[pex54] Discretized FJC model I: force-extension characteristics

One unphysical feature of the FJC model discussed in [pex53] was that the heat capacity did not approach zero in the limit $T \to 0$. It stayed nonzero instead in violation of the third law of thermodynamics. This defect can be removed by discretizing the polar angle θ_i between the bond vector $\vec{a}_i$ and the direction of the applied force $\vec{F}$. We thus modify the Hamiltonian of [pex53] as follows:

$$\mathcal{H} = -Fa\sum_{i=1}^{N}\cos\theta_i = -Fa\sum_{i=1}^{N}\frac{m_i}{s}, \quad m_i = -s, -s+1, \ldots, s-1, s, \tag{1}$$

where s can assume any positive integer or half-integer value $\frac{1}{2}, 1, \frac{3}{2}, \ldots$. In the context of the Brillouin paramagnet [tex86], which is a different application of the same mathematical model, this discretization is very natural and represents spin quantization. The canonical partition function again factorizes and now involves the evaluation of a sum instead of an integral:

$$Z_N \doteq \mathrm{Tr}[e^{-\beta\mathcal{H}}] = Z_1^N, \quad Z_1 = \sum_{m=-s}^{+s} e^{\beta Fam/s}, \quad \beta \doteq 1/k_BT. \tag{2}$$

(a) Evaluate Z_N and infer the following expression for the Gibbs free energy from it:

$$G(T,F,N) = -k_BT\ln\left(\frac{\sinh\big(\beta Fa(1+1/2s)\big)}{\sinh(\beta Fa/2s)}\right). \tag{3}$$

(b) Calculate expressions for the average end-to-end distance via $\langle L\rangle \doteq \beta^{-1}\partial(\ln Z_N)/\partial F$ and the mean-square end-to-end distance $\langle\langle L^2\rangle\rangle \doteq \beta^{-2}\partial^2(\ln Z_N)/\partial F^2$. Show that in the limit $s \to \infty$ the expression derived in [pex53] for the same quantities naturally emerge.
(c) Plot a set of curves with $s = \frac{1}{2}, 1, \frac{3}{2}, 5, 10, 50$ for both quantities over the range $0 < \beta FA < 10$ as solid lines. Then add dashed curves for the results representing the original (continuum) FJC model. Interpret the results.

Solution: