable droplet/bubble is induced only by the numerical errors caused by the discretization, interpolations, etc., in such simple assessment. Thus, only the linearly unstable droplet/bubble can be detected. Stability against large fluctuations, for instance, is not within the scope of the present simulations. Since the process of collapse depends on those errors, numerical convergence with respect to the discrete resolution or the size of the truncated spatial domain was not aimed at in the present simulations.

⁷This is a parameter setting for the Sutherland model with the sixth inverse power potential and hard core of radius σ .

5.5.1 Single droplet/bubble in the metastable region

As a stability test of the solution in the metastable region, simulations are conducted for the single droplets with the radial density distributions shown in Fig. 5.11(a) in the case $D = 2$. The far-field parameters are $(\eta_\infty, \tilde{T}_\infty) = (0.15, 0.9)$ and $(0.17, 0.9)$, respectively. The corresponding Gibbs radius is larger for the former; see open and closed circles in Fig. 5.10(a). Figs. 5.12 and 5.13 show the results obtained by setting $L_d/\sigma = 50$ with 200×200 uniform divisions in the quadrant $0 \leq X_1, X_2 \leq L_d$ and 128×128 uniform divisions in molecular velocity. The droplet is maintained in the long time evolution for the case $(\eta_\infty, \tilde{T}_\infty) = (0.15, 0.9)$ where the corresponding Gibbs radius is larger, while it collapses for the case $(\eta_\infty, \tilde{T}_\infty) = (0.17, 0.9)$ where the corresponding Gibbs radius is smaller.

The difference of stability with respect to the Gibbs radius is also observed in the case of bubbles. Figs. 5.14 and 5.15 show the results for the bubbles with the radial density distributions shown in Fig. 5.11(b) in the case $D = 2$. The computational parameters are the same as those used in the droplet cases in Figs. 5.12 and 5.13. Again, the bubble is maintained for a long time in the case $(\eta_\infty, \tilde{T}_\infty) = (0.542, 0.9)$ where the corresponding Gibbs radius is larger, while it collapses in the case $(\eta_\infty, \tilde{T}_\infty) = (0.52, 0.9)$ where the corresponding Gibbs radius is smaller; see the open and closed circles in Fig. 5.10(b).

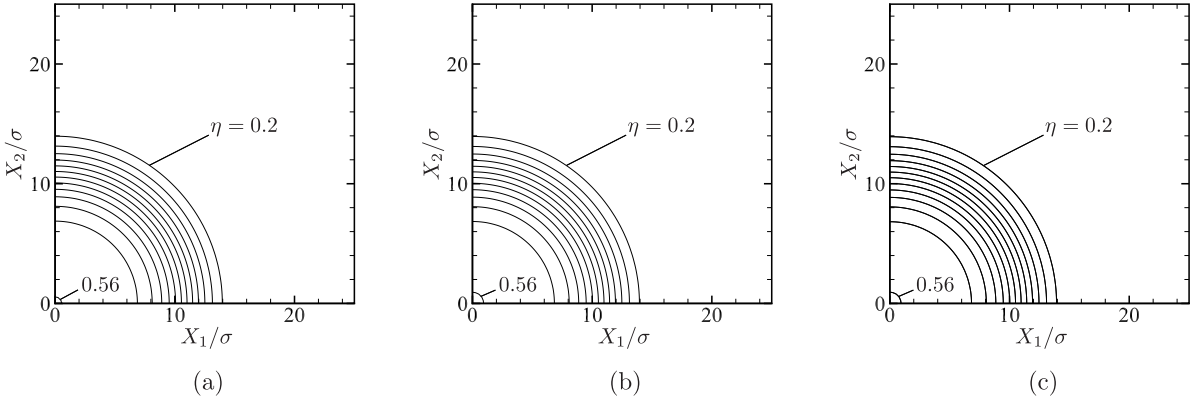


Figure 5.12: Simulation of stability for the droplet with the radial density distribution indicated by the solid line in Fig. 5.11(a), i.e., the case $(\eta_\infty, \tilde{T}_\infty) = (0.15, 0.9)$ and $D = 2$. Contours of $\eta (= b\rho) = 0.2 + 0.03m$ ($m = 0, 1, \dots$) are plotted. (a) $t/t_c = 0$. (b) $t/t_c = 3000$. (c) $t/t_c = 5000$.

Irrespective of whether droplet or bubble, the pair of far-field parameters for the steady single droplet/bubble lies near the binodal curve in the metastable region. It is thus suggested that single stable droplets/bubbles are formed only near the binodal curve in the metastable

