Physics 130C Lecture Notes
Chapter 2: The emergence of classical mechanics from quantum mechanics

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The purpose of this chapter is to think about why the world seems like it is classical, although we have every reason to believe that it is in fact quantum mechanical.

The world seems classical to us, and apparently not quantum mechanical. Similarly, it can seem like the Sun is orbiting the Earth. As in the Wittgenstein story related by Coleman, we'd like to try to ask "And how would it have looked if it had looked the other way?" In the Wittgenstein story, he is asking how it would have looked if the Earth were orbiting the Sun, which it is. Here we will ask: how would it have looked if the world were quantum mechanical, which it is. As Coleman says: "Welcome home."

We will give three classes of answer to this question. In order of increasing degree of difficulty, and increasing explanatory power, they can be called: Ehrenfest's Theorem, stationary phase, and decoherence.

2.1 Ehrenfest's Theorem

[Shankar, Chapter 6] But first, a simple way in which we can see that some of classical mechanics is correct, even in quantum mechanics, is the following. (It is actually the same manipulation we did when we studied time evolution of the density matrix of a closed system.)

Consider the time evolution of expectation values of operators in a pure state $|\psi\rangle$:

$$\partial_t \langle \mathbf{A} \rangle_\psi = \partial_t \left(\langle \psi | \mathbf{A} | \psi \rangle \right) = \left\langle \dot{\psi} \middle| \mathbf{A} | \psi \rangle + \langle \psi | \mathbf{A} \middle| \dot{\psi} \right\rangle + \langle \psi | \dot{\mathbf{A}} | \psi \rangle .$$

If operator $\mathbf{A}$ has no explicit time dependence, *i.e.* it is the same operator at all times, then we can drop the last term. Axiom 3 says:

$$\left| \dot{\psi} \right\rangle = -\frac{\mathbf{i}}{\hbar} \mathbf{H} | \psi \rangle , \quad \left\langle \dot{\psi} \right| = +\frac{\mathbf{i}}{\hbar} \langle \psi | \mathbf{H}$$

so

$$\partial_t \langle \mathbf{A} \rangle_\psi = -\frac{\mathbf{i}}{\hbar} \langle \psi | \left(\mathbf{A}\mathbf{H} - \mathbf{H}\mathbf{A} \right) | \psi \rangle = -\frac{\mathbf{i}}{\hbar} \langle [\mathbf{A}, \mathbf{H}] \rangle_\psi .$$

This is called Ehrenfest's theorem.[1]

If you have encountered Poisson brackets in classical mechanics, you will recognize the similarity of this equation with the classical evolution equation

$$\partial_t a = \{a, H\}_{PB} .$$

To make closer contact with more familiar classical mechanics, consider the case where $\mathbf{A} = \mathbf{x}$, the position operator for a 1d particle, whose Hamiltonian is

$$\mathbf{H} = \frac{\mathbf{p}^2}{2m} + V(\mathbf{x}).$$

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[1] This was not the most impressive thing that Ehrenfest did during his career as a physicist.

So:
$$\partial_t \langle \mathbf{x} \rangle = -\frac{\mathbf{i}}{\hbar} \langle [\mathbf{x}, \mathbf{H}] \rangle = -\frac{\mathbf{i}}{\hbar} \langle [\mathbf{x}, \frac{\mathbf{p}^2}{2m}] \rangle.$$

An opportunity for commutator algebra: $[\mathbf{x}, \mathbf{p}^2] = \mathbf{p}[\mathbf{x}, \mathbf{p}] + [\mathbf{x}, \mathbf{p}]\mathbf{p} = 2\mathbf{i}\hbar\mathbf{p}$. So

$$\partial_t \langle \mathbf{x} \rangle = -\frac{\mathbf{i}}{\hbar} \langle \frac{2\mathbf{i}\hbar\mathbf{p}}{2m} \rangle = +\frac{\langle \mathbf{p} \rangle}{m}. \tag{1}$$

Surely you recognize the relation $\dot{x} = p/m$ from classical mechanics. In QM it's true as a relation among expectation values.

Consider
$$\partial_t \langle \mathbf{p} \rangle = -\frac{\mathbf{i}}{\hbar} \langle [\mathbf{p}, \mathbf{H}] \rangle = -\frac{\mathbf{i}}{\hbar} \langle [\mathbf{p}, V(\mathbf{x})] \rangle$$

To find this commutator, use the position basis:

$$[\mathbf{p}, V(\mathbf{x})] = \int dx \, |x\rangle \langle x| [-\mathbf{i}\hbar\partial_x, V(x)] = -\mathbf{i}\hbar \int dx \, |x\rangle \langle x| \partial_x V(x) = -\mathbf{i}\hbar V'(\mathbf{x})$$

– unsurprisingly, $\mathbf{p}$ acts as a derivative. So

$$\partial_t \langle \mathbf{p} \rangle = -\frac{\mathbf{i}}{\hbar} \langle -\mathbf{i}\hbar V'(\mathbf{x}) \rangle = \langle -\frac{\partial \mathbf{H}}{\partial \mathbf{x}} \rangle$$

Compare this with the other Hamilton's equation of classical mechanics, $\dot{p} = -\frac{\partial H}{\partial x}$.

(Notice by the way that for more general $\mathbf{H}$, we would find

$$\partial_t \langle \mathbf{x} \rangle = \langle \partial_{\mathbf{p}} \mathbf{H} \rangle$$

instead of (1).)

Beware the following potential pitfall in interpreting Ehrenfest's theorem. Just because the average value of $\mathbf{x}$ evolves according to $\partial \langle \mathbf{p} \rangle = \langle -\partial_{\mathbf{x}} \mathbf{H} \rangle$, does not mean that it satisfies the classical equations of motion! The issue is that in general $\langle -\partial_{\mathbf{x}} \mathbf{H} \rangle$ is not linear in $\mathbf{x}$ (only for a harmonic oscillator), and

$$\langle \mathbf{x}^2 \rangle \neq \langle \mathbf{x} \rangle^2 .$$

Fluctuations about the mean values can matter!

I am skipping here some valuable remarks in Shankar pages 182-183 discussing when classical evolution is valid, and why it requires heavy particles. We'll see a bit of this in the next subsection.

2.2 Measurement, first pass

[Preskill 3.1.1[2]] Here is a simple model of how measurement happens (due to von Neumann), first in summary form and then more concretely. To measure an observable $\mathbf{M}$ of some system A, we couple it to something we can see, a "pointer." This means tensoring with the Hilbert space of the pointer $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_{\text{pointer}}$, and adding a term to the Hamiltonian which couples the observable of interest to an observable of the pointer:

$$\mathbf{H} = ... + \Delta\mathbf{H} = ... + \lambda\mathbf{M} \otimes \mathbf{P} \tag{2}$$

where the ... are the terms that were there before, and include the dynamics of the pointer system. The time evolution by this Hamiltonian then acts by a unitary operator on the whole world (system $\otimes$ pointer), and creates entanglement between the two parts – that is, it will produce a state which is a superposition of different eigenstates of the observable tensored with states of the pointer that we can distinguish from each other:

$$|\psi\rangle \sim a_1 |m_1\rangle \otimes |p_1\rangle + a_2 |m_2\rangle \otimes |p_2\rangle \ .$$

The measurement occurs when system A becomes *entangled* with the pointer. (We are going to postpone the discussion of how we see the pointer!)

To be more concrete, let's focus on an example where the pointer is the position of a particle which would be free if not for its coupling to $\mathbf{M}$.

This means the Hamiltonian for the full system is

$$\mathbf{H} = \mathbf{H}_0 + \mathbb{1} \otimes \frac{\mathbf{P}^2}{2m} + \lambda\mathbf{M} \otimes \mathbf{P}$$

where now $\mathbf{P}$ is the momentum of the pointer particle and m is its mass; we get to pick λ. You might worry that the observable $\mathbf{M}$ will change while we are trying to measure it, because of evolution by $\mathbf{H}_0$. This problem doesn't arise if either we pick an observable which is a conserved quantity $[\mathbf{M}, \mathbf{H}_0] = 0$ or if we don't take too long.

Here's why we want the pointer-particle to be heavy (large m) to use our classical intuition. We want to be able to wait for a bit and then measure the position of the particle. You'll recall that in quantum mechanics this is not trivial: we don't want it to start in a position eigenstate, because time evolution will cause it to spread out instantly (a position eigenstate is a superposition of momentum eigenstates with equal amplitude for arbitrarily-large momentum). We want to start it out in a wavepacket with some finite width Δx, which we can optimize.

In this case, its initial uncertainty in its velocity is $\sim \Delta v = \Delta p/m \sim \frac{\hbar}{m\Delta x}$; after time t its width becomes

$$\Delta x(t) \sim \Delta x + \frac{\hbar t}{m\Delta x} \ .$$

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[2]Skip the scary sections of Preskill (3.1.2-3.1.5) about generalized measurement and 'POVM's.

If the experiment will take a time t, we should minimize $\Delta x(t)$ over the initial width Δx; that gives $(\Delta x)^2 \sim \hbar t/m$, which also gives the uncertainty in the final position

$$\Delta x(t) \geq \sqrt{\frac{\hbar t}{m}} \ .$$

Consistent with your intuition, we can avoid this issue by taking a really heavy particle as our pointer.

