Homework 4: Phys 7230 (Spring 2022)

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Due: March 14, 2022

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

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

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

$$\left\langle e^{-x} \right\rangle \geq e^{-\langle x \rangle}. \tag{1.2}$$

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

Solution.
At the limit that $x \to 0$ and $\langle x \rangle \to 0$, $\left\langle e^{-x} \right\rangle \approx \langle 1 - x \rangle = 1 - \langle x \rangle \approx e^{-\langle x \rangle}$. 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

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

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

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

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 $k(\alpha/k_BT)$. Then solve this equation for the function $k(\alpha/k_BT)$ numerically and/or graphically, giving its two limits, the critical value of $(\alpha/k_BT)_c$ 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 $k(\alpha/k_BT)$. From this solution show that the variational theory predicts a phase transition in this problem in the solution for k as a function of α/k_BT, namely that the thermodynamics (free energy, etc) has two distinct phases, corresponding to high and low α/k_BT. 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

$$Z_{\text{tr}} = \int \frac{dxdp}{2\pi\hbar} \exp\left(-\frac{1}{2}\frac{\beta}{m}p^2 - \frac{1}{2}\beta kx^2\right) = \frac{k_BT}{\hbar\omega_0}, \tag{1.5}$$

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

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

Thus, the variational free energy is

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

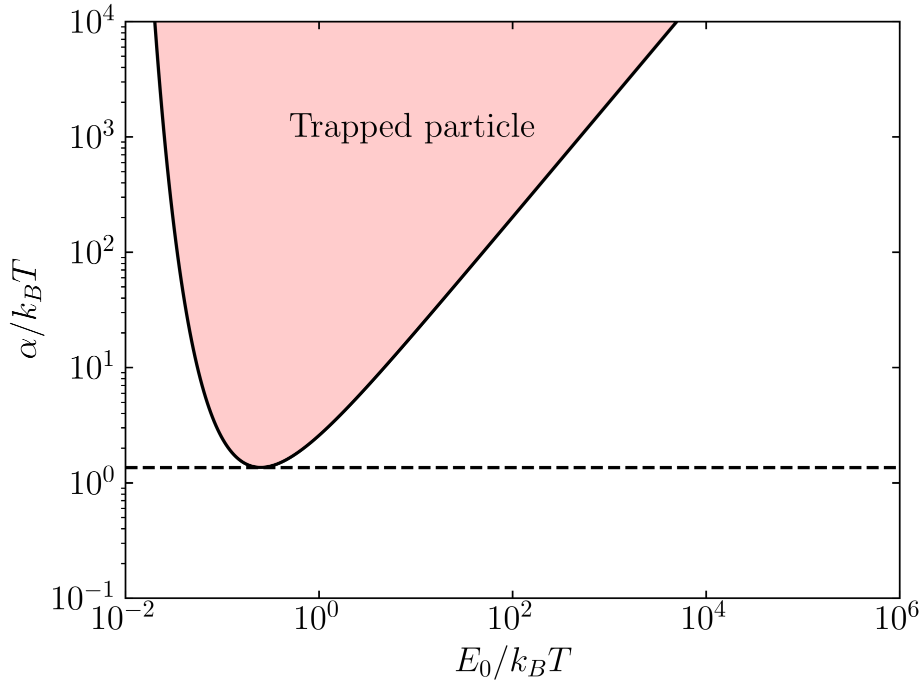
In normalized units,

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

Now, the spring constant k minimizing F_{v} satisfies $\partial F_{\mathrm{v}}(k)/\partial k = 0$, which results in the following transcendental equation

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

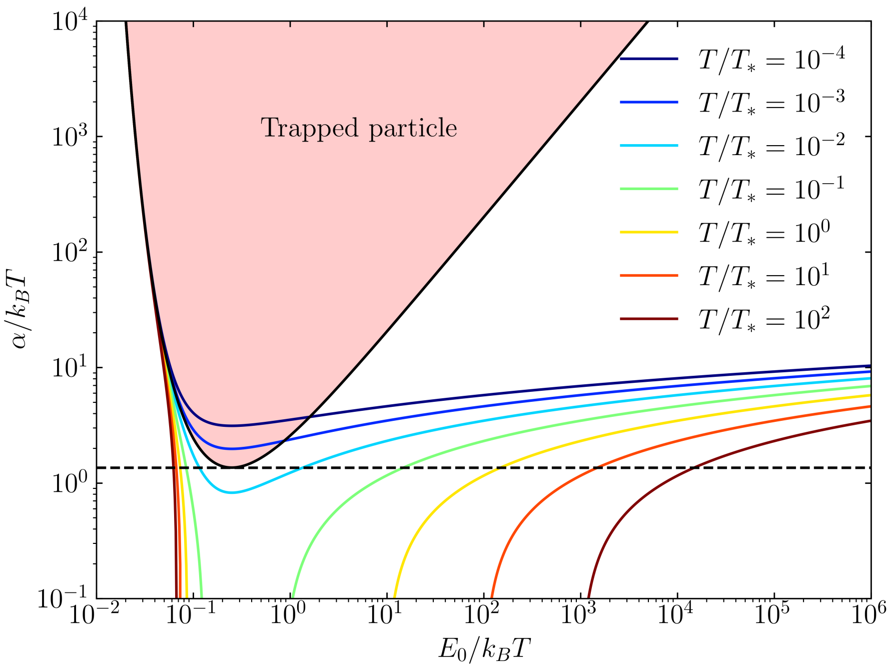
where α/k_BT determines the amplitude of the periodic potential, and $E_0 = (1/2)kx_0^2$ is the spring potential energy. In the following, we plot $f(E_0)$.



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

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

where k_m is the solution of (1.9). Below, we overlay F_v/k_BT onto the previous plot from $T/T_* = 10^{-4}$ (blue) to $T/T_* = 10^2$ (red). Note that $F_v(k_m)/k_BT$ is only valid for $\alpha/k_BT \gtrsim 1$. 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,

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

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

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

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

Solution.
From the LHS of (2.1),

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

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

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

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

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

□

(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, illutrated 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, $n \to s$, the probability of its conformation $\mathbf{R}(s)$ in a d-dimensional space is given by

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

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.

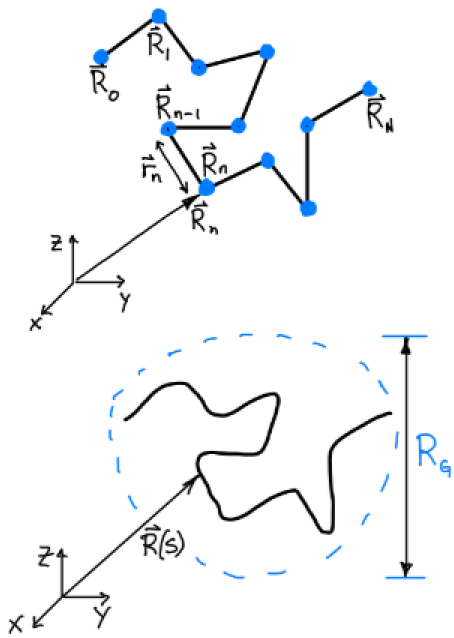


Figure 1: Edward's "phantom" polymer model executing an ideal random walk in d-dimensional space, characterized by $N+1$ monomer positions, $\mathbf{R}_n$.

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,

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

where $\mathbf{u} = \Big(\mathbf{R}_1 \quad \dots \quad \mathbf{R}_{N-1}\Big)^T$, $\mathbf{h} = \Big(\mathbf{R}_0 \quad \dots \quad \mathbf{R}_N\Big)^T$ 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

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

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

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

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

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

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

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

which resembles the 1-link PDF. □

(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 $\sqrt{N}$. □

***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

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

and path-integral

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

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

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

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),

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

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

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

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

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

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

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

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

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

□

(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 $x \in \big[-L/2, L/2\big]$ is

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

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

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

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

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

Thus, taking the limit that $L \to \infty$, 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

$$x(\tau) = x_{\rm cl}(\tau) + y(\tau), \tag{3.12}$$

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

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

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

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

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

- The key observation in Eq. (3.14) is that for quadratic action $S_E\big[x(\tau)\big]$, the kernel $S_E''[x_{\rm cl}]$ in the exponential is independent of $x_{\rm cl}(\tau)$. 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* not on x,x'. We can therefore not worry about this prefactor $\mathcal{N}(\beta\hbar)$ and focus on $\exp\Big(-S_E\big[x_{\rm cl}(\tau)\big]/\hbar\Big)$ 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 $x_{\rm cl}(0) = x, x_{\rm cl}(\beta\hbar) = x'$, and evaluate

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

thereby obtaining

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

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

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

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

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

Then, from (3.14),

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

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.

Plugging (3.19) into (3.3), we get the following differential equation for $\mathcal{N}$

$$\frac{d\mathcal{N}}{d\tau} = -\frac{1}{2\tau}\mathcal{N}, \qquad (3.20)$$

where $\tau = \beta\hbar$. The general solution is

$$\mathcal{N}(\tau) = \frac{N_0}{\sqrt{\beta\hbar}}, \tag{3.21}$$

with some constant N_0. By normalization condition, we find $N_0 = \sqrt{m/2\pi\hbar}$ such that

$$\rho(x, x'; \beta) = \sqrt{\frac{m}{2\pi\hbar^2\beta}} \exp\left[-\frac{m(x-x')^2}{2\hbar^2\beta}\right]. \tag{3.22}$$

□

(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

$$Z = \int d\mathbf{x}\rho(\mathbf{x}, \mathbf{x}; \beta) = \left(\frac{m}{2\pi\hbar^2\beta}\right)^{d/2} \int d\mathbf{x}. \tag{3.23}$$

Viewing the free particle as a particle in a large infinite square well, if the domain is $[-L, L]^d$ for $L \to \infty$, then $Z \to \infty$ as well and (ii) it follows that $P(x) \to \infty$. 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 equilibriation. 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

$$P(\mathbf{x}) = \frac{1}{V(L)} \exp\left[-\frac{m(\mathbf{x}-\mathbf{x}')^2}{2m\hbar^2\beta}\right], \tag{3.24}$$

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 oscilator.

(a) Calculate $\rho^u(x, x'; \beta)$ from the path-integral analysis, by finding $x_{\rm cl}(\tau)$ and the corresponding $S_E\big[x_{\rm cl}(\tau)\big] = S_{\rm cl}(x, x', \beta\hbar)$, 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

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

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

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

where

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

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

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

□

(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

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

But the trace of ρ^u is also Z

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

Thus,

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

□

(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,

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

□

(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,

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

□

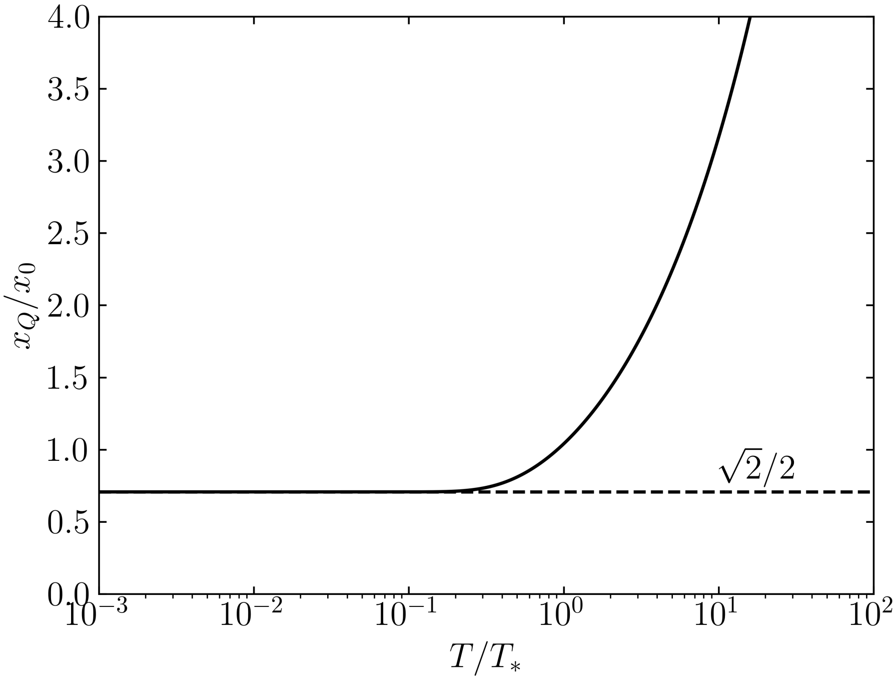
(e) Study high- and low-temperature limits of $x_Q(T)$, and make arguments for the resulting limiting forms, by thinking about the purely classical and purely quantum limits of the harmonic oscillator.

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

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

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 $\left\langle x^2 \right\rangle = x_0^2 \left\langle e^{i\omega_0 t} \right\rangle = x_0^2/2$. 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 $x_Q \to \infty$. □

***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

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

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 $\hat{\rho}_{AB} = \sum_{s,s'=1}^{4} \rho_{ss'} |s\rangle\langle s'| = \sum_{\sigma,\sigma'=0,1} \rho_{ss'} |\sigma_A\rangle \otimes |\sigma_B\rangle \langle\sigma'_A| \otimes \langle\sigma'_B|$.

(i) Verify that this is indeed a density matrix for a pure state by showing $\mathrm{Tr}[\hat{\rho}_{AB}] = \mathrm{Tr}\big[\hat{\rho}^2_{AB}\big] = 1$. *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,

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

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

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

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

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

$$S_{vN} = -\langle \ln \hat{\rho}_{AB}\rangle = -\mathrm{Tr}\left(\hat{\rho}_{AB} \ln \hat{\rho}_{AB}\right) = 0, \tag{5.4}$$

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 $\det\left(\hat{\rho}_{AB} - \sigma\mathbb{1}\right) = \sigma^4 - \sigma^3 = \sigma^3(\sigma - 1)$, which are 0 and 1. Thus indeed,

$$S_{vN} = -\mathrm{Tr}\left[\hat{\rho}_{AB} \ln \hat{\rho}_{AB}\right] = -\sum_{\sigma=0,1} \sigma \ln \sigma = 0. \tag{5.5}$$

□

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

$$\hat{\rho}_A = \mathrm{Tr}\, \hat{\rho}_{AB} = \sum_{\sigma_B} \langle \sigma_B | \hat{\rho}_{AB} | \sigma_B \rangle \,, \tag{5.6}$$

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

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

Thus,

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

□

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

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.,

$$S_E = -\left\langle \ln \hat{\rho}_A \right\rangle_A = -\,\mathrm{Tr}\left(\hat{\rho}_A \ln \hat{\rho}_A \right) = 0, \tag{5.9}$$

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 $\det\left(\hat{\rho}_A - \sigma_A \mathbb{1}\right) = \lambda(\lambda - 1)$, which are still 0 and 1. Thus, $S_E = -\sum_{\sigma_A = 0,1} \sigma_A \ln \sigma_A = 0$. □

(b) *entangled* "cat" state

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

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 $\hat{\rho}_{AB} = \sum_{s,s'=1}^{4} \rho_{ss'} \,|s\rangle \langle s'| = \sum_{\sigma,\sigma'=0,1} \rho_{ss'} \,|\sigma_A\rangle \otimes |\sigma_B\rangle \left\langle \sigma'_A \right| \otimes \left\langle \sigma'_B \right|$.

(i) Verify that this is indeed a density matrix for a pure state by showing $\mathrm{Tr}[\hat{\rho}_{AB}] = \mathrm{Tr}\left[\hat{\rho}_{AB}^2\right] = 1$. *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

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

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

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

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

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

$$S_{vN} = -\langle \ln \hat{\rho}_{AB}\rangle = -\,\mathrm{Tr}\left(\hat{\rho}_{AB} \ln \hat{\rho}_{AB}\right) = 0, \tag{5.13}$$

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 $\hat{\rho}^2_{AB} - \hat{\rho}_{AB} = 0$, $\sigma^2 - \sigma = 0$ 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, $S_{vN} = 0$. □

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

$$\hat{\rho}_A = \mathrm{Tr}_B\, \hat{\rho}_{AB} = \sum_{\sigma_B} \langle \sigma_B | \hat{\rho}_{AB} | \sigma_B \rangle\,, \tag{5.14}$$

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, $\hat{\rho}_A = \frac{1}{2}\mathbb{1}$. □

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

Solution.

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

(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.

$$S_E = -\langle \ln \hat{\rho}_A \rangle_A = -\operatorname{Tr}_A \left(\hat{\rho}_A \ln \hat{\rho}_A \right) = \ln 2, \tag{5.15}$$

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. $\square$