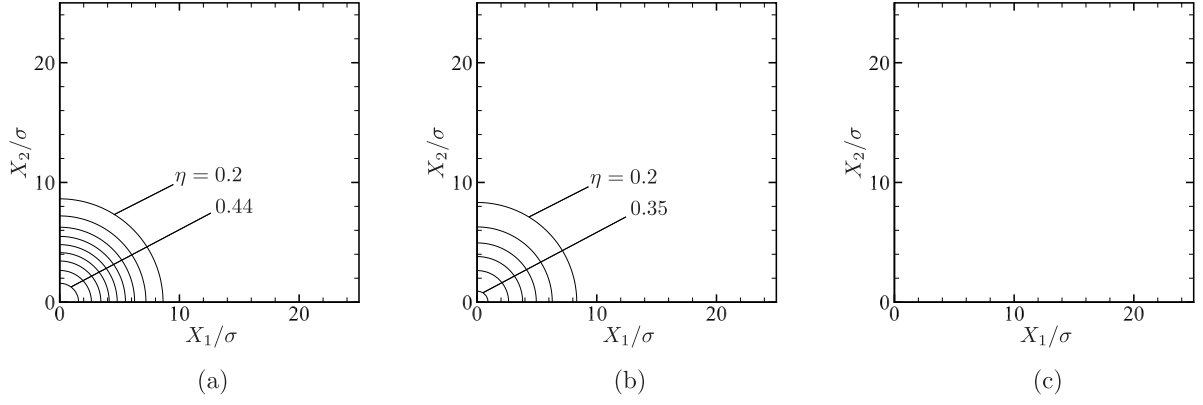


Figure 5.13: Simulation of stability for the droplet with the radial density distribution indicated by the dashed-dotted line in Fig. 5.11(a), i.e., the case $(\eta_\infty, \tilde{T}_\infty) = (0.17, 0.9)$ and $D = 2$. Contours of $\eta(=b\rho) = 0.2 + 0.03m$ ($m = 0, 1, \dots$) are plotted. (a) $t/t_c = 0$. (b) $t/t_c = 3000$. (c) $t/t_c = 5000$. In panel (c), $0.17 < \eta < 0.173$ entirely and no contour is plotted accordingly.

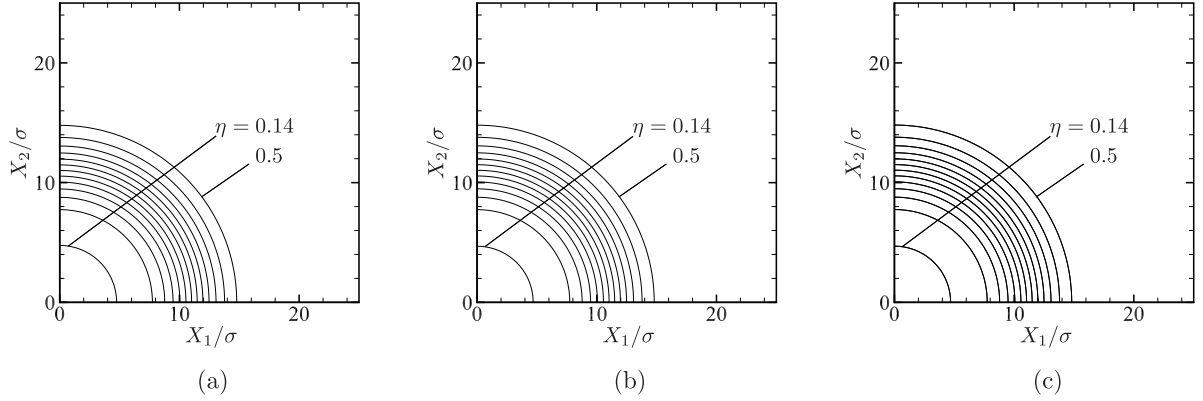


Figure 5.14: Simulation of stability for the bubble with the radial density distribution indicated by the solid line in Fig. 5.11(b), i.e., the case $(\eta_\infty, \tilde{T}_\infty) = (0.542, 0.9)$ and $D = 2$. Contours of $\eta(=b\rho) = 0.5 - 0.03m$ ($m = 0, 1, \dots$) are plotted. (a) $t/t_c = 0$. (b) $t/t_c = 500$. (c) $t/t_c = 1000$.

region.

Finally, it should be noted that both droplet and bubble collapse in the case of closed circles in Fig. 5.10, while they are maintained for a long time in the case of open circle in Fig. 5.10. Since the YL relation breaks down for closed circles in Fig. 5.10 and is still valid for open circles, it is strongly suggested that the YL relation holds for stable single droplet/bubble. Indeed, MD simulation results in the literature such as [5,6] have reported the generation of nano-sized bubbles, further confirming the validity of the YL relation for those bubbles. At the same time, [5] has reported difficulties in keeping much smaller bubbles for a long time.

