

Problem Set #4

①

1.) Multivariate Gaussian

$$P_{x_1, \dots, x_N}(x_1, \dots, x_N) = \frac{\sqrt{\det(\bar{G})}}{(2\pi)^N} \exp\left[-\frac{\vec{x}^T \cdot \bar{G} \cdot \vec{x}}{2}\right]$$

$$\vec{x}^T \cdot \bar{G} \cdot \vec{x} = \sum_{i,j} x_i g_{ij} x_j$$

diagonalize: $\vec{x} = \vec{U} \vec{Y} \Rightarrow x_i = \sum_j U_{ij} Y_j$

$$\vec{x}^T \cdot \bar{G} \cdot \vec{x} = \vec{Y}^T \cdot \vec{U}^T \cdot \bar{G} \cdot \vec{U} \cdot \vec{Y}$$

$$= \sum_{j,k,l,m} Y_j U_{jk} g_{kl} U_{lm} Y_m$$

$$\text{since } \sum_{k,l} U_{jk} g_{kl} U_{lm} = \lambda_j \delta_{jm}$$

$$\vec{x}^T \cdot \bar{G} \cdot \vec{x} = \sum_{j,m} x_j \lambda_j \delta_{jm} Y_m = \sum_j \lambda_j Y_j^2$$

$$\begin{aligned} \int dx_1 \dots dx_N P_{x_1, \dots, x_N}(x_1, \dots, x_N) &= \int dx_1 \dots dx_N \frac{\sqrt{\det(\bar{G})}}{(2\pi)^N} \exp\left[-\frac{\vec{x}^T \cdot \bar{G} \cdot \vec{x}}{2}\right] \\ &= \int dx_1 \dots dx_N \frac{\sqrt{\det(\bar{G})}}{(2\pi)^N} \exp\left(-\frac{1}{2} \sum_j \lambda_j x_j^2\right) \end{aligned}$$

since $\sum_i x_i U_{ji} U_{jh} x_h = \sum_i x_i^2 = 1$

$$\vec{U}^T \vec{U} = 1 \Rightarrow \det(\vec{U}) \det(\vec{U}) = 1$$

$$\det(\vec{U}) = 1$$

$\det(\vec{U})$ - Jacobian determinant

$$\begin{aligned} &= \prod_i \left[\int dy_i e^{-\frac{\lambda_i}{2} y_i^2} \right] \frac{\sqrt{\det(\bar{G})}}{(2\pi)^N} = \prod_{i=1}^N \frac{1}{\sqrt{\lambda_i}} \frac{\sqrt{\det(\bar{G})}}{(2\pi)^N} \\ &= \frac{\sqrt{(2\pi)^N}}{(\prod_j \lambda_j)^{1/2}} \frac{\sqrt{\det(\bar{G})}}{(2\pi)^N} = 1 \end{aligned}$$

- characteristic function

$$f_{x_1, \dots, x_N}(k_1, \dots, k_N) = \int e^{i(k_1 x_1 + \dots + k_N x_N)} P_{x_1, \dots, x_N}(x_1, \dots, x_N) \quad j = \sqrt{-1}$$

$$= \sqrt{\frac{\det(\bar{G})}{(2\pi)^N}} \int dx_1, \dots, dx_N \exp \left[-\frac{1}{2} \vec{x}^T \bar{G} \vec{x} + j \vec{b} \cdot \vec{x} \right]$$

$$= \sqrt{\frac{\det(\bar{G})}{(2\pi)^N}} \int dy_1 \cdot dy_N \exp \left[-\frac{1}{2} \sum_i y_i^2 \lambda_i + j \tilde{b}_i y_i \right]$$

$$\vec{b} = \vec{b} \cdot \vec{1}$$

$$= \sqrt{\frac{\det(\bar{G})}{(2\pi)^N}} \int dy_1 \cdot dy_N \prod \exp \left[-\frac{\lambda_i y_i^2}{2} + j \tilde{b}_i y_i \right]$$

