Advanced Quantum Mechanics

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Lecture #21

Path Integrals and QM

Recap of Last Class

- Quadratic Lagrangians: Separation classical and quantum contribution

$$U(x_f,t_f;x_i,t_i) = e^{iS_{cl}(x_i,t_i;x_f,t_f)}A(t_f,t_i)\int_{y(t_i)=y(t_f)=0}\mathcal{D}[y(t)]e^{i\int_{t_i}^{t_f}\frac{1}{2}m\dot{y}^2 - V_2 y^2}$$

$$= e^{iS_{cl}(x_i,t_i;x_f,t_f)}A^{'}(t_f,t_i)$$

- Evaluation of the classical action for free particle and Harmonic Oscillator

- Evaluation of quantum fluctuation contribution for free particle and Harmonic Oscillator

- Matrix element of time-ordered operators ⟶ Sources and Generating Functionals

- Variation with respect to paths ⟶ Ehrenfest Theorem and Schrodinger Equation

A Brief Detour : Quantum Statistical Mechanics

A quantum system weakly interacting with a "heat bath", i.e. a very large system with which the system under consideration can exchange energy.

The exchange of energy does not change the properties of the "bath".

The coupling to the bath is weak so that it does not change the spectrum of the system.

Interested in long time, time averaged behaviour of the system ⟶ equilibrium in the canonical ensemble with a temperature T determined by temp. of the bath.

Probability of the system being found in an energy eigenstate:

$$P(n) = \frac{e^{-\beta E_n}}{Z}$$

Partition Function:

$$Z = \sum_n e^{-\beta E_n} = Tr\ e^{-\beta \hat{H}}$$

Free Energy :

$$Z = e^{-\beta F} \qquad F = -\frac{1}{\beta} \ln Z$$

Can obtain all thermodynamic properties from the Free energy / Partition Fn.

Eqbm Stat Mech : Calculate the partition function from microscopic Hamiltonian

Path Integrals and Partition function

Partition Function $$Z = Tr\ e^{-\beta \hat{H}} = \int dx \langle x | e^{-\beta \hat{H}} | x \rangle$$

Remember: $$U(x_f, t_f; x_i, t_i) = \langle x_f | e^{-i(t_f - t_i)\hat{H}} | x_i \rangle$$

If we take take $t_f - t_i \longrightarrow -i\beta$, and $x_f = x_i$, we should recover the matrix element required in the calculation of Z. We need an additional integral over the x co-ord.

Now: $$U(x_f, t_f; x_i, t_i) = \left(\frac{mN}{2\pi i (t_f - t_i)} \right)^{1/2} \int \mathcal{D}[x(t)] e^{iS[x(t)]}$$

$$S[x(t)] = \int_{t_i}^{t_f} dt \left[\frac{1}{2} m \dot{x}^2(t) - V(x(t)) \right] = \int_{t_i}^{t_f} dt \mathcal{L}[x(t), \dot{x}(t)]$$

What does this look like when we make the substitution $t_f - t_i \longrightarrow -i\beta$?

We need to look at path integral formulation in imaginary time $\tau = it$

Path Integrals in Imaginary Time

Start with the more general expression

$$U(x_f, \tau_f; x_i, \tau_i) = \langle x_f | e^{-(\tau_f - \tau_i)\hat{H}} | x_i \rangle$$

where $\tau_f - \tau_i$ will be identified with β at the end.

Let us follow the steps we took in deriving the path integral in real time

1) Break up into products of evolution over infinitesimal imaginary time intervals

$$U(x_f, \tau_f; x_i, \tau_i) = \langle x_f | \hat{U}[\tau_f, \tau_i + (N-1)\epsilon] \hat{U}[\tau_i + (N-1)\epsilon, \tau_i + (N-2)\epsilon] ... \hat{U}[\tau_i + 2\epsilon, \tau_i + \epsilon] \hat{U}[\tau_i + \epsilon, \tau_i] | x_i \rangle$$

2) Introduce resolution of identity at each step

$$= \int dx_1 \int dx_2 .. \int dx_{N-1} \langle x_f | \hat{U}[\tau_f, \tau_i + (N-1)\epsilon] | x_{N-1} \rangle \langle x_{N-1} | \hat{U}[\tau_i + (N-1)\epsilon, \tau_i + (N-2)\epsilon] | x_{N-2} \rangle \langle x_{N-2} | ...$$

$$... | x_2 \rangle \langle x_2 | \hat{U}[\tau_i + 2\epsilon, \tau_i + \epsilon] | x_1 \rangle \langle x_1 | \hat{U}[\tau_i + \epsilon, \tau_i] | x_i \rangle$$

Infinitesimal Evolution in Imaginary Time

$$\langle x_{k+1}|e^{-\hat{H}(\hat{p},\hat{x})\epsilon}|x_k\rangle = \int dp_{k+1}\langle x_{k+1}|p_{k+1}\rangle\langle p_{k+1}|e^{-\hat{H}(\hat{p},\hat{x})\epsilon}|x_k\rangle \; \frac{1}{2\pi}$$

$$= \int dp_{k+1}e^{ip_{k+1}\cdot x_{k+1}}\langle p_{k+1}|e^{-\hat{H}(\hat{p},\hat{x})\epsilon}|x_k\rangle \; \frac{1}{2\pi}$$

$$= \int dp_{k+1}e^{ip_{k+1}\cdot x_{k+1}}\langle p_{k+1}| : e^{-\hat{H}(\hat{p},\hat{x})\epsilon} : |x_k\rangle \; \frac{1}{2\pi}$$

$$= \int dp_{k+1}e^{ip_{k+1}\cdot x_{k+1}}e^{-H(p_{k+1},x_k)\epsilon}\langle p_{k+1}|x_k\rangle\frac{1}{2\pi}$$

$$= \int dp_{k+1}e^{ip_{k+1}\cdot(x_{k+1}-x_k)}e^{-H(p_{k+1},x_k)\epsilon}\frac{1}{2\pi}$$

The momentum integral is a Gaussian integral

$$\int dp_{k+1}e^{-\frac{\epsilon}{2m}\left[p^2-ip_{k+1}\cdot\frac{2m(x_{k+1}-x_k)}{\epsilon}\right]}\frac{1}{2\pi}$$

$$= \left(\frac{m}{2\pi\epsilon}\right)^{1/2} e^{-\frac{m}{2}\frac{(x_{k+1}-x_k)^2}{\epsilon}}$$

Path Integral in Imaginary Time

$$U(x_f,\tau_f;x_i,\tau_i) = \left(\frac{m}{2\pi\epsilon}\right)^{N/2} \int dx_1 \int dx_2 .. \int dx_{N-1} e^{-\epsilon \sum_{k=0}^{N-1}\left[\frac{m}{2}\frac{(x_{k+1}-x_k)^2}{\epsilon^2} + V(x_k)\right]}$$

Take continuum limit ⟶ paths in imaginary time

$$U(x_f,\tau_f;x_i,\tau_i) = \left(\frac{m}{2\pi\epsilon}\right)^{1/2} \int \mathcal{D}[x(\tau)] e^{-S_E[x(\tau)]} \qquad S_E[x(\tau)] = \int_{\tau_i}^{\tau_f} d\tau \frac{m}{2}\left(\frac{dx(\tau)}{d\tau}\right)^2 + V[x(\tau)]$$

Note that we could have obtained it by the substitution τ = it in

$$U(x_f,t_f;x_i,t_i) = \left(\frac{mN}{2\pi i(t_f - t_i)}\right)^{1/2} \int \mathcal{D}[x(t)] e^{iS[x(t)]}$$

$$S[x(t)] = \int_{t_i}^{t_f} dt \left[\frac{1}{2} m\dot{x}^2(t) - V(x(t))\right] = \int_{t_i}^{t_f} dt \mathcal{L}[x(t),\dot{x}(t)]$$

i ∫ dt ⟶ ∫ dτ

The substitution changes the sign of the time derivative term in the Lagrangian.

Statistical Mechanics and path integrals

$$Z = \int dx U(x, \beta; x, 0)$$

$$U(x_f, \tau_f; x_i, \tau_i) = \left(\frac{m}{2\pi\epsilon}\right)^{1/2} \int \mathcal{D}[x(\tau)] e^{-S_E[x(\tau)]} \qquad S_E[x(\tau)] = \int_{\tau_i}^{\tau_f} d\tau \frac{m}{2}\left(\frac{dx(\tau)}{d\tau}\right)^2 + V[x(\tau)]$$

The partition function is a path integral over all β-periodic paths in imaginary time, with each path contributing exp(-S_E), where S_E is the Classical Euclidean Action (i.e. in imaginary time).

Quadratic Lagrangians and Classical-Quantum Separation

We can follow the same steps as we took for real time path-integrals to show that

For Quadratic Lagrangians, the path integral separates into a classical and quantum contribution

$$U(x_f, \tau_f; x_i, \tau_i) = e^{-S_E^{cl}(x_f, \tau_f; x_i, \tau_i)} A'(\tau_f, \tau_i)$$

The "Classical" path is the one satisfying the Euler Lagrange Equations in imaginary time

$$m\frac{d^2x}{d\tau^2} = \frac{\partial V}{\partial x}$$

and the quantum contribution

$$A'(\tau_f, \tau_i) = \left(\frac{m}{2\pi\epsilon}\right)^{1/2} \int_{y(\tau_i)=y(\tau_f)=0} \mathcal{D}[y(\tau)] e^{-\int_{\tau_i}^{\tau_f} d\tau \frac{1}{2}m\dot{y}^2 + V_2 y^2}$$

Partition Fn. for free particle and H.O.

Since we have obtained the dictionary to go back and forth between real and imaginary time, we can use the real time propagators already calculated to get this.

Free Particle: $$U(x_f, t_f; x_i, t_i) = \left(\frac{m}{2\pi i(t_f - t_i)}\right)^{1/2} e^{i\frac{m}{2}\frac{(x_f - x_i)^2}{(t_f - t_i)}}$$

The dictionary: $i\,(t_f - t_i) \longrightarrow \beta = 1/T$, $x_f = x_i = x$, Integrate over x

$$Z = \left(\frac{mT}{2\pi}\right)^{1/2} \int dx = \Omega \left(\frac{mT}{2\pi}\right)^{1/2}$$

Harmonic Oscillator: $$U(x_f, t_f; x_i, t_i) = \left(\frac{m\omega_0}{2\pi i \sin[\omega_0(t_f - t_i)]}\right)^{1/2} e^{i\frac{m\omega_0}{2\sin[\omega_0(t_f - t_i)]}[(x_f^2 + x_i^2)\cos\omega_0(t_f - t_i) - 2x_i x_f]}$$

$$\sin[\omega_0(t_f - t_i)] \to -i\sinh[\beta\omega_0] \qquad \cos[\omega_0(t_f - t_i)] \to \cosh[\beta\omega_0]$$

$$Z = \left(\frac{m\omega_0}{2\pi\sinh[\beta\omega_0]}\right)^{1/2} \int dx e^{-\frac{m\omega_0 x^2}{\sinh[\beta\omega_0]}(\cosh[\beta\omega_0] - 1)} = \left(\frac{m\omega_0}{2\pi\sinh[\beta\omega_0]}\right)^{1/2} \int dx e^{-m\omega_0\tanh[\beta\omega_0/2]x^2}$$

$$= \left(\frac{m\omega_0}{2\pi\sinh[\beta\omega_0]}\right)^{1/2} \left(\frac{2\pi}{2m\omega_0\tanh[\beta\omega_0/2]}\right)^{1/2} = \frac{1}{2\sinh[\beta\omega_0/2]}$$

Density Matrix and Thermal Averages

The thermal average of an observable A $A_{th} = \frac{1}{Z}\sum_n \langle n|\hat{A}|n\rangle e^{-\beta E_n} = \frac{1}{Z} Tr\ \hat{A}e^{-\beta \hat{H}} = Tr\ \hat{A}\hat{\rho}$

$\hat{\rho} = \frac{e^{-\beta\hat{H}}}{Z}$ is the density operator and $\rho(x,x') = \langle x|\hat{\rho}|x'\rangle$ is called the density matrix

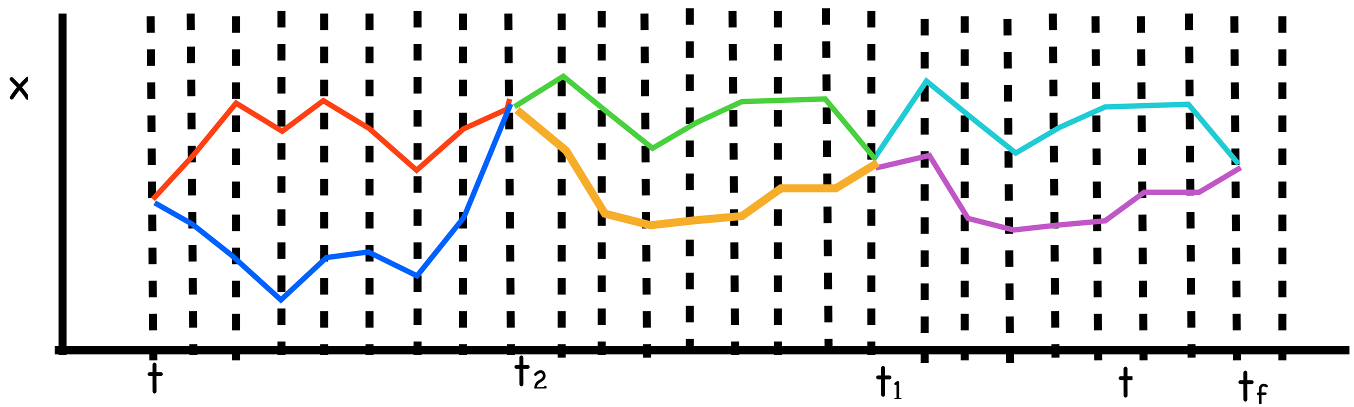
$$\rho(x,x') = \frac{\int_{x_0=x'}^{x_\beta=x} \mathcal{D}'[x(\tau)]e^{-S_E[x(\tau)]}}{\int_{x_0=x}^{x_\beta=x} \mathcal{D}[x(\tau)]e^{-S_E[x(\tau)]}}$$

' indicates that the numerator does not have the additional integral over x which Z has

Define Heisenberg operators in imaginary time $x(\tau) = e^{\tau H}\ x\ e^{-\tau H}$

Thermal Average of (Imaginary) Time ordered products of x can be written in the usual way

$$\langle T[x(\tau_1)x(\tau_2)..x(\tau_n)]\rangle_{th} = \frac{\int_{x_0=x}^{x_\beta=x} \mathcal{D}[x(\tau)]x(\tau_1)x(\tau_2)..x(\tau_n)e^{-S_E[x(\tau)]}}{\int_{x_0=x}^{x_\beta=x} \mathcal{D}[x(\tau)]e^{-S_E[x(\tau)]}}$$



What about QM and real time ?

$$\langle x_f|T[x(t_1)x(t_2)..x(t_n)]|x_i\rangle = \int \mathcal{D}[x(t)]x(t_1)x(t_2)..x(t_n)e^{iS[x(t)]}$$

$$\langle T[x(\tau_1)x(\tau_2)..x(\tau_n)]\rangle_{th} = \frac{\int_{x_0=x}^{x_\beta=x} \mathcal{D}[x(\tau)]x(\tau_1)x(\tau_2)..x(\tau_n)e^{-S_E[x(\tau)]}}{\int_{x_0=x}^{x_\beta=x} \mathcal{D}[x(\tau)]e^{-S_E[x(\tau)]}}$$

$$Z\langle T[x(\tau_1)x(\tau_2)..x(\tau_n)]\rangle_{th} = \int_{x_0=x}^{x_\beta=x} \mathcal{D}[x(\tau)]x(\tau_1)x(\tau_2)..x(\tau_n)e^{-S_E[x(\tau)]}$$

Other than the constant multiplicative factor Z , and the additional x integral, this looks like what we want to calculate if we can analytically continue back to real time.

$$Z\langle x_f|T[x(\tau_1)x(\tau_2)..x(\tau_n)]|x_i\rangle_{th} = \int_{x_0=x_i}^{x_\beta=x_f} \mathcal{D}[x(\tau)]x(\tau_1)x(\tau_2)..x(\tau_n)e^{-S_E[x(\tau)]} = F(\tau_1,\tau_2,..\tau_n,\beta)$$

$$\langle x_f|T[x(t_1)x(t_2)..x(t_n)]|x_i\rangle = F[\tau_1 \to -it_1, \tau_2 \to -it_2, ..\tau_n \to -it_n, \beta \to -i(t_f - t_i)]$$

We will soon see that calculating expectations in imaginary time is easier, and hence we often work in imaginary time formalism (e.g. to develop pert. theory) and analytically continue to real time if needed.

A Detour : Probability Distributions, Expectations, Moments

Consider a continuous real random variable X

The probability that X lies between the values x and x+dx is given by P(x) dx

The function P(x) is called the probability distribution function of X.

The avg. value of a random variable (expectation value) is given by $\bar{X} = \int xP(x)dx$

The expectation of a function F[X] of the random variable is given by $\bar{F[X]} = \int f(x)P(x)dx$

The expectation of +ve powers of the random variable are called its moments (1st moment is avg.)

$\bar{X^n} = \int x^n P(x)dx$ is called the n^{th} moment of the distribution

Moment Generating Function:
$$F[\alpha] = \bar{e^{\alpha X}} = \int e^{\alpha x} P(x)dx = 1 + \sum_n \frac{\alpha^n}{n!}\bar{X^n}$$

$$\bar{X^n} = \left.\frac{\partial^n F[\alpha]}{\partial \alpha^n}\right|_{\alpha=0}$$

A Detour : Cumulants and Cumulant Generating Functions

The cumulant generating function is defined as the logarithm of the moment generating fn.

$$G[\alpha] = \ln F[\alpha]$$

Cumulants are defined from the expansion of G

$$G[\alpha] = \sum_n \kappa_n \frac{\alpha^n}{n!}$$

Cumulants are related to moments through the recursion formula

$$\kappa_n = \mu_n - \sum_{m=1}^{n-1} {}^{n-1}C_{m-1} \kappa_m \mu_{n-m}$$

First Few Cumulants :

$$\kappa_1 = \mu_1 = \bar{X}$$

$$\kappa_2 = \mu_2 - \kappa_1^2 = \bar{X^2} - (\bar{X})^2$$

$$\kappa_3 = \mu_3 - 3\kappa_2\kappa_1 - \kappa_1^3$$

Gaussian Distribution : Moments and Cumulants

$$P(x) = \frac{1}{\sqrt{2\pi\sigma}} e^{-\frac{(x-\mu)^2}{2\sigma^2}}$$

Moment Generating Function:

$$F[\alpha] = \int_{-\infty}^{\infty} e^{\alpha x} P(x) dx = \frac{1}{\sqrt{2\pi\sigma}} \int_{-\infty}^{\infty} e^{\alpha x} e^{-\frac{(x-\mu)^2}{2\sigma^2}}$$

$$F[\alpha] = e^{\mu\alpha + \frac{1}{2}\alpha^2\sigma^2}$$

Cumulant Generating Function: $$G[\alpha] = \mu\alpha + \frac{1}{2}\alpha^2\sigma^2$$

It is evident that all cumulants beyond n=2 vanishes in this case.