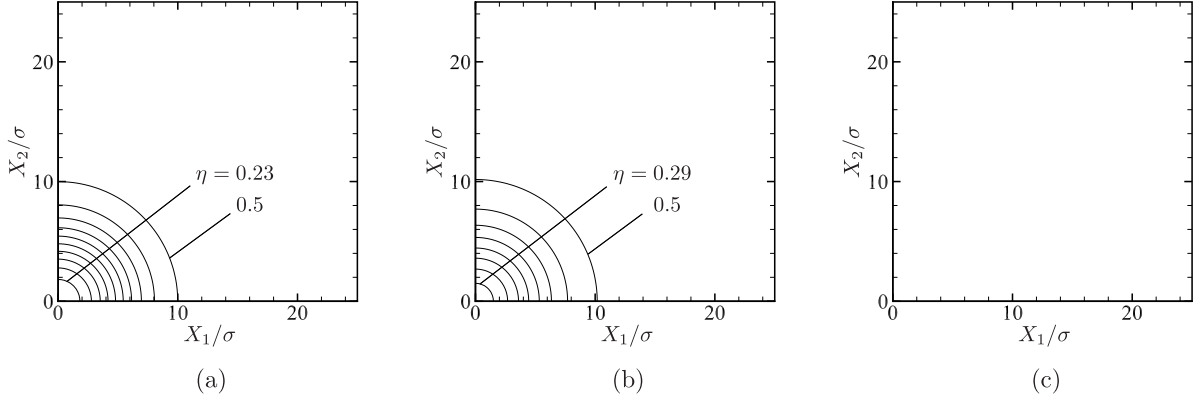


Figure 5.15: Simulation of stability for the bubble with the radial density distribution indicated by the dashed-dotted line in Fig. 5.11(b), i.e., the case $(\eta_\infty, \tilde{T}_\infty) = (0.52, 0.9)$ and $D = 2$. Contours of $\eta(= b\rho) = 0.5 - 0.03m$ ($m = 0, 1, \dots$) are plotted. (a) $t/t_c = 0$. (b) $t/t_c = 500$. (c) $t/t_c = 1000$. In panel (c), $0.500 < \eta < 0.52$ entirely and no contour is plotted accordingly.

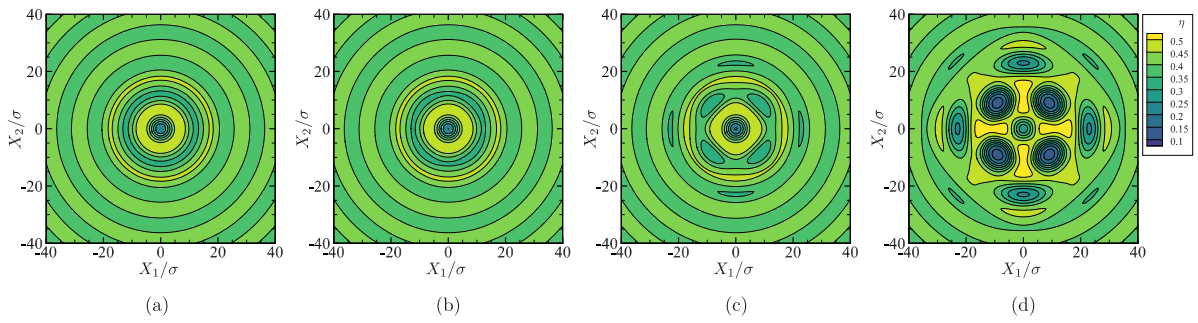


Figure 5.16: Simulation for the collapse of the solution in the unstable region with the radial density distribution indicated by the solid line in Fig. 5.7(a): $(\eta_O, \eta_\infty, \tilde{T}_\infty) = (0.2, 0.4, 0.8)$ in the case $D = 2$. Contour plots of $\eta(= b\rho)$ are shown. (a) $t/t_c = 0$. (b) $t/t_c = 100$. (c) $t/t_c = 150$. (d) $t/t_c = 200$.

Note that there are no terms representing fluctuations in our one-particle distribution model (5.1a). Nevertheless, the above observations are consistent with the MD simulation results. The trigger of the collapse in the present simulations is the numerical errors occurring in the discretization and approximation procedure. Therefore, the detected collapse is not related to the type of fluctuations, but rather to the structure of the droplet/bubble itself. Our dynamical system approach combined with the numerical simulations enables us to make clear this point, since unstable droplet/bubble cannot be obtained by the MD approach with fluctuations.

5.5.2 Single droplet/bubble in the unstable region

As a stability test of the solution in the unstable region, simulations are conducted for the solution with the radial density distributions shown in Fig. 5.7(a) in the case $D = 2$. The set of origin and far-field parameters is $(\eta_O, \eta_\infty, \tilde{T}_\infty) = (0.2, 0.4, 0.8)$. Figure 5.16 shows the results obtained by setting $L_d/\sigma = 120$ with 480×480 uniform divisions in the quadrant $0 \leq X_1, X_2 \leq L_d$ and 192×192 uniform divisions in molecular velocity. This setting offers the highest resolution in discretization and the largest spatial domain (thus the least influence of truncation of space) in the present computational work. Simulations have been performed with other settings as well but they are omitted to report here.

As a whole, the speed of collapse is faster than those observed in the metastable region, see Figs. 5.13 and 5.15, suggesting the difficulties to find a stable droplet/bubble of the Bessel/spherical Bessel function-type structure shown in Fig. 5.7. This may be connected with the fact that unstable small droplets/bubbles in the metastable region are found closer to the spinodal than to the binodal curve. However, the process of collapse is more complicated in the unstable and induces new centers of many droplets and bubbles. This feature looks supporting the scenario of spinodal decomposition in the literature (see also Sec. 5.B).

5.6 Concluding remarks

In the present paper, we have discussed the steady single droplet/bubble and its stability on the basis of the kinetic model equation proposed in [19]. After the presentation of kinetic model in Sec. 5.2, the problem is reduced to a problem of the radial density distribution, assuming the resting Maxwellian with a uniform temperature and isotropic field with re-

spect to the origin of the coordinates in Sec. 5.3. The reduced problem is treated as a low dimensional dynamical system in Sec. 5.4 and is studied by using the concept of the phase space vector field, fixed point, and *flow*. The trajectories in phase space are found to change qualitatively whether the set of parameters of the far-field uniform state falls into the unstable region or the metastable region. In particular, the structure of the single droplet/bubble in the unstable region is found to be well described by the family of the Bessel and the spherical Bessel functions for spatially two- and three-dimensional cases. In the metastable region, the droplet/bubble is always of a radially monotone structure in density. Its inside is not necessarily at a fully developed uniform state and accordingly the YL relation may be broken in such a case.

