

Homework 4: Phys 7230 (Spring 2022)

Tien Vo

Due: March 14, 2022

Problem 1 (Variational approximation): In the lectures we derived the classical variational bound for the free energy, given by

$$F \leq F_{\text{tr}} + \langle \mathcal{H} - \mathcal{H}_{\text{tr}} \rangle_{\text{tr}}, \quad (1.1)$$

where H_{tr} is the variational trial Hamiltonian that best approximates \mathcal{H} . To prove this result we utilize the convexity of a decaying exponential function, namely for a random variable x

$$\langle e^{-x} \rangle \geq e^{-\langle x \rangle}. \quad (1.2)$$

(a) Prove above convexity inequality at least to lowest order in Taylor series expansion.

Solution.

At the limit that $x \rightarrow 0$ and $\langle x \rangle \rightarrow 0$, $\langle e^{-x} \rangle \approx \langle 1 - x \rangle = 1 - \langle x \rangle \approx e^{-\langle x \rangle}$. Thus, (1.2) is true to the lowest order in x and $\langle x \rangle$. \square

(b) Show that the variational inequality (1.1) is equivalent to $F \leq F_{\text{v}} = \langle \mathcal{H} \rangle_{\text{tr}} - TS_{\text{tr}}$, where S_{tr} is the Shannon's entropy for the probability distribution $P = Z_{\text{tr}}^{-1} e^{-\beta \mathcal{H}_{\text{tr}}}$, with an extra factor of k_B to make units consistent with our thermodynamics.

Solution.

By definition, Shannon's entropy is

$$\begin{aligned} S_{\text{tr}} &= -k_B \sum_q P_q \ln P_q \\ &= k_B \sum_q P_q (\beta \mathcal{H}_{\text{tr}} + \ln Z_{\text{tr}}) \\ &= \frac{1}{T} \sum_q \mathcal{H}_{\text{tr}} P_q + k_B \ln Z_{\text{tr}} \sum_q P_q \quad (Z_{\text{tr}} = \text{const}) \\ &= \frac{1}{T} \langle \mathcal{H}_{\text{tr}} \rangle_{\text{tr}} - \frac{1}{T} F_{\text{tr}}. \end{aligned} \quad (1.3)$$

Thus, rearranging, we get $F_{\text{tr}} + \langle \mathcal{H} - \mathcal{H}_{\text{tr}} \rangle_{\text{tr}} = \langle \mathcal{H} \rangle_{\text{tr}} + F_{\text{tr}} - \langle \mathcal{H}_{\text{tr}} \rangle_{\text{tr}} = \langle \mathcal{H} \rangle_{\text{tr}} - TS_{\text{tr}}$, as desired. \square

(c) Consider a particle in a periodic potential described by a Hamiltonian

$$\mathcal{H} = \frac{p^2}{2m} + \alpha(1 - \cos x), \quad (1.4)$$

where I took x to be dimensionless, i.e., measured in units of another length x_0 to simplify the notation. Motivated by the physical expectation that at low T , a particle that starts at $x = 0$ may be trapped in the minimum of the cosine, use $\mathcal{H}_{\text{tr}} = (1/2)kx^2$ to treat this problem variationally.

Specifically, please use the variational procedure to get an implicit equation for the variational parameter function $k(\alpha/k_B T)$. Then solve this equation for the function $k(\alpha/k_B T)$ numerically and/or graphically, giving its two limits, the critical value of $(\alpha/k_B T)_c$ at which the transition occurs, and sketching the function. You will find Mathematica useful.

Hint: (1) You will find our Gaussian integral calculus very useful. (2) You will obtain an implicit equation for the variational parameter k . You can solve this equation numerically or graphically finding the behavior of $k(\alpha/k_B T)$. From this solution show that the variational theory predicts a phase transition in this problem in the solution for k as a function of $\alpha/k_B T$, namely that the thermodynamics (free energy, etc) has two distinct phases, corresponding to high and low $\alpha/k_B T$. Just for the record, this intriguing finding is an example of a failure of the variational approximation for this single particle (0d) problem, that will, however, become correct for higher dimensional problem, e.g., an extended d -dimensional $u(d > 1)$ object, e.g., a fluctuating membrane trapped in a periodic potential.

Solution.

Let $\mathcal{H}_{\text{tr}} = p^2/2m + (1/2)kx^2$. Then the trial partition function is

$$Z_{\text{tr}} = \int \frac{dx dp}{2\pi\hbar} \exp\left(-\frac{1}{2}\frac{\beta}{m}p^2 - \frac{1}{2}\beta kx^2\right) = \frac{k_B T}{\hbar\omega_0}, \quad (1.5)$$

where $\omega_0^2 = k/m$. Then $F_{\text{tr}} = -k_B T \ln Z_{\text{tr}}$ and $\langle \mathcal{H}_{\text{tr}} \rangle_{\text{tr}} = k_B T$, by partition theorem on \mathcal{H}_{tr} (2 quadratic degrees of freedom). Also,

$$\begin{aligned} \langle \mathcal{H} \rangle_{\text{tr}} &= \left\langle \frac{p^2}{2m} \right\rangle + \alpha - \alpha \langle \cos(x/x_0) \rangle \\ &= \frac{k_B T}{2} + \alpha - \frac{\alpha\omega_0}{2\pi k_B T} \sqrt{\frac{2\pi}{\beta/m}} \int_{-\infty}^{\infty} dx \cos(x/x_0) \exp\left(-\frac{1}{2}\beta kx^2\right) \\ &= \frac{k_B T}{2} + \alpha \left[1 - \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} du \cos\left(\frac{u}{x_0\sqrt{\beta k}}\right) e^{-u^2/2} \right] \quad (u = \sqrt{\beta k}x) \\ &= \frac{k_B T}{2} + \alpha \left[1 - \exp\left(-\frac{k_B T}{2kx_0^2}\right) \right]. \end{aligned} \quad (1.6)$$

Thus, the variational free energy is

$$F_v(k) = \langle \mathcal{H} \rangle_{\text{tr}} + F_{\text{tr}} - \langle \mathcal{H}_{\text{tr}} \rangle_{\text{tr}} = -\frac{k_B T}{2} + \alpha \left[1 - \exp\left(-\frac{k_B T}{2kx_0^2}\right) \right] - k_B T \ln\left(\frac{k_B T}{\hbar\omega_0}\right). \quad (1.7)$$

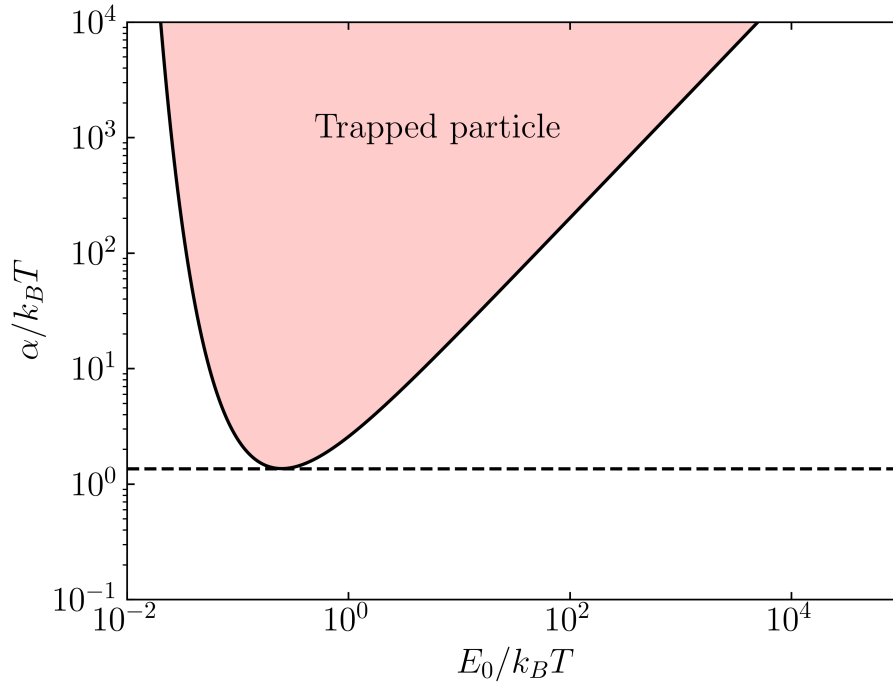
In normalized units,

$$\frac{F_v(k)}{k_B T} = -\frac{1}{2} + \frac{\alpha}{k_B T} \left[1 - \exp\left(-\frac{k_B T}{2kx_0^2}\right) \right] - \ln\left(\frac{k_B T}{\hbar\omega_0}\right). \quad (1.8)$$

Now, the spring constant k minimizing F_v satisfies $\partial F_v(k)/\partial k = 0$, which results in the following transcendental equation

$$\frac{\alpha}{k_B T} = \frac{kx_0^2}{k_B T} \exp\left(\frac{k_B T}{2kx_0^2}\right) = 2E_0 \exp\left(\frac{1}{4E_0}\right) = f(E_0), \quad (1.9)$$

where $\alpha/k_B T$ determines the amplitude of the periodic potential, and $E_0 = (1/2)kx_0^2$ is the spring potential energy. In the following, we plot $f(E_0)$.

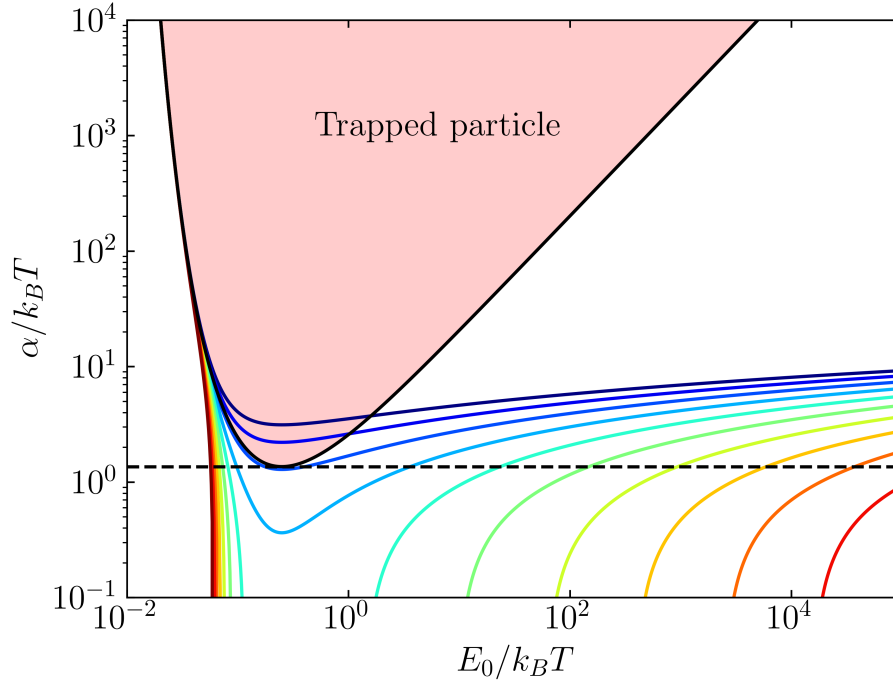


For $\alpha/k_B T \lesssim 1$, the potential is too small compared to the thermal motion of the particle, not being able to trap it. When $\alpha/k_B T \gtrsim 1$, there exists a range of E_0 (shaded red) in which the particle follows harmonic motion described by \mathcal{H}_{tr} . The horizontal dashed line marks the critical value of $\alpha/k_B T \sim 1.5$ and $E_0/k_B T \sim 0.2$ where this phase transition occurs. Furthermore, we can define the degeneracy temperature $k_B T_* = 4\pi^2 \hbar^2 / 2mx_0^2$ and rewrite

the variational free energy as

$$\begin{aligned}\frac{F_v(k_m)}{k_B T} &= -\frac{1}{2} + \frac{\alpha}{k_B T} \left[1 - \exp\left(-\frac{k_B T}{2kx_0^2}\right) \right] - \ln\left(\pi\sqrt{\frac{T/T_*}{E_0}}\right) \\ &= -\frac{1}{2} + 2E_0\left(e^{1/4E_0} - 1\right) - \ln\left(\pi\sqrt{\frac{T/T_*}{E_0}}\right),\end{aligned}\tag{1.10}$$

where k_m is the solution of (1.9). Below, we overlay $F_v/k_B T$ onto the previous plot from $T/T_* = 10^{-4}$ (blue) to $T/T_* = 10^4$ (red). Note that $F_v(k_m)/k_B T$ is only valid for $\alpha/k_B T \gtrsim 1$. A low T particle (blue) has significant free energy for all E_0 , while a high T particle (red) only has significant free energy for low E_0 or high E_0 .



□

Problem 2 (Propagation in imaginary time, random walk and phantom polymer): (a) Using Gaussian integral calculus demonstrate an important and very useful (e.g., for path integrals and our applications below) Gaussians “propagation” relation,

$$\int_{-\infty}^{\infty} dx_2 \frac{1}{\sqrt{2\pi\tau_2}} e^{-\frac{(x_3-x_2)^2}{2\tau_2}} \frac{1}{\sqrt{2\pi\tau_1}} e^{-\frac{(x_2-x_1)^2}{2\tau_1}} = \frac{1}{\sqrt{2\pi(\tau_2+\tau_1)}} e^{-\frac{(x_3-x_1)^2}{2(\tau_2+\tau_1)}}, \quad (2.1)$$

and thereby prove unnormalized density matrix the “propagator” property for the *free-particle*,

$$\rho^u(x_3, x_1; \tau_1 + \tau_2) = \int dx_2 \rho^u(x_3, x_2; \tau_2) \rho^u(x_2, x_1; \tau_1), \quad (2.2)$$

that, as discussed in class is satisfied by all $\rho^u(x, x', \tau)$.

Solution.

From the LHS of (2.1),

$$\begin{aligned} \text{LHS} &= \frac{1}{2\pi\sqrt{\tau_1\tau_2}} \int_{-\infty}^{\infty} dx_2 \exp \left[-\frac{(x_3-x_2)^2}{2\tau_2} - \frac{(x_2-x_1)^2}{2\tau_1} \right] \\ &= \frac{1}{2\pi\sqrt{\tau_1\tau_2}} \exp \left[-\frac{x_3^2\tau_1 + x_1^2\tau_2}{2\tau_1\tau_2} \right] \int_{-\infty}^{\infty} dx_2 \exp \left[-\frac{1}{2} \frac{\tau_1 + \tau_2}{\tau_1\tau_2} x_2^2 + \frac{x_3\tau_1 + x_1\tau_2}{\tau_1\tau_2} x_2 \right] \\ &= \frac{1}{\sqrt{2\pi(\tau_1 + \tau_2)}} \exp \left[\frac{1}{2\tau_1\tau_2(\tau_1 + \tau_2)} (2x_1x_3\tau_1\tau_2 - x_1^2\tau_1\tau_2 - x_3^2\tau_1\tau_2) \right] \\ &= \frac{1}{\sqrt{2\pi(\tau_1 + \tau_2)}} \exp \left[-\frac{(x_3-x_1)^2}{2(\tau_1 + \tau_2)} \right] \\ &= \text{RHS}. \end{aligned} \quad (2.3)$$

