Lattice-gas model of two-component fluid

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We consider a simple lattice-gas model of the two-component fluid with the Hamiltonian

$$H(\{n_i\}) = \sum_{i=1}^{V} \left(V_i^A n_i^A + V_i^B n_i^B\right)$$
$$+ \sum_{(ij)} \left(V_{ij}^{AA} n_i^A n_j^A + V_{ij}^{AB} n_i^A n_j^B + V_{ij}^{BA} n_i^B n_j^A + V_{ij}^{BB} n_i^B n_j^B\right), \qquad (1)$$

where $n_i^A + n_i^B = \{0, 1\}$, the second sum runs over all lattice bonds denoted by (ij), and $V_{ij}^{AB} = V_{ij}^{BA}$. Using the Gibbs-Bogolyubov inequality [1], we obtain the following density functional for the grand potential:

$$\Omega(T, \mu^A, \mu^B, V; \{\rho_i^A\}, \{\rho_i^B\})$$
$$= T \sum_{i=1}^{V} \left[\rho_i^A \ln \rho_i^A + \rho_i^B \ln \rho_i^B + (1 - \rho_i^A - \rho_i^B) \ln(1 - \rho_i^A - \rho_i^B)\right]$$
$$+ \sum_{i=1}^{V} \left[(V_i^A - \mu^A)\rho_i^A + (V_i^B - \mu^B)\rho_i^B\right]$$
$$+ \sum_{(ij)} \left(V_{ij}^{AA} \rho_i^A \rho_j^A + V_{ij}^{AB} \rho_i^A \rho_j^B + V_{ij}^{BA} \rho_i^B \rho_j^A + V_{ij}^{BB} \rho_i^B \rho_j^B\right). \qquad (2)$$

Moreover, $\Omega \equiv \Omega(T, \mu^A, \mu^B, V; \{\rho_i^A\}, \{\rho_i^B\})$ (2) must be minimized with respect to the local mean-field densities, i.e., ρ_i^A and ρ_i^B, $i = 1, \ldots, V$ satisfy the set of equations $\partial\Omega/\partial\rho_m^A = 0$, $\partial\Omega/\partial\rho_m^B = 0$.

We use this approach to discuss the liquid-vapor surface tension of the system at hand.

[1] A. P. Hughes, U. Thiele, and A. J. Archer, Am. J. Phys. **82**, 1119 (2014).