The stability of thus obtained steady single droplet/bubble is also tested numerically by a simple assessment. The results suggest that the single droplet/bubble becomes unstable away from the binodal curve in the metastable region. This is consistent with the MD simulation results in the literature. Since there are no terms representing fluctuations in our one-particle distribution model, the observed instability is due to the structure of the droplet/bubble itself. We have discussed this feature in view of the YL relation and the size of droplet/bubble. The process of collapse of the droplet/bubble, in particular the difference of qualitative features in the metastable and the unstable region, is also demonstrated.

5.A Maxwellian as a time asymptotic solution

In this Appendix, we will show that, under suitable assumptions at a far distance, there is a functional monotonically decreasing in time and that the solution of (5.1) approaches a local resting Maxwellian with uniform temperature T_∞ . This feature is one of the chief merits of our kinetic model over the original Enskog–Vlasov equation.

Consider the problem (5.1). Let us denote the uniform resting Maxwellian and Φ_S at a far distance by f_∞ and $\Phi_{S\infty}$, respectively. We first integrate (5.1a) multiplied by $\ln(f/f_\infty) - \Phi_{S\infty}/(RT_\infty)$ with respect to $\boldsymbol{\xi}$ and then further integrate the resulting with respect to $\boldsymbol{X}$ over a control volume $\mathcal{D}$, where $\mathcal{D}$ is the spherical domain centered at the origin with a

sufficiently large radius $\mathcal{R}_d$. After some manipulations [11,19], we obtain

$$\frac{d}{dt} \int_{\mathcal{D}} (H[f] - H[f_\infty]) d\mathbf{X} \quad (5.48a)$$

$$\begin{aligned} &= \int_{\partial\mathcal{D}} \int \xi_i n_i f \left(\ln \frac{f}{f_\infty} - 1 \right) d\boldsymbol{\xi} dS + \int_{\partial\mathcal{D}} H_i[f] n_i dS \\ &\quad + \int_{\mathcal{D}} \left\{ \int \left(\ln \frac{f}{f_\infty} \right) Q_c^b[f] d\boldsymbol{\xi} - \frac{\lambda_P}{RT^2} \left(\frac{\partial T}{\partial X_k} \right)^2 \right. \\ &\quad \left. - \frac{\mu_P}{2RT} \left(\frac{\partial v_i}{\partial X_j} \right)^2 - \frac{\mu_B}{RT} \left(\frac{\partial v_k}{\partial X_k} \right)^2 \right\} d\mathbf{X}, \end{aligned} \quad (5.48b)$$

where n_i is the inward normal unit to the surface $\partial\mathcal{D}$ and

$$\begin{aligned} H[f] &= \int f \left(\ln \frac{f}{f_\infty} - 1 \right) d\boldsymbol{\xi} + \frac{T_\infty - T}{RT_\infty} \int \frac{\partial \Phi_S}{\partial T} d\rho \\ &\quad + \frac{1}{RT_\infty} \left(\rho(\Phi_S - \Phi_{S_\infty}) - \int \rho \frac{\partial \Phi_S}{\partial \rho} d\rho \right) + \frac{\kappa}{2RT_\infty} \left(\frac{\partial \rho}{\partial X_k} \right)^2, \end{aligned} \quad (5.48c)$$

$$\begin{aligned} H_i[f] &= \frac{v_i}{RT_\infty} \left[(T_\infty - T) \int \frac{\partial \Phi_S}{\partial T} d\rho - \rho(\Phi_S - \Phi_{S_\infty} + \Phi_L) \right] \\ &\quad - \frac{v_j}{RT_\infty} \left(\mu_P \frac{\partial v_i}{\partial X_j} + \mu_B \frac{\partial v_k}{\partial X_k} \delta_{ij} \right) - \frac{T - T_\infty}{RTT_\infty} \lambda_P \frac{\partial T}{\partial X_i} + \frac{\kappa}{RT_\infty} \frac{\partial \rho v_k}{\partial X_k} \frac{\partial \rho}{\partial X_i}. \end{aligned} \quad (5.48d)$$

Note that the constant $H[f_\infty]$ is subtracted from $H[f]$ in (5.48a) to avoid the integral diverging in the limit $\mathcal{R}_d \rightarrow \infty$. Thanks to the property of Q_c^b [23], all the four terms in the last integral on the right-hand side of (5.48a) are nonpositive, and thus the following inequality holds:

$$\frac{d}{dt} \int_{\mathcal{D}} (H[f] - H[f_\infty]) d\mathbf{X} \leq \int_{\partial\mathcal{D}} H_i[f] n_i dS + \int_{\partial\mathcal{D}} \int \xi_i n_i f \left(\ln \frac{f}{f_\infty} - 1 \right) d\boldsymbol{\xi} dS, \quad (5.49)$$

where the equality holds if and only if f is a Maxwellian with uniform T and v_i . By the far-field condition (5.1b), these uniform T and v_i ought to be T_∞ and zero, respectively.