Now, for a 1-d free particle, the density matrix is

$$\begin{aligned} \rho^u(x, x'; \beta = \tau/\hbar) &= \frac{1}{\lambda_T} \exp \left[-\pi \frac{(x-x')^2}{\lambda_T^2} \right] \quad (\lambda_T = \hbar\sqrt{\beta/2\pi m}) \\ &= \frac{1}{\hbar} \sqrt{\frac{m}{2\pi\beta}} \exp \left[-\frac{m}{\hbar^2} \frac{(x-x')^2}{2\beta} \right] \\ &= \sqrt{\frac{m}{\hbar}} \frac{1}{\sqrt{2\pi\tau}} \exp \left[-\frac{m}{\hbar} \frac{(x-x')^2}{2\tau} \right] \\ &= \frac{1}{\sqrt{2\pi\bar{\tau}}} \exp \left[-\frac{(x-x')^2}{2\bar{\tau}} \right], \end{aligned} \quad (2.4)$$

where we have set $\bar{\tau} = \tau\hbar/m$ for simplification. Then, it follows from the RHS of (2.2) that

$$\begin{aligned}
\text{RHS} &= \int dx_2 \frac{1}{\sqrt{2\pi\bar{\tau}_2}} \exp\left[-\frac{(x_3 - x_2)^2}{2\bar{\tau}_2}\right] \frac{1}{\sqrt{2\pi\bar{\tau}_1}} \exp\left[-\frac{(x_2 - x_1)^2}{2\bar{\tau}_1}\right] \\
&= \frac{1}{\sqrt{2\pi(\bar{\tau}_1 + \bar{\tau}_2)}} \exp\left[-\frac{(x_3 - x_1)^2}{2(\bar{\tau}_1 + \bar{\tau}_2)}\right] \\
&= \rho^u(x_3, x_1; \tau_1 + \tau_2) \\
&= \text{LHS}.
\end{aligned} \tag{2.5}$$

□

(b) Edward's "phantom" polymer model, coupled harmonic oscillators, and a random walk

As we may discuss in more detail in a few lectures, a simplest model of a polymer (a giant flexible linear molecule of N monomers strung together, illustrated in Fig. 1 below) is that of a freely-joined chain of N links $\mathbf{r}_n = \mathbf{R}_n - \mathbf{R}_{n-1}$. In the continuum, $n \rightarrow s$, the probability of its conformation $\mathbf{R}(s)$ in a d -dimensional space is given by

$$P[\mathbf{R}(s)] = \left(\frac{d}{2\pi b_0^2}\right)^{dN/2} \exp\left[-\frac{d}{2b_0^2} \int_0^N ds \left(\frac{\partial \mathbf{R}}{\partial s}\right)^2\right], \tag{2.6}$$

where b_0 is the preferred link length and prefactor is a normalization, much like in Eq. (2.1) for 2 links. We can view this system as described by an ideal polymer Hamiltonian

$$\mathcal{H} = \frac{\sigma}{2} \int_0^N ds \left(\frac{\partial \mathbf{R}}{\partial s}\right)^2, \tag{2.7}$$

where $\sigma = k_B T d / (\pi b_0^2)$ is the entropic polymer free energy per unit of length, i.e., tension, notably proportional to thermal energy $k_B T$.

(i) By discretizing above probability distribution into product of N 1-link probability distributions,

$$p(\mathbf{r}_n) = \left(\frac{d}{2\pi b_0^2}\right)^{d/2} \exp\left[-\frac{d}{2b_0^2} (\mathbf{R}_n - \mathbf{R}_{n-1})^2\right], \tag{2.8}$$

written in terms of the position \mathbf{R}_n of n -th monomer, and by integrating over all N *intermediate* monomer positions, \mathbf{R}_n for $1 < n < N$ compute the probability distribution $P[\mathbf{R}_N - \mathbf{R}_0]$, for the end-to-end displacement $\mathbf{R}_N - \mathbf{R}_0$.

Hint: Surprise! You have just computed a path-integral for a single polymer statistical mechanics, computing its partition function $Z = \exp(-\beta F)$, for fixed ends $\mathbf{R}_N, \mathbf{R}_0$ of the polymer.

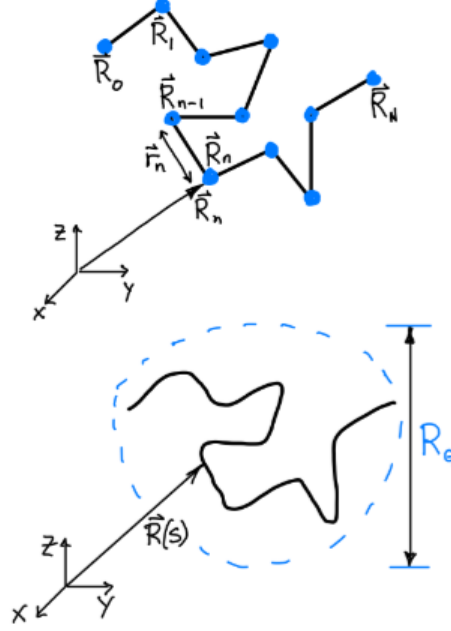


Figure 1: Edward's “phantom” polymer model executing an ideal random walk in d -dimensional space, characterized by $N + 1$ monomer positions, \mathbf{R}_n .

Solution.

From (2.6), we discretize $\int_0^N ds \mapsto \sum_{n=1}^N$

$$\begin{aligned}
 P[\mathbf{R}(s)] &\approx \left(\frac{d}{2\pi b_0^2} \right)^{dN/2} \exp \left[-\frac{d}{2b_0^2} \sum_{n=1}^N (\mathbf{R}_n - \mathbf{R}_{n-1})^2 \right] \\
 &= \left(\frac{d}{2\pi b_0^2} \right)^{dN/2} \prod_{n=1}^N \exp \left[-\frac{d}{2b_0^2} (\mathbf{R}_n - \mathbf{R}_{n-1})^2 \right] \\
 &= \prod_{n=1}^N \left(\frac{d}{2\pi b_0^2} \right)^{d/2} \exp \left[-\frac{d}{2b_0^2} (\mathbf{R}_n - \mathbf{R}_{n-1})^2 \right] \\
 &= \prod_{n=1}^N p(\mathbf{r}_n).
 \end{aligned} \tag{2.9}$$

Then,

$$\begin{aligned}
P[\mathbf{R}_N - \mathbf{R}_0] &= \int d^d \mathbf{R}_1 \dots d^d \mathbf{R}_{N-1} \prod_{n=1}^N p(\mathbf{r}_n) \\
&= \left(\frac{d}{2\pi b_0^2} \right)^{dN/2} \exp \left[-\frac{d}{2b_0^2} (\mathbf{R}_0^2 + \mathbf{R}_N^2) \right] \int d^d \mathbf{R}_1 \dots d^d \mathbf{R}_{N-1} \\
&\quad \times \exp \left[-\frac{d}{b_0^2} (\mathbf{R}_1^2 - \mathbf{R}_0 \cdot \mathbf{R}_1 + \mathbf{R}_2^2 - \mathbf{R}_1 \cdot \mathbf{R}_2 + \dots + \mathbf{R}_{N-1}^2 - \mathbf{R}_N \cdot \mathbf{R}_{N-1}) \right] \\
&= \left(\frac{d}{2\pi b_0^2} \right)^{dN/2} \exp \left[-\frac{d}{2b_0^2} (\mathbf{R}_0^2 + \mathbf{R}_N^2) \right] \int d\mathbf{u} \exp \left[-\frac{d}{b_0^2} (\mathbf{u}^T \cdot \mathbf{A} \cdot \mathbf{u} - \mathbf{h}^T \cdot \mathbf{u}) \right],
\end{aligned} \tag{2.10}$$

where $\mathbf{u} = (\mathbf{R}_1 \dots \mathbf{R}_{N-1})^T$, $\mathbf{h} = (\mathbf{R}_0 \dots \mathbf{R}_N)^T$ are $d(N-1)$ -dimensional vectors.