So the only disturbance of the system caused by the coupling to this heavy particle is from the term we added (we'll ignore the $\frac{\mathbf{P}^2}{2m}$ term because the particle is heavy and we don't wait long):

$$\mathbf{H}_p \equiv \lambda \mathbf{M} \otimes \mathbf{P} \ .$$

(I will stop writing the $\otimes$ now: $\mathbf{MP} \equiv \mathbf{M} \otimes \mathbf{P}$.) The time evolution operator is

$$\mathbf{U}(t) = e^{-i\lambda t \mathbf{MP}} \ .$$

In the $\mathbf{M}$ eigenbasis $\mathbf{M} = \sum_n |m_n\rangle \langle m_n|m_n$, this is

$$\mathbf{U}(t) = \sum_n |m_n\rangle \langle m_n| e^{-i\lambda t m_n \mathbf{P}} \ .$$

But recall from Taylor's theorem that $\mathbf{P}$ generates a translation of the position of the pointer particle:

$$e^{-ix_0\mathbf{P}} \psi(x) = e^{-x_0 \partial_x} \psi(x) = \psi(x - x_0).$$

Acting on a wavepacket, this operator $e^{-ix_0\mathbf{P}}$ moves the whole thing by $-x_0$.

So: if we start the system in an arbitrary state of A, initially unentangled with the pointer, in some wavepacket $\psi(x)$:

$$|\alpha\rangle_A \otimes |\psi(x)\rangle = \sum_n \alpha_n |m_n\rangle \otimes |\psi(x)\rangle$$

then this evolves to

$$\mathbf{U}(t)\Big(\Big(\sum_n \alpha_n |m_n\rangle\Big) \otimes |\psi(x)\rangle\Big) = \sum_n \alpha_n |m_n\rangle \otimes |\psi(x - m_n \lambda t)\rangle$$

the pointer moves by an amount which depends on the value of the observable m_n! So if we can resolve the position of the particle within $\delta x < \lambda t \Delta m_n$, we can put the system in an eigenstate of $\mathbf{M}$. The probability for finding the pointer shifted by $\lambda t m_n$ is $|\alpha_n|^2$; we conclude that the initial state $|\alpha\rangle$ is found in eigenstate m_n with probability $|\langle m_n|\alpha\rangle|^2$, as we would have predicted from Axiom 4.

[End of Lecture 12]

I would like to amplify this last remark. Suppose we choose the initial wavepacket for the pointer particle to be $\psi_{\text{packet}}(x)$ as in the figure, so that its support is entirely within a 'bin', a range of x, determined by our measuring resolution (the size of the bin should be larger than $\Delta x(t)$). That is: $\psi_{\text{packet}}(x) = 0$ for x outside 'Bin 0'. Because the particle lives in the continuum, the probability of its being at any one value of x is infinitesimal : so that $|\psi_{\text{packet}}(x)|^2$ is a probability *distribution*. To get a finite probability we must integrate. The probability to find a particle in the state $\psi_{\text{packet}}(x)$ inside 'Bin 0' is
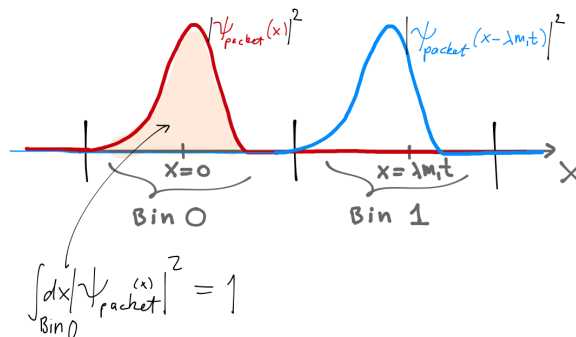
$$\int_{\text{Bin } 0} dx |\psi_{\text{packet}}(x)|^2 = 1.$$

So far we've just talked about the wavefunction of the pointer. In the initial state of the whole system,

$$|\psi_0\rangle = |\alpha\rangle \otimes |\psi_{\text{packet}}\rangle = \left(\left(\sum_n \alpha_n |m_n\rangle\right) \otimes |\psi_{\text{packet}}\rangle\right)$$

how do we determine the probability of finding the pointer particle in Bin 0? The operator we are measuring when we look for the pointer at x is $\mathbb{1}_A \otimes \mathbf{x}$ – we are not looking directly at the system, only at the pointer particle. So if the answer is x, the projector onto the outcome space is

$$\mathbb{1}_A \otimes |x\rangle\langle x|$$

and the probability density is (AS ALWAYS) the expectation value of the projector onto the outcome space:

$$\langle\psi_0| \left(\mathbb{1}_A \otimes |x\rangle\langle x|\right) |\psi_0\rangle = \langle\alpha|\alpha\rangle \cdot |\psi_{\text{packet}}(x)|^2 = |\psi_{\text{packet}}(x)|^2$$

so the answer (in this product state) is the same as if the system weren't there at all.

But the state of the whole system (system plus pointer) at time t is:

$$|\psi_t\rangle = \mathbf{U}(t)\left(\left(\sum_n \alpha_n |m_n\rangle\right) \otimes |\psi_{\text{packet}}(x)\rangle\right) = \sum_n \alpha_n |m_n\rangle \otimes |\psi_{\text{packet}}(x - m_n\lambda t)\rangle$$

In this state, the probability density for the pointer particle location is

$$p_t(x) = \langle\psi_t| \left(\mathbb{1}_A \otimes |x\rangle\langle x|\right) |\psi_t\rangle = \sum_n |\alpha_n|^2 |\psi_{\text{packet}}(x - \lambda m_n t)|^2 \ .$$

Assume for simplicity that one of the eigenvalues of $\mathbf{M}$ is $m_0 = 0$; then the probability of finding the particle in Bin 0 is now

$$\int_{\text{Bin } 0} dx\, p_t(x) = \int_{\text{Bin } 0} dx |\psi_{\text{packet}}(x)|^2 = |\alpha_0|^2.$$

Measuring spins (Stern-Gerlach)

I need to comment on how one measures spins, to make it clear that it can really be done, and as an example of the preceding discussion.

If we want to measure $\boldsymbol{\sigma}^z$ of a spin-$\frac{1}{2}$ particle, we send it through a region of inhomogeneous magnetic field. Its magnetic moment is $\mu\vec{\sigma}$, and so the term coupling the system A ($=$ the spin of the particle) to the pointer variable (which will turn out to be the z-momentum of the particle) is

$$\mathbf{H}_p = \vec{\mu} \cdot \vec{B} = -\lambda\mu\mathbf{z}\boldsymbol{\sigma}^z .$$

where we have chosen $\vec{B}(\vec{x}) = -\lambda z\hat{z}$ to vary linearly in z.

The point of having an inhomogeneous field is so that this exerts a force on the particle. The direction of the force depends on its spin. To connect with the previous discussion: Here the observable we want to measure is $\mathbf{M} = \boldsymbol{\sigma}^z$. Redoing the previous analysis, we encounter the operator

$$e^{-im\mathbf{z}} = e^{-m\frac{d}{dp_z}}$$

which generates a translation in p_z, the momentum of the particle, by m: it imparts an impulse to the pointer system (which is the translational degree of freedom of the particle itself). We then watch where the particle goes – if it goes higher/lower than where it was headed, its spin was up/down.

To measure $\boldsymbol{\sigma}^x$ instead, we rotate the magnets by $\pi/2$. More generally, we can measure $\vec{\sigma} \cdot \hat{n}$ for some unit vector $\hat{n}$ in the xz plane by tilting the magnets so the field points along $\hat{n}$ and depends on $\vec{x} \cdot \hat{n}$.

If we attenuate the beam so that one particle passes through during a macroscopic amount of time, it still hits one or the other spot. If the initial state isn't an eigenstate of $\boldsymbol{\sigma}^z$, no one has figured out a way to predict which spot it will hit. The discussion above on Bell's inequalities was intended to demonstrate that *there is experimental evidence that it is not possible even in principle to make this prediction.*

Notice that it is very convenient (perhaps *too* convenient) that observables in QM are represented by Hermitian operators, since this means that we can always add them to the Hamiltonian as in (2) (multiplied by some operators from the measuring device) to describe measuring devices.

Orthogonal measurements and generalized measurements

A brief and ignorable side-comment about why there are those scary 'POVM' sections in Preskill's notes, for your future reference: the kind of measurement we described above is called 'orthogonal measurement'. This is fully general, as long as we have access to the whole system. If we must forget about part of the system – just as in that case states are not rays and time evolution is not unitary – measurement is not orthogonal projection onto eigenstates. One reason that this becomes tricky is that we can consistently assign mutually exclusive probabilities to two observations only if there is no possibility of their interference. Those scary sections straighten this out by answering the question: "What does a projection onto an eigenstate in the full Hilbert space look like to the reduced density matrix of a subspace?"

2.3 Decoherence and the interpretation of QM

[Le Bellac 6.4.1, Preskill §3.4] So far in our discussion of quantum mechanics, the measurement axiom is dramatically different from the others, in that it involves non-linear evolution. The discussion of von Neumann's model of measurement did not fix this problem, but merely postponed it.

To see that there is still a problem, suppose we have a quantum system whose initial state is either $|+\rangle$ or $|-\rangle$ (*e.g.* an electron whose spin is up or down along the z direction), and we do some von Neumann measurement on it (*e.g.* we send the electron through a Stern-Gerlach apparatus also oriented along z) as a result of which it becomes entangled with the measuring apparatus (*e.g.* the electron's position at some detector) according to the rule

$$|+\rangle \otimes |\Psi_0\rangle \to |+\rangle \otimes |\Psi_+\rangle \,, \quad |-\rangle \otimes |\Psi_0\rangle \to |-\rangle \otimes |\Psi_-\rangle \,,$$

where $|\Psi_0\rangle$ is the initial state of the pointer and the measuring apparatus and $\langle \Psi_+|\Psi_-\rangle = 0$.

