[pex47] Phase diagram of two-component fluid

The free-energy density describing the phase separation of a two-component fluid as derived in a mean-field lattice model has the form

$$f(T,\phi) = \frac{k_B T}{v_c}\Big[\phi\ln\phi + (1-\phi)\ln(1-\phi) + \chi\phi(1-\phi)\Big], \quad \chi = -\frac{z\Delta\epsilon}{2k_B T} > 0,$$

where ϕ is the volume fraction of the solute, v_c is the specific volume of solute and solvent particles, z is the coordination number, and $\Delta\epsilon$ is a measure of the (attractive) interaction between solute particles and between solvent particles.

(a) Derive explicit expressions for the spinodal line $\chi_{sp}(\phi)$ as the locations of inflection points and the coexistence curve $\chi_{co}(\phi)$ as the locations of local minima.

(b) Plot the phase diagram in the (ϕ,χ) plane with proper labels and the proper identifications of regions where the mixed macrostate is stable, unstable, or metastable.

(c) For a certain realization of this model the energy parameter assumes the value $\chi = 600/T$, where T is the temperature measured in units of Kelvin. What is the highest temperature for which phase separation is a possibility? In the phase-separated state at temperature 273K what are the solute volume fractions ϕ_{co} on the coexistence curve and ϕ_{sp} on the spinodal line?

Solution: