Self-assembly of a dimer system

From the combinatorics of dancing couples to the favorable binding of biomolecules

1 Introduction

Say that $2N$ initially paired people enter a dance hall. Within the hall, the paired people split up and mingle, such that at a later time some people are paired and other people are alone. Let the intensity of the dance hall music correlate inversely with how likely people are to be paired; low intensity leading to more pairing, high intensity leading to less pairing. Also assume that people generally like to be paired rather than alone, and, when paired, they prefer to be so with the partners they entered the hall with. Presuming we could quantitatively parameterize intensity and people's affinities for pairing, under what conditions do all people settle into a state consisting of the original pairs?

This seemingly arbitrary combinatorics problem can be used as the basis for studying the favorable binding between DNA and protein, ssDNA strands with each other, and proteins with each other. In this work, we built a statistical physics model to do so.

2 Main Result

We begin with a physical system containing $2N$ distinguishable monomers labeled $\alpha_1, \alpha_2, \ldots, \alpha_{2N}$. Each monomer has a mass m_0, and the monomers exist at thermal equilibrium temperature T in a volume V. Each monomer can bind to any other monomer, and when monomer α_k binds to monomer α_ℓ, the two form the dimer (α_k, α_ℓ) where the ordering within the pair is not important.

We define "correct dimers" as those consisting of an α_k binding with α_{N+k} where $k \leq N$; all other dimers are considered incorrect. We take the incorrect dimers to form with binding energy $-E_0$, and the correct dimers to form with binding energy $-(E_0 + \Delta)$ where $E_0, \Delta > 0$.

Computing the partition function for this system at temperature T, yields the exact result

$$Z_N(V, T, E_0, \Delta) = \frac{1}{2\sqrt{\pi}\,\Gamma\left(N + 1/2\right)} \left(\frac{V}{\lambda_0^3}\right)^{2N} \int_0^\infty \int_0^\infty dx\, dy\, \frac{e^{-x-y}}{\sqrt{xy}} \left(\mathcal{M}_+{}^{2N} + \mathcal{M}_-{}^{2N}\right), \tag{1}$$

where

$$\mathcal{M}_\pm \equiv \sqrt{x} \;\pm\; \left(\frac{2\sqrt{2}\,\lambda_0^3}{V}\right)^{1/2} e^{\beta E_0/2} \sqrt{y\,(e^{\beta\Delta} + 2x - 1)}. \tag{2}$$

with Γ being the Gamma function. Taking the large N limit of Eq.(1) and using the resulting approximation to compute the average number of total dimers $\langle k \rangle$ and the average number of correct dimers $\langle m \rangle$ we find the system of equations

$$\frac{4\sqrt{2}\,\lambda_0^3}{V}\, e^{\beta E_0} = \frac{\langle k \rangle - \langle m \rangle (1 - e^{-\beta\Delta})}{\left(N - \langle k \rangle\right)^2}, \qquad \frac{e^{\beta\Delta}}{2} = \langle m \rangle \frac{N - \langle m \rangle (1 - e^{-\beta\Delta})}{\langle k \rangle - \langle m \rangle (1 - e^{-\beta\Delta})}. \tag{3}$$

This system of equations provide the means for answering our starting question (originally phrased in terms of dance hall couples): Under what conditions does the system settle into a state consisting entirely of correct dimers? We find that the two necessary (but not sufficient) conditions that the parameters must satisfy in order for the system to be in such a state are

$$2N < e^{\beta\Delta}, \qquad NV < \sqrt{2}\,\lambda_0^3\, e^{\beta(E_0 + \Delta)}. \tag{4}$$

The conditions in Eq.(4) allow us to place approximate limits on particle number and particle energy for systems where the completely correct binding state is functionally important.