But now what if the initial state of the spin is not just up or down along z? The von Neumann evolution is still linear:

$$(\lambda\,|+\rangle + \mu\,|-\rangle) \otimes |\Psi_0\rangle \to \lambda\,|+\rangle \otimes |\Psi_+\rangle + \mu\,|-\rangle \otimes |\Psi_-\rangle$$

which we are supposed to picture as a superposition of macroscopically different states of the measuring apparatus, a Schrödinger's cat state.

To understand why in practice we end up with one or the other macroscopic state (and don't see any effects of *interference* between the outcomes) something has to pick a basis.

The thing that picks the basis is a phenomenon called *decoherence* which results from the coupling of the system to its environment. By the 'environment' here I mean all the rest of

the world, like the dust particles in the room and the air molecules and the photons from the overhead lights and the photons from the Cosmic Microwave Background; what these all have in common is that we don't keep track of their quantum state.

The choice of basis is determined by how the system is coupled to the environment. Generally, this coupling is via local interactions, and this is *why* we experience macroscopic objects as having a definite location.

The idea is that the environment is making (von Neumann) measurements of our system – it interacts with it and becomes entangled with it. But because we don't keep track of the state of the environment, we must trace out the Hilbert space of the environment. And (I claim and will explain below that) the off-diagonal entries of the resulting reduced density matrix for the system rapidly become small as a result of the interactions with the environment:

$$\boldsymbol{\rho}_{\text{before decoherence}} = |\psi\rangle\langle\psi| = (\lambda|1\rangle + \mu|2\rangle)(\lambda^\star\langle1| + \mu^\star\langle2|)$$

$$\boldsymbol{\rho}_{\text{during decoherence}} = |\lambda|^2|1\rangle\langle1| + |\mu|^2|2\rangle\langle2| + e^{-t\gamma}(\lambda\mu^\star|1\rangle\langle2| + \mu\lambda^\star|2\rangle\langle1|) \tag{3}$$

'Rapidly' here means much faster than other natural time scales in the system (like $\hbar/\Delta E$). For practical purposes, this process is irreversible, since the correlations (*e.g.* the information about the relative phase between $|1\rangle$ and $|2\rangle$ in an initial pure state) are lost in the huge Hilbert space of the environment; it leaves the system in a classical mixture,

$$\boldsymbol{\rho}_{\text{after decoherence}} = |\lambda|^2|1\rangle\langle1| + |\mu|^2|2\rangle\langle2|.$$

So the claim is that most of the states in the Hilbert space of any system with an environment (any system we encounter outside an ultracold vacuum chamber) are fragile and decay rapidly to a small subset of states that have a classical limit. (These are sensibly called 'classical states'.) We will see this very explicitly in a simple model, below.

[End of Lecture 13]

2.3.1 A simple way to think about how interactions with the environment destroy interference effects

You can prevent interference effects by measurements. As a paradigmatic example of interference effects, consider yet again the double slit experiment. If you measure which hole the particle goes through, you will not see the interference pattern. I will illustrate this claim next, but first, consider who is 'you' in the preceding sentences? 'You' could just as well be the dust particles in the room. So this discussion provides a model of how to think about why quantum interference is destroyed by coupling to the environment.

Consider the following description of the double-slit (this next paragraph is just setting up notation and I hope is familiar!). If the particle goes through the upper path (call this state

$|\uparrow\rangle$), the resulting wavefunction at the detector screen is $\psi_\uparrow(x)$; the probability of seeing the particle hit the location x is $P_\uparrow(x) = |\psi_\uparrow(x)|^2$. Similarly, the lower path state $|\downarrow\rangle$ produces the wavefunction $\psi_\downarrow(x)$, with resulting distribution of hits at the detector $P_\downarrow(x) = |\psi_\downarrow(x)|^2$. A superposition of the two states $\mu|\uparrow\rangle + \lambda|\downarrow\rangle$ produces the superposition of wavefunctions $|\text{superposition}\rangle = \mu\psi_\uparrow + \lambda\psi_\downarrow$. Now the detector records the interference pattern:

$$P_{\text{superposition}}(x) = |\mu\psi_\uparrow(x) + \lambda\psi_\downarrow(x)|^2 = |\mu^2|P_\uparrow(x) + |\lambda|^2 P_\downarrow(x) + \underbrace{\left(\mu\lambda^\star\psi_\uparrow(x)\psi_\downarrow^\star(x) + cc\right)}_{\text{interference terms}}$$

where 'cc' stands for complex conjugate. The last two terms represent the consequences of interference (e.g. they are the ones that oscillate in x).

Now suppose that the particle is coupled to some environment which is influenced by which slit it traverses; in particular an initial product state evolves via interactions into

$$(\mu|\uparrow\rangle + \lambda|\downarrow\rangle) \otimes |\psi\rangle_E \overset{\text{wait}}{\rightarrow} \mu|\uparrow\rangle \otimes |a\rangle + \lambda|\downarrow\rangle \otimes |b\rangle \equiv |E\rangle$$

where a, b are some states of the environment. This is just like our description of von Neumann measurement: the system becomes entangled with the measuring device.

But now what's the resulting pattern on the detector screen, $\text{Prob}_{\text{this entangled state, E}}(x)$?

$$\begin{aligned}\text{Prob}_E(x) &= \| \mu\psi_\uparrow(x)|a\rangle + \lambda\psi_\downarrow(x)|b\rangle \|^2 \\ &= |\mu\psi_\uparrow(x)|^2\langle a|a\rangle + |\lambda\psi_\downarrow(x)|^2\langle b|b\rangle + \underbrace{\left(\mu\lambda^\star\psi_\uparrow(x)\psi_\downarrow^\star(x)\langle a|b\rangle + cc\right)}_{\text{interference terms}} \quad . \end{aligned} \qquad (4)$$

The crucial point is that the size of the interference terms is multiplied by the number $\langle a|b\rangle$ – the overlap between the two different states into which the environment is put by looking at the particle path. For example, if the states are orthogonal, the interference effects are completely gone; this is the case where the environment has successfully measured the path of the particle, since $|a\rangle$ and $|b\rangle$ can be distinguished for sure. The extent to which the state of the environment is a useful pointer for the which-way information is exactly the extent to which the interference is destroyed!

(Thanks to Eric Michelsen for provoking me to add this discussion. You may enjoy his slides on decoherence, here.)

2.3.2   Time evolution of open systems

[The intimidating Le Bellac Chapter 15.2] You shouldn't be satisfied with the discussion of decoherence so far. Where did the $e^{-\gamma t}$ in Eq. (3) come from?

Given a pure state in $\mathcal{H}_A \otimes \mathcal{H}_B$ evolving according to some Hamiltonian evolution, how does the reduced state operator ρ_A evolve? Given any example we could (in principle) figure

it out by explicit computation of the reduced density matrix. We saw in Chapter 1 that if the two subsystems A and B don't interact, its evolution is unitary. If the systems do interact, I claim that the reduced state operator evolves over a finite time interval in the following way, by *Kraus superoperators*:

$$\boldsymbol{\rho}_A \to \mathcal{K}(\boldsymbol{\rho}) = \sum_{\mu=1}^{K} \mathbf{M}_\mu \boldsymbol{\rho}_A \mathbf{M}_\mu^\dagger, \tag{5}$$

where unitary evolution of the whole system is guaranteed by

$$\sum_{\mu=1}^{K} \mathbf{M}_\mu^\dagger \mathbf{M}_\mu = \mathbb{1}_A,$$

and K is some number which depends on the system and its coupling to the environment. On the other hand, $\sum_\mu \mathbf{M}_\mu \mathbf{M}_\mu^\dagger$ can be some crazy thing. (Note that the object $\mathcal{K}$ is called a 'superoperator' because it is an operator that acts on operators.)

The statement that the evolution of $\boldsymbol{\rho}_A$ can be written this way is very general. In fact any linear operation which keeps $\boldsymbol{\rho} \otimes \frac{1}{\dim \mathcal{H}_C} \mathbb{1}_C$ a density matrix for any C has a such a form. Such a thing is called a *completely positive map*. You might think it is enough for us to consider evolution maps which keep $\boldsymbol{\rho}$ positive (and not the stronger demand that $\boldsymbol{\rho} \otimes \mathbb{1}_C$ is positive). As an example which shows that this is a real condition: The transpose operation $\rho \to \rho^T$ is positive but not completely positive. From the point of view we have taken, that we are describing the evolution of a subsystem which interacts with a larger system, this demand (that extending the evolution by doing nothing to the larger system should still be positive) is quite natural. It is a fancy theorem (the *Kraus representation theorem*)[3] that any completely positive map may be written in the form (5).

A little more on Kraus superoperators

To see a little more explicitly where these operators come from, imagine again that $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_E$ and we begin in an initial unentangled state

$$\boldsymbol{\rho} = \boldsymbol{\rho}_A \otimes |0\rangle_E \langle 0|_E.$$

(Note that we're not going to keep track of the state of the environment – in fact, that's its point in life. So we don't need an accurate model of what it's doing, just an accurate model of what it's doing to our system. This is why we can make this simplifying step of acting just on $|0\rangle_E$.) Time evolution acts by

$$\boldsymbol{\rho} \to \mathbf{U} \boldsymbol{\rho} \mathbf{U}^\dagger$$

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[3]where 'fancy' means 'we will not prove it here'

where $\mathbf{U} = e^{-\mathbf{i}\mathbf{H}t}$ is the (unitary!) time evolution operator on the *whole* system. This means it acts on the reduced density matrix for subsystem A (namely $\boldsymbol{\rho}_A \equiv \operatorname{tr}_{\mathcal{H}_E}\boldsymbol{\rho}$) by

$$\boldsymbol{\rho}_A \to \boldsymbol{\rho}'_A = \operatorname{tr}_{\mathcal{H}_E}\mathbf{U}\boldsymbol{\rho}\mathbf{U}^\dagger.$$

More explicitly

$$(\boldsymbol{\rho}'_A)_{mn} = \sum_{\mu kl} \mathbf{U}_{m\mu,k0}\boldsymbol{\rho}_{kl}\mathbf{U}^\dagger_{l0,n\mu}$$

with

$$\mathbf{U}_{m\mu,k\nu} = {}_A\langle m| \otimes {}_E\langle\mu|\mathbf{U}|k\rangle_A \otimes |\nu\rangle_E.$$

So we have

$$\boldsymbol{\rho}_A \to \boldsymbol{\rho}'_A = \operatorname{tr}_{\mathcal{H}_E}\mathbf{U}\boldsymbol{\rho}\mathbf{U}^\dagger = \sum_\mu \mathbf{M}_\mu\boldsymbol{\rho}_A\mathbf{M}^\dagger_\mu$$

with

$$\mathbf{M}_\mu = {}_E\langle\mu|\mathbf{U}|0\rangle_E$$

From this we see that

$$\sum_\mu \mathbf{M}^\dagger_\mu\mathbf{M}_\mu = \sum_\mu {}_E\langle 0|\mathbf{U}^\dagger \underbrace{|\mu\rangle_E {}_E\langle\mu|}_{=\mathbb{1}_E} \mathbf{U}|0\rangle_E = \mathbb{1}_A$$

while

$$\sum_\mu \mathbf{M}_\mu\mathbf{M}^\dagger_\mu = \sum_\mu {}_E\langle\mu|\mathbf{U}|0\rangle_E {}_E\langle 0|\mathbf{U}^\dagger|\mu\rangle_E = \text{something we can't determine without more information.}$$

A useful expression for the time evolution for extracting $\mathbf{M}_\mu$ is

$$\mathbf{U}|\varphi\rangle_A \otimes |0\rangle_E = \sum_\mu \mathbf{M}_\mu \otimes \mathbb{1}_E |\varphi\rangle_A \otimes |\mu\rangle_E = \sum_\mu \mathbf{M}_\mu|\varphi\rangle_A \otimes |\mu\rangle_E. \tag{6}$$

This will guarantee that

$$\boldsymbol{\rho} \to \operatorname{tr}_{\mathcal{H}_E}\left(\mathbf{U}_{AE}|\phi\rangle_A \otimes |0\rangle_E {}_A\langle\phi| \otimes {}_E\langle 0|\mathbf{U}^\dagger_{AE}\right) = \sum_\mu \mathbf{M}_\mu\boldsymbol{\rho}\mathbf{M}^\dagger_\mu.$$

Note that $\mathcal{K}$ is not unique: Making a change of basis on the environment E doesn't change our evolution of $\boldsymbol{\rho}$, but will change the appearance of $\mathcal{K}$.

The phase-damping channel

Let us consider an example of how a qbit may be coupled to an environment, where we can see decoherence in action. It has the fancy name of "the phase-damping channel". We'll

model the environment as a 3-state system $\mathcal{H}_E = \text{span}\{|0\rangle_E, |1\rangle_E, |2\rangle_E\}$, and suppose that the result of (linear, unitary) time evolution of the coupled system over a time dt acts by

$$\mathbf{U}_{AE}|0\rangle_A\otimes|0\rangle_E = \sqrt{1-p}\,|0\rangle_A\otimes|0\rangle_E + \sqrt{p}\,|0\rangle_A\otimes|1\rangle_E\,,\quad \mathbf{U}_{AE}|1\rangle_A\otimes|0\rangle_E = \sqrt{1-p}\,|1\rangle_A\otimes|0\rangle_E + \sqrt{p}\,|1\rangle_A\otimes|2\rangle_E\,,$$

[4] [5] Notice that the system A of interest actually doesn't evolve at all in this example!

A bit of interpretation here is appropriate. Suppose the two states we are considering represent positions some heavy particle in outer space, $|0\rangle_A = |x_0\rangle, |1\rangle_A = |x_1\rangle$, where x_1 and x_2 are far apart; we'd like to understand why we don't encounter such a particle in a superposition $a\,|x_0\rangle + b\,|x_1\rangle$. The environment is described by $e.g.$ black-body photons bouncing off of it (even in outer space, there is a nonzero background temperature associated to the cosmic microwave background). It is reasonable that these scatterings don't change the state of the heavy particle, because it is so heavy. But photons scattering off the particle in different positions get scattered into different states, so the evolution of the environment should be distinct for the two different states of the heavy particle A. The probability p is determined by the scattering rate of the photons: how long does it take a single photon to hit the heavy particle.

To find the Kraus operators, $\mathbf{M}_\mu$, we can use the expression:

$$\mathbf{U}_{AE}|\phi\rangle_A\otimes|0\rangle_E = \sum_{\mu=0}^{2}(\mathbf{M}_\mu\otimes\mathbb{1}_B)|\phi\rangle_A\otimes|\mu\rangle_E\,.$$

We can read off the $\mathbf{M}$s:

$$\mathbf{M}_0 = \sqrt{1-p}\,\mathbb{1}_A,\quad \mathbf{M}_1 = \sqrt{p}\,|0\rangle_{A\,A}\langle 0|,\quad \mathbf{M}_2 = \sqrt{p}\,|1\rangle_{A\,A}\langle 1|.$$

So the reduced density matrix evolves according to

$$\boldsymbol{\rho}_A \to \mathcal{K}(\rho_A) = (1-p)\boldsymbol{\rho} + p\begin{pmatrix} \rho_{00} & 0 \\ 0 & \rho_{11} \end{pmatrix} = \begin{pmatrix} \rho_{00} & (1-p)\rho_{01} \\ (1-p)\rho_{10} & \rho_{11} \end{pmatrix}$$

Suppose we wait twice as long? Then the density matrix becomes

$$(\star)\qquad \mathcal{K}^2(\rho_A) = \mathcal{K}(\mathcal{K}(\boldsymbol{\rho}_A)) = \begin{pmatrix} \rho_{00} & (1-p)^2\rho_{01} \\ (1-p)^2\rho_{10} & \rho_{11} \end{pmatrix}\,.$$

You see where this is going. After a time $t \equiv n \cdot dt$, the density matrix is

$$\boldsymbol{\rho}_A(t) = \mathcal{K}^n(\boldsymbol{\rho}_A) = \begin{pmatrix} \rho_{00} & (1-p)^n\rho_{01} \\ (1-p)^n\rho_{10} & \rho_{11} \end{pmatrix} = \begin{pmatrix} \rho_{00} & e^{-\gamma t}\rho_{01} \\ e^{-\gamma t}\rho_{10} & \rho_{11} \end{pmatrix}$$

---

[4]Le Bellac (whose judgement is usually impeccable and I don't think this is his fault) calls this operation a 'quantum jump operator'; this seems like totally unnecessary and confusing jargon to me. The reason there is any kind of 'jump' is because we are waiting a finite amount of time, dt.

[5]What if the initial state of the environment is something other than $|0\rangle_E$? We don't need to know.

– as promised the off-diagonal terms decay exponentially in time, like $e^{-\gamma t}$, with $\gamma = -\log(1-p)/dt \sim p/dt$ (the last step is true if p is small using the Taylor expansion of $\log(1-p)$). Nothing happens to the diagonal elements of $\boldsymbol{\rho}$ *in this basis*. The choice of special classicalizing basis was made when we said that the states $|0\rangle$ and $|1\rangle$ of the qbit caused the environment to evolve differently.

So notice that it is the scattering rate with the environment (via p) that determines the decoherence rate γ – it's just the frequency with which the system interacts with its environment. Getting hit by these photons (which don't do anything to it!) happens much much faster than anything else that happens to the particle. This is why Schrödinger's cat seems so absurd: it gets hits with lots photons (or other aspects of its environment with similar effect) before we even look at it.

I must comment on a crucial assumption we made at the step ($\star$) where we iterated the evolution $\mathcal{K}$. In stating the model above, I've only told you how to evolve the whole system if the environment is in the ground state $|0\rangle_E$. In order for ($\star$) to be the correct rule for evolving twice as long, we must assume that the environment relaxes to its ground state over the time dt. It is natural that the environment would forget what it's been told by the system in such a short time if the environment is some enormous thing. Big things have fast relaxation times.

[End of Lecture 14]

Under unitary time evolution that we've seen for closed systems, the time dependence is always periodic: it always comes back to its initial state eventually, and never forgets. How does a quantum system relax to its groundstate (like we assumed in our model of the environment)? A model of this is given by our second example, next:

Amplitude-damping channel

[Preskill 3.4.3, Le Bellac §15.2.4] This is a very simple model for a two-level atom, coupled to an environment in the form of a (crude rendering of a) radiation field.

The atom has a groundstate $|0\rangle_A$; if it starts in this state, it stays in this state, and the radiation field stays in its groundstate $|0\rangle_E$ (zero photons). If it starts in the excited state $|1\rangle_A$, it has some probability p per time dt to return to the groundstate and emit a photon, exciting the environment into the state $|1\rangle_E$ (one photon). This is described by the time evolution

$$\mathbf{U}_{AE} |0\rangle_A \otimes |0\rangle_E = |0\rangle_A \otimes |0\rangle_E$$

$$\mathbf{U}_{AE} |1\rangle_A \otimes |0\rangle_E = \sqrt{1-p} \, |1\rangle_A \otimes |0\rangle_E + \sqrt{p} \, |0\rangle_A \otimes |1\rangle_E \,.$$

The environment has two states so there are two Kraus operators, which (using (6)) are

$$\mathbf{M}_0 = \begin{pmatrix} 1 & 0 \\ 0 & \sqrt{1-p} \end{pmatrix}, \mathbf{M}_1 = \begin{pmatrix} 0 & \sqrt{p} \\ 0 & 0 \end{pmatrix}.$$

Unitary of the evolution of the whole system is recovered because

$$\mathbf{M}_0^\dagger \mathbf{M}_0 + \mathbf{M}_1^\dagger \mathbf{M}_1 = \begin{pmatrix} 1 & 0 \\ 0 & 1-p \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ 0 & p \end{pmatrix} = \mathbb{1}.$$

So the density matrix evolves according to

$$\begin{aligned}
\boldsymbol{\rho} \to \mathcal{K}(\boldsymbol{\rho}) &= \mathbf{M}_0 \boldsymbol{\rho} \mathbf{M}_0^\dagger + \mathbf{M}_1 \boldsymbol{\rho} \mathbf{M}_1^\dagger \\
&= \begin{pmatrix} \rho_{00} & \sqrt{1-p}\rho_{01} \\ \sqrt{1-p}\rho_{10} & (1-p)\rho_{11} \end{pmatrix} + \begin{pmatrix} p\rho_{11} & 0 \\ 0 & 0 \end{pmatrix} = \begin{pmatrix} \rho_{00}+p\rho_{11} & \sqrt{1-p}\rho_{01} \\ \sqrt{1-p}\rho_{10} & (1-p)\rho_{11} \end{pmatrix}
\end{aligned}$$

After n steps (in time $t = n \cdot dt$), the 11 matrix element has undergone $\rho_{11} \to (1-p)^n \rho_{11} = e^{-\gamma t}$, again exponential decay with rate $-\log(1-p)/dt \sim p/dt$ (for small p). Using $\rho_{00}+\rho_{11} = 1$, the whole matrix is:

$$\mathcal{K}^n(\boldsymbol{\rho}) = \begin{pmatrix} 1 + (1-p)^n \rho_{11} & (1-p)^{n/2} \rho_{01} \\ (1-p)^{n/2} \rho_{10} & (1-p)^n \rho_{11} \end{pmatrix} \quad .$$

If you wait long enough, the atom ends up in its groundstate:

$$\lim_{n \to \infty} \mathcal{K}^n(\boldsymbol{\rho}) = \begin{pmatrix} \rho_{00} + \rho_{11} & 0 \\ 0 & 0 \end{pmatrix} = |0\rangle_A \langle 0|_A \ .$$

This example of open-system evolution takes a mixed initial state (say some incoherent sum of ground and excited state) to a (particular) pure final state. (Note that the off-diagonal elements (the 'coherences') decay at half the rate of ρ_{11} (the population of the excited state).

We'll see some more examples of couplings to the environment on HW 7.

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2.3.3   Interpretations of quantum mechanics and the origin of the Born rule

[Weinberg 3.7] The measurement axiom 4 we gave at the beginning of this class is called *the Copenhagen interpretation*, and is due to Max Born with much philosophical baggage added by Niels Bohr. Max Born's version can be called the "shut up and calculate" interpretation of quantum mechanics, and Niels Bohr's version can be called the "shut up and calculate" interpretation minus the shutting-up part[6]. It involves a distinction, some sort of boundary, between quantum (the system) and classical (the measuring device). The latter involves non-linear evolution which is not described within quantum mechanics.

In the discussion above we have seen that it is possible to improve upon this situation by including the effects of decoherence. We have, however, not derived the Born rule (that in a measurement of an observable $\mathbf{A} = \sum_a a |a\rangle \langle a|$ in the state $\boldsymbol{\rho}$, we get the answer a with

___

[6]The first part of this apt description is due to David Mermin and the second is due to Scott Aaronson.

probability tr $\boldsymbol{\rho} |a\rangle \langle a|$). There are two still-viable (classes of) points of view on how this might come about, which can generally be called *ontological* and *epistemological*. The crux of the issue is how we think about the wavefunction: is it a complete description of all there is to know about physical reality? or is it a statement about (someone's, whose?) knowledge (about reality?)?

The meaning attached to probability can itself be divided along the same lines (of ontology and epistemology) as QM interpretations, in this context called *frequentist* and *Bayesian* notions of probability theory. The frequentist way of thinking about probability is that we imagine we have a large collection of identically-prepared copies of the system; a statement about probability then is a statement about what fraction of these copies realize the outcome in question. This definition is great when it is available, but there are some situations where we'd like to use the machinery of probability theory but cannot imagine making an ensemble (*e.g.*, the increase in global temperatures on the Earth is *probably* due to the behavior of humans). Then we are forced to use a Bayesian interpretation, which is a statement about the most reasonable expectations given current information.

The latter (Bayesian) point of view is appealing because it would instantly remove any issue about the 'collapse of the wavefunction'. If the wavefunction were merely a book-keeping device about the information held by an observer, then of course it must be updated when that observer makes a measurement! [7] However, this point of view (sometimes called *quantum Bayesianism*) requires us to give up the notion of an objective state of the system and allows the possibility that we might get in trouble in our accounting of the states kept in the books of different observers. I will not say more about it but it is interesting.

The former point of view (that the wavefunction is real and has all the possible information) leads pretty directly to the "many worlds interpretation". This is an absurd-seeming name given to the obviously-correct description of the measurement process that we've given in subsection 2.2: as a result of interactions, the state of the system becomes entangled with that of the measuring device, and with the air in the room, and with the eyeballs and brain of the experimenter. So of course when the experimenter sees the needle of the measuring device give some answer, that is the answer. That is the answer on the observer's *branch of the wavefunction*[8]:

$$|\Psi\rangle_{\text{universe}} = \frac{1}{\sqrt{2}} \left(\left| \text{🐱} \right\rangle + | \text{🐱} \rangle \right) \otimes \left| \text{👤} \right\rangle \xrightarrow{\text{wait}} \frac{1}{\sqrt{2}} \left| \text{🐱} \right\rangle \otimes \left| \text{👤} \right\rangle + \frac{1}{\sqrt{2}} | \text{🐱} \rangle \otimes \left| \text{👤} \right\rangle$$

---

[7] For example, J. B. Hartle, *Quantum mechanics of individual systems,* Am. J. Phys. 36 (1968) 704 makes the claim that a quantum "state is not an objective property of an individual system, but is that information, obtained from a knowledge of how the system was prepared, which can be used for making predictions about future measurements . . . The 'reduction of the wave packet' does take place in the consciousness of the observer, not because of any unique physical process which takes place there, but only because the state is a construct of the observer and not an objective property of the physical system."

[8] You may (should) recognize the observer depicted here from xkcd. The cat pictures are of unknown provenance.

As we have seen above, the inevitable phenomenon of decoherence picks out particular *classical states*, determined by the coupling of the system to its environment, which are the ones that are observed by a classical observer, *i.e.* by someone who fails to keep track of all the detailed correlations between the system and every speck of dust and photon in its environment.

Does this solve all the problems of interpreting measurement in QM? No, we haven't really derived the Born rule for how we should interpret matrix elements of operators in terms of probabilities.

Can we derive the Born rule from the first three Axioms of QM? If not, something additional to QM is required, even within the many-worlds interpretation. The answer is 'sort of'.

Suppose we adopt a frequentist interpretation, and give ourselves many ($N \gg 1$, non-interacting) copies of our quantum system.[9] (The question of how to prepare such a thing consistent with no-quantum-Xerox we will ignore here.) So the state of the whole system, in $\mathcal{H}^{\otimes N}$, is

$$|\Psi_0\rangle = \left(\sum_{n_1} c_{n_1}|n_1\rangle\right) \otimes \left(\sum_{n_2} c_{n_2}|n_2\rangle\right) \otimes \cdots \otimes \left(\sum_{n_N} c_{n_N}|n_N\rangle\right) = \sum_{n_1,n_2\ldots n_N} c_{n_1}c_{n_2}\cdots c_{n_N}|n_1,n_2\cdots n_N\rangle.$$

We assume for convenience that these states are ON: $\langle n_1', n_2', \ldots n_N'|n_1, n_2, \ldots n_N\rangle = \delta_{n_1'n_1}\delta_{n_2'n_2}\cdots\delta_{n_N'n_N}$, so normalization is guaranteed by $\sum_n |c_n|^2 = 1$.

Let us further assume that the states $|n_s\rangle$ are classical states, into which the system decoheres. (We are assuming that each of the copies of the system is coupled to an environment in the same appropriate way.) This means that after a short time, the state of the combined system will be

$$|\Psi_1\rangle = \sum_{n_1,n_2\ldots n_N} c_{n_1}c_{n_2}\cdots c_{n_N} e^{i(\varphi_1+\varphi_2+\ldots+\varphi_N)}|n_1,n_2\cdots n_N\rangle$$

where φ_s are totally random phases, which when we average over them will set to zero any off-diagonal matrix elements:

$$\rightarrow \boldsymbol{\rho} = \sum_{n_1,n_2\ldots n_N} |c_{n_1}c_{n_2}\cdots c_{n_N}|^2 |n_1,n_2\cdots n_N\rangle \langle n_1,n_2\cdots n_N| \ .$$

Now an observer who is part of this system will find herself after a while on some branch of the wavefunction in some definite basis state, $|n_1, n_2\ldots n_N\rangle$ (this is what decoherence does for us). If she finds N_n copies in the state n, she will sensibly declare that the probability that any one copy is in state n is

$$P_n = N_n/N.$$

---

[9]This discussion is due to J. Hartle, 1968.