$$\mathbf{A} = \begin{pmatrix} \mathbb{1} & -(1/2)\mathbb{1} & \dots & 0 & 0 \\ (-1/2)\mathbb{1} & \mathbb{1} & -(1/2)\mathbb{1} & \dots & 0 \\ \vdots & -(1/2)\mathbb{1} & \ddots & \ddots & \vdots \\ 0 & 0 & \ddots & \mathbb{1} & -(1/2)\mathbb{1} \\ 0 & 0 & \dots & -(1/2)\mathbb{1} & \mathbb{1} \end{pmatrix} \tag{2.11}$$

is a symmetric block matrix of d -dimensional identity matrices $\mathbb{1}$. By Gaussian integration that we derived in Homework 2,

$$Z_0 = \int d\mathbf{u} \exp \left[-\frac{1}{2} \frac{2d}{b_0^2} \mathbf{u}^T \cdot \mathbf{A} \cdot \mathbf{u} \right] = \frac{1}{(\det \mathbf{A})^{d/2}} \left(\frac{\pi b_0^2}{d} \right)^{d(N-1)/2}, \tag{2.12}$$

where $\det \mathbf{A} = N/2^{N-1}$, by construction and note the power of d in the determinant comes from the fact that it is a block matrix. Now, we also need to calculate

$$\frac{d}{4b_0^2} \mathbf{h}^T \cdot \mathbf{A}^{-1} \cdot \mathbf{h} = \frac{d}{4b_0^2} \left(A_{1,1}^{-1} \mathbf{R}_0^2 + 2\mathbf{A}_{1,N-1}^{-1} \mathbf{R}_0 \cdot \mathbf{R}_N + A_{N-1,N-1}^{-1} \mathbf{R}_N^2 \right). \tag{2.13}$$

The inverse of \mathbf{A} is defined as $\mathbf{A}^{-1} = \text{cof}(\mathbf{A}) / \det \mathbf{A}$ where $\text{cof}(\mathbf{A})$ is the cofactor matrix of \mathbf{A} with elements defined by

$$(\text{cof} \mathbf{A})_{i,j} = (-1)^{i+j} \det \mathbf{A}_{ij}, \tag{2.14}$$

where \mathbf{A}_{ij} is the i, j minor of \mathbf{A} , not the i, j element. Thus,

$$A_{1,1}^{-1} = A_{N-1,N-1}^{-1} = \frac{2}{N}(N-1), \quad \text{and} \quad A_{1,N-1}^{-1} = \frac{2}{N}. \tag{2.15}$$

Putting all of this together, we can finally write the probability distribution function of $\mathbf{R}_N - \mathbf{R}_0$ as

$$\begin{aligned}
P[\mathbf{R}_N - \mathbf{R}_0] &= \left(\frac{d}{2\pi b_0^2}\right)^{dN/2} \exp\left[-\frac{d}{2b_0^2}(\mathbf{R}_0^2 + \mathbf{R}_N^2)\right] \frac{2^{d(N-1)/2}}{N^{d/2}} \left(\frac{\pi b_0^2}{d}\right)^{d(N-1)/2} \\
&\quad \times \exp\left[\frac{d}{2b_0^2 N}[(N-1)(\mathbf{R}_0^2 + \mathbf{R}_N^2) + 2\mathbf{R}_0 \cdot \mathbf{R}_N]\right] \\
&= \left(\frac{d}{2\pi b_0^2 N}\right)^{d/2} \exp\left[-\frac{d}{2b_0^2 N}(\mathbf{R}_N - \mathbf{R}_0)^2\right],
\end{aligned} \tag{2.16}$$

which resembles the 1-link PDF. \square

(ii) Compute the “radius of gyration” $R_g(N)$, defined by

$$R_g^2 = \left\langle (\mathbf{R}_N - \mathbf{R}_0)^2 \right\rangle, \tag{2.17}$$

which characterizes the root-mean-squared radius occupied by a polymer in the d -dimensional embedding space.

Note that, in thinking of the links of the polymer as random steps executed as a function of “time” s , this polymer statistics reproduces the random walk result that after N steps the random walker is only \sqrt{N} away from where she started. All this is of course a consequence of central limit theorem.

Solution.

Let $\mathbf{X} = \mathbf{R}_N - \mathbf{R}_0$, then

$$\begin{aligned}
R_g^2 = \langle \mathbf{X}^2 \rangle &= \left(\frac{d}{2\pi b_0^2 N}\right)^{d/2} \int d^d \mathbf{X} \exp\left[-\frac{1}{2} \frac{d}{b_0^2 N} \mathbf{X}^2\right] \mathbf{X}^2 \\
&= \left(\frac{d}{2\pi b_0^2 N}\right)^{d/2} \prod_{i=1}^d \left[\int_{-\infty}^{\infty} dX_i \left(\sum_{j=1}^d X_j^2 \right) \exp\left(-\frac{1}{2} \frac{d}{b_0^2 N} X_i^2\right) \right] \\
&= \left(\frac{d}{2\pi b_0^2 N}\right)^{d/2} \sqrt{\frac{(2\pi)^{d-1}}{d/b_0^2 N}} \frac{1}{d/b_0^2 N} \sqrt{\frac{2\pi}{d/b_0^2 N}} \\
&= b_0^2 \frac{N}{d}.
\end{aligned} \tag{2.18}$$

Thus, R_g indeed grows as \sqrt{N} . \square

Problem 3 (Free particle density matrix in coordinate representation): In lectures we discussed many properties and forms of the coordinate-space density matrix $\rho(x, x'; \beta)$, including its expected low- and high- T limits, as well as its eigenstates

$$\rho^u(x, x'; \beta) = \sum_n \psi_n(x) \psi_n^*(x') e^{-\beta E_n}, \quad (3.1)$$

and path-integral

$$\rho^u(x, x'; \beta) = \int_{x(0)=x; x(\beta\hbar)=x'} [dx(\tau)] e^{-S_E[x(\tau)]/\hbar} \quad (3.2)$$

formulations, as well as the “imaginary-time” Schrödinger-like equation in β

$$\partial_\beta \rho^u(x, x'; \beta) = -\mathcal{H}(\hat{\rho}, x) \rho^u(x, x'; \beta), \quad (3.3)$$

that it satisfies, where $\hat{\rho} = -i\hbar\partial_x$, i.e., giving the coordinate representation Schrödinger equation in imaginary time. Let us explore the details of this for a free particle here.

(a) For a free particle, use its Hamiltonian inside (3.3), solve the resulting diffusion equation (in “time” β) solve, taking into account the appropriate “initial condition” for $\beta = 0$, discussed in class, required by the general definition of $\hat{\rho}^u$.

Hint: The solution is as simple as solving free-particle Schrödinger equation in imaginary “time” or a real diffusion equation in infinite space.

Solution.

First, by separation of variables, we write $\rho(x, x'; \beta) = X(\mathbf{x}, \mathbf{x}') B(\beta)$. Then from (3.3),

$$\frac{1}{B} \frac{dB}{d\beta} = \frac{\hbar^2}{2m} \frac{1}{X} \nabla^2 X = -E, \quad (3.4)$$

where E is some constant. This separates into two ordinary differential equations in \mathbf{x} and β , in which the general solutions are $B = e^{-\beta E}$ and

$$X(x, x') = f(\mathbf{k}) \sin(\mathbf{k} \cdot \mathbf{x}) + g(\mathbf{k}) \cos(\mathbf{k} \cdot \mathbf{x}), \quad (3.5)$$

where $E = \hbar^2 k^2 / 2m$. However, by normalization condition, $\rho(\mathbf{x}, \mathbf{x}, \beta = 0) = 1$, so we must require $f(\mathbf{k}) = 0$. The general solution for ρ is then a linear combination of these basis functions

$$\rho(\mathbf{x}, \mathbf{x}'; \beta) = \int d^d \mathbf{k} g(\mathbf{k}) \cos(\mathbf{k} \cdot \mathbf{x}) e^{-\beta \hbar^2 k^2 / 2m}. \quad (3.6)$$

Now, note that for $\beta \rightarrow 0$ and $\mathbf{x}, \mathbf{x}' \in \mathbb{R}^d$,

$$\rho(\mathbf{x}, \mathbf{x}'; \beta = 0) = \int d^d \mathbf{k} g(\mathbf{k}) \cos(\mathbf{k} \cdot \mathbf{x}) = \delta(\mathbf{x} - \mathbf{x}') = \frac{1}{(2\pi)^d} \int d^d \mathbf{k} e^{i\mathbf{k} \cdot (\mathbf{x} - \mathbf{x}')}. \quad (3.7)$$

Thus, we can solve for $g(\mathbf{k})$ and write the final solution as

$$\begin{aligned}\rho(\mathbf{x}, \mathbf{x}'; \beta) &= \frac{1}{2\pi} \int d^d \mathbf{k} \exp \left[-\frac{1}{2} \frac{\beta \hbar^2}{m} k^2 + i(\mathbf{x} - \mathbf{x}') \cdot \mathbf{k} \right] \\ &= \frac{1}{(2\pi)^d} \left(\frac{2\pi}{\beta \hbar^2 / m} \right)^{d/2} \exp \left[-\frac{(\mathbf{x} - \mathbf{x}')^2}{2\beta \hbar^2 / m} \right] \\ &= \left(\frac{m}{2\pi \hbar^2 \beta} \right)^{d/2} \exp \left[-\frac{1}{2} \frac{m(\mathbf{x} - \mathbf{x}')^2}{\hbar^2 \beta} \right].\end{aligned}\tag{3.8}$$

□

(b) Use Hamiltonian eigenbasis representation, Eq. (3.1) and your knowledge of what the free-particle eigenstates are, to rederive the above result for $\rho^u(x, x'; \beta)$, also quoted in the lectures. Note that if you properly take the eigenstates to be normalized in a large box of size L (most convenient with periodic boundary conditions), this analysis automatically gives the correct prefactor for $\rho^u(x, x'; \beta)$.

Solution.

The eigenstate of a particle in an infinite square well for $x \in [-L/2, L/2]$ is

$$\psi_n(x) = \sqrt{\frac{2}{L}} \sin \left[\frac{n\pi x}{2} + \frac{n\pi}{2} \right],\tag{3.9}$$

with energy $E_n = n^2 \pi^2 \hbar^2 / 2mL^2$. Thus, from (3.1),

$$\rho(x, x'; \beta) = \frac{2}{L} \sum_{n=0}^{\infty} \sin \left[\frac{n\pi x}{L} + \frac{n\pi}{2} \right] \sin \left[\frac{n\pi x'}{L} + \frac{n\pi}{2} \right] \exp \left[-\beta \frac{n^2 \pi^2 \hbar^2}{2mL^2} \right].\tag{3.10}$$

Letting $\sum_n \mapsto \sum_0^{\infty} dn$, we can calculate this infinite series with Mathematica

$$\rho(x, x'; \beta) = \sqrt{\frac{m}{2\pi \hbar^2 \beta}} \left\{ \exp \left[-\frac{1}{2} \frac{m(x - x')^2}{\hbar^2 \beta} \right] - \exp \left[-\frac{1}{2} \frac{m(L + x + x')^2}{\hbar^2 \beta} \right] \right\}.\tag{3.11}$$

Thus, taking the limit that $L \rightarrow \infty$, the second exponent vanishes, leaving the 1-dimensional form of the answer in part (a). □

(c) Now we will use, perhaps a bit less familiar path-integral formulation. One useful approach to evaluate a path-integral is that of a semi-classical saddle-point approximation.

- An amazing fact, however, that we will see below is that this semi-classical approach is in fact *exact* for a quadratic action, as for e.g., a free particle and harmonic oscillator (the following problem).

- Examining Eq. (3.2), we see that all dependence of $\rho^u(x, x'; \beta)$ on x, x' is in the boundary conditions on $x(0), x(\beta\hbar)$. So let's introduce new time-dependent coordinates $y(\tau)$, with

$$x(\tau) = x_{\text{cl}}(\tau) + y(\tau), \quad (3.12)$$

where $x_{\text{cl}}(\tau)$ is the classical path satisfying the Euler-Lagrange equation

$$\left. \frac{\delta S_E[x(\tau)]}{\delta x(\tau)} \right|_{x_{\text{cl}}(\tau)} = 0, \quad (3.13)$$

and satisfying $x_{\text{cl}}(0) = x, x_{\text{cl}}(\beta\hbar) = x'$. Thus, $y(0) = y(\beta\hbar) = 0$.

- Inserting Eq. (3.12) into the action in Eq. (3.2) and expanding to lowest nontrivial order in $y(\tau)$ we find

$$\rho^u(x, x'; \beta) \approx e^{-S_E[x_{\text{cl}}(\tau)]/\hbar} \int_{y(0)=y(\beta\hbar)=0} [dy(\tau)] \exp \left[-\frac{1}{2\hbar} \int_0^{\beta\hbar} d\tau y(\tau) S_E''[x_{\text{cl}}] y(\tau) \right], \quad (3.14)$$

where first functional derivative term is absent because it vanishes by virtue of the equation of motion Eq. (3.13) satisfied by $x_{\text{cl}}(\tau)$.

- The key observation in Eq. (3.14) is that for quadratic action $S_E[x(\tau)]$, the kernel $S_E''[x_{\text{cl}}]$ in the exponential is independent of $x_{\text{cl}}(\tau)$. Thus, for such quadratic theory, the remaining functional integral over $y(\tau) \mathcal{N}(\beta\hbar)$ is just a “constant” that only depends on $\beta\hbar$, but *not* on x, x' . We can therefore not worry about this prefactor $\mathcal{N}(\beta\hbar)$ and focus on $\exp \left(-S_E[x_{\text{cl}}(\tau)]/\hbar \right)$ that contains all the key dependence on x, x' , giving us $\rho^u(x, x'; \beta)$ up to the factor $\mathcal{N}(\beta\hbar)$.

Solution.

See part (d). □

(d) For a free particle, solve the (Euclidean) classical Euler-Lagrange equation of motion Eq. (3.13) for $x(\tau, x, x')$ with initial conditions $x_{\text{cl}}(0) = x, x_{\text{cl}}(\beta\hbar) = x'$, and evaluate

$$S_E[x_{\text{cl}}(\tau)] \equiv S_{\text{cl}}(x, x', \beta\hbar), \quad (3.15)$$

thereby obtaining

$$\rho^u(x, x'; \beta) = \mathcal{N}(\beta\hbar) e^{-S_{\text{cl}}(x, x', \beta\hbar)/\hbar}. \quad (3.16)$$

Demonstrate that up to the unknown prefactor $\mathcal{N}(\beta\hbar)$, you obtain exactly the result found in (a) and (b).

Solution.

The Lagrangian of a free particle is $\mathcal{L} = (1/2)m\dot{x}^2$. Thus, the action is $S_E[x(\tau)] = (m/2) \int_0^{\beta\hbar} d\tau \dot{x}^2$. Then it follows that

$$\begin{aligned}
\frac{\delta S_E[x(\tau)]}{\delta x(\tau)} &= \lim_{\epsilon \rightarrow 0} \frac{1}{\epsilon} \left\{ S_E[x(t) + \epsilon \delta(t - \tau)] - S_E[x(t)] \right\} \\
&= \frac{m}{2} \int_0^{\beta\hbar} dt \lim_{\epsilon \rightarrow 0} \frac{1}{\epsilon} \left\{ [\dot{x} + \epsilon \delta'(t - \tau)]^2 - \dot{x}^2 \right\} \\
&= \frac{m}{2} \int_0^{\beta\hbar} dt \lim_{\epsilon \rightarrow 0} [2\dot{x} \delta'(t - \tau) + \epsilon \delta'^2] \\
&= m \int_0^{\beta\hbar} \dot{x} \delta'(t - \tau) \\
&= -m\ddot{x}.
\end{aligned} \tag{3.17}$$

Extremizing S_E , it follows that the classical trajectory is $x_{\text{cl}}(\tau) = a\tau + b$ for some constant $a, b \in \mathbb{R}$. Now, using the initial conditions $x_{\text{cl}}(0) = x$ and $x_{\text{cl}}(\beta\hbar) = x'$, we can write

$$x_{\text{cl}}(\tau) = -\frac{x - x'}{\beta\hbar} \tau + x. \tag{3.18}$$

Then, from (3.14),

$$\begin{aligned}
\rho^u(x, x'; \beta) &\approx \mathcal{N}(\beta\hbar) \exp \left[-\frac{S_E[x_{\text{cl}}(\tau)]}{\hbar} \right] \\
&= \mathcal{N}(\beta\hbar) \exp \left[-\frac{m}{2} \frac{(x - x')^2}{\beta^2 \hbar^3} \int_0^{\beta\hbar} d\tau \right] \\
&= \mathcal{N}(\beta\hbar) \exp \left[-\frac{1}{2} \frac{m(x - x')^2}{\hbar^2 \beta} \right],
\end{aligned} \tag{3.19}$$

which is the same as previous results, up to a factor $\mathcal{N}(\beta\hbar)$. □

(e) As a non-required bonus, you can determine the prefactor $\mathcal{N}(\beta\hbar)$, by discretizing the path integral in (3.14) as you did for a polymer in problem 2 (note mathematically it is exactly the same path integral) and then requiring the $\mathcal{N}(\Delta\tau)$ (with $\beta\hbar = N\Delta\tau$) to be special function such that the “propagator” relation, (2.1) is satisfied.

