Physics 212b, Ken Intriligator lecture 1, Jan 8, 2018

• Briefly recap the usual description of QM: observables are replaced with operators, with classical Poisson brackets replaced with commutators, in particular $[\widehat{q}_a, \widehat{p}_b] = i\hbar\delta_{ab}$. The operators act in some Hilbert space $\mathcal{H}$, and the state of the system is a vector $|\psi\rangle \in \mathcal{H}$. Measuring an observable $\mathcal{O}$ magically (one can say better words) projects $|\psi\rangle$ on to an eigenstate $|o\rangle$ of $\widehat{\mathcal{O}}$ with probability amplitude $\langle o|\psi\rangle$, and probability $|\langle o|\psi\rangle|^2$. More generally, we can compute correlation functions and expectation values, getting amplitudes like $\mathcal{M} = \langle\chi| \prod_j \widehat{\mathcal{O}}_j|\psi\rangle$, and then probability via $|\mathcal{M}|^2$. Probability amplitudes of different options, like going through one slit or another, add, so squaring to get probabilities leads to interference effects. Time evolution is generated by a unitary operator $U(t, t_0)$ that satisfies $i\hbar\partial_t U(t, t_0) = HU(t, t_0)$; for time independent H, integrating gives $U(t, t_0) = e^{-i\widehat{H}(t-t_0)/\hbar}$; more generally, $U(t, t_0) = T\exp(-i\int_{t_0}^t \widehat{H}dt/\hbar)$. Likewise, spatial translation is generated by $U(\vec{a}) = e^{-i\vec{a}\cdot\widehat{\vec{P}}/\hbar}$, which acts as $U(\vec{a})|\vec{x}\rangle = |\vec{x} + \vec{a}\rangle$ and rotation is generated by $U(\vec{\phi}) = e^{-i\vec{\phi}\cdot\widehat{\vec{J}}/\hbar}$. In Schrodinger's picture we put the time dependence in the states, $i\hbar\partial_t|\psi(t)\rangle_S = \widehat{H}|\psi(t)\rangle_S$, whereas in Heisenberg's picture we instead put the time dependence in the operators, $\frac{d}{dt}\widehat{\mathcal{O}}^H(t) = (i\hbar)^{-1}[\widehat{\mathcal{O}}^H, \widehat{H}] + \frac{\partial}{\partial t}\widehat{\mathcal{O}}^H$.

• Let's start with a bit of a detour, which I find fascinating: Feynman's path integral description of quantum mechanics. We do not need operators in this description. Instead, we compute amplitudes by integrating over all possible paths between the initial and final states, weighted by a phase that is the path's action:

$$\mathcal{M} = \int [dq(t)] \exp(iS[q(t)]/\hbar) \prod_j \mathcal{O}_j(t_j)$$

His intuitive idea was to consider double slit interference, and then extrapolate to infinitely many tiny slits in infinitely many pretend barriers filling space.

The classical limit is recovered if $S/\hbar \gg 1$, and then the rapidly varying phase integral cancels except where the action is stationary, recovering the classical principle of least action. In classical physics, S is not a physical observable; in this description of QM it takes on some physical meaning as the path-weighting phase factor.

A nice thing about the path integral description of QM is that it generalizes immediately to quantum field theory, where we integrate over all values of the quantum fields (gauge fields, Fermion fields, Higgs field, etc, even the metric field if we're doing quantum gravity (though that's tricky)) with e.g. $S = \int d^dx\mathcal{L}$ in d space-time dimensions:

$$\mathcal{M} = \int [dA_\mu(x)][d\Psi(x)][d\Phi(x)][dg_{\mu\nu}(x)]\ldots\exp(iS/\hbar)\prod \mathcal{O}(x^\mu).$$

The integral over all paths (or field configurations) can be evaluated by taking time (or space-time) to be a lattice, and then taking the lattice mesh size to zero. Non-zero mesh size can be put on a computer: this is what e.g. Julius Kuti does to study quantum field theory.

• Define the propagator: $K(x_2,t_2;x_1,t_1) \equiv \langle x_2|U(t_2,t_1)|x_1\rangle$. Then

$$K(x_3,t_3;x_1,t_1) = \int dx_2 K(x_3,t_3;x_2,t_2)K(x_2,t_2;x_1,t_1),$$

$$\psi(x_2,t_2) = \int dx_1 K(x_2,t_2;x_1,t_1)\psi(x_1,t_1).$$

K (sometimes called the Kernal) depends on the theory, but not the initial state condition. The wavefunction $\psi(x,t)$ depends on the initial state. It follows from $i\hbar\partial_t U(t,t_0) = HU(t,t_0)$ that K is a Green's function for the S.E.

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

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

Also note that

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

This is naturally interpreted as coming from making time periodic. Taking $\beta = it/\hbar$, this is the thermal partition function. Also, the Fourier transform is nice:

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

• Consider first a free particle, and we can easily evaluate

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

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

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, $S[x_{cl},\dot{x}_{cl}] = \int dt(\frac{1}{2}A^2m\omega^2)(\sin^2(\omega t+\phi)-\cos^2(\omega t+\phi)) = \ldots$ 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}:

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

- Now let's consider Feynman's description:

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

where the integral is over all paths from the initial state to the final state and $\mathcal{N}$ is a normalization factor. This is called a functional integral. Break it up into lots of ordinary integrals on a mesh, and then take the mesh size to zero: $x_0 \equiv x_i$ and $x_{N+1} \equiv x_f$. Consider the free particle case:

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

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. and is properly normalized:

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

• 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.

A similar derivation leads to e.g.

$$\langle q_4, t_4|T\widehat{q}(t_3)\widehat{q}(t_2)|q_1, t_1\rangle = \int[dq(t)]q(t_3)q(t_2)e^{iS/\hbar},$$

where the integral is over all paths, with endpoints at (q_1, t_1) and (q_4, t_4).

The functional integral automatically accounts for time ordering: the LHS involves time ordered operators, while the RHS has a functional integral, which does not involve operators (so there is no need to worry about time ordering – it is automatic).

- 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

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

Now do the gaussian integrals and collect the $\mathcal{O}(\epsilon)$ terms to get the SE.