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Course: **8.333 - Statistical Mechanics I**
Problem set: **#2**

1. Random deposition.

(a) Consider a site. Assume that the gold atoms arrive at this site over time via a Poisson process. The deposition rate is d layers per second, so this Poisson process has rate d. Over time t, the average number of deposition at a site is dt. With this, we have

$$\Pr(m \text{ atoms in time } t) = \boxed{\frac{(dt)^m e^{-dt}}{m!}}$$

Glass is not covered if there is no deposition, i.e., $m = 0$. The fraction of the glass not covered by the atoms is the probability of zero deposition:

$$\Pr(0 \text{ atoms in time } t) = \boxed{e^{-dt}}$$

We see that the fraction of the glass not covered decreases exponentially in time.

(b) From Part (a), we know that the average thickness is $\langle x \rangle = dt$. To find the variance we need to compute the second moment:

$$\langle x^2 \rangle = \sum_{i=0}^{\infty} x^2 \frac{(dt)^x e^{-dt}}{x!} = dt + d^2t^2.$$

Therefore, the variance in thickness is

$$\sigma^2 = \langle x^2 \rangle - \langle x \rangle^2 = \boxed{dt}$$

2. Semi-flexible polymer in two dimensions.

(a) It's nicer to work with the ϕ-dependent $\mathcal{H}$, so let us write $\mathbf{t}_m \cdot \mathbf{t}_n$ in terms of angles:

$$\mathbf{t}_m \cdot \mathbf{t}_n = a^2 \cos(\theta_m + \theta_{m+1} + \cdots + \theta_{n-1}).$$

The summed form for the angles is not very convenient to work with, as there is no clear way to find $\langle \mathbf{t}_m \cdot \mathbf{t}_n \rangle$ written in this form. Instead, let us find $a^2 \langle \exp(i(\theta_m + \theta_{m+1} + \cdots + \theta_{n-1})) \rangle$ and then take the real part. This, written in this form, is still cumbersome. However, we may assume that the angles ϕ_i are independent, and therefore

$$\langle \mathbf{t}_m \cdot \mathbf{t}_n \rangle = \text{Re}\left[a^2 \langle \exp(i(\theta_m + \theta_{m+1} + \cdots + \theta_{n-1})) \rangle\right] = \text{Re}\left[a^2 \prod_{j=m}^{n-1} \langle e^{i\phi_j} \rangle\right] = a^2 \prod_{j=m}^{n-1} \langle \cos \phi_j \rangle.$$

Moreover, since the angles ϕ_i's are independent, the probability for each configuration is simply the product of the individual probabilities:

$$\Pr(\phi_1, \dots, \phi_{N-1}) = \exp\left[\frac{a^2\kappa}{k_BT} \sum_{i=1}^{N-1} \cos \phi_i\right] = \prod_{i=1}^{N-1} \exp\left[\frac{a^2\kappa}{k_BT} \cos \phi_i\right].$$

And so we may write

$$\Pr(\phi_i) = \exp\left[\frac{a^2\kappa}{k_BT} \cos \phi_i\right]$$

With this we have

$$\langle \mathbf{t}_m \cdot \mathbf{t}_n \rangle = a^2 \prod_{j=m}^{n-1} \frac{\int d\phi \cos\phi \exp\left[\frac{a^2\kappa}{k_B T}\cos\phi_i\right]}{\int d\phi \exp\left[\frac{a^2\kappa}{k_B T}\cos\phi_i\right]} = a^2 \left\{ \frac{\int d\phi \cos\phi \exp\left[\frac{a^2\kappa}{k_B T}\cos\phi\right]}{\int d\phi \exp\left[\frac{a^2\kappa}{k_B T}\cos\phi\right]} \right\}^{|n-m|}.$$

So $\langle \mathbf{t}_m \cdot \mathbf{t}_n \rangle$ has the form $a^2[f(T)]^{|n-m|}$ where $f(T)$ is the fraction in the curly brackets. We may write $\langle \mathbf{t}_m \cdot \mathbf{t}_n \rangle$ as an exponential:

$$\langle \mathbf{t}_m \cdot \mathbf{t}_n \rangle = a^2 \exp\left[|n-m| \ln f(T)\right] = a^2 \exp\left[\frac{|n-m|}{1/\ln f(T)}\right] \equiv a^2 \exp\left[\frac{-|n-m|}{\xi}\right],$$

as desired. The persistence length is thus

$$\boxed{l_p = a\xi = \frac{a}{-\ln f(T)} = \frac{a}{\ln\left[\frac{\int d\phi \exp\left[\frac{a^2\kappa}{k_B T}\cos\phi\right]}{\int d\phi \cos\phi \exp\left[\frac{a^2\kappa}{k_B T}\cos\phi\right]}\right]}}$$

(b) By definition, we have

$$\mathbf{R} = \sum_{i=1}^{N} \mathbf{t}_i \implies \langle R^2 \rangle = \langle \mathbf{R} \cdot \mathbf{R} \rangle = \sum_{m,n=1}^{N} \langle \mathbf{t}_m, \mathbf{t}_n \rangle = \sum_{m,n=1}^{N} a^2 \exp\left[\frac{-|n-m|}{\xi}\right].$$

Now we consider what happens when $N \to \infty$. We see that $\mathbf{R}$ has the form

$$\langle R^2 \rangle = a^2 \left[N + N_1 e^{-1/\xi} + N_2 e^{-2/\xi} + N_3 e^{-3/\xi} + \dots\right]$$

where $N_1, N_2, N_3, \dots$ are natural numbers. In the limit $N \to \infty$, we have $N_j \approx 2N$ for small j's (swapping n, m gives an extra factor of 2), and N_j's for large j's don't really matter because of the exponential decay $e^{-j/\xi}$. So, we may very well write this as

$$\langle R^2 \rangle \approx a^2 \left[N + 2N\left(e^{-1/\xi} + e^{-2/\xi} + e^{-3/\xi} + \dots\right)\right]$$

We now recall that

$$\frac{x}{1-x} = x + x^2 + x^3 + \dots$$

So, we have a rather compact formula for $\langle R^2 \rangle$:

$$\boxed{\langle R^2 \rangle = a^2 N \left(1 + 2\frac{e^{-1/\xi}}{1 - e^{-1/\xi}}\right), \qquad N \to \infty}$$

(c) $\mathbf{R}$ is a sum of iid's $\mathbf{t}_i$. In view of the central limit theorem, $p(\mathbf{R})$ is a Gaussian. To determine the form of $p(\mathbf{R})$, we must find the first and second moments. Since each $\mathbf{t}_i$ is random, we can conclude that $\langle \mathbf{R} \rangle = 0$. The second moment is given by Part (b), and so the variance of this distribution is $\sigma^2 = \langle R^2 \rangle - 0 = \langle R^2 \rangle$ which is what we found in Part (b). To find the normalization constant, we look at the covariance matrix C. Its determinant $|\det(C)|$ will be the product of $\langle R_x^2 \rangle$ and $\langle R_y^2 \rangle$, each of which is $\langle R^2 \rangle/2$ (by symmetry, and the fact that variances of independent variables add). With these,

$$p(\mathbf{R}) = \frac{1}{\sqrt{(2\pi)^2 |\det(C)|}} \exp\left(-\frac{\mathbf{R}^\top C^{-1} \mathbf{R}}{2}\right) = \boxed{\frac{1}{\pi \langle R^2 \rangle} \exp\left(-\frac{\mathbf{R} \cdot \mathbf{R}}{\langle R^2 \rangle}\right)}$$

where we have used the fact that $C = \langle R^2 \rangle \mathbb{I}/2$.

(d) We shall "formally" consider the modified probability weight:

$$\exp(-\mathcal{H}/k_BT) \to \exp(\mathbf{F}\cdot\mathbf{R}/k_BT)\exp(-\mathcal{H}/k_BT).$$

Taking the average of $\mathbf{R}$ under these new weights yields

$$\langle \mathbf{R} \rangle = \frac{\int \mathbf{R}\exp(\mathbf{F}\cdot\mathbf{R}/k_BT)\exp(-\mathcal{H}/k_BT)}{\int \exp(\mathbf{F}\cdot\mathbf{R}/k_BT)\exp(-\mathcal{H}/k_BT)}.$$

We may treat $\mathbf{R}\exp(\mathbf{F}\cdot\mathbf{R}/k_BT)$ and $\exp(\mathbf{F}\cdot\mathbf{R}/k_BT)$ as input functions whose averages we wish to find and write

$$\langle R \rangle = \frac{\langle \mathbf{R}\exp(\mathbf{F}\cdot\mathbf{R}/k_BT)\rangle'}{\langle \exp(\mathbf{F}\cdot\mathbf{R}/k_BT)\rangle'}$$

where the new average $\langle\cdot\rangle'$ are essentially averages for when $\mathbf{F}=0$. The denominator becomes unity, while the numerator can be expanded as

$$\langle \mathbf{R}_i \exp(\mathbf{F}\cdot\mathbf{R}/k_BT)\rangle' \approx \langle \mathbf{R}_i\rangle' + \frac{\langle \mathbf{R}_i\mathbf{F}\cdot\mathbf{R}\rangle'}{k_BT} + \frac{\langle \mathbf{R}_i(\mathbf{F}\cdot\mathbf{R})^2\rangle'}{2k_BT} + \frac{\langle \mathbf{R}_i(\mathbf{F}\cdot\mathbf{R})^3\rangle'}{6k_BT} + \dots$$

where (1) $\mathbf{R}_i$'s are the components of $\mathbf{R}$ (i.e., i is x and y), and that $\langle R\rangle$ at $\mathbf{F}=0$ is simply $\langle R^2\rangle$ which we already know. Moreover, terms with odd-powered $\mathbf{R}$'s will vanish by symmetry. We are thus interested in the term

$$\langle \mathbf{R}_i\mathbf{F}\cdot\mathbf{R}\rangle' = \langle \mathbf{R}_i\mathbf{F}_j\mathbf{R}_j\rangle' = \mathbf{F}_j\langle \mathbf{R}_i\mathbf{R}_j\rangle' = F_j\delta_{ij}\langle R^2\rangle/2 = F_i\langle R^2\rangle/2.$$

With this we have

$$\boxed{\langle \mathbf{R}\rangle = \frac{\langle R^2\rangle}{2k_BT}\mathbf{F} + \mathcal{O}(F^3) = K^{-1}\mathbf{F} + \mathcal{O}(F^3), \qquad K = \frac{2k_BT}{\langle R^2\rangle}}$$

3. Foraging. We have

$$p(r|t) = \frac{r}{2Dt}\exp\left(-\frac{r^2}{4Dt}\right) \quad \text{and} \quad p(t) \propto \exp\left(-\frac{t}{\tau}\right).$$

Normalizing $p(t)$ give the leading factor equal $1/\tau$. So, we can write

$$p(t) = \frac{1}{\tau}\exp\left(-\frac{t}{\tau}\right).$$

The (unconditional) probability of finding the searcher at a distance r from the nest is

$$p(r) = \int_0^\infty p(r|t)p(t)\,dt = \int_0^\infty \frac{r}{2D\tau t}\exp\left(-\frac{r^2}{4Dt} - \frac{t}{\tau}\right)dt.$$

We may compute this using saddle-point approximation. Let $f(t) = r^2/4Dt + t/\tau$. Then we see that f attains a maximum at $t_0 = r\sqrt{\tau}/2\sqrt{D}$. Let $g(t) = r/2D\tau t$. The saddle point approximation reads

$$p(r) \approx e^{-f(t_0)}g(t_0)\sqrt{\frac{2\pi}{f''(t_0)}} = \exp\left(\frac{-r}{\sqrt{D\tau}}\right)\frac{1}{\sqrt{D}\tau^{3/2}}\sqrt{\frac{2\pi r t^{3/2}}{4\sqrt{D}}} \implies \boxed{p(r) \propto \sqrt{r}\exp\left(\frac{-r}{\sqrt{D\tau}}\right)}$$

We could also say that asymptotically the exponential decay in r dominates over the $\sqrt{r}$ growth, and so in the large r limit, $p(r) \sim \exp\left(-r/\sqrt{D\tau}\right)$.

4. Jensen's inequality and Kullback–Liebler divergence.

(a) Claim: Jensen's inequality: For a convex function $\langle f(x) \rangle \geq f(\langle x \rangle)$.

Proof. blah □

(b)

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