10/12/09

Functional Integral Formulation

- We turn to functional integrals for many-body systems for several reasons: to generate a perturbation series in the interaction, to construct non-perturbative approximations, and to be able to do full numerical simulations of the system.

We'll start by constructing the path integral for the familiar case of a quantum mechanical particle and then generalize to many particles.
- we will not discuss these in great detail, although we will look at how to do numerical simulations
- instead we will move on to the field theory representation, which will look like a generalization of our model partition function.

- Usually texts start in "real time" and then later connect to the mathematically better defined "imaginary time, (also called "Euclidean")
  - We will do the opposite: start with partition functions (which means the equivalent of imaginary time) and then consider the real time version after.
  - We note that simulations require the Euclidean formulation.

- So we start with a quantum mechanical particle with Hamiltonian $\hat{H}(\hat{p},\hat{q})$, where these can be generalized momentum and space coordinates.
  - The most familiar version is a single particle in a potential:

$$\boxed{\hat{H}(\hat{p},\hat{q}) = \frac{\hat{p}^2}{2m} + V(\hat{q})}$$

where we have in mind $\hat{q} \to \hat{x}$ usually.

- Note: there's no need to get metaphysical about what imaginary time means; it is sufficient to consider it a useful trick to extract physical observables.

10/12/89

So start with the partition function $Z = \mathrm{Tr}\, e^{-\beta\hat{H}}$, which we can evaluate in any basis. Let's choose the coordinate basis, so

$$\boxed{Z = \mathrm{Tr}\, e^{-\beta\hat{H}} = \int dx \, \langle x | e^{-\beta\hat{H}} | x \rangle}$$

where we'll consider $\hat{H}(\hat{p},\hat{x}) = \frac{\hat{p}^2}{2m} + V(\hat{x})$.

- From our discussions of evaluating $\mathrm{Tr}\, e^{-\beta\hat{H}} = \mathrm{Tr}\, e^{-\beta(\hat{T}+\hat{V})}$ where $\hat{T}$ and $\hat{V}$ do not commute (as $\frac{\hat{p}^2}{2m}$ and $V(\hat{x})$ do not commute), we have in mind breaking up $e^{-\beta\hat{H}}$ into small pieces.

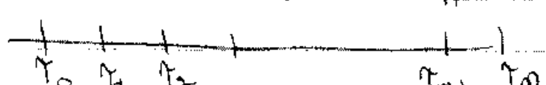
- Then it is natural to consider the Euclidean evolution operator U_E:

$$\boxed{U_E(x_f\tau_f, x_i\tau_i) = \langle x_f | e^{-(\tau_f-\tau_i)\hat{H}/\hbar} | x_i \rangle}$$

so that Z is just a sum with $x_i = x_f$ (diagonal) and $\tau_f - \tau_i = \beta\hbar$. [Note: We'll use units in which $\hbar = 1$ but sometimes the $\hbar$'s will be explicit and sometimes not. Sorry!]

- We break up $\tau_i = 0$ to $\tau_f = \beta$ (or $-\beta/2$ to $+\beta/2$) in small enough intervals $\Delta\tau = \epsilon$ so that $e^{-\epsilon(\hat{T}+\hat{V})} \doteq e^{-\epsilon\hat{T}} e^{-\epsilon\hat{V}}$ is a sufficiently accurate approximation.
  - So take M equal steps with $\beta = M\epsilon = \tau_f - \tau_i$ (we'll keep τ_i and τ_f for generality — this will make it easy to connect to real time).

- Label the "times" in between as τ_n:



so that $\boxed{\tau_0 \equiv \tau_i}$ and $\boxed{\tau_M \equiv \tau_f}$

and $\boxed{\tau_n = \tau_0 + n\epsilon \qquad n = 0, 1, \ldots, M.}$

10/12/09

For convenience, let $\boxed{X_0 \equiv X_i}$ and $\boxed{X_M \equiv X_f}$

So into $e^{-\hat{H}(\tau_f - \tau_i)} = (e^{-\epsilon \hat{H}})^M$, insert $\int dx_i |x_i\rangle\langle x_i| = 1$ in between each $e^{-\epsilon\hat{H}} \underset{\text{insert here}}{\wedge} e^{-\epsilon\hat{H}}$ term

[Note that $|x\rangle$ can stand for $|\vec{x}\,\alpha\rangle$ if there is a spin index, or something more general.

$$\Rightarrow \int dx\, |x\rangle\langle x| \rightarrow \sum_\alpha \int d^3\vec{x}\, |\vec{x}\,\alpha\rangle\langle \vec{x}\,\alpha| = 1]$$

Then

$$\boxed{\begin{aligned} U_E(x_f\tau_f; x_i\tau_i) &\doteq \langle x_f|(e^{-\epsilon\hat{H}})^M|x_i\rangle \\ &= \int\left(\prod_{k=1}^{M-1} dx_k\right)\langle x_M|e^{-\epsilon\hat{H}}|x_{M-1}\rangle\langle x_{M-1}|e^{-\epsilon\hat{H}}|x_{M-2}\rangle \\ &\quad \times \cdots \langle x_{M-2}|\cdots\; e^{-\epsilon\hat{H}}|x_2\rangle\langle x_1|e^{-\epsilon\hat{H}}|x_0\rangle \end{aligned}}$$

- Now if all the $\hat{p}$'s in $e^{-\epsilon\hat{H}}$ were to the left and all of the $\hat{x}$'s to the right, then we could insert $\int |p\rangle\langle p|\, dp$ and use $\boxed{\langle p_n|\hat{H}(\hat{p},\hat{x})|x_{n-1}\rangle = H(p_n, x_{n-1})\langle p_n|x_{n-1}\rangle}$

$\Rightarrow$ normal order $e^{-\epsilon\hat{H}}$ (not just $\hat{H}$!) just a function now, not an operator

- Note that $\hat{H}_r = \frac{\hat{p}^2}{2m} + V(\hat{x})$ is in the right form, but these get mixed up in $e^{-\epsilon\hat{H}} = e^{-\epsilon(\frac{\hat{p}^2}{2m} + V(\hat{x}))} \neq e^{-\epsilon\frac{\hat{p}^2}{2m}} e^{-\epsilon V(\hat{x})}$ since $[\hat{p},\hat{x}] \neq 0$.
  - But as we've noted before, they are <u>approximately</u> equal with the error proportional to ϵ^2 $\Rightarrow$ we can make the error as small as we want.

- Note that seeing $e^{(A+B)} \doteq e^A e^B$ when $[A,B] \neq 0$ is easiest by expanding each:

e^{A+B}: $1 + (A+B) + \frac{1}{2}(A+B)^2 = 1 + (A+B) + \frac{1}{2}(A^2 + \underline{AB+BA} + B^2) + \ldots \neq (1 + A + A^2/2)(1 + B + B^2/2)$
$= 1 + (A+B) + \frac{1}{2}(A^2 + \underline{2AB} + B^2/2) + \ldots$

10/12/09

We define "normal ordering" or "normal form" on a operator $\hat{O}(\hat{p},\hat{x})$ as the result of moving all the $\hat{p}$'s to the left and all the $\hat{x}$'s to the right.

- It is designated $:\hat{O}(\hat{p},\hat{x}):$
- We will encounter other types of normal ordering (that is, with other operators) later on.

- For $\hat{H}_V(\hat{p},\hat{x}) = \frac{\hat{p}^2}{2m} + V(\hat{x}) = :\hat{H}_V(\hat{p},\hat{x}):$, (since $\hat{p}$'s are to the left!) we get

$$\boxed{:e^{-\epsilon \hat{H}(\hat{p},\hat{x})}: = \sum_{n=0}^{\infty} (-\epsilon)^n \sum_{k=0}^{n} \frac{1}{k!(n-k)!} \left(\frac{\hat{p}^2}{2m}\right)^k \left(V(\hat{x})\right)^{n-k}}$$

- You can verify by some rearrangement that this is equivalent to $e^{-\epsilon \frac{\hat{p}^2}{2m}} e^{-\epsilon V(\hat{x})}$ [expand both]

- When we say the difference is $O(\epsilon^2)$ between the original and normal-ordered exponentials we should be a bit more explicit. We mean that the $\epsilon \to 0$ limit is well behaved because when acting on a normalizable, differentiable wave function, the difference is ϵ^2 times a <u>finite</u> number.

- We can use the normal form directly in U_E:

$$\boxed{\begin{aligned}\langle x_n | :e^{-\epsilon \hat{H}(\hat{p},\hat{x})}: | x_{n-1}\rangle &= \int d^3p_n \langle x_n | p_n\rangle \langle p_n | :e^{-\epsilon \hat{H}(\hat{p},\hat{x})}: | x_{n-1}\rangle \\ &= \int \frac{d^3p_n}{(2\pi)^3} e^{ip_n(x_n - x_{n-1})} e^{-\epsilon H(p_n, x_{n-1})}\end{aligned}}$$

where the 2nd line has no operators left and $\langle x_n|p_n\rangle = \frac{1}{(2\pi)^{3/2}} e^{ip_n x_n}$, $\langle p_n | x_{n-1}\rangle = \frac{e^{-ip_n x_{n-1}}}{(2\pi)^{3/2}}$

- This works for any $\hat{H}$. Here we specialize to H_V.

10/12/09

$$\langle x_n| e^{-\epsilon\left(\frac{\hat{p}^2}{2m}+V(\hat{x})\right)}|x_{n-1}\rangle = \langle x_n| :e^{-\epsilon\left(\frac{\hat{p}^2}{2m}+V(\hat{x})\right)}: |x_{n-1}\rangle + O(\epsilon^2)$$

$$= \int \frac{d^3 p_n}{(2\pi)^3} e^{ip_n(x_n-x_{n-1})} e^{-\epsilon\frac{p_n^2}{2m}} e^{-\epsilon V(x_{n-1})} + O(\epsilon^2)$$

- Note that the p_n integral is a Gaussian, which we can do. Once again...

$$\int \frac{d^3p_n}{(2\pi)^3} e^{-\epsilon\frac{p_n^2}{2m}+ip_n(x_n-x_{n-1})} = \int \frac{d^3p_n}{(2\pi)^3} e^{-\frac{\epsilon}{2m}\left[p_n^2 - \frac{i2m}{\epsilon}p_n(x_n-x_{n-1})\right]}$$

$$= \int \frac{d^3p_n}{(2\pi)^3} e^{-\frac{\epsilon}{2m}\left(p_n - \frac{im}{\epsilon}(x_n-x_{n-1})\right)^2} e^{-\frac{\epsilon}{2m}\frac{m^2}{\epsilon^2}(x_n-x_{n-1})^2} \quad \leftarrow \text{From completing the square}$$

$$= e^{-\epsilon\frac{m}{2}\left(\frac{x_n-x_{n-1}}{\epsilon}\right)^2} \frac{1}{(2\pi)^3} \underbrace{\int d^3p'\, e^{-\frac{\epsilon}{2m}p'^2}}_{4\pi\int_0^\infty p'^2 dp'\, e^{-\frac{\epsilon}{2m}p'^2} = \left(\frac{2m\pi}{\epsilon}\right)^{3/2}} \quad \leftarrow \text{shifting integral, Jacobian} = 1$$

$$= \left(\frac{m}{2\pi\epsilon}\right)^{3/2} e^{-\epsilon\frac{m}{2}\left(\frac{x_n-x_{n-1}}{\epsilon}\right)^2}$$

- Note that the factor out front depends only on m and ϵ (and $\hbar$ if we included it explicitly). Since it doesn't have any dependence on parameters in V, we will often cancel it by dividing by a noninteracting evolution operator or partition function.

- What if we had chosen another approximation to $e^{-\epsilon\left(\frac{\hat{p}^2}{2m}+V(\hat{x})\right)}$ that was also $O(\epsilon^2)$ accurate? For example: $1-\epsilon\left(\frac{\hat{p}^2}{2m}+V(\hat{x})\right)+O(\epsilon^2)$. The problem is that the momentum integration would diverge, in contrast to the Gaussian integral.
  - There is still some freedom left because we could have placed $V(\hat{x})$ differently. On the left, we would have $V(x_n)$ instead of $V(x_{n-1})$, or we could split the difference: $\frac{1}{2}[V(x_{n-1})+V(x_n)]$. Negele and Orland Chap. 8 has a discussion of when this can make a difference.

- Note that the quantum mechanics issue of operator ordering (how to arrange the $\hat{p}$'s and $\hat{x}$'s in this case) shows up in path integrals as different ways to discretize.

10/12/09

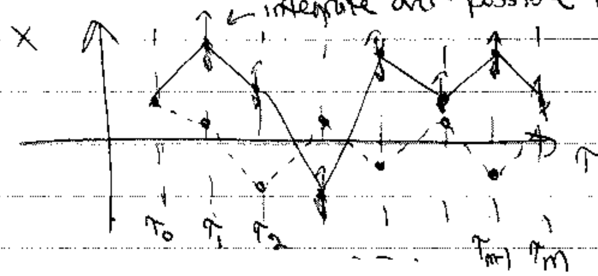
If we put together all the pieces of $U_E(x_f\tau_f; x_i\tau_i)$:

$$\boxed{U_E(x_f\tau_f; x_i\tau_i) = \lim_{M\to\infty} \int dx_1 \cdots dx_{M-1} \left(\frac{m}{2\pi\epsilon}\right)^{\frac{3M}{2}} e^{-\epsilon \sum_{k=1}^{M}\left[\frac{m}{2}\left(\frac{x_k - x_{k-1}}{\epsilon}\right)^2 + V(x_{k-1})\right]}}$$

mass

if we take the "continuum limit"

← integrate over possible intermediate x_k's.



two possible "trajectories"

- We may designate the "trajectory" $\{x_0, x_1, \ldots, x_M\}$ as $x(\tau)$, with $x(\tau_i) = x_i$ and $x(\tau_f) = x_f$ in the $M\to\infty$ limit.
  - but note that $x(\tau)$ is not continuous or differentiable in general: as $\tau_i \to \tau_{i+1}$, nothing says $x_i \to x_{i+1}$!

- We'll also write $\frac{x_k - x_{k-1}}{\epsilon} \to \frac{dx}{d\tau}$ with similar caveats.

** When there is an issue about interpreting an expression, always return to the discrete definition!
  - And M is finite for numerical simulations.

Using the "continuum" notation ($M\to\infty$), then

$$\boxed{\epsilon \sum_{k=1}^{M} \frac{m}{2}\left(\frac{x_k - x_{k-1}}{\epsilon}\right)^2 \longrightarrow \int_{\tau_i}^{\tau_f} d\tau\, \frac{m}{2}\left(\frac{dx}{d\tau}\right)^2} \qquad \boxed{\epsilon \sum_{k=1}^{M} V(x_{k-1}) \to \int_{\tau_i}^{\tau_f} d\tau\, V(x(\tau))}$$

so that:

$$\boxed{U_E(x_f\tau_f; x_i\tau_i) = \int_{(x_i\tau_i)}^{(x_f\tau_f)} \mathcal{D}[x(\tau)]\, e^{-\frac{1}{\hbar}\int_{\tau_i}^{\tau_f}\left\{\frac{m}{2}\left(\frac{dx(\tau)}{d\tau}\right)^2 + V(x(\tau))\right\}}}$$

← $\hbar$ restored!

with the $\mathcal{D}$ notation hiding the scary measure!

$$\boxed{\int_{(x_i,\tau_i)}^{(x_f\tau_f)} \mathcal{D}[x(\tau)] \equiv \lim_{M\to\infty} \int \left(\prod_{k=1}^{M-1} dx_k\right)\left(\frac{m}{2\pi\epsilon\hbar}\right)^{3M/2}}$$

10/12/19

We identify the combination

$$\boxed{S_E[x(\tau)] = \int_{\tau_i}^{\tau_f} d\tau \left[\frac{m}{2}\left(\frac{dx(\tau)}{d\tau}\right)^2 + V[x(\tau)]\right]}$$

as the Euclidean action. This is the imaginary time version of the convention action

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

is the Lagrangian.

Note the sign change, which comes from $t \to -i\tau$ (and an overall sign). All the manipulations have a real time form, which defines a path integral for the evolution operator:

$$\boxed{U(x_f t_f, x_i t_i) = \lim_{M\to\infty} \int dx_1 \cdots dx_{M-1} \left(\frac{m}{2\pi i\epsilon\hbar}\right)^{\frac{3M}{2}} e^{\frac{i}{\hbar}\epsilon \sum_{k=1}^{M}\left(\frac{m}{2}\left(\frac{x_k - x_{k-1}}{\epsilon}\right)^2 - V(x_{k-1})\right)}}$$

So we just have some i's. The interpretation is that the matrix element of U is found by summing over all "paths" that start at x_i at time t_i and end at x_f at time t_f.

- Each path is weighted by $e^{i/\hbar \cdot \text{action}}$
- As $\hbar \to 0$, a stationary phase approximation implies that neighboring paths interfere destructively unless the phase $i/\hbar\, S$ doesn't change ($\delta S = 0$)

$\Rightarrow$ This is the condition for the classical trajectory.

The "continuum" version is

$$\boxed{U(x_f t_f, x_i t_i) = \int_{(x_i t_i)}^{(x_f t_f)} \mathcal{D}[x(t)]\, e^{i/\hbar\, S[x(t)]}}$$

where $U(x_f t_f, x_i t_i) = \langle x_f | e^{-\frac{i}{\hbar}\hat{H}(t_f - t_i)} | x_i \rangle$

Recall that $i\hbar \frac{\partial}{\partial t} |\Psi(t)\rangle = \hat{H} |\Psi(t)\rangle$

$\Rightarrow |\Psi(t_f)\rangle = e^{-i/\hbar \hat{H}(t_f - t_i)} |\Psi(t_i)\rangle.$

(62)

10/12/09

We note that the Euclidean and real time versions of the evolution operator contain the same information. We can verify this by inserting a complete set of eigenstates of $\hat{H}$ $\Rightarrow$ $\hat{H}|\varphi_n\rangle = E_n|\varphi_n\rangle$ and $\langle x|\varphi_n\rangle = \varphi_n(x)$ so

$$\boxed{\begin{aligned} U(x_f t_f, x_i t_i) = \langle x_f| e^{\frac{i\hat{H}}{\hbar}(t_f-t_i)}|x_i\rangle &= \sum_n \langle x_f|\varphi_n\rangle\langle\varphi_n| e^{\frac{-i\hat{H}}{\hbar}(t_f-t_i)}|x_i\rangle \\ &= \sum_n \varphi_n(x_f)\,\varphi_n^*(x_i)\, e^{-iE_n(t_f-t_i)/\hbar} \end{aligned}}$$

$$\boxed{U_E(x_f \tau_f; x_i \tau_i) = \langle x_f| e^{\frac{\hat{H}}{\hbar}(\tau_f-\tau_i)}|x_i\rangle = \sum_n \varphi_n(x_f)\,\varphi_n^*(x_i)\, e^{-E_n(\tau_f-\tau_i)/\hbar}}$$

so either one contains the eigenvalues and eigenvectors of $\hat{H}$.

These are called "spectral representations"

- Consider U_E with $\tau_i = 0$, $\tau_f = T$ and the limit $T \to \infty$. Then the ground state φ_0 will dominate the sum and we can find E_0 by taking the $\ln$ and dividing by T.

$$\Rightarrow \boxed{E_0 = \lim_{T\to\infty}\left(-\frac{1}{T}\ln\int_{(x_i,0)}^{(x_f,T)} \mathcal{D}[x(\tau)]\, e^{-\frac{1}{\hbar}\int_0^T d\tau\left[\frac{m\dot{x}^2}{2}+V(x)\right]} + \underbrace{\lim_{T\to\infty}\frac{1}{T}\cancel{\ln \varphi_0(x_f)\varphi_0^*(x_i)}}_{0}\right)}$$

so the dependence on x_i and x_f drops out!

For the partition function, we just set $x_i = x(0) = x$, $x_f = x(\beta) = x$ and integrate ("trace") over x:

$$\boxed{\begin{aligned} Z = \mathrm{Tr}\, e^{-\beta\hat{H}} &= \int dx\, \langle x| e^{-\beta\hat{H}}|x\rangle \\ &= \int dx \int_{x(0)=x}^{x(\beta)=x} \mathcal{D}(x(\tau))\, e^{-\frac{1}{\hbar}\int_0^\beta d\tau\left(\frac{m}{2}\left(\frac{dx(\tau)}{d\tau}\right)^2 + V(x(\tau))\right)} \\ &\equiv \int_{x=x(\beta)=x(0)} \mathcal{D}[x(\tau)]\, e^{-\frac{1}{\hbar}\int_0^\beta d\tau\left[\frac{m}{2}\left(\frac{dx}{d\tau}\right)^2 + V(x(\tau))\right]} \end{aligned}}$$