Notice that $\sum_n N_n = N$ guarantees that this distribution is normalized. This is actually what people do to measure probability distributions for outcomes of quantum systems in practice. To be absolutely sure of the probability distribution it is necessary to take $N \to \infty$.

If we are willing to accept *part* of the measurement axiom, we can now go the rest of the way. (After all, we have to say something about what we should do with the state vector to get physics out of it.) In particular, let's accept the following **Weak version of Axiom 4:**

If the state vector is an eigenstate of an observable $\mathbf{A}$ with eigenvalue a, then for sure the system has the value a of that observable.

(Pretty reasonable.) Now consider the family of hermitean operators $\mathbf{P}_n$ called *frequency operators*, defined to be linear and to act on the basis states by

$$\mathbf{P}_n \left| n_1...n_N \right\rangle \equiv \frac{N_n}{N} \left| n_1...n_N \right\rangle \quad ,$$

where as above N_n is the number of the indices $n_1..n_N$ which is equal to n.

So Born's rule would be derived from the weak axiom 4 above if we could show that

$$\mathbf{P}_n \left| \Psi_1 \right\rangle \overset{?}{=} |c_n|^2 \left| \Psi_1 \right\rangle \quad .$$

This is not true. But it becomes truer as N gets larger:

$$\| \left(\mathbf{P}_n - |c_n|^2 \right) \left| \Psi_1 \right\rangle \|^2 = \frac{1}{N} |c_n|^2 \left(1 - |c_n|^2 \right) \leq \frac{1}{4N}. \tag{7}$$

For a derivation of this statement, see Weinberg page 91. Weinberg mentions an important hidden loophole here: the fact that the 2-norm $\| \left| \psi \right\rangle \|^2 \equiv \left\langle \psi | \psi \right\rangle$ is what appears in the Born rule in this derivation is a consequence of the fact that we used it in measuring the distance between states in (7).

There is a lot more to say about this subject, and there probably always will be, but we have to shut up and calculate now.

2.4   Path integrals

[Shankar, Chapter 8 and 21; Feynman; Kreuzer, Chapter 11]

The path integral will offer us another route to classical physics.

The path integral formulation of quantum mechanics is the ultimate logical conclusion from the double-slit experiment. The basic lesson from that discussion is that the two paths the

particle could have taken *interfere.* More precisely: to find the amplitude for some quantum process (whose absolute-square is the probability), we must sum over all ways that it can occur.

If we send a quantum particle through a wall with two little holes, we obtain a probability amplitude for where it will land which is obtained by summing the contributions from each of the holes.

$$\text{one wall, two slits:} \quad \psi_1(y) = \frac{1}{\sqrt{2}} \left(\psi_{\text{from hole 1}}(y) + \psi_{\text{from hole 2}}(y) \right).$$

Now suppose that instead of the detector, we put another wall with two holes. We compute the probability amplitude at each of the spots in the same way. (there is an important issue of normalization, to which we'll return.) Let's figure out the probability amplitude for a detector placed after the second wall, like this:

Two walls two slits:
$$\psi_2(y) \quad = \quad \frac{1}{\sqrt{2}} \left(\psi_{\text{from hole 1 of wall 2}}(y) + \psi_{\text{from hole 2 of wall 2}}(y) \right)$$

Further we can write

$$\psi_{\text{from hole } i \text{ of wall 2}}(y) = U_{yi}^{(2)} \psi_{\text{at hole } i \text{ of wall 2}}$$

where $U^{(2)}$ is an appropriate evolution operator. In turn

$$\psi_{\text{at hole } i \text{ of wall 2}} = \sum_j U_{ij}^{(1)} \psi_{\text{at hole } j \text{ of wall 1}} \cdot$$

Altogether, we are adding together a bunch of complex numbers in a pattern you have seen before: it is matrix multiplication:

$$\psi_2(y) = \sum_{j,k} U_{ij}^{(2)} U_{jk}^{(1)} \psi_k$$

where
$$U_{ij}^{(\alpha)} = \text{ the contribution } i \text{ from hole } j \text{ of wall } \alpha$$

What this formula is saying is that the wavefunction at the final detector is constructed by a *sum over paths* that the particle could have taken. More dramatically, it is a *sum over all the possible paths.* Don't forget that the contribution from each path is a complex number.

If we had one wall with three holes we would sum the contributions from each of the three holes.

$$\text{one wall, three slits:} \quad \psi(y) = \frac{1}{\sqrt{3}} \left(\psi_{\text{from hole 1}} + \psi_{\text{from hole 2}} + \psi_{\text{from hole 3}} \right).$$

You can imagine adding more holes. And you can imagine more walls.

Now imagine that the world is totally full of walls and that *all the walls are totally full of holes*. Even if there is no wall, we must sum over the paths. [10]

<div align="right">[End of Lecture 15]</div>

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[10]This wonderful device is due to Feynman. Take a look at Volume III of the Feynman Lectures. A more elaborate treatment appears in Feynman and Hibbs, *Quantum Mechanics and Path Integrals*.

2.4.1 A more formal statement of the path integral formulation

It will turn out that the previous formulations of quantum mechanics is to Hamiltonian mechanics as the path integral formulation is to Lagrangian mechanics (for a particle in 1d, this is $L = p\dot{x} - H$). Just as in the classical case, a big advantage of the Lagrangian formulation is that symmetries are sometimes more explicit.

[Shankar Chapter 8] Here is a statement of the rules. Suppose we want to construct the *propagator* for a 1d particle:

$$U(x, t; x', 0) \equiv \langle x|\mathbf{U}(t)|x'\rangle .$$

We assume that the hamiltonian is time-independent, so the time evolution operator is $\mathbf{U}(t) = e^{-\mathbf{iH}t/\hbar}$. A path integral representation of U is obtained by:

1. Find all paths $x(s)$ the particle could take from x' to x in time t.

2. For each path, evaluate the *action* $S[x] = \int_0^t ds L(x(s), \dot{x}(s))$. For a free particle, this is $S[x] = \int_0^t ds \left(\frac{1}{2}m\dot{x}^2 - V(x(s))\right) .$[11]

3. Add them up:
$$U(x, t; x', 0) = A \sum_{\text{all paths, } x(s)} e^{\frac{\mathbf{i}}{\hbar}S[x(s)]} . \tag{8}$$

   A is a normalization constant. The paths in the sum begin at x' at $s = 0$ and end at x at $s = t$.

Notice that this was what $\hbar$ was designed for all along: it is the 'quantum of action', the basic unit of action.

2.4.2 A derivation of the path integral from the canonical formalism of QM

[Kreuzer, chapter 11.2, Shankar chapter 21.1, 8.5]

Let us consider the propagator in a possibly-more general quantum system – the amplitude for the system to transition from state α at time 0 to state β at time t:

$$U(\beta, t; \alpha, 0) \equiv \langle \beta, t|e^{-\mathbf{iH}t}|\alpha, 0\rangle .$$

---

[11] For those of you who have been classical-mechanics-deprived, the purpose-in-life of the action is that it is extremized by the classical path. That is, Hamilton's equations are satisfied by the path of least (or most) action:
$$0 = \frac{\delta S[x]}{\delta x(s)} \propto m\ddot{x} + \partial_x V.$$

In the previous expression, I've assumed for simplicity that $\mathbf{H}$ is time-independent. Here we just require that we have a resolution of the identity of the form

$$\mathbb{1} = \int d\alpha \, |\alpha\rangle \, \langle \alpha|.$$

(If you want, think x wherever you see α, but it's much more general; for example, it could be a discrete variable.)

We're going to chop up the time evolution into a bunch (N) of little steps of size dt: $t = N dt$.

$$e^{-i\mathbf{H}t} = \underbrace{e^{-i\mathbf{H}dt} e^{-i\mathbf{H}dt} e^{-i\mathbf{H}dt} \cdots e^{-i\mathbf{H}dt}}_{N \text{ times}} = \prod_{i=1}^{N} e^{-i\mathbf{H}dt}$$

The basic strategy is to insert lots of resolutions of the identity in the time evolution operator. You should think of this as placing screens with infinitely many slits; the sum over states is the sum over which slit the particle goes through. Then

$$
\begin{aligned}
& e^{-i\mathbf{H}t} \\
= \ & e^{-i\mathbf{H}dt} \int d\alpha_{N-1} \, |\alpha_{N-1}\rangle \, \langle \alpha_{N-1}| e^{-i\mathbf{H}dt} \int d\alpha_{N-2} \, |\alpha_{N-2}\rangle \, \langle \alpha_{N-2}| e^{-i\mathbf{H}dt} \cdots \\
& \qquad \cdots \int d\alpha_2 \, |\alpha_2\rangle \, \langle \alpha_2| e^{-i\mathbf{H}dt} \int d\alpha_1 \, |\alpha_1\rangle \, \langle \alpha_1| e^{-i\mathbf{H}dt} \\
= \ & \prod_{i=1}^{N-1} \left(\int d\alpha_i e^{-i\mathbf{H}dt} \, |\alpha_i\rangle \, \langle \alpha_i| \right)
\end{aligned}
$$

We can regard the collection $\{\alpha_i \equiv \alpha(t_i)\}$ as parametrizing the possible 'paths' that the system can take as time passes. We will have to take a limit $N \to \infty, dt \to 0$; sometimes this is subtle.

