Advanced Thermodynamics

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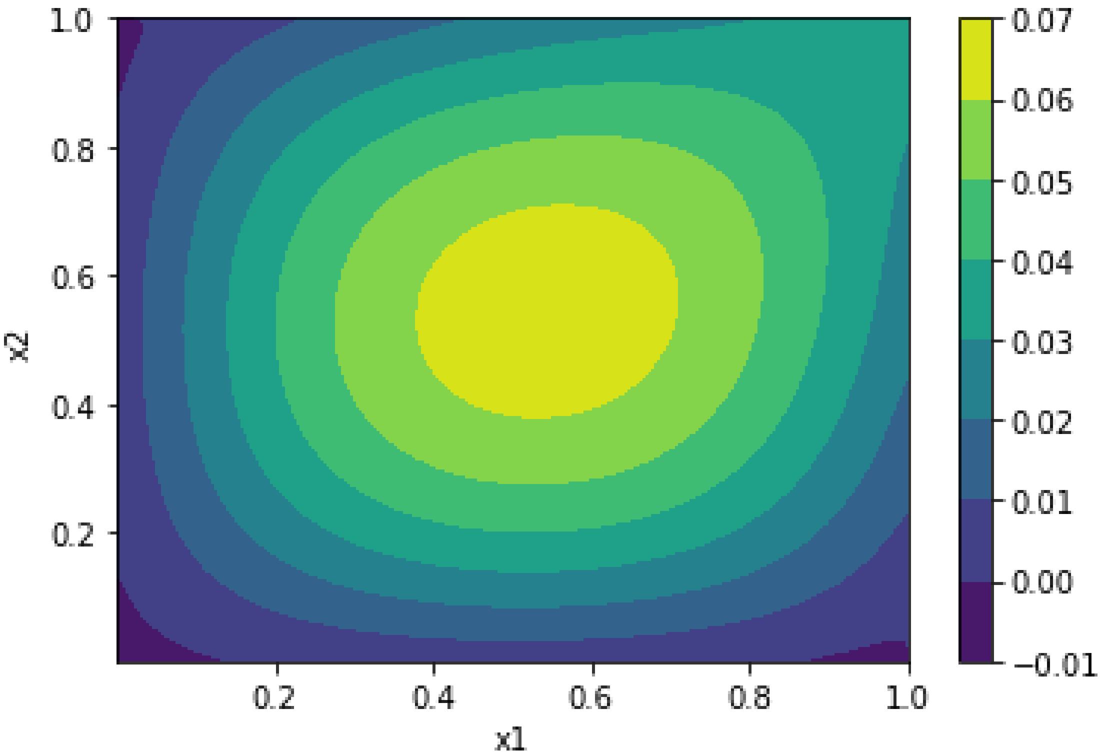
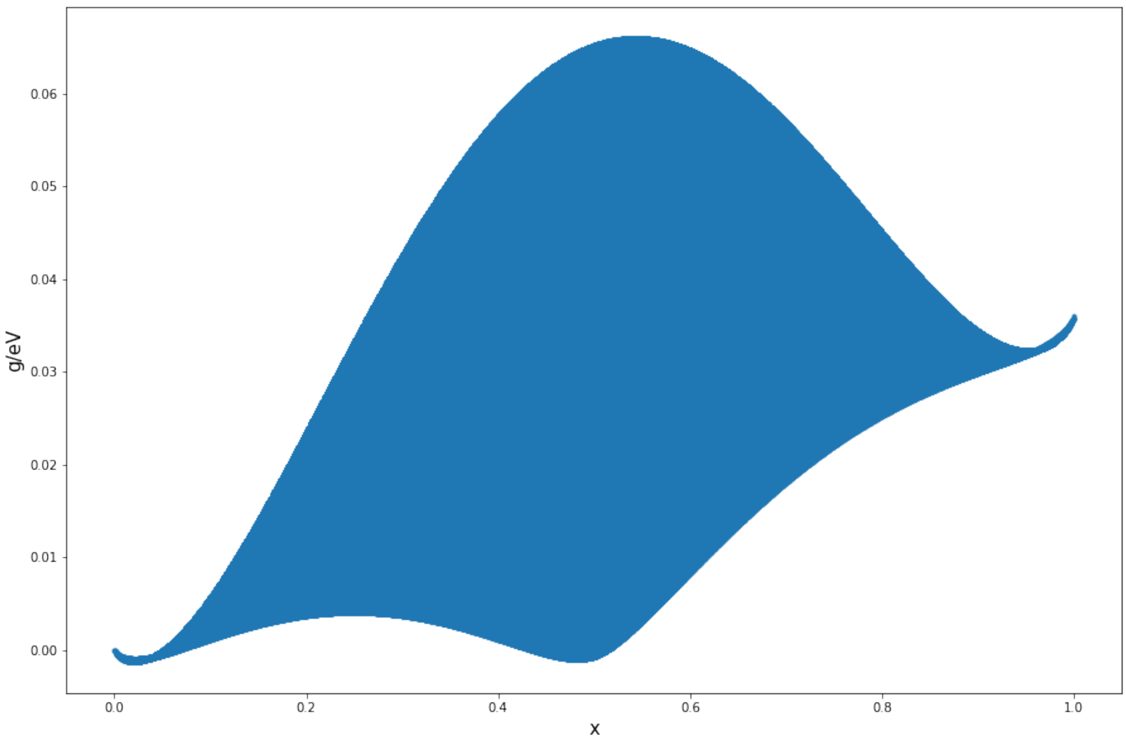
1.

$$g(x_1, x_2) = h - Ts = \Omega_a x_1(1-x_1) + \Omega_a x_2(1-x_2) + \Omega_b x_1 x_2 + \Omega_c x_1(1-x_1)x_2(1-x_2)$$
$$+ k_B T\left[x1 \ln x_1 + (1-x_1)\ln(1-x_1) + x_2 \ln x_2 + (1-x_2)\ln(1-x_2)\right]$$

2. The contour plot is shown as following:



3. The ensemble plot is shown as following:

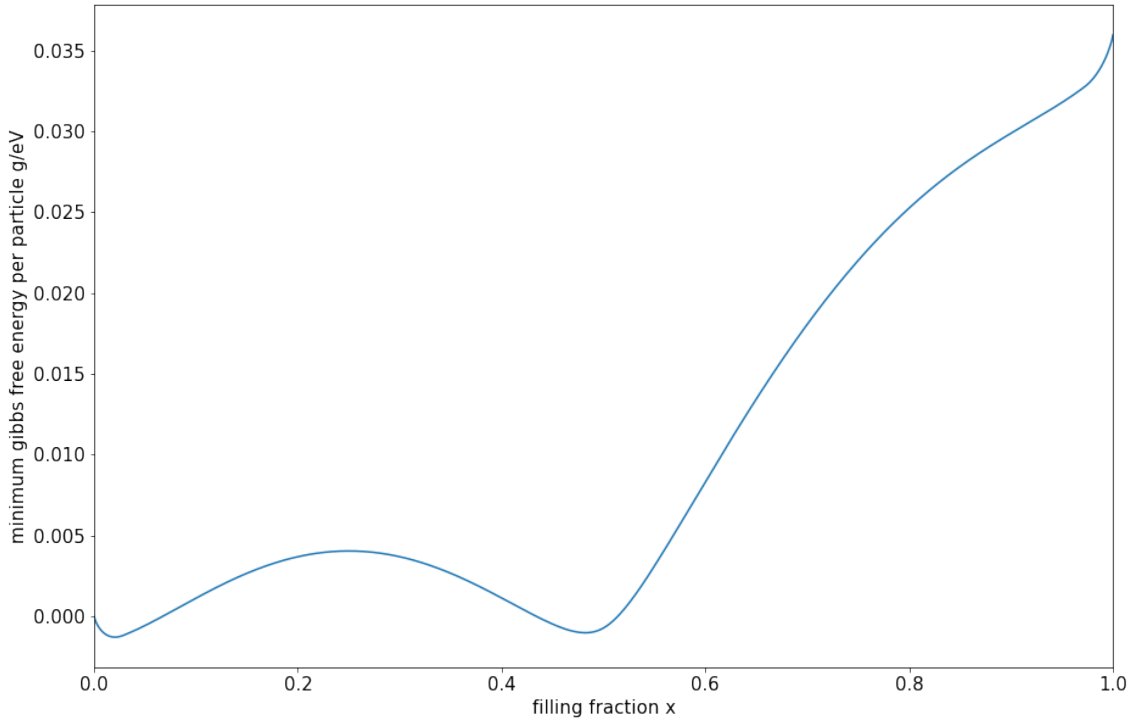


4. At equilibrium, we have $S = S_{max}$. For an (N, p, T) ensemble, the thermodynamic potential is $G = G(N, p, T)$. For this system, the pressure and temperature remains constant, while N is not. Taking the second derivative of G in respect of N, we have

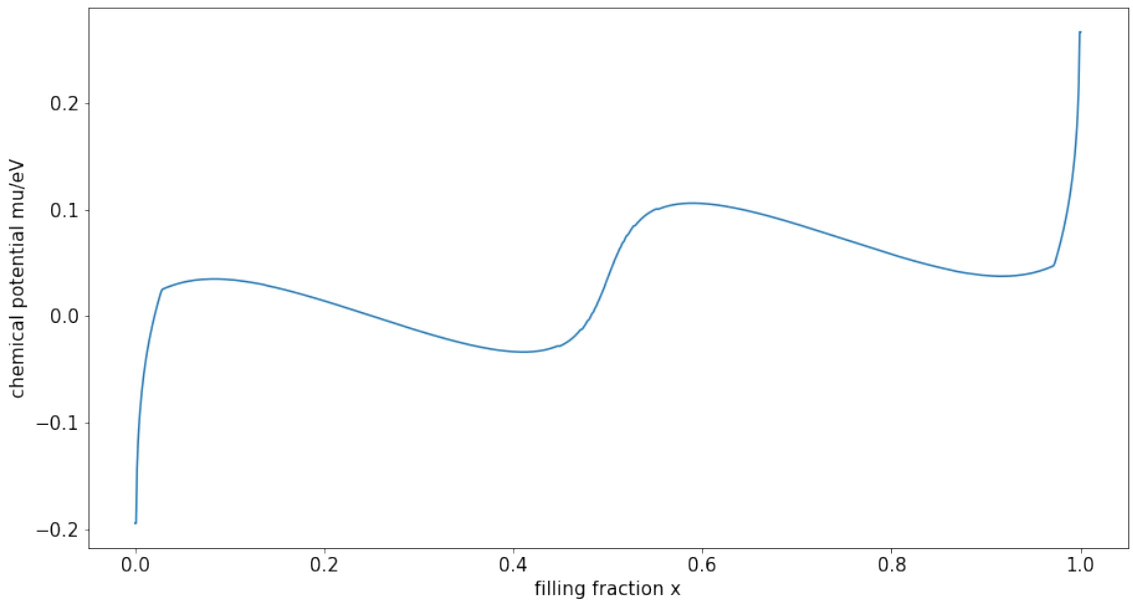
$$\left(\frac{\partial^2 G}{\partial N^2}\right)_{p,T} = \frac{\partial}{\partial N}\left(\frac{\partial G}{\partial N}\right)_{p,T} = \left(\frac{\partial \mu}{\partial N}\right)_{p,T} > 0$$

Therefore the Gibbs Free Energy is minimum at equilibrium, and so is the gibbs free energy per particle g.

5. The plot is shown as following:

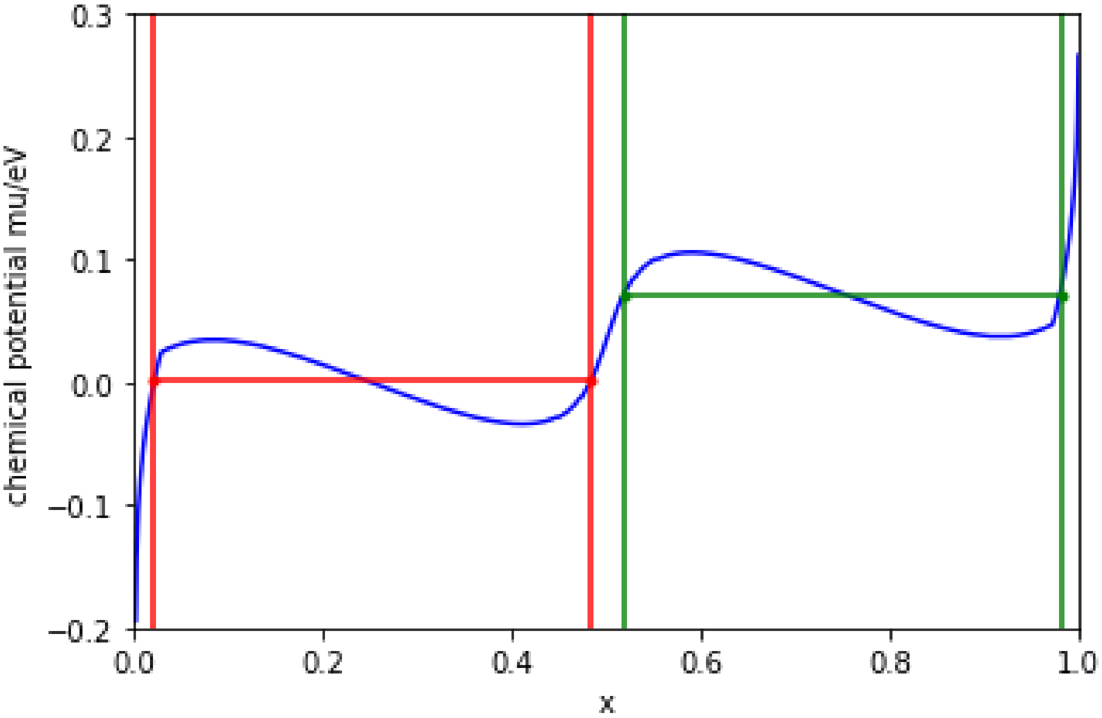


6. $\mu(x) = \frac{\partial g}{\partial x}$, and the plot is shown as following:



7. There are two phase co-existence regions for this system

8. The coexistence region are denoted in red and green respectively:



Region 1: $x_{b1} - x_{a1} = 0.462, \mu_{coex} = 0.002eV$
Region 2: $x_{b2} - x_{a2} = 0.462, \mu_{coex} = 0.072eV$