Alternatively, you can determine $\mathcal{N}(\tau)$ by requiring that (3.16) satisfies the diffusion equation, (3.3), thereby obtaining and solving a differential equation for $\mathcal{N}(\tau)$.

Solution.

□

(f) Now that we have obtained $\rho^u(x, x'; \beta)$ by three methods above, calculate the corresponding (i) partition function $Z(\beta)$ and the (ii) probability $P(x) = \rho^u(x, x, \beta)/Z(\beta)$ of finding a free particle at position x .

Hint: The answer makes sense and is trivial.

Solution.

(i) By definition, the partition function Z is the trace

$$Z = \int d\mathbf{x} \rho(\mathbf{x}, \mathbf{x}; \beta) = \left(\frac{m}{2\pi\hbar^2\beta} \right)^{d/2} \int d\mathbf{x}. \quad (3.20)$$

Viewing the free particle as a particle in a large infinite square well, if the domain is $[-L, L]^d$ for $L \rightarrow \infty$, then $Z \rightarrow \infty$ as well and (ii) it follows that $P(x) \rightarrow \infty$. Mathematically, this makes sense because the continuous probability distribution function $P(\mathbf{x}) = \rho/Z$ is infinitely dense. So the probability is only non-zero in any non-zero measure subset of the support of P ($\{\mathbf{x}\}$ is a zero measure set).

But physically, it is due to equilibration. Diffusion in an infinite space with the ergodicity hypothesis blows up the uncertainty in x . But we know precisely the momentum (or energy). Now, this would no longer be true for finite L , in which the energy eigenvalues are discretized. So the probability in this limit may be finite and equates to

$$P(\mathbf{x}) = \frac{1}{V(L)} \exp \left[-\frac{m(\mathbf{x} - \mathbf{x}')^2}{2m\hbar^2\beta} \right], \quad (3.21)$$

where $V = \int_{[-L, L]^d} d\mathbf{x}$ is the volume of the square well. □

Problem 4 (Particle in harmonic potential density matrix in coordinate representation): Here we want to calculate $\rho^u(x, x'; \beta)$ and the corresponding partition function Z and $P(x)$ for a quantum harmonic oscillator. The first two methods (a) and (b), above are in fact a bit challenging to utilize, though the solution of the imaginary-time Schrödinger equation (a) is quite straightforward, but technically grungy. So below we will focus on the path-integral approach.

Carefully following the path-integral procedure in problem 3, above, now for a quantum harmonic oscillator.

(a) Calculate $\rho^u(x, x'; \beta)$ from the path-integral analysis, by finding $x_{\text{cl}}(\tau)$ and the corresponding $S_E[x_{\text{cl}}(\tau)] = S_{\text{cl}}(x, x', \beta\hbar)$, and using (3.16), up to a prefactor $\mathcal{N}(\beta\hbar)$.

Solution.

The Lagrangian is $\mathcal{L} = (1/2)m\dot{x}^2 - (1/2)m\omega_0^2 x^2$ where $\omega_0^2 = k/m$. Thus, the E-L equation of motion is

$$m\ddot{x} = \frac{\partial \mathcal{L}}{\partial x} = -m\omega_0^2 x \Rightarrow \frac{d^2 x}{dt^2} = -\omega_0^2 x \Rightarrow \frac{d^2 x}{d\tau^2} = \omega_0^2 x, \quad (4.1)$$

where we have written $t = -i\tau$. The general solution to this differential equation is

$$x(\tau) = Ae^{\omega_0\tau} + Be^{-\omega_0\tau}, \quad (4.2)$$

where

$$A = \frac{x - e^{\beta\hbar\omega_0} x'}{1 - e^{2\beta\hbar\omega_0}}, \quad \text{and} \quad B = -e^{\beta\hbar\omega_0} \frac{e^{\beta\hbar\omega_0} x - x'}{1 - e^{2\beta\hbar\omega_0}} \quad (4.3)$$

satisfy the initial conditions $x(0) = x, x(\beta\hbar) = x'$. It follows that the unnormalized density matrix is

$$\begin{aligned} \rho^u(x, x'; \beta) &= \mathcal{N}(\beta\hbar) \exp \left[-\frac{m}{2\hbar} \int_0^{\beta\hbar} d\tau (\dot{x}^2 - \omega_0^2 x^2) \right] \\ &= \mathcal{N} \exp \left[\frac{m}{2\hbar} \int_0^{\beta\hbar} d\tau ((dx/d\tau)^2 + \omega_0^2 x^2) \right] \\ &= \mathcal{N} \exp \left[-\frac{m\omega_0}{2\hbar} \left[A^2 (1 - e^{2\beta\hbar\omega_0}) - B^2 (1 - e^{-2\beta\hbar\omega_0}) \right] \right] \\ &= \mathcal{N} \exp \left[-\frac{m\omega_0}{4\hbar} \left[(x + x') \tanh \left(\frac{\beta\hbar\omega_0}{2} \right) + (x - x')^2 \coth \left(\frac{\beta\hbar\omega_0}{2} \right) \right] \right] \end{aligned} \quad (4.4)$$

□

(b) Compute the canonical partition function Z (that you have done in an earlier homework) to determine the prefactor $\mathcal{N}(\beta\hbar)$.

Solution.

The Hamiltonian is $\mathcal{H} = p^2/2m + (1/2)m\omega_0^2 x^2$ with eigenvalues $E_n = \hbar\omega_0(n + 1/2)$. Thus, the partition function is

$$Z = \sum_{n=0}^{\infty} \exp \left[-\beta \hbar \omega_0 \left(n + \frac{1}{2} \right) \right] = e^{-\beta \hbar \omega_0 / 2} \sum_{n=0}^{\infty} \left(e^{-\beta \hbar \omega_0} \right)^n = \frac{1}{2 \sinh(\beta \hbar \omega_0 / 2)}. \quad (4.5)$$

But the trace of ρ^u is also Z

$$Z = \mathcal{N} \int_{-\infty}^{\infty} dx \exp \left[-\frac{m\omega_0}{\hbar} \tanh \left(\frac{\beta \hbar \omega_0}{2} \right) x^2 \right] = \mathcal{N} \sqrt{\frac{\pi \hbar}{m\omega_0 \tanh(\beta \hbar \omega_0 / 2)}}. \quad (4.6)$$

Thus,

$$\mathcal{N} = \frac{1}{2 \sinh(\beta \hbar \omega_0 / 2)} \sqrt{\frac{m\omega_0 \tanh(\beta \hbar \omega_0 / 2)}{\pi \hbar}} = \sqrt{\frac{m\omega_0}{2\pi \hbar \sinh(\beta \hbar \omega_0)}}. \quad (4.7)$$

□

(c) Compute the probability density $P(x) = \rho^u(x, x, \beta) / Z(\beta) = \rho(x, x, \beta)$ of finding the particle in a harmonic potential at position x .

Solution.

From previous results,

$$P(x) = \frac{\rho^u}{Z} = \sqrt{\frac{m\omega_0 \tanh(\beta \hbar \omega_0 / 2)}{\pi \hbar}} \exp \left(-\frac{m\omega_0 \tanh(\beta \hbar \omega_0 / 2)}{\hbar} x^2 \right). \quad (4.8)$$

□

(d) Using $P(x)$, compute the root-mean-squared length $x_Q(T)$, defined by the variance $x_Q^2(T) = \langle x^2 \rangle$.

Solution.

By definition,

$$\begin{aligned} x_Q^2 &= \sqrt{\frac{m\omega_0 \tanh(\beta \hbar \omega_0 / 2)}{\pi \hbar}} \int_{-\infty}^{\infty} dx x^2 \exp \left(-\frac{m\omega_0 \tanh(\beta \hbar \omega_0 / 2)}{\hbar} x^2 \right) \\ &= \frac{\hbar}{2m\omega_0 \tanh(\beta \hbar \omega_0 / 2)}. \\ \Rightarrow x_Q &= \sqrt{\frac{\hbar}{2m\omega_0 \tanh(\beta \hbar \omega_0 / 2)}}. \end{aligned} \quad (4.9)$$

□

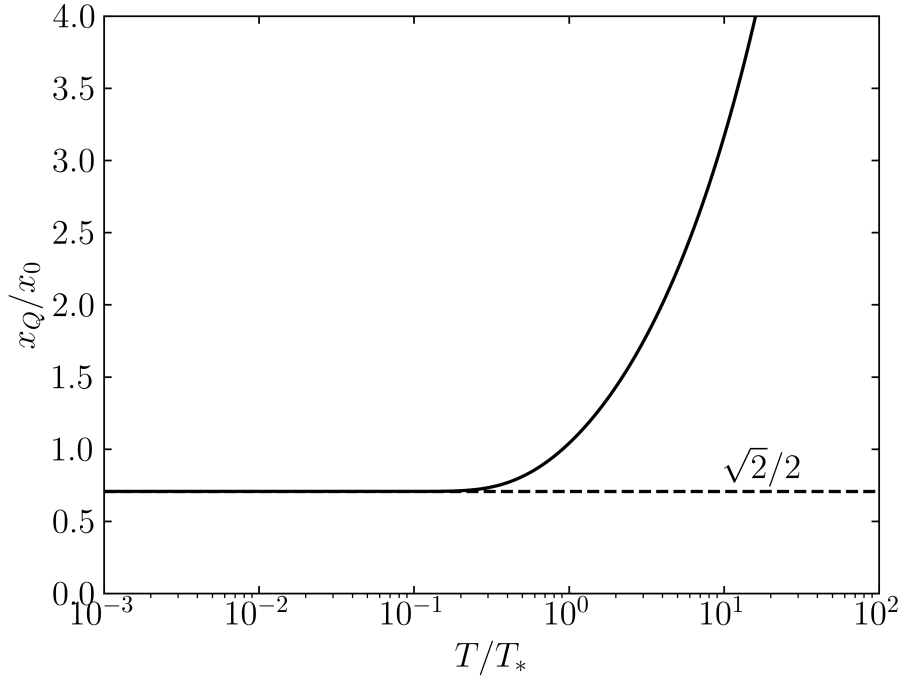
(e) Study high- and low-temperature limits of $x_Q(T)$, and make arguments for the resulting limiting forms, by thinking about the purely classical and purely quantum limits of the harmonic oscillator.

Solution.

Let the crossover temperature be $T_* = \hbar\omega_0/k_B$ and $x_0 = \hbar/m\omega_0$ such that the maximum spring potential energy is exactly one quantum of energy $(1/2)kx_0^2 = \hbar\omega_0/2$. Then x_Q can be rewritten as

$$x_Q = x_0 \frac{1}{\sqrt{2 \tanh(T^*/2T)}}. \quad (4.10)$$

Below, we plot this function.



In the low temperature limit ($T/T_* \ll 1$), x_Q approaches the limit of $x_0/\sqrt{2}$. Recall the time-dependent solution of a harmonic oscillator $x \sim x_0 e^{i\omega_0 t}$. Thus $\langle x^2 \rangle = x_0^2 \langle e^{i\omega_0 t} \rangle = x_0^2/2$. So this limit makes sense. In the classical regime ($T/T_* \gg 1$), the available energy is much larger than $\hbar\omega_0/2$. Also, the scale of the oscillation in x is much larger than that defined by the quantum scale x_0 . So it makes sense that $x_Q \rightarrow \infty$. \square

Problem 5 (Density matrix and entanglement entropy): Consider a system consisting of two qubits (“quantum bit”, each realized as any two-level system e.g., a double-well potential or a spin-1/2 or just two atomic levels, a basic element of a quantum computer) A and B , with each taking on two possible values, designated by, say 0 and 1. Take this 2-qubit “computer” to be in a pure

(a) *unentangled*, i.e., product state

$$|\psi_{AB}\rangle = \frac{1}{2}(|0\rangle + |1\rangle) \otimes (|0\rangle + |1\rangle). \quad (5.1)$$

Construct the two-qubit density matrix $\hat{\rho}_{AB} = |\psi_{AB}\rangle \langle \psi_{AB}|$ for the whole system and extract its corresponding (4×4) matrix representation $\rho_{ss'}$ in this $|s\rangle = |\sigma_A\rangle \otimes |\sigma_B\rangle$ ($\sigma_{A,B} = 0, 1 \mapsto s = 1, 2, 3, 4$) basis, namely $\hat{\rho}_{AB} = \sum_{s,s'=1}^4 \rho_{ss'} |s\rangle \langle s'| = \sum_{\sigma,\sigma'=0,1} \rho_{\sigma\sigma'} |\sigma_A\rangle \otimes |\sigma_B\rangle \langle \sigma'_A| \otimes \langle \sigma'_B|$.

(i) Verify that this is indeed a density matrix for a pure state by showing $\text{Tr}[\hat{\rho}_{AB}] = \text{Tr}[\hat{\rho}_{AB}^2] = 1$. *Hint*: You can do this by working directly with the matrix $\rho_{\sigma\sigma'}$ or more formally working in a representation-independent way.

Solution.

First, we write $|1\rangle = |0, 0\rangle$, $|2\rangle = |0, 1\rangle$, $|3\rangle = |1, 0\rangle$, and $|4\rangle = |1, 1\rangle$. Now, by assumption,

$$\begin{aligned} |\psi_{AB}\rangle \langle \psi_{AB}| &= \frac{1}{4}(|0, 0\rangle + |0, 1\rangle + |1, 0\rangle + |1, 1\rangle)(\langle 0, 0| + \langle 0, 1| + \langle 1, 0| + \langle 1, 1|) \\ &= \frac{1}{4}(|1\rangle + |2\rangle + |3\rangle + |4\rangle)(\langle 1| + \langle 2| + \langle 3| + \langle 4|). \end{aligned} \quad (5.2)$$

Reading off directly from this, we can write the density matrix as

$$\hat{\rho}_{AB} = \frac{1}{4} \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \end{pmatrix}, \quad \text{and} \quad \hat{\rho}_{AB}^2 = \hat{\rho}_{AB} = \frac{1}{4} \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \end{pmatrix}. \quad (5.3)$$

Thus, by definition, the trace is the sum of the diagonals and it is obvious that $\text{Tr}[\hat{\rho}_{AB}] = \text{Tr}[\hat{\rho}_{AB}^2] = 1$. \square

(ii) Show that the von Neumann entropy of this state vanishes, i.e.,

$$S_{vN} = -\langle \ln \hat{\rho}_{AB} \rangle = -\text{Tr}(\hat{\rho}_{AB} \ln \hat{\rho}_{AB}) = 0, \quad (5.4)$$

as it must for any pure state. *Hint*: One way to define a function of an operator (e.g., $\ln \hat{O}$) is by its eigenvalues by going to its diagonal basis.

Solution.