The propagator is then

$$U(\beta, t; \alpha, 0) = \int \prod_{i=1}^{N-1} d\alpha_i \langle \alpha_i| e^{-i\mathbf{H}dt} \, |\alpha_{i-1}\rangle$$

with $\alpha_0 = \alpha$ and $\alpha_N = \beta$.

What happened here? Let's take the case where we divide the interval up into two parts, $N = 2$. So we're using

$$e^{-i\mathbf{H}(t_a - t_b)} = e^{-i\mathbf{H}(t_a - t)} e^{-i\mathbf{H}(t - t_b)}$$

which follows from the deep fact $t_a - t_b = (t_a - t) + (t - t_b)$. Now stick a 'wall full of holes,' $\mathbb{1} = \int dx \, |x\rangle \, \langle x|$ in between the two factors:

$$e^{-i\mathbf{H}(t_a - t_b)} = \int dx e^{-i\mathbf{H}(t_a - t)} \, |x\rangle \, \langle x| e^{-i\mathbf{H}(t - t_b)}$$

and now take matrix elements:

$$
\begin{aligned}
U(x_b, t_b; x_a, t_a) &\equiv \langle x_b | e^{-i\mathbf{H}(t_b - t_a)} | x_a \rangle \\
&= \int dx \langle x_b | e^{-i\mathbf{H}(t_b - t)} | x \rangle \langle x | e^{-i\mathbf{H}(t - t_a)} | x_a \rangle \\
&= \int dx\, U(x_b, t_b; x, t) U(x, t; x_a, t_a).
\end{aligned} \tag{9}
$$

In words: the amplitude to propagate from x_a, t_a to x_b, t_b is equal to the sum over x of amplitudes to get from x_a, t_a to x and from there to x_b, t_b, all in time $t_b - t_a$.

To be more concrete, let's think about a 1d particle in a potential. The Hamiltonian is

$$
\mathbf{H} = \frac{\mathbf{p}^2}{2m} + V(\mathbf{x}) \, ,
$$

and a useful resolution of the identity is in position space $\int dx\, |x\rangle \langle x| = \mathbb{1}, \mathbf{x}\, |x\rangle = x\, |x\rangle$. We must consider the amplitude from which $\mathbf{U}$ is made:

$$
U(x_{j+1}, dt; x_j, 0) = \langle x_{j+1} | e^{-i\mathbf{H}dt} | x_j \rangle = \langle x_{j+1} | e^{-i\left(\frac{\mathbf{p}^2}{2m} + V(\mathbf{x})\right)dt} | x_j \rangle \, . \tag{10}
$$

Using the identity

$$
e^{\mathbf{A}} e^{\mathbf{B}} = e^{\mathbf{A} + \mathbf{B} + \frac{1}{2}[\mathbf{A}, \mathbf{B}] + \cdots}
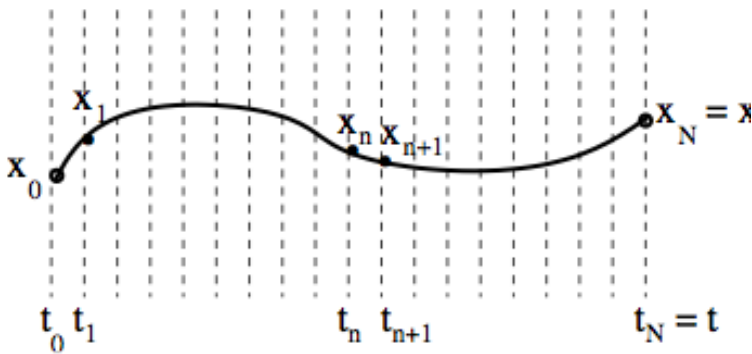$$

and the fact that the time step dt is small, we can split up the evolution:

$$
e^{-i\mathbf{H}dt} = e^{-idt\frac{\mathbf{p}^2}{2m}} e^{-idt V(\mathbf{x})} + \mathcal{O}(dt^2)
$$

Then we can act with $V(\mathbf{x})$ on the right ket and have for the amplitude

$$
\langle x_{j+1} | e^{-i\mathbf{H}dt} | x_j \rangle = \langle x_{j+1} | e^{-\frac{i}{\hbar}dt\frac{\mathbf{p}^2}{2m}} | x_j \rangle e^{-\frac{i}{\hbar}dt V(x_j)}
$$

using the fact that $V(\mathbf{x})$ is diagonal in position space.

[from Herman Verlinde]

Next we turn the $\mathbf{p}^2$ into a number by further inserting a resolution of the identity in momentum space: $\mathbb{1} = \int dp \, |p\rangle \langle p|, \mathbf{p} \, |p\rangle = p \, |p\rangle$.

$$e^{-\mathbf{i} \frac{\mathbf{p}^2}{2m} dt} = \int dp \, e^{-\mathbf{i} dt \frac{p_j^2}{2m}} \, |p_j\rangle \langle p_j|$$

Putting these things together, the propagator is:

$$U(x_f, t; x_0, 0) = \int [dpdx] \prod_{j=1}^{N-1} e^{-\mathbf{i} dt \frac{p^2(t_j)}{2m} - \mathbf{i} dt V(x_j)} \langle x_j | p_j \rangle \langle p_j | x_{j-1} \rangle$$

where we defined the *path-integral measure*

$$[dpdx] \equiv \prod_{j=1}^{N-1} \frac{dp(t_j) dx(t_j)}{2\pi} \ .$$

The integral has a boundary condition that $x(t_N) = x_f, x(t_0 = 0) = x_0$. Now we use

$$\langle p | x \rangle = \frac{1}{\sqrt{2\pi}} e^{-\mathbf{i} px/\hbar}$$

to write the path integral as:

$$\begin{aligned} U(x_f, t; x_0, 0) &= \int [dxdp] \prod_{j=1}^{N-1} e^{\frac{\mathbf{i}}{\hbar} dt p_j (x_j - x_{j-1}) - \frac{\mathbf{i}}{\hbar} dt H(p_j, x_j)} \\ &\simeq \int [dxdp] \, e^{\frac{\mathbf{i}}{\hbar} \int dt (p\dot{x} - H(p,x))} = \int [dxdp] \, e^{\frac{\mathbf{i}}{\hbar} S} \ . \end{aligned} \quad (11)$$

This is a sum over the configurations in *phase space*, weighted by $e^{\frac{\mathbf{i}}{\hbar} S}$, the action in units of Planck's constant.

The information about the initial and final states are in the boundary conditions on the path integral: we only integrate over paths where $x(t = 0) = x_0, x(t_j = t) = x_f$.

We can turn this into an integral just over real-space configurations (as described above), since the ps only enter quadratically in the exponent. The Gaussian integrals we need to do are:

$$\prod_{i=1}^{N-1} \int_{-\infty}^{\infty} \frac{dp_i}{2\pi\hbar} e^{-\frac{\mathbf{i} dt}{2m\hbar} p_i^2 - \frac{\mathbf{i}}{\hbar} p_i (x_i - x_{i-1})} = \prod_{i=1}^{N-1} \sqrt{\frac{m}{2\pi \mathbf{i} dt}} e^{\frac{\mathbf{i} m (x_i - x_{i-1})^2}{2\hbar dt}} \ .$$

You can check that this gives the formula claimed above in (8), with $\sum_{\text{all paths}} \cdot \equiv \prod_{i=1}^{N-1} dx_i \cdot$.

[Beware factors of $\sqrt{2\pi}$ in the measure. Exercise: restore all factors of $\hbar$.]

The path integral solves the Schrödinger equation

Consider the wave function $\psi(y, t) = \langle y | \psi(t) \rangle$. y here is just a value of x.

At the next time-step $t + dt$ it evolves to

$$\psi(x, t + dt) = \langle x | \mathbf{U}(dt) \underbrace{\cdot}_{\mathbb{1} = \int dy |y\rangle\langle y|} |\psi(t)\rangle = \int dy \underbrace{\langle x | \mathbf{U}(dt) |y\rangle}_{U(x, t+dt; y, t)} \psi(y, t). \tag{12}$$

So we need the propagator for one time step, which we have seen in (10). Let's redo the manipulation which gets rid of the p integrals for just this one time step:

$$
\begin{aligned}
U(x, t + dt; y, t) &= \langle y | e^{-\frac{i}{\hbar}\frac{\mathbf{p}^2}{2m}} | x \rangle \, e^{-\frac{i}{\hbar}dt V(x)} = \int dp \langle y | p \rangle \langle p | x \rangle e^{-\frac{i}{\hbar}dt\frac{p^2}{2m}} e^{-\frac{i}{\hbar}dt V(x)} \\
&= \int \frac{dp}{2\pi} e^{-ipy + ipx} e^{-idt\frac{p^2}{2m}} e^{-idt V(x)} = \sqrt{\frac{m}{2\pi i dt}} e^{\frac{im}{2\hbar dt}(x-y)^2 - idt V(x)} \;.
\end{aligned}
$$

Now let's plug this into (12). Change integration variables $y = x + \eta, dy = d\eta$.

$$\psi(x, t + dt) = \int d\eta \frac{1}{Z} e^{\frac{idt}{\hbar}\left(m\left(\frac{\eta}{dt}\right)^2 - V(x, t)\right)} \left(\psi(x) + \eta\psi'(x) + \frac{1}{2}\eta^2\psi''(x) + \ldots\right)$$

The normalization constant is $Z = \sqrt{\frac{2\pi i dt}{m}}$. So, keeping terms to first order in dt and doing the gaussian integrals over η, we have

$$\psi(x, t) + dt \partial_t \psi(x, t) = \psi(x, t) - \frac{i dt}{\hbar} V(x, t)\psi(x, t) - \frac{\hbar dt}{2im}\partial_x^2 \psi(x, t).$$

This means

$$-\frac{\hbar}{i}\partial_t \psi = \mathbf{H}\psi.$$

So here's a fancy way to think about the path integral: it is a formal solution of the Schrödinger equation.