$$= \sqrt{\frac{\det(\bar{G})}{(2\pi)^N}} \prod_{i=1}^N \left[\int dy_i \exp \left[-\frac{\lambda_i y_i^2}{2} + j \tilde{b}_i y_i \right] \right]$$

$$= \sqrt{\frac{\det(\bar{G})}{(2\pi)^N}} \prod_{i=1}^N \left[\int dy_i \exp \left[-\frac{\lambda_i}{2} \left(y_i^2 - 2 \frac{j \tilde{b}_i}{\lambda_i} y_i + \frac{j^2 \tilde{b}_i^2}{\lambda_i^2} - \frac{j^2 \tilde{b}_i^2}{\lambda_i^2} \right) \right] \right]$$

$$= \sqrt{\frac{\det(\bar{G})}{(2\pi)^N}} \left(\prod_{i=1}^N \exp \left[-\frac{\tilde{b}_i^2}{2\lambda_i} \right] \right) \left(\prod_{i=1}^N \int dy_i \exp \left[-\frac{\lambda_i}{2} \left(y_i - \frac{j \tilde{b}_i}{\lambda_i} \right)^2 \right] \right)$$

$$= \prod_{i=1}^N \exp \left[-\frac{\tilde{b}_i^2}{2\lambda_i} \right] = \prod_{i=1}^N \exp \left[-\frac{\tilde{b}_i^2}{2\lambda_i} \right] \prod_{i=1}^N \exp \left[-\frac{j^2 \tilde{b}_i^2}{2\lambda_i} \right]$$

- moments: $j \frac{\partial}{\partial n_i} f_{x_1, \dots, x_N}(k_1, \dots, k_N) \Big|_{\vec{k}=0} = \langle x_i \rangle = 0$

$$\left(j \frac{\partial}{\partial n_i} \right) \left(j \frac{\partial}{\partial n_i} \right)$$

rewrite characteristic function

$$A_{ij} = \sum_m \frac{u_{mi} u_{mj}}{\lambda_m}$$

↓

$$f_{x_1, \dots, x_n}(h_1, \dots, h_n) = \prod_{i=1}^n \exp\left(-\frac{\mathbf{h}^T \cdot \bar{\mathbf{A}}_{ij} \mathbf{h}}{2}\right)$$

moments:

$$\langle x_i \rangle = -j \partial_{h_i} f \Big|_{\mathbf{h}=0} = \langle x_i \rangle = 0$$

$$\langle x_i x_j \rangle = \partial_{h_i}^2 \partial_{h_j}^2 f \Big|_{\mathbf{h}=0} = - \partial_{h_i} \partial_{h_j} f \Big|_{\mathbf{h}=0}$$

$$= - \partial_{h_i} \left[\exp\left(-\frac{\mathbf{h}^T \cdot \bar{\mathbf{A}} \cdot \mathbf{h}}{2}\right) \left(\sum_k \frac{A_{jk} h_k}{2} + \sum_l \frac{h_l A_{li}}{2} \right) \right] \Big|_{\mathbf{h}=0}$$

$$= \frac{A_{ji} + A_{ij}}{2} = \frac{A_{ij} + A_{ij}}{2} = A_{ij}$$

Other moments will be products of the matrix elements A_{ij}

2.) Thermal Fluctuations in rubber band

$$E[y(x)] = \frac{1}{2} \int_0^L dx (y'(x))^2$$

$$Q(\beta) = \int_{y(0)=0}^{y(L)=0} \mathcal{D}[y(x)] e^{-\frac{\beta}{2} \int_0^L dx (y'(x))^2}$$

discretize: $y(x) \rightarrow$ $x_0 = 0$
 $x_N = L$ $\Delta x = \frac{L}{N}$

choose equally spaced grid

$$\int_0^L dx (y'(x))^2 \Rightarrow \sum_{i=0}^{N-1} \left(\frac{y_{i+1} - y_i}{\Delta x} \right)^2 \Delta x$$

$$Q(\beta) = \int dy_1 \dots dy_{N-1} \exp \left[-\frac{\beta}{2} \sum_{i=0}^{N-1} \frac{(y_{i+1} - y_i)^2}{\Delta x} \right] \quad \begin{matrix} y_0 = 0 \\ y_N = 0 \end{matrix}$$

to calculate $\langle y(x_1) y(x_2) \rangle$ is

use identity: $\int \exp \left(-\frac{\beta}{2\Delta x} (y - y')^2 \right) \exp \left(-\frac{\beta}{2\Delta x} (y' - y'')^2 \right) dy'$

$$= \int dy' \exp \left[-\frac{\beta}{2\Delta x} (y^2 - 2yy' + y'^2) - \frac{\beta}{2\Delta x} (y'^2 - 2y'y'' + y''^2) \right]$$

$$= \exp \left[-\frac{\beta}{2\Delta x} y^2 - \frac{\beta}{2\Delta x} y''^2 \right] \times$$

$$\int dy' \exp \left[-\frac{\beta}{2} \left(\frac{y'^2}{\Delta x + \Delta x'} + 4y' \left(\frac{y}{\Delta x} + \frac{y''}{\Delta x'} \right) \right) \right]$$

$$= \exp \left[-\frac{\beta}{2\Delta x} y^2 - \frac{\beta}{2\Delta x'} y''^2 \right] \int dy' \exp \left[-\frac{\beta}{2} \frac{(\Delta x + \Delta x')}{\Delta x \Delta x'} \left(y'^2 - \frac{2y'(\Delta x y + \Delta x' y'')}{\Delta x + \Delta x'} \right) \right]$$

$$= \exp \left[-\frac{\beta}{2} \left(\frac{y^2}{\Delta x} + \frac{y''^2}{\Delta x'} \right) \right]$$

$$\left[\frac{2\pi \Delta x \Delta x'}{\beta(\Delta x + \Delta x')} \right] \exp \left[+\frac{\beta}{2} \frac{(\Delta x + \Delta x')}{\Delta x \Delta x'} \frac{(\Delta x y + \Delta x' y'')^2}{(\Delta x + \Delta x')^2} \right]$$

$$\int dy_1 dy_2 e^{-A y_1^2 - B(y_2 - y_1)^2 - C y_2^2}$$

$$A = \frac{\beta}{2x_1} \quad B = \frac{\beta}{2(x_2 - x_1)} \quad C = \frac{\beta}{2(1 - x_1)^2}$$

$$\int dy_1 e^{-A y_1^2} y_1 \left[\int dy_2 e^{-C y_2^2 - B(y_2 - y_1)^2} y_2 \right]$$

$$\int dy_2 y_2 e^{-C y_2^2 - B y_2^2 + 2B y_1 y_2 - B y_1^2}$$

$$e^{-B y_1^2} \int dy_2 y_2 e^{-(C+B) y_2^2 + 2B y_1 y_2}$$

$$= e^{-B y_1^2} \int dy_2 y_2 e^{-(B+C) \left[y_2^2 - \frac{2B y_1 y_2}{(B+C)} + \frac{B^2 y_1^2}{(B+C)^2} - \frac{B^2 y_1^2}{(B+C)^2} \right]}$$

$$= e^{-B y_1^2} \int dy_2 y_2 e^{-(B+C) \left[y_2^2 - \frac{2B y_1 y_2}{(B+C)} + \frac{B^2 y_1^2}{(B+C)^2} - \frac{B^2 y_1^2}{(B+C)^2} \right]}$$

$$= e^{-B y_1^2 + \frac{B^2 y_1^2}{(B+C)}} \int dy_2 y_2 e^{-(B+C) \left[y_2 - \tilde{y} \right]^2}$$

$$\tilde{y} = \frac{B y_1}{B+C}$$

$$\tilde{y}_2 = y_2 - \tilde{y}$$

$$= e^{-B y_1^2 + \frac{B^2 y_1^2}{(B+C)}} \int d\tilde{y}_2 \tilde{y}_2 e^{-(B+C) \tilde{y}_2^2}$$