To evaluate each term on the right-hand side of (5.49), we will make two reasonable assumptions: (i) the net mass flux and the net heat flux on the control surface are finite, so that the mass flow and heat flow normal to the surface decays at most with the rate of $|\mathbf{X}|^{-2}$ at a far distance. Moreover, we further assume that mass and heat flow are also at the same order, since the far field is a given resting uniform Maxwellian; (ii) because of (i), the deviation of f from f_∞ is expected to vanish very slowly ($\sim |\mathbf{X}|^{-m}$ with m being some positive number), which implies that the length scale of change around the control surface $\partial\mathcal{D}$ is $\mathcal{R}_d$ and thus the effective Knudsen number there defined by the ratio of the reference

mean-free-path $\ell_\infty = (2RT_\infty)^{1/2}/A_\infty^b$, where $A_\infty^b = A^b(\rho_\infty, T_\infty)$, to the scale length $\mathcal{R}_d$ is small, i.e., $\epsilon \equiv \ell_\infty/\mathcal{R}_d \ll 1$ [34]. Therefore, the VDF around the control surface can be well evaluated by the Chapman–Enskog (CE) expansion.

Under these reasonable assumptions, we can show that

$$\lim_{\mathcal{R}_d \rightarrow \infty} \int_{\partial\mathcal{D}} H_i[f] n_i dS = 0, \quad (5.50)$$

$$\lim_{\mathcal{R}_d \rightarrow \infty} \int_{\partial\mathcal{D}} \int \xi_i n_i f \left(\ln \frac{f}{f_\infty} - 1 \right) d\xi dS = 0. \quad (5.51)$$

To prove (5.50), first consider (5.48d). Keeping in mind that the heat flow at a far distance is well described by the gradient of temperature, the first term on the right-hand side of (5.49) can be well evaluated by the assumption (i). Indeed, since $v_i \sim |\mathbf{X}|^{-2}$ and $q_i(\propto \partial T/\partial X_i) \sim |\mathbf{X}|^{-2}$, each term on the right-hand side of (5.48d) is estimated as a small quantity multiplied by $|\mathbf{X}|^{-2}$, where the small quantity is the one that tends to vanish as $|\mathbf{X}| \rightarrow \infty$, such as $T_\infty - T$, $\Phi_S - \Phi_{S_\infty}$, $\Phi_L(\propto \partial^2 \rho/\partial X_i^2)$, $\partial v_i/\partial X_j$, and $\partial \rho/\partial X_i$. Therefore, once integrated over the control surface, the integral of each term multiplied by n_i is estimated as the same size as the small quantity. Hence, each term vanishes in the limit $\mathcal{R}_d \rightarrow \infty$, the estimate (5.50) is obtained.

Next, to prove (5.51), consider the last term on the right-hand side of (5.49). Compared with the case of (5.50), we need more details about the asymptotic behavior at a far field and thus make use of the CE expansion based on the assumption (ii). We present the outline of the analyses below.

To make clear the ordering in the CE expansion, we use the dimensionless notation

$$\begin{aligned} \hat{t} &= \frac{(2RT_\infty)^{1/2}}{\mathcal{R}_d} t, \quad x_i = \frac{X_i}{\mathcal{R}_d}, \quad \zeta_i = \frac{\xi_i}{(2RT_\infty)^{1/2}}, \quad \hat{f} = \frac{(2RT_\infty)^{3/2}}{\rho_\infty} f, \\ \hat{F}_i &= -\frac{\partial}{\partial x_i} (\hat{\Phi}_S + \hat{\Phi}_L), \quad \hat{\Phi}_S = \frac{\Phi_S}{2RT_\infty}, \quad \hat{\Phi}_L = \frac{\Phi_L}{2RT_\infty}, \\ \hat{Q}_c^b &= \frac{(2RT_\infty)^{3/2}}{\rho_\infty A_\infty^b} Q_c^b, \quad \hat{Q}_d + \epsilon \hat{Q}_d^b = \frac{2\mathcal{R}_d RT_\infty}{\rho_\infty} Q_d^b, \quad \hat{A}^b = \frac{A^b}{A_\infty^b}, \\ \hat{\alpha}_i &= \frac{\mathcal{R}_d}{2RT_\infty} \alpha_i, \quad \hat{\beta} = \frac{\mathcal{R}_d}{(2RT_\infty)^{1/2}} \beta, \\ \hat{\rho} &= \frac{\rho}{\rho_\infty}, \quad \hat{T} = \frac{T}{T_\infty}, \quad \hat{v}_i = \frac{v_i}{(2RT_\infty)^{1/2}}, \quad \hat{c}_i = \frac{c_i}{(2RT_\infty)^{1/2}}, \\ \check{\mu}_P &= \frac{A_\infty^b \mu_P}{\rho_\infty RT_\infty}, \quad \check{\mu}_B = \frac{A_\infty^b \mu_B}{\rho_\infty RT_\infty}, \quad \check{\lambda}_P = \frac{A_\infty^b \lambda_P}{\rho_\infty RT_\infty 2R}, \end{aligned}$$

and rewrite (5.1a) into

$$\frac{\partial \hat{f}}{\partial \hat{t}} + \zeta_i \frac{\partial \hat{f}}{\partial x_i} + \hat{F}_i \frac{\partial \hat{f}}{\partial \zeta_i} = \frac{1}{\epsilon} \hat{Q}_c^b + \hat{Q}_d + \epsilon \hat{Q}_d^b. \quad (5.52a)$$

Here the original Q_d^b has been decomposed into dimensionless $\hat{Q}_d$ and $\hat{Q}_d^b$ in such a way that

$$\hat{Q}_d = - \frac{\partial}{\partial \zeta_i} [(\hat{\alpha}_i + \hat{\beta} \hat{c}_i) \hat{f}], \quad (5.52b)$$

$$\hat{Q}_d^b = - \frac{1}{3 \hat{\rho} \hat{T}} \frac{\partial}{\partial \zeta_i} \left(\left\{ \frac{3}{2} \hat{T} \frac{\partial \check{S}_{ij}}{\partial x_j} + \hat{c}_i \left[\frac{\partial}{\partial x_k} \left(\check{\lambda}_P \frac{\partial \hat{T}}{\partial x_k} \right) + \frac{\partial \hat{v}_j}{\partial x_k} \check{S}_{jk} \right] \right\} \hat{f} \right), \quad (5.52c)$$

$$\check{S}_{ij} = \check{\mu}_P \frac{\partial \hat{v}_i}{\partial x_j} + \check{\mu}_B \frac{\partial \hat{v}_k}{\partial x_k} \delta_{ij}. \quad (5.52d)$$

By following the standard procedure of the CE expansion, we seek the solution of (5.52a) in the form

$$\hat{f} = \hat{f}^{(0)} + \epsilon \hat{f}^{(1)} + \epsilon^2 \hat{f}^{(2)} + \dots. \quad (5.53)$$

The details of the calculation for the present kinetic model can be found in the Appendix of [19]. Here we summarize the results up to $O(\epsilon)$:

$$\hat{f}^{(0)} = \frac{\hat{\rho}}{(\pi \hat{T})^{3/2}} \exp \left(- \frac{\hat{c}_k^2}{\hat{T}} \right), \quad (5.54a)$$

$$\hat{f}^{(1)} = (\hat{A}_i \hat{c}_i + \hat{B} \hat{c}_k^2 + \hat{C}_{ij} \hat{c}_i \hat{c}_j + \hat{D}_i \hat{c}_i \hat{c}_k^2) \frac{\hat{f}^{(0)}}{\hat{A}^b}, \quad (5.54b)$$

where $\hat{A}_i$, $\hat{B}$, $\hat{C}_{ij}$, and $\hat{D}_i$ are the following dimensionless version of the quantities to be defined later in (5.56b)–(5.56e):

$$\hat{A}_i = \mathcal{R}_d A_i, \quad \hat{B} = \frac{\mathcal{R}_d}{2} (2RT_\infty)^{1/2} B, \quad \hat{C}_{ij} = \frac{\mathcal{R}_d}{2} (2RT_\infty)^{1/2} C_{ij}, \quad \hat{D}_i = \mathcal{R}_d RT_\infty D_i.$$

Now let us evaluate the last term on the right-hand side of (5.49). Since $f = [\rho_\infty (2RT_\infty)^{-3/2}] \hat{f}$,

$$\begin{aligned} & \int \xi_i n_i f [\ln(f/f_\infty) - 1] d\xi \\ &= \rho_\infty (2RT_\infty)^{1/2} \int \zeta_i n_i \hat{f} [\ln(\hat{f}/\hat{f}_\infty) - 1] d\zeta \\ &= \rho v_i n_i \left[\ln \frac{\rho T^{-3/2}}{\rho_\infty T_\infty^{-3/2}} + \frac{v_k^2}{2RT_\infty} + \frac{5}{2} \frac{T - T_\infty}{T_\infty} \right] \\ & \quad + \frac{\rho v_j n_i}{RT_\infty} \left[- \frac{RT}{(1-\nu)A^b} \frac{\partial v_i}{\partial x_j} + O(\epsilon^2) \right] \\ & \quad + \frac{T - T_\infty}{T_\infty} \left[- \frac{5}{2} \frac{\rho R}{A^b} \frac{\partial T}{\partial x_i} n_i + O(\epsilon^2) \right] \end{aligned}$$

$$+ \rho_\infty (2RT_\infty)^{1/2} \frac{\epsilon^2}{2} \int \zeta_i n_i \frac{(\hat{f}^{(1)})^2}{\hat{f}^{(0)}} d\zeta + O(\epsilon^3), \quad (5.55)$$

where $\hat{f}_\infty = [(2RT_\infty)^{3/2}/\rho_\infty] f_\infty$.

If we integrate (5.55) over the control surface $\partial\mathcal{D}$, then each term is multiplied by $O(\mathcal{R}_d^2)$ (the order of the surface area). But using the assumption (i) again and recalling that $\epsilon = \ell_\infty/\mathcal{R}_d$, the contributions of the first three lines on the most right-hand side of (5.55) are estimated as small quantities that tend to vanish as $\mathcal{R}_d \rightarrow \infty$. Since $\epsilon^3 \mathcal{R}_d^2 = \ell_\infty^2 \epsilon$, the contribution of the last term $O(\epsilon^3)$ on the most right-hand side of (5.55) also tends to vanish in the same limit. Therefore, we are left with the term

$$\rho_\infty (2RT_\infty)^{1/2} \frac{\epsilon^2}{2} \int \zeta_i n_i \frac{(\hat{f}^{(1)})^2}{\hat{f}^{(0)}} d\zeta.$$