We diagonalize $\hat{\rho}_{AB}$ by finding the roots of $\det(\hat{\rho}_{AB} - \sigma \mathbb{1}) = \sigma^4 - \sigma^3 = \sigma^3(\sigma - 1)$, which are 0 and 1. Thus indeed,

$$S_{vN} = -\text{Tr}[\hat{\rho}_{AB} \ln \hat{\rho}_{AB}] = -\sum_{\sigma=0,1} \sigma \ln \sigma = 0. \quad (5.5)$$

\square

(iii) Compute the reduced (2×2) density matrix

$$\hat{\rho}_A = \text{Tr} \hat{\rho}_{AB} = \sum_{\sigma_B} \langle \sigma_B | \hat{\rho}_{AB} | \sigma_B \rangle, \quad (5.6)$$

by tracing over the states of the B qubit, that describes the density matrix for the A qubit subsystem.

Solution.

From (5.2), we find that

$$\langle 0 | \hat{\rho}_{AB} | 0 \rangle = \langle 0 | \hat{\rho}_{AB} | 1 \rangle = \langle 1 | \hat{\rho}_{AB} | 0 \rangle = \langle 1 | \hat{\rho}_{AB} | 1 \rangle = \frac{1}{4} [|0\rangle + |1\rangle] [\langle 0| + \langle 1|] = \frac{1}{2}. \quad (5.7)$$

Thus,

$$\hat{\rho}_A = \frac{1}{2} \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}, \quad \text{and} \quad \hat{\rho}_A^2 = \frac{1}{2} \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}. \quad (5.8)$$

□

(iv) Verify that this reduced density matrix describes a pure state, by showing $\text{Tr}[\hat{\rho}_A] = \text{Tr}[\hat{\rho}_A^2] = 1$.

Solution.

The trace is just the sum of the diagonal elements, which is 1 for both, obviously. □

(v) Show that consistent with above, the *entanglement* entropy (von Neumann entropy of $\hat{\rho}_A$) for subsystem A , described by this reduced density matrix, $\hat{\rho}_A$ still vanishes, i.e.,

$$S_E = -\langle \ln \hat{\rho}_A \rangle_A = -\text{Tr}(\hat{\rho}_A \ln \hat{\rho}_A) = 0, \quad (5.9)$$

demonstrating that the qubits A and B are not entangled, since $\hat{\rho}_{AB}$ was constructed from a *product* state.

Solution.

Again we find the eigenvalues from the roots of $\det(\hat{\rho}_A - \sigma_A \mathbb{1}) = \lambda(\lambda - 1)$, which are still 0 and 1. Thus, $S_E = -\sum_{\sigma_A=0,1} \sigma_A \ln \sigma_A = 0$. □

(b) *entangled* “cat” state

$$\langle \psi_{AB} | = \frac{1}{\sqrt{2}} (|0\rangle \otimes |0\rangle + |1\rangle \otimes |1\rangle). \quad (5.10)$$

Construct the two-qubit density matrix $\hat{\rho}_{AB} = |\psi_{AB}\rangle \langle \psi_{AB}|$ for the whole system and extract its corresponding (4×4) matrix representation $\rho_{ss'}$ in this $|s\rangle = |\sigma_A\rangle \otimes |\sigma_B\rangle$ ($\sigma_{A,B} = 0, 1 \mapsto s = 1, 2, 3, 4$) basis, namely $\hat{\rho}_{AB} = \sum_{s,s'=1}^4 \rho_{ss'} |s\rangle \langle s'| = \sum_{\sigma,\sigma'=0,1} \rho_{\sigma\sigma'} |\sigma_A\rangle \otimes |\sigma_B\rangle \langle \sigma'_A| \otimes \langle \sigma'_B|$.

(i) Verify that this is indeed a density matrix for a pure state by showing $\text{Tr}[\hat{\rho}_{AB}] = \text{Tr}[\hat{\rho}_{AB}^2] = 1$. *Hint:* You can do this by working directly with the matrix $\rho_{\sigma\sigma'}$ or more formally working in a representation-independent way.

Solution.

Keeping the same definitions as in part (a-i), now the density matrix is

$$\begin{aligned} |\psi_{AB}\rangle \langle \psi_{AB}| &= \frac{1}{2}(|0,0\rangle + |1,1\rangle)(\langle 0,0| + \langle 1,1|) \\ &= \frac{1}{2}(|1\rangle + |4\rangle)(\langle 1| + \langle 4|). \end{aligned} \quad (5.11)$$

Thus, the only non-trivial elements are $\rho_{11} = \rho_{44} = \rho_{14} = \rho_{41} = 1/2$. We can also write

$$\hat{\rho}_{AB} = \frac{1}{2} \begin{pmatrix} 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 \end{pmatrix}, \quad \text{and} \quad \hat{\rho}_{AB}^2 = \hat{\rho}_{AB} = \frac{1}{2} \begin{pmatrix} 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 \end{pmatrix}, \quad (5.12)$$

Thus, it is trivial that $\text{Tr}[\hat{\rho}_{AB}] = \text{Tr}[\hat{\rho}_{AB}^2] = 1$, from the diagonal elements. \square

(ii) Show that the von Neumann entropy of this state vanishes, i.e.,

$$S_{vN} = -\langle \ln \hat{\rho}_{AB} \rangle = -\text{Tr}(\hat{\rho}_{AB} \ln \hat{\rho}_{AB}) = 0, \quad (5.13)$$

as it must for any pure state. *Hint:* One way to define a function of an operator (e.g., $\ln \hat{O}$) is by its eigenvalues by going to its diagonal basis.

Solution.

By Cayley-Hamilton theorem, since $\hat{\rho}_{AB}$ follows the polynomial $\hat{\rho}_{AB}^2 - \hat{\rho}_{AB} = 0$, $\sigma^2 - \sigma = 0$ is the characteristic polynomial of \mathbf{A} , which has roots at $\sigma = 0$ and $\sigma = 1$. These are the eigenvalues and similar to the previous part, $S_{vN} = 0$. \square

(iii) Compute the reduced density (2×2) matrix

$$\hat{\rho}_A = \text{Tr}_B \hat{\rho}_{AB} = \sum_{\sigma_B} \langle \sigma_B | \hat{\rho}_{AB} | \sigma_B \rangle, \quad (5.14)$$

by tracing over the states of the B qubit, that describes the density matrix for the A qubit subsystem.

Solution.

By definition, $\langle 0 | \hat{\rho}_A | 0 \rangle = \frac{1}{2} \langle 0 | 0 \rangle = \frac{1}{2}$, and $\langle 1 | \hat{\rho}_A | 1 \rangle = \frac{1}{2} \langle 1 | 1 \rangle = \frac{1}{2}$. Also, $\langle 1 | \hat{\rho}_A | 0 \rangle = \langle 0 | \hat{\rho}_A | 1 \rangle = \frac{1}{2} \langle 0 | 1 \rangle = 0$. Thus, $\hat{\rho}_A = \frac{1}{2} \mathbb{1}$. \square

(iv) Verify that this reduced density matrix describes a mixed state, by showing $\text{Tr}[\hat{\rho}_A] = 1$, but $\text{Tr}[\hat{\rho}_A^2] < 1$.

Solution.

From the previous part, it is clear that $\text{Tr}[\hat{\rho}_A] = 1$. However, $\hat{\rho}_A^2 = (1/4)\mathbb{1}$, so $\text{Tr}[\hat{\rho}_A^2] = 1/2 < 1$. \square

(v) Show that, consistent with above, the *entanglement* entropy (von Neumann entropy of $\hat{\rho}_A$) for subsystem A , described by this reduced density matrix, $\hat{\rho}_A$ is nonzero, i.e.

$$S_E = -\langle \ln \hat{\rho}_A \rangle_A = -\text{Tr}_A (\hat{\rho}_A \ln \hat{\rho}_A) = \ln 2, \quad (5.15)$$

demonstrating that the qubits A and B are *entangled*, since $\hat{\rho}_{AB}$ was constructed from a maximally *entangled* “cat” state.

Solution.

Since $\hat{\rho}_A$ is already diagonal, we can tell that the eigenvalue of $\hat{\rho}_A$ is $\sigma_A = 1/2$, which is degenerate. So $S_E = -2\sigma_A \ln \sigma_A = \ln 2$, meaning A and B are entangled. \square