$$= e^{-\frac{B y_1^2}{B+C}} \frac{B y_1}{B+C} \frac{\sqrt{\pi}}{B+C}$$

$$\int dy_1 e^{-A y_1^2} \frac{y_1^2 \beta}{B+C} e^{-\frac{BC y_1^2}{B+C}} = \frac{\beta}{B+C} \int dy_1 e^{-\frac{(AB+AC+BC) y_1^2}{B+C}}$$

$$= \frac{\beta}{B+C} \frac{\sqrt{\pi}}{2 (AB+AC+BC)^{3/2}} = \frac{\beta \sqrt{\pi}}{2 (AB+AC+BC)^{3/2}}$$

denominator: $\int dy_i dy_j e^{-A y_i^2 - B(y_j - y_i)^2 - C y_j^2}$

$$\begin{aligned}
 &= \int dy_i \int dy_j e^{-A y_i^2} \left[\int dy_j e^{-(B+C)y_j^2 + 2B y_i y_j} \right] e^{-B y_i^2} \\
 &= \int dy_i e^{-(A+B)y_i^2} \left[\int dy_j e^{-(B+C)y_j^2 - \frac{2B y_i y_j}{(B+C)} + \frac{B^2 y_i^2}{(B+C)^2} - \frac{B^2 y_i^2}{(B+C)^2}} \right] \\
 &= \int dy_i e^{-(A+B)y_i^2 + \frac{B^2}{B+C} y_i^2} \sqrt{\frac{B}{B+C}} \\
 &= \int dy_i e^{-\frac{(A+B)(B+C) - B^2}{B+C} y_i^2} \sqrt{\frac{B}{B+C}} \\
 &= \int dy_i e^{-\frac{(AB + BC + AC) y_i^2}{B+C}} \sqrt{\frac{B}{B+C}} \\
 &= \frac{\sqrt{\pi}}{\sqrt{AB + BC + AC}}
 \end{aligned}$$

numerator
denominator

$$\frac{B}{2(AB + AC + BC)}$$

$$\begin{aligned}
 &= \frac{B}{2} \frac{B^2}{4} \left(\frac{1}{x_i(x_j - x_i)} + \frac{1}{x_i(L - x_j)} \right. \\
 &\quad \left. + \frac{1}{(x_j - x_i)(L - x_j)} \right) \\
 &= \frac{B^2}{4} \left[\frac{L}{x_i(x_j - x_i)(L - x_j)} \right]
 \end{aligned}$$

$$\begin{aligned}
 &\frac{4B}{4B^2} \frac{x_i(L - x_j)}{L} \\
 &\frac{x_i(L - x_j)}{BL}
 \end{aligned}$$

4.2

$$\sum_{N_r} Z^{N_r} Q_{N_r}$$

$$Z = e^{\beta \mu}$$

- approximate by largest term in sum and justify
- consider $\ln$ of probability density

$$f(N_r) = N_r \ln Z + \ln Q_{N_r}$$

- find maximum

$$f'(N_r) = \ln Z + \frac{1}{Q_{N_r}} \frac{\partial Q_{N_r}}{\partial N_r} = 0$$

$$\Rightarrow \beta \mu = - \frac{1}{Q_{N_r}} \frac{\partial Q_{N_r}}{\partial N_r} = \beta \left\langle \frac{\partial E_s}{\partial N_r} \right\rangle$$

$$\text{since } Q_{N_r}(N_r) = \sum_s e^{-\beta E_s}$$

$$\Rightarrow \mu = \left\langle \frac{\partial E_s}{\partial N_r} \right\rangle \rightarrow \text{defines } \bar{N}_r \text{ (maximum)}$$