But the substitution of (5.54), after some manipulations, gives

$$\begin{aligned} & \rho_\infty (2RT_\infty)^{1/2} \frac{\epsilon^2}{2} \int \zeta_i n_i \frac{(\hat{f}^{(1)})^2}{\hat{f}^{(0)}} d\zeta \\ &= -\frac{1}{4} \frac{\rho RT}{(1-\nu)(A^b)^2} \frac{\overline{\partial v_i}}{\partial X_j} (2A_i n_j + C_{ij} v_k n_k) \\ & \quad - \frac{5}{4} \frac{\rho R^2 T}{(A^b)^2} \frac{\partial T}{\partial X_i} (B n_i + D_i v_k n_k) + \frac{35}{8} \frac{\rho (RT)^3}{(A^b)^2} D_i B n_i \\ & \quad + \frac{1}{4} \frac{\rho (RT)^2}{(A^b)^2} (C_{ii} A_j n_j + 2C_{ij} A_i n_j) + \frac{7}{4} \frac{\rho (RT)^3}{(A^b)^2} (C_{ii} D_j n_j + 2C_{ij} D_i n_j), \end{aligned} \quad (5.56a)$$

where

$$A_i = \frac{5}{2} \frac{1}{T} \frac{\partial T}{\partial X_i}, \quad (5.56b)$$

$$B = \frac{2}{3RT} \frac{\partial v_i}{\partial X_i}, \quad (5.56c)$$

$$C_{ij} = -\frac{1}{RT} \left(\frac{\nu}{1-\nu} \frac{\overline{\partial v_i}}{\partial X_j} + \frac{\partial v_i}{\partial X_j} + \frac{\partial v_j}{\partial X_i} \right), \quad (5.56d)$$

$$D_i = -\frac{1}{RT^2} \frac{\partial T}{\partial X_i}. \quad (5.56e)$$

Because of the assumption (i), the first two lines on the right-hand side of (5.56a) is $O(\mathcal{R}_d^{-2})$ multiplied by small quantities that tend to vanish as $\mathcal{R}_d \rightarrow \infty$. By the same assumption, the remaining terms are also at most $O(\mathcal{R}_d^{-2})$ multiplied by small quantities that tend to vanish as $\mathcal{R}_d \rightarrow \infty$, since they are multiplications among A_i , B , C_{ij} , and D_i . Therefore, integrating (5.56a) over the control surface $\partial\mathcal{D}$ and taking the limit $\mathcal{R}_d \rightarrow \infty$ results in (5.51). This

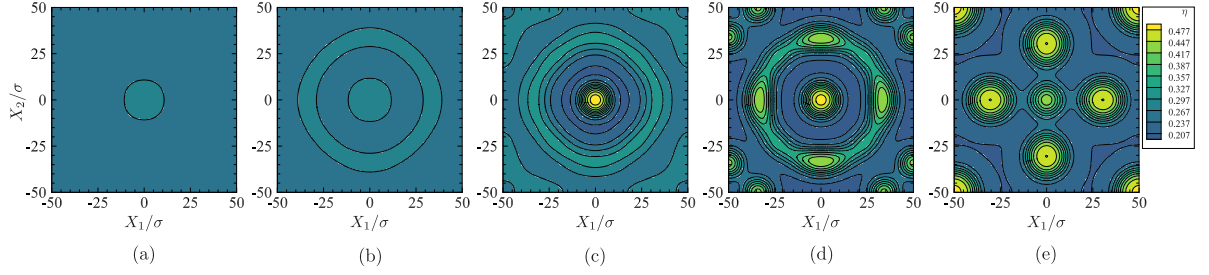


Figure 5.17: Time evolution of the phase change caused by a density disturbance from the resting uniform equilibrium state with density ρ_* and temperature T_* under a spatially periodic condition in the case of $(b\rho_*, T_*/T_c) = (4/15, 0.9) = (0.266\dots, 0.9)$ (unstable case). Contour plots of $\eta(= b\rho)$ are shown. (a) $t/t_c = 0$. (b) $t/t_c = 500$. (c) $t/t_c = 1000$. (d) $t/t_c = 2000$. (e) $t/t_c = 5000$.

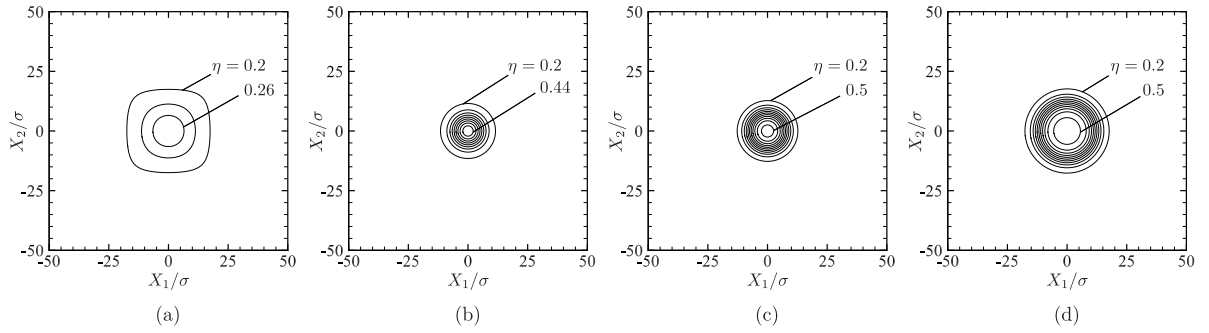


Figure 5.18: Time evolution of the phase change caused by a density disturbance from the resting uniform equilibrium state with density ρ_* and temperature T_* under a spatially periodic condition in the case of $(b\rho_*, T_*/T_c) = (0.2, 0.9)$ (metastable case). Contours of $\eta(= b\rho) = 0.2 + 0.03m$ ($m = 0, 1, \dots$) are plotted. (a) $t/t_c = 0$. (b) $t/t_c = 500$. (c) $t/t_c = 1500$. (d) $t/t_c = 20000$.

concludes that (5.49) is reduced to

$$\frac{d}{dt} \int_{\mathbb{R}^3} (H[f] - H[f_\infty]) d\mathbf{X} \leq 0, \quad (5.57)$$

and the equality holds if and only if f is a resting Maxwellian with uniform temperature T_∞ .

