11/9/16 Lecture 13 outline

- Last time: propagator: $K(\vec{x}_2,t_2;\vec{x}_1,t_1)\equiv\langle\vec{x}_2|U(t_2,t_1)|\vec{x}_1\rangle$. E.g. for free particle:

$$K_{free}=\int\frac{d^3p}{(2\pi)^3\hbar}\exp[i(\vec{p}\cdot(\vec{x}_2-\vec{x}_1)-\vec{p}^2(t_2-t_1)/2m)/\hbar]=$$

$$=\left(\frac{m}{2\pi i\hbar(t_2-t_1)}\right)^{3/2}\exp[im(\vec{x}_2-\vec{x}_1)^2/2\hbar(t_2-t_1)].$$

For the 1d SHO get

$$K_{SHO}=\sum_n u_n(x_2)u_n^*(x_1)e^{-iE_n(t_2-t_1)/\hbar}=$$

$$\sqrt{\frac{m\omega}{2\pi i\hbar\sin(\omega(t_2-t_1))}}\exp[im\omega\left((x_2^2+x_1^2)\cos\omega(t_2-t_1)-2x_2x_1\right)/2\hbar\sin(\omega(t_2-t_1))].$$

These look a bit disgusting but are actually nice: the exponentials are the expected Hamilton functions from classical mechanics, fitting with our discussion before. The fact that they are precisely the classical result, without additional quantum corrections, is special to cases where every term in the Hamiltonian is at most quadratic. In terms of the path integral, the WKB approximation is related to a saddle point approximation of integrals, and the integrals reduce to Gaussians for the case of quadratic actions, and the saddle point approximation in such special cases happens to be exact.

E.g. for a free particle we can evaluate $S[x_{cl},\dot{x}_{cl}]=\int_{t_1,x_1}^{t_2,x_2}dt\frac{1}{2}m\dot{\vec{x}}^2=\frac{1}{2}m(\vec{x}_2-\vec{x}_1)^2/(t_2-t_1)$. For a SHO, $S[x_{cl},\dot{x}_{cl}]=\int dt(\frac{1}{2}A^2m\omega^2)(\sin^2(\omega t+\phi)-\cos^2(\omega t+\phi))=\dots$ where we eliminate A and ϕ in terms of (x_1,t_1) and (x_2,t_2). Some interesting general properties of S_{cl}:

$$\frac{\partial S_{cl}}{\partial t_2}=-E,\qquad\frac{\partial S_{cl}}{\partial\vec{x}_2}=\vec{p}.$$

We will use these soon.

- Note that it follows from the above definition that

$$K(\vec{x}_3,t_3;\vec{x}_1,t_1)=\int d^3\vec{x}_2K(\vec{x}_3,t_3;\vec{x}_2,t_2)K(\vec{x}_2,t_2;\vec{x}_1,t_1),$$

$$\psi(\vec{x}_2,t_2)=\int d^3\vec{x}_1K(\vec{x}_2,t_2;\vec{x}_1,t_1)\psi(\vec{x}_1,t_1).$$

The Kernal K depends on the theory, but not the initial state condition. The wavefunction $\psi(x,t)$ depends on the initial state.

- Can show that K is a Green's function for the S.E.

$$\left(\frac{-\hbar^2}{2m}\partial_{\vec{x}_2}^2 + V(\vec{x}_2) - i\hbar\partial_{t_2}\right)K(\vec{x}_2,t_2;\vec{x}_1,t_1) = -i\hbar\delta^3(\vec{x}_2-\vec{x}_1)\delta(t_2-t_1),$$

$$K(\vec{x}_2,t;\vec{x}_1,t) = \delta^3(\vec{x}_2-\vec{x}_1)\delta(t_2-t_1), \qquad K(\vec{x}_2,t_2;\vec{x}_1,t_1) \equiv 0 \quad \text{if } t_2 < t_1.$$

- Also

$$G(t) \equiv \int d^3\vec{x} K(\vec{x},t;\vec{x},0) = \sum_E e^{-iEt/\hbar}.$$

Taking $\beta = it/\hbar$ this is like the partition function. Also, Fourier transform

$$\tilde{G}(E) = -i\int_0^\infty G(t)e^{iEt/\hbar}/\hbar = -i\int_0^\infty dt \sum_{E_a} e^{i(E-E_a)t/\hbar}/\hbar = \sum_{E_a}\frac{1}{E-E_a}.$$

- Feynman:

$$K(\vec{x}_2,t_2;\vec{x}_1,t_1) = \int [d\vec{x}(t)]e^{iS[\vec{x}(t)]/\hbar},$$

- Free particle example, take $x_0 \equiv x_i$ and $x_{N+1} \equiv x_f$.

$$K(x_f,t_f;x_i,t_i) = \left(\frac{-im}{2\pi\hbar\epsilon}\right)^{N/2}\int\prod_{i=1}^N dx_i \exp[\frac{im}{2\hbar\epsilon}\sum_{i=1}^{N+1}(x_i - x_{i-1})^2]$$

Where we take $\epsilon \to 0$ and $N \to \infty$, with $N\epsilon = T$ held fixed. Do integral in steps. Apply expression for real gaussian integral (valid: analytic continuation):

$$\int_{-\infty}^\infty d\phi \exp(ia\phi^2) = \sqrt{\frac{i\pi}{a}}.$$

where we analytically continued from the case of an ordinary gaussian integral. Think of a as being complex. Then the integral converges for $\mathrm{Im}(a) > 0$, since then it's damped.

More generally, use Gaussian integrals:

$$Z(J_i) \equiv \prod_{i=1}^N \int d\phi_i \exp(-A_{ij}\phi_i\phi_i + B_i\phi_i) = \pi^{N/2}(\det A)^{-1/2}\exp(A_{ij}^{-1}B_iB_j/4).$$

After integrating over x_1, x_2, ..., x_{n-1}, get:

$$\left(\frac{2\pi i\hbar n\epsilon}{m}\right)^{-1/2}\exp[\frac{m}{2\pi i\hbar n\epsilon}(x_n - x_0)^2].$$

So by induction the final answer for the free particle case is

$$K(x_f, t_f; x_i; t_i) = \left(\frac{2\pi i\hbar T}{m}\right)^{-1/2} \exp[im(x_b - x_a)^2/2\hbar T].$$

which agrees with the answer that we obtained (via just one dp Gaussian integral in the usual formulation of QM).

We can check that it satisfies the S.E. Note that

$$\lim_{T\to 0} \sqrt{\frac{m}{2\pi i\hbar T}} e^{imx^2/2\hbar T} = \delta(x).$$

• Comment on x_2 and t_2 dependence and connection with $\psi \sim e^{i(px-Et)/\hbar}$ for free particle example: fits with $\partial S_{cl}/\partial t_2 = -E$ and $\partial S_{cl}/\partial x_2 = p$.

• Derivation of PI from the S.E.: $\langle \vec{x}_2, t_2 | U(t_2, t_1) | \vec{x}_1, t_1 \rangle$ can be evaluated from $U \sim e^{-iHT/\hbar}$ by breaking up the $T = (t_2 - t_1)$ interval as $T = N\delta t$, taking $N \to \infty$ and $\delta t \to 0$. In each interval we insert a complete set of both $\vec{x}$ and $\vec{p}$ projectors, and use $\langle \vec{x} | \vec{p} \rangle \sim e^{i\vec{p}\cdot\vec{x}/\hbar}$:

$$\langle \vec{x} + d\vec{x}, t + dt | e^{-i\widehat{H}dt/\hbar} | \vec{x}, t \rangle = \int \frac{d^3\vec{p}}{(2\pi\hbar)^3} \langle \vec{x} + d\vec{x}, t + dt | e^{-i\widehat{H}dt/\hbar} | \vec{p} \rangle \langle \vec{p} | \vec{x}, t \rangle$$

$$= \int \frac{d^3\vec{p}}{(2\pi\hbar)^3} e^{i(-Hdt + \vec{p}\cdot d\vec{x})/\hbar} \propto e^{iLdt/\hbar},$$

where in the last step we did the Gaussian momentum integral by analytic continuation and completing the square; in the end, this gives the Legendre transformation: $\int (\vec{p}\cdot\dot{\vec{x}} - H)dt \to \int Ldt$. Note that the path integral does not involve operators, they have been replaced by the integrals over complete sets of eigenstates and eigenvalues.

• Derivation of the SE from the path integral:

$$\psi(x, t+\epsilon) = \int dy K(x, t+\epsilon; x', t)\psi(x', t)dx'$$

$$\approx \int d\eta A \exp(i\hbar^{-1}[\tfrac{1}{2}m\eta^2\epsilon^{-1} - \epsilon V(\tfrac{1}{2}(x+\eta))])\psi(x+\eta, t)$$

where $\eta \equiv x' - x$ and A is a normalization factor, that can be determined by considering the $\epsilon \to 0$ limit; this gives $A = (2\pi i\hbar\epsilon/m)$, as found above. For $\epsilon \to 0$, the oscillating exponential gives zero unless the exponent $\sim \eta^2/\epsilon$ is within one phase oscillation, so η is also small. If we take η small and expand both sides in small ϵ, we get the SE for $\psi(x,t)$ from

$$\psi(x,t) + \epsilon\frac{\partial\psi}{\partial t} \approx A \int d\eta e^{im\eta^2/2\hbar\epsilon}(1 - \frac{i\epsilon}{\hbar}V(x,t))(\psi + \eta\partial_x\psi + \tfrac{1}{2}\eta^2\partial_x^2\psi).$$

- Recall WKB: in the different regions,

$$\psi(x,t) \approx \psi(x_0)\sqrt{\frac{p(x_0)}{p(x)}}\exp(\pm\frac{i}{\hbar}\int_{x_0}^{x} p(x')dx').$$

The exponent is essentially $iS_{cl}/\hbar$, which is the saddle point approximation to $K(x,t;x_0,t_0)$ as computed from the path integral. The $1/\sqrt{p}$ comes from doing the Gaussian integral for quadratic deviations in the Taylor series expansion around the extremal value.