

[pex55] Discretized FJC model II: entropy and heat capacity

Here we examine how the unphysical features of the original (continuum) FJC detected in [pex53] are removed in the discretized version as solved in [pex54]. We begin with the expression for the Gibbs free energy:

$$G(T, F, N) = -k_B T \ln \left(\frac{\sinh(\beta F a(1 + 1/2s))}{\sinh(\beta F a/2s)} \right) \quad (1)$$

(a) Calculate expressions for the entropy via $S \doteq -(\partial G/\partial T)_{F,N}$ and for the heat capacity via $C_F \doteq T(\partial S/\partial T)_{F,N}$. Show that in the limit $s \rightarrow \infty$ the expressions derived in [pex53] for the same quantities naturally emerge, except for an additive term in the entropy.

(b) Plot a set of curves with $s = \frac{1}{2}, 1, \frac{3}{2}, 5, 10, 50$ for $S/[Nk_B \ln(2s)]$ over the range $0 < (\beta F a)^{-1} < 2$ as solid lines. The extra scaling factor ensures convergence in the limit $s \rightarrow \infty$. Add a dashed line representing the same function for $s = 10000$ to represent a case much closer to the continuum limit. Describe what happens to entropy in the continuum limit. How does this result connect the result produced in [pex53]?

(c) Plot a set of curves with $s = \frac{1}{2}, 1, \frac{3}{2}, 5, 10, 50$ for $C_F/(Nk_B)$ over the range $0 < (\beta F a)^{-1} < 2$ as solid lines. Add a dashed line representing the result for $s \rightarrow \infty$ from [pex53]. Interpret what you observe.

Solution: