1. **Correlated Gaussian random variables**

A set of random variables $\{x_1, x_2, \ldots, x_N\}$, each with zero mean, is Gaussian distributed according to the energy function

$$U_0[\{x_j\}] = \frac{1}{2}k_{\rm B}T\sum_{j=1}^{N}\sum_{k=1}^{N} x_j K_{jk} x_k,$$

where $\mathbf{K}$ is a real, symmetric, nonsingular matrix whose off-diagonal terms couple fluctuations of different variables.

In the following problems you may find it useful to consider fluctuations of the normal modes

$$\eta^{(n)} = \sum_{j=1}^{N} \xi_j^{(n)} x_j,$$

where $\xi_k^{(n)}$ is the $n^{\rm th}$ eigenvector of K with corresponding eigenvalue $\lambda^{(n)}$:

$$\sum_k K_{jk}\ \xi_k^{(n)} = \lambda^{(n)}\xi_j^{(n)}.$$

Notice that we are using subscripts to index the $\{x_i\}$ variables, and superscripts to index normal modes.

Recall that $\mathbf{K}$ is diagonal in the basis of its eigenvectors, and therefore can be inverted trivially in that basis:

$$K_{jk} = \sum_{n=1}^{N} \xi_j^{(n)}\lambda^{(n)}\xi_k^{(n)}, \qquad K_{jk}^{-1} = \sum_{n=1}^{N} \xi_j^{(n)}\frac{1}{\lambda^{(n)}}\xi_k^{(n)}$$

Finally, note that the set of eigenvectors is orthonormal and complete:

$$\sum_{k=1}^{N} \xi_k^{(n)}\xi_k^{(m)} = \delta_{nm}, \qquad \sum_{n=1}^{N} \xi_j^{(n)}\xi_k^{(n)} = \delta_{jk}.$$

Here, $\delta_{j,k}$ is the Kronecker delta, which vanishes when $j \neq k$ and is unity for $j = k$.

(i) Show that the $\{x_i\}$ variables can be expressed as linear combinations of the normal mode coordinates:

$$x_i = \sum_n \xi_i^{(n)}\eta^{(n)}$$

(ii) For a single normal mode n, calculate the equilibrium probability distribution $p(\eta^{(n)})$. (You could begin by writing βU_0 in terms of the $\{\eta^{(m)}\}$ variables.)

(iii) Show that

$$\left\langle e^{b\eta^{(n)}}\right\rangle = \exp\left[\frac{b^2}{2\lambda^{(n)}}\right],$$

where b is a constant. Using this result, calculate

$$\left\langle \exp\left[\sum_{n=1}^{N} c^{(n)}\eta^{(n)}\right]\right\rangle,$$

where $\{c^{(1)}, c^{(2)}, \dots, c^{(N)}\}$ is an array of constants.

(iv) Show that

$$\left\langle \exp\left[\sum_{j=1}^{N} a_j x_j\right]\right\rangle = \exp\left[\frac{1}{2}\sum_{j=1}^{N}\sum_{k=1}^{N} a_j K^{-1}_{jk} a_k\right],$$

where $\langle \cdots \rangle$ denotes an average over the $\{x_i\}$ variables, and K^{-1}_{jk} is the (j,k) element of the inverse of the matrix **K**.

In carrying out this calculation, you might find it useful to define $c^{(n)} = \sum_j a_j \xi_j^{(n)}$

(v) The average you computed in part (iv) can be viewed as a function of the coefficients $\{a_j\}$. By differentiating with respect to these coefficients, show that the elements of K^{-1} determine correlations between the $\{x_i\}$ variables:

$$K^{-1}_{jk} = \langle \delta x_j \delta x_k \rangle$$

(vi) Now imagine that the $\{x_i\}$ variables are subjected to a set of external forces $\{f_1, f_2, \dots, f_N\}$, giving a total energy

$$U[\{x_j\}] = U_0 - \sum_{j=1}^{N} f_j x_j.$$

By first calculating the partition function

$$Q(\mathbf{f}) = \int dx_1 \int dx_2 \cdots \int dx_N \, e^{-\beta U},$$

show that the induced response $\langle x_i \rangle_{\mathbf{f}}$ of variable i is given by

$$\langle x_i \rangle_{\mathbf{f}} = \beta \sum_{j=1}^{N} \langle \delta x_i \delta x_j \rangle f_j$$

2. **Computing radial distribution functions from simulation**

In class we defined the pair distribution function $g(r) = \langle \rho(r) \rangle_{\mathbf{r}_1=0}/\bar{\rho}$ of a liquid in terms of the average density field $\langle \rho(r) \rangle_{\mathbf{r}_1=0}$ surrounding a tagged particle at the origin. Here you will use Monte Carlo simulations of a hard sphere fluid to obtain numerical results for $g(r)$.

(i) Let N_{R_1,R_2} be the fluctuating number of particles in a spherical shell, with inner radius R_1 and outer radius R_2, centered on a tagged particle. Show that

$$\langle N_{R_1,R_2} \rangle = \bar{\rho} \int_{R_1<|\mathbf{r}|<R_2} d\mathbf{r}\; g(r),$$

and as a result

$$\langle N_{R,R+dR} \rangle \approx 4\pi R^2 \, dR \, \bar{\rho} g(R)$$

for a very thin shell of width dR.

(ii) Show that the average number of particles in a thin shell can also be written in terms of the probability distribution $P(R)$ for the distance R between a pair of particles,

$$\langle N_{R,R+dR} \rangle \approx (N-1) P(R) \, dR.$$

(iii) Adapt your hard sphere Monte Carlo simulation program to calculate $g(r)$. You might find the results from parts (i) and (ii) useful for this purpose, since they relate $g(r)$ to a histogram that can be computed very straightforwardly. Make sure to take advantage of particles' statistical equivalence. (More specifically, note that the distribution of distance between particles #1 and #2 is exactly the same as for any other pair of particles).

Perform calculations for systems of at least $N = 200$ particles, at densities $N/V = 0.9d^{-3}$, $0.8d^{-3}$, $0.7d^{-3}$, $0.6d^{-3}$, $0.5d^{-3}$, $0.4d^{-3}$, $0.3d^{-3}$, $0.2d^{-3}$, $0.1d^{-3}$, and $0.02d^{-3}$. Plot your results.