- expand $f(N_r)$ to second order

$$f(N_r) = f(\bar{N}_r) + \frac{1}{2} f''(\bar{N}_r) (N_r - \bar{N}_r)^2$$

$$f''(\bar{N}_r) = \frac{\partial}{\partial \bar{N}_r} f'(\bar{N}_r) = \frac{\partial}{\partial \bar{N}_r} \left[\ln Z + \frac{1}{Q_{\bar{N}_r}} \frac{\partial Q_{\bar{N}_r}}{\partial \bar{N}_r} \right]$$

$$= -\beta \frac{\partial \mu}{\partial \bar{N}_r}$$

$$\text{since } \frac{\partial \bar{N}_r}{\partial \mu} = \frac{\langle \Delta N^2 \rangle}{\beta} \quad (\text{Eq. 4.5.2, 4.5.3 in book})$$

$$\Rightarrow f(N_r) = f(\bar{N}_r) - \frac{\beta^2}{\langle \Delta N^2 \rangle} (N_r - \bar{N}_r)^2$$

$$Z^{N_r} Q_{N_r} = Z^{\bar{N}_r} Q_{\bar{N}_r} e^{-\frac{\beta^2}{\langle \Delta N^2 \rangle} (N_r - \bar{N}_r)^2}$$

$\Rightarrow$ sharply peaked distribution

4.3

probability that one particle is in the box

$$p \Rightarrow \frac{V}{V^{(0)}} \quad N\text{-particles} \left(\frac{V}{V^{(0)}}\right)^N$$

$$\Delta V = V^{(0)} - V$$

$$P(N, V) = \frac{1}{N!} \left(\frac{V}{V^{(0)}}\right)^N \frac{N^{(0)}!}{(N^{(0)} - N)!} = q^{N^{(0)}} p^N \frac{N^{(0)}!}{N! (N^{(0)} - N)!}$$

$$a.) \bar{N} = \sum_{N=0}^{\infty} N P(N, V)$$

$$= \sum_{N=0}^{\infty} N q^{N^{(0)}} p^N \frac{N^{(0)}!}{N! (N^{(0)} - N)!} = \sum_{N=0}^{\infty} q^{N^{(0)}} p^N \frac{N^{(0)}!}{(N-1)! (N^{(0)} - N)!}$$

$$= N^{(0)} p \sum_{N=0}^{\infty} q^{N^{(0)}} p^{N-1} \frac{(N^{(0)} - 1)!}{(N-1)! (N^{(0)} - N)!}$$

$$= N^{(0)} p (p + q)^{N^{(0)} - 1} = N^{(0)} p$$

$$(\Delta N)_{r.m.s} \Rightarrow \sum_{N=0}^{\infty} N^2 P(N, V) = \sum_{N=0}^{\infty} N^2 q^{N^{(0)}} p^N \frac{N^{(0)}!}{N! (N^{(0)} - N)!}$$

$$= \sum_{N=0}^{\infty} N q^{N^{(0)}} p^N \frac{N^{(0)}!}{(N-1)! (N^{(0)} - N)!}$$

$$= \sum_{N=0}^{\infty} (N-1) q^{N^{(0)}} p^N \frac{N^{(0)}!}{(N-1)! (N^{(0)} - N)!}$$

$$+ p \sum_{N=0}^{\infty} q^{N^{(0)}} p^{N-1} \frac{N^{(0)}!}{(N-1)! (N^{(0)} - N)!}$$

