# Homework 4: Phys 7230 (Spring 2022)

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

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

where $H_{\rm tr}$ 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.*

□

(b) Show that the variational inequality (1.2) is equivalent to $F \leq F_{\rm v} = \langle \mathcal{H} \rangle_{\rm tr} - TS_{\rm tr}$, where $S_{\rm tr}$ is the Shannon's entropy for the probability distribution $P = Z_{\rm tr}^{-1} e^{-\beta \mathcal{H}_{\rm tr}}$, with an extra factor of $k_B$ to make units consistent with our thermodynamics.

*Solution.*

□

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

$$\mathcal{H} = \frac{p^2}{2m} + \alpha(1 - \cos x), \tag{1.3}$$

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 $\mathcal{H}_{\rm tr} = (1/2)kx^2$ 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 $\alpha/k_BT$, namely that the thermodynamics (free energy, etc) has two distinct phases, corresponding to high and low $\alpha/k_BT$. 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 ($d > 1$) object, e.g., a fluctuating membrane trapped in a periodic potential.

***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.*

□

(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

$$P\big[\mathbf{R}(s)\big] = \left(\frac{d}{2\pi b_0^2}\right)^{dN/2} \exp\left[-\frac{d}{2b_0^2}\int_0^N ds \left(\frac{\partial \mathbf{R}}{\partial s}\right)^2\right], \tag{2.3}$$

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

$$\mathcal{H} = \frac{\sigma}{2}\int_0^N ds \left(\frac{\partial \mathbf{R}}{\partial s}\right)^2, \tag{2.4}$$

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,

$$p(\mathbf{r}_n) = \left(\frac{d}{2\pi b_0^2}\right)^{d/2} \exp\left[-\frac{d}{2b_0^2}(\mathbf{R}_n - \mathbf{R}_{n-1})^2\right], \tag{2.5}$$

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.

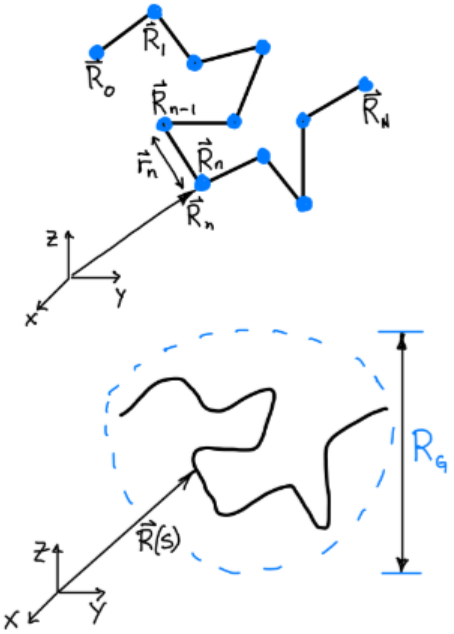


Figure 1: Edward's "phantom" polymer model executing an ideal random walk in $d$-dimensional space, characterized by $N+1$ monomer positions, $\mathbf{R}_n$.

*Solution.*

□

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

$$R_g^2 = \left\langle (\mathbf{R}_N - \mathbf{R}_0)^2 \right\rangle , \tag{2.6}$$

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.*

□

***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

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

formulations, as well as the "imaginary-time" Schrödinger-like equation in $\beta$

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

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" $\beta$) 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.*

□

(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.*

□

(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

$$x(\tau) = x_{\rm cl}(\tau) + y(\tau), \tag{3.4}$$

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

$$\left.\frac{\delta S_E\big[x(\tau)\big]}{\delta x(\tau)}\right|_{x_{\rm cl}(\tau)} = 0, \tag{3.5}$$

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

- Inserting Eq. (3.4) into the action in Eq. (3.2) and expanding to lowest nontrivial order in $y(\tau)$ we find

$$\rho^u(x,x';\beta) \approx e^{-S_E\left[x_{\rm cl}(\tau)\right]/\hbar} \int_{y(0)=y(\beta\hbar)=0} \big[dy(\tau)\big] \exp\left[-\frac{1}{2\hbar}\int_0^{\beta\hbar} d\tau y(\tau) S_E''[x_{\rm cl}] y(\tau)\right], \tag{3.6}$$

where first functional derivative term is absent because it vanishes by virtue of the equation of motion Eq. (3.5) satisfied by $x_{\rm cl}(\tau)$.

- The key observation in Eq. (3.6) 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.*

□

(d) For a free particle, solve the (Euclidean) classical Euler-Lagrange equation of motion Eq. (3.5) for $x(\tau, x, x')$ with initial conditions $x_{\rm cl}(0) = x, x_{\rm cl}(\beta\hbar) = x'$, and evaluate

$$S_E\big[x_{\rm cl}(\tau)\big] \equiv S_{\rm cl}(x,x',\beta\hbar), \tag{3.7}$$

thereby obtaining

$$\rho^u(x,x';\beta) = \mathcal{N}(\beta\hbar) e^{-S_{\rm cl}(x,x',\beta\hbar)/\hbar}. \tag{3.8}$$

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

*Solution.*

□

(e) As a non-required bonus, you can determine the prefactor $\mathcal{N}(\beta\hbar)$, by discretizing the path integral in (3.6) 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, (**??**) is satisfied.

Alternatively,you can determine $\mathcal{N}(\tau)$ by requiring that (3.8) 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.

***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 (3.8), up to a prefactor $\mathcal{N}(\beta\hbar)$.

*Solution.*

□

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

*Solution.*

□

(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.*

□

(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.*

□

(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.

***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 $(4 \times 4)$ 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.*

□

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

$$S_{vN} = -\langle \ln \hat{\rho}_{AB} \rangle = -\,\mathrm{Tr}\,(\hat{\rho}_{AB} \ln \hat{\rho}_{AB}) = 0, \tag{5.2}$$

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.*

□

(iii) Compute the reduced $(2 \times 2)$ density matrix

$$\hat{\rho}_A = \mathrm{Tr}\,\hat{\rho}_{AB} = \sum_{\sigma_B} \langle\sigma_B|\hat{\rho}_{AB}|\sigma_B\rangle\,, \tag{5.3}$$

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

*Solution.*

□

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

*Solution.*

□

(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.,

$$S_E = -\left\langle \ln \hat{\rho}_A \right\rangle_A = -\operatorname{Tr}\left(\hat{\rho}_A \ln \hat{\rho}_A\right) = 0, \tag{5.4}$$

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

*Solution.*

□

(b) *entangled* "cat" state

$$\langle \psi_{AB}| = \frac{1}{\sqrt{2}}\big(|0\rangle \otimes |0\rangle + |1\rangle \otimes |1\rangle\big). \tag{5.5}$$

Construct the two-qubit density matrix $\hat{\rho}_{AB} = |\psi_{AB}\rangle \langle \psi_{AB}|$ for the whole system and extract its corresponding $(4 \times 4)$ 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 $\operatorname{Tr}[\hat{\rho}_{AB}] = \operatorname{Tr}\left[\hat{\rho}_{AB}^2\right] = 1$. *Hint*: You can do this by working directly with the matrix $\rho_{\sigma\sigma'}$ or more formally working in a representation-independent way.

*Solution.*

□

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

$$S_{vN} = -\left\langle \ln \hat{\rho}_{AB} \right\rangle = -\operatorname{Tr}\left(\hat{\rho}_{AB} \ln \hat{\rho}_{AB}\right) = 0, \tag{5.6}$$

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.*

□

(iii) Compute the reduced density $(2 \times 2)$ matrix

$$\hat{\rho}_A = \operatorname{Tr}_B \hat{\rho}_{AB} = \sum_{\sigma_B} \langle \sigma_B | \hat{\rho}_{AB} | \sigma_B \rangle, \tag{5.7}$$

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

*Solution.*

□

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

*Solution.*

□

(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.

$$S_E = -\left\langle \ln \hat{\rho}_A \right\rangle_A = -\operatorname{Tr}_A \left( \hat{\rho}_A \ln \hat{\rho}_A \right) = \ln 2, \tag{5.8}$$

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