5.B Generation of droplet/bubble induced by a periodic disturbance

In Sec. 5.4.4.1, the single droplet/bubble in the unstable region of parameters $(\eta_\infty, \tilde{T}_\infty)$ shows slow damping of the ripple of density. The feature of the slow damping might look unnatural as a physical picture. Indeed, one of the conclusions drawn in the present paper is that such a single droplet/bubble is unlikely stable and eventually collapses in a long run. However, if we pursue the time evolution from the uniform equilibrium state on the basis of the kinetic

model equation after adding a disturbance at the initial time, then a similar density ripple pattern appears transiently in the unstable region. We here address such an example.

Figure 5.17 shows the results of a simulation that starts from an equilibrium state in the unstable region initiated by a periodic disturbance with period $2L_d$. The initial equilibrium state with the disturbance in the unit domain $|X_1|, |X_2| \leq L_d$ is given by

$$f = \frac{\rho}{(2\pi RT_*)^{3/2}} \exp\left(-\frac{\xi^2}{2RT_*}\right), \quad (5.58)$$

$$\rho/\rho_* = 1 + [\delta_\sigma(X_1)\delta_\sigma(X_2) - 1/(2L_d)^2]C\sigma^2, \quad (5.59)$$

$$\delta_\sigma(x) = \begin{cases} \frac{1}{40\sigma} \left[1 + \cos\left(\frac{\pi x}{20\sigma}\right)\right], & (|x| \leq 20\sigma), \\ 0, & (|x| > 20\sigma), \end{cases} \quad (5.60)$$

where $b\rho_* = 4/15 (= 0.266\dots)$, $T_*/T_c = 0.9$, and $C = 1$. The present pair of parameters $(b\rho_*, T_*/T_c)$ lies deep inside the unstable region, if $(b\rho_*, T_*/T_c)$ is regarded as $(\eta_\infty, \tilde{T}_\infty)$ in Fig. 5.2. The computation is conducted by the same numerical code as that used in Sec. 5.5, except that the periodic condition is applied at $|X_1|, |X_2| = L_d$ and that a correction step of the total mass, momentum and energy is inserted at every time step to retain their conservations better. In practice, the correction step had little effect on the results, but slightly improved the convergence with respect to resolution. The computational data are as follows. The quadrant of the periodic domain, $0 \leq X_1, X_2 \leq L_d$, is divided into 200×200 uniform squares with $L_d/\sigma = 50$, the truncated molecular velocity space is divided into 128×128 uniform squares, and the step size of time is $0.025t_c$. Because of the periodic condition, the system merely obeys the energy conservation and the temperature is, in general, different between the initial and the final equilibrium state at rest in the present simulation.

The radial ripple pattern of density emerges in Fig. 5.17(b), followed by its growth in amplitude as shown in Fig. 5.17(c). As the time further goes on, the pattern changes into multiple droplets with their center at the resonant points of interactions by periodicity as in Figs. 5.17(d) and 5.17(e). During this process, the temperature in the system rises from $T/T_c = 0.9$ to $T/T_c \simeq 0.95$ and the droplets creation decreases the surrounding density to $\eta \simeq 0.21 - 0.22$, causing the shift of the system from the unstable to the metastable parameter region. The pattern in Fig. 5.17(e) is not yet in the final stage and the temperature is not enough uniform. After Fig. 5.17(e), the center droplet first collapses, and then the surrounding four droplets move to the center, unite into one droplet, and further absorb the

corner droplets. The process after Fig. 5.17(e) was sensitive to the resolution of simulation, but in any case was finished with a single droplet in a unit periodic domain.

Figure 5.18 shows the results of the simulation for $b\rho_* = 0.2$, $T_*/T_c = 0.9$, and $C = 100$ for comparison. The computational domain, the discretization of space and molecular velocity, and the time step size are the same as those used in Fig. 5.17. A relatively large disturbance is necessary to initiate the phase change, since the new pair of parameters $(b\rho_*, T_*/T_c) = (0.2, 0.9)$ lies in the metastable region. Throughout the time evolution, the ripple of density is not observed at least at a visible level in this figure. A droplet with a radial monotone density distribution grows gradually from the initial state to the state in Fig. 5.18(d). During the process, the temperature in the system rises from $T/T_c = 0.9$ to $T/T_c \simeq 0.936$. In Fig. 5.18(d), the system has almost reached its final steady state.

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List of publications

Chapter 2

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Chapter 3

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Chapter 4

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Chapter 5

T. Miyauchi and S. Takata, “Single droplet or bubble and its stability: Kinetic theory and dynamical system approaches,” *Phys. Rev. E* **110**, 025102 (2024).

Additional information

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