$$= \sum_{N=0}^{\infty} q^{N^{(0)}} p^N \frac{N^{(0)}!}{(N-2)! (N^{(0)} - N)!}$$

$$+ p \sum_{N=0}^{\infty} N^{(0)}$$

$$= N^{(0)} (N^{(0)} - 1) p^2 + N^{(0)} p$$

$$\sqrt{(\Delta N)_{r.m.s}^2} = \sqrt{N^{(0)} (p)(p-1)}$$

4.3.b
4.3.c

see lecture notes on binomial distribution

$$p \ll 1 \quad N^{(0)} \gg N$$

$$P(N) = q^{N^{(0)}-N} p^N \frac{N^{(0)}!}{N! (N^{(0)}-N)!}$$

$$p \ll 1 \Rightarrow q \approx 1 \quad N^{(0)} p = \bar{N}$$

$$P(N) = (N^{(0)} p)^N \frac{N^{(0)}!}{N! N^{(0)N} (N^{(0)}-N)!}$$

$$\text{since } N^{(0)} \gg N \quad \frac{N^{(0)}!}{(N^{(0)}-N)!} = N^{(0)N}$$

$$P(N) = \frac{\bar{N}^N}{N!}$$

normalization

$$\sum_{N=0}^{\infty} P(N) = 1$$

$$\sum_{N=0}^{\infty} \frac{\bar{N}^N}{N!} = e^{\bar{N}}$$

normalized distribution: $P(N) = e^{-\bar{N}} \frac{\bar{N}^N}{N!}$

4.4

$$P(N) = \frac{Z^N Q_N(V, T)}{\tilde{Q}(Z, V, T)}$$

- verification: probability of particle number N and energy E

$$P(N, E) = \frac{e^{\beta \mu N - \beta E}}{\sum_{N, E} e^{\beta \mu N - \beta E}} = \frac{e^{-\beta \mu N - \beta E}}{\tilde{Q}(Z, V, T)}$$

$$P(N) = \sum_E P(N, E) = \frac{e^{\beta \mu N} \sum_E e^{-\beta E}}{\tilde{Q}(Z, V, T)} = \frac{Z^N Q_N(V, T)}{\tilde{Q}(Z, V, T)}$$

- for ideal gas (classical)

$$Q_N(V, T) = \frac{Q_1(V, T)^N}{N!} \Rightarrow P(N) = \frac{Z^N Q_1^N(V, T)}{N! \tilde{Q}(Z, V, T)} = \frac{[Z Q_1]^N}{N!} \frac{1}{\tilde{Q}}$$

f.m.s.

$$P(N) = \frac{a^N}{N!} \frac{1}{\sum_N \frac{a^N}{N!}} \Rightarrow \text{normalised Poisson distribution}$$

$$\bar{N} = \sum_{N=0}^{\infty} N P(N) = \frac{\sum_{N=0}^{\infty} N a^N}{\sum_{N=0}^{\infty} \frac{a^N}{N!}} = \frac{\sum_{N=1}^{\infty} \frac{a^N}{(N-1)!}}{\sum_{N=0}^{\infty} \frac{a^N}{N!}} = \frac{a \sum_{N=0}^{\infty} \frac{a^{N-1}}{(N-1)!}}{\sum_{N=0}^{\infty} \frac{a^N}{N!}} = a$$

$$\bar{N} = a = Z Q_1$$

$$P(N) = \frac{a^N}{N!} \frac{1}{\sum_N \frac{a^N}{N!}} = \exp(-a) \frac{a^N}{N!}$$

For Poisson distribution:

$$\sum_{N=0}^{\infty} N P(N) = a = \bar{N}$$

$$\sum_{N=0}^{\infty} N^2 P(N) = \sum_{N=0}^{\infty} \frac{N^2 a^N}{N!} = \sum_{N=0}^{\infty} \frac{N a^N}{(N-1)!} = \frac{\sum_{N=1}^{\infty} \frac{(N-1) a^N}{(N-2)!}}{\bar{N}} + \frac{\sum_{N=1}^{\infty} \frac{a^N}{(N-1)!}}{\bar{N}}$$

$$= a^2 + a$$

$$\Rightarrow \langle \Delta N^2 \rangle = \langle N^2 \rangle - \langle N \rangle^2 = a = \langle N \rangle$$

since $a = \sum Q_i = e^{\beta \mu} Q_1 = \bar{N}$

it holds that

$$\langle N^2 \rangle - \langle N \rangle^2 = \frac{1}{\beta} \frac{\partial}{\partial \mu} \bar{N} = \frac{1}{\beta} \frac{\partial}{\partial \mu} e^{\beta \mu} Q_1 = e^{\beta \mu} Q_1 = \bar{N}$$