Dynamic van der Waals Theory: A Phase Field Model of Fluids

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Dynamic van der Waals Theory
A Phase Field Model of Fluids

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In usual theories of phase transitions, the fluctuations of the temperature \( T \) are assumed to be small and are neglected. However, there can be situations in which phase transitions occur in inhomogeneous \( T \). For example, wetting properties near the gas-liquid critical point are very sensitive to applied heat flux and boiling processes remain largely unexplored [A. Onuki, Phase Transition Dynamics (Cambridge, 2002)]. To treat such problems we propose to start with a coarse-grained entropy rather than a Ginzburg-Landau free energy. For one-component fluids, let an entropy functional \( S \) be determined by the local number density \( n = n(r,t) \) and the local internal energy density \( e = e(r,t) \) as

\[
S = \int dr \left[ ns - \frac{1}{2} C |\nabla n|^2 \right]
\]

(1)

We assume that \( s = s(n,e) \) is the entropy per particle defined as a function of \( n \) and \( e \). The gradient term represents a decrease of the entropy due to inhomogeneity of \( n \). We introduce the local temperature \( T' = T(n,e) \) by

\[
\frac{1}{T'} = \frac{\delta}{\delta e} S
\]

(2)

where \( n \) is fixed in the derivative. For the special form of Eq.1 we simply obtain \( 1/T = n(\partial s/\partial e)_n \). Maximization of \( S \) under a fixed total particle number \( \int dr n \) and a fixed total energy \( \int dr e \) leads to the equilibrium conditions \( T' = \text{const.} \) and \( h/T' \equiv \delta S/\delta n = \text{const.} \). As first derived by van der Waals, the equilibrium interface density profile \( n = n(x) \) is determined by \( h = \mu(n,T') - C T \delta^2 n/dx^2 = \text{const.} \) [J.S. Rowlinson, J. Stat. Phys. 20, 197 (1979)]. In the van der Waals theory \( s = s(n,e) \) is given by

\[
s = k_B \ln[(e/n + \epsilon v_0 n)^{d/2}(1/v_0 n - 1)] + \text{const.}
\]

(3)

where \( v_0 \) and \( \epsilon \) are positive constants representing the molecular volume and the magnitude of the attractive potential, respectively, and \( d \) is the space dimensionality.

The reversible part of the stress tensor reads

\[
\Pi_{ij} = p \delta_{ij} + CT \left[ \nabla_i n \nabla_j n - (n \nabla^2 n + |\nabla n|^2/2) \delta_{ij} \right]
\]

(4)

where \( p = n(\mu + s') - e \) is the van der Waals pressure. The mass density \( \rho = mn \) obeys the continuity equation. The momentum density \( J = \rho v \) and the energy density obey appropriate dynamic equations.
including the gradient part of the stress tensor. The entropy production rate $dS/dt$ within the fluid is non-negative-definite if there is no heat flow from outside.

We give a numerical solution of our phase field model imposing a wetting boundary condition on all the boundaries. At $t = 0$ we placed a gas droplet at the center of the cell in equilibrium at $T' = 0.875T_c$. The bottom boundary was then increased by a constant $\Delta T = 0.054T_c$ for $t > 0$, while the top boundary was held at the initial temperature. There is no gravity, while we use "bottom" and "top". Fig.1 shows droplet migration toward the bottom, caused by a Marangoni effect. See a first report: N. O. Young et al., J. Fluid Mech. 6, 350 (1959) (where bubbles and liquid were different fluids and there was no first-order transition at the interface). Fig.2 displays the velocity and the temperature in the steady state. It is a new finding that the velocity component through the interface is nonvanishing, leading to latent heat transport. Because it is highly efficient, a flat temperature or no temperature gradient appears inside the droplet. In the steady state the gas droplet apparently wets the bottom partially, while a very thin liquid layer is sandwiched between the bottom boundary and the droplet. We can define an apparent contact angle $\theta_{\text{eff}}$, which is a decreasing function of $\Delta T'$. Garrabos et al. observed in space that gas spreads on a heated wall initially wetted by liquid and exhibits an apparent contact angle even larger than $\pi/2$ [Phys. Rev. E 64, 051602 (2001)]. With further increasing $\Delta T'$ the heated wall is completely covered by gas, eventually leading to film boiling in gravity.