2.4.3 Classical mechanics (and WKB) from stationary-phase configurations

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Aside: The Saddle Point Method

Consider an integral of the form above

$$I = \int dx \ e^{-Nf(x)}$$

where $N \gg 1$ is a big number and $f(x)$ is a smooth function. As you can see from the example in the figure (where N is only 10), $e^{-Nf(x)}$ is hugely peaked around the absolute minimum of $f(x)$, which I'll call x_0. We can get a good approximation to the integral by just considering a region near $x = x_0$, and Taylor expanding $f(x)$ about this point:

$$f(x) = f(x_0) + \frac{1}{2}(x - x_0)^2 f''(x_0) + \dots$$

where there's no linear term since x_0 is a critical point, and we assume a minimum $f''(x_0) > 0$. It is also important that $x = x_0$ is in the range of integration. Then

$$I = \int dx e^{-Nf(x)} \approx \int dx e^{-N\left(f(x_0) + \frac{1}{2}(x-x_0)^2 f''(x_0) + \dots\right)}$$

Figure 1: Top: $f(x) = (x^2 - 1)^2 - \frac{1}{2}x^3$. Bottom: $e^{-Nf(x)}$ with $N = 10$.

$$= e^{-Nf(x_0)} \int dy e^{-\frac{N}{2}f''(x_0)y^2 + \dots} \approx e^{-Nf(x_0)}\sqrt{\frac{2\pi}{Nf''(x_0)}}.$$

The important bit is that the integral is well-approximated by $e^{-Nf(x_0)}$, *i.e.* just plugging in the value at the critical point. (Actually, for values of N as small as I've chosen in the example, the bit with the f'' is important for numerical accuracy; for the example in the figure, including this factor, the saddle point method gives $\int_{-2}^{2} dx e^{-Nf(x)} = 206.7$, while numerical integration gives 209.3. Without the gaussian integral correction, saddle point gives 816.6. For values of $N \sim 10^{24}$ we can just keep the leading term.)

Now, I claim that this kind of trick also works for integrals of the form

$$I = \int dx e^{iNf(x)} \ . \tag{13}$$

Then it has a different name: 'stationary phase'. The description of why it works is slightly different. Recall that $\int_0^{2\pi} d\theta e^{i\theta} = 0$; thinking of complex numbers as 2d vectors, this vanishes because we are adding up arrows pointing in all directions. They interfere destructively.
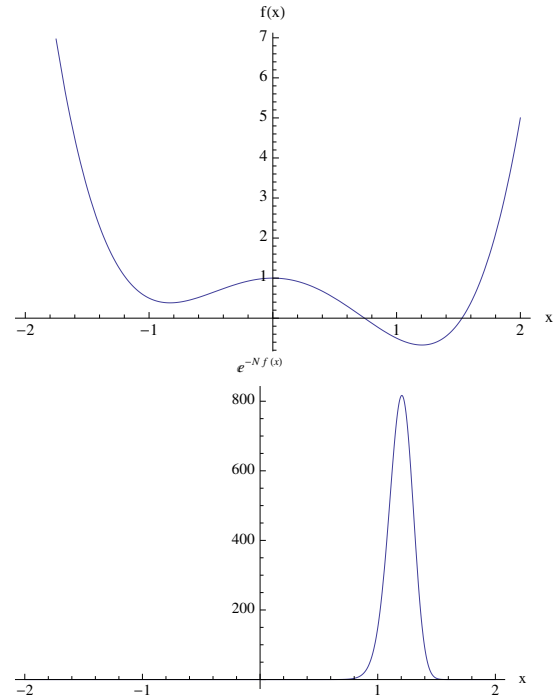
If $f'(x) \neq 0$, the phase in (13) is rapidly varying as x varies, and the phase goes around many times, and the sum of arrows goes nowhere. Only when $f'(x) = 0$ (when the phase is stationary) do the arrows point in the same direction and add together. So the biggest contributions to the integral come from the values of x where $f'(x) = 0$. The contribution is proportional to $e^{iNf(x_0)}$.

The analog of the gaussian integral correction above is now:

$$\int du e^{i\alpha u^2} = \sqrt{\frac{\pi}{\alpha}} e^{i\pi/4}.$$

(You may recall this $\pi/4$ from WKB.)

The thing that will play the role of the large number N will be $1/\hbar$. The stationary-phase approximation in this context is called the semi-classical approximation.

Calculus of Variations

To apply the previous discussion to the path integral, we need to think about functionals – things that eat functions and give numbers – and how they vary as we vary their arguments.

The basic equation of the calculus of variations is:

$$\frac{\delta x(t)}{\delta x(s)} = \delta(t-s).$$

This the statement that $x(t)$ and $x(s)$ for $t \neq s$ are independent. From this rule and integration by parts we can get everything we need. For example, let's ask how does the potential term in the action $S_V[x] = \int dt V(x(t))$ vary if we vary the path of the particle. Using the chain rule, we have:

$$\delta S_V = \int ds \delta x(s) \frac{\delta \int dt V(x(t))}{\delta x(s)} = \int ds \delta x(s) \int dt \partial_x V(x(t)) \delta(t-s) = \int dt \delta x(t) \partial_x V(x(t)).$$

We could rewrite this information as :

$$\frac{\delta \int dt V(x(t))}{\delta x(s)} = V'(x(s)).$$

[12] What about the kinetic term $S_T[x] \equiv \int dt \frac{1}{2} m \dot{x}^2$? Here we need integration by parts:

$$\frac{\delta}{\delta x(s)} S_T[x] = \frac{2}{2} m \int dt \dot{x}(t) \partial_t \frac{\delta x(t)}{\delta x(s)} = m \int dt \dot{x}(t) \partial_t \delta(t-s) = -m \int dt \ddot{x}(t) \delta(t-s) = -m \ddot{x}(s).$$

---

[12] If you are unhappy with thinking of what we just did as a use of the chain rule, think of time as taking on a discrete set of values t_i (this is what you have to do to define calculus anyway) and let $x(t_i) \equiv x_i$. Now instead of a functional $S_V[x(t)]$ we just have a function of several variables $S_V(x_i) = \sum_i V(x_i)$. The basic equation of calculus of variations is even more obvious now:

$$\frac{\partial x_i}{\partial x_j} = \delta_{ij}$$

and the manipulation we did above is

$$\delta S_V = \sum_j \delta x_j \partial_{x_j} S_V = \sum_j \delta x_j \partial_{x_j} \sum_i V(x_i) = \sum_j \sum_i \delta x_j V'(x_i) \delta_{ij} = \sum_i \delta x_i V'(x_i).$$

So: the stationary phase condition for our path integral is

$$0 = \delta S = \int dt \delta x(t) \frac{\delta S}{\delta x(t)}$$

Since this must be true for all $\delta x(t)$, this is equivalent to

$$0 = \frac{\delta S}{\delta x(t)},$$

which for the free particle is

$$0 = \frac{\delta S}{\delta x(t)} = -m\ddot{x}(t) - V'(x(t)) \tag{14}$$

which you recognize as Newton's law.

In classical mechanics, we just care about one trajectory, the one satisfying the classical equations of motion, (14). In QM, we must sum over all trajectories, but the trajectories satisfying the classical equations of motion are special: the classical paths (paths near which the variation of the action is small compared to $\hbar$) make contributions that interfere constructively. Sometimes they dominate.

The approximation we get to the wave function from stationary phase is the WKB approximation:

$$\psi_{\text{WKB}}(x,t) = \frac{C}{\sqrt{|p(x)|}} e^{\frac{i}{\hbar} S(x,t)} \; .$$

In this expression,

$$S(x,t) = \int_0^t ds L(x,\dot{x})|_{\underline{x}|x(0)=x_0,x(t)=x} \quad ,$$

p is determined by $x, \dot{x}$ (as $p = \frac{\delta S}{\delta x(t)}$), and C is a normalization constant.

I have described this in terms of a solution $\underline{x}$ with fixed boundary conditions at $0, t$; it is more useful to have an expression for the wave function of a definite energy. This is obtained as follows (basically another Legendre transform, using $L = p\dot{x} - H$):

$$S(x,t) = \int_0^t ds \left(p \frac{dx}{dt} - H \right)|_{\underline{x}|x(0)=x_0,x(t)=x} = \int_{x_0}^x p(x')dx' - E(t - t_0)$$

Here E is given by $E = H(x,p) = \frac{p^2}{2m} + V(x)$. We can solve this for $p(x)$:

$$p(x) \equiv \sqrt{2m\left(E - V(x)\right)}$$

so the WKB wave function is

$$\psi_{\text{WKB}}(x,t) = \frac{C}{\sqrt{|p(x)|}} e^{\frac{i}{\hbar} \int_{x_0}^x p(x')dx' - Et} \; .$$

which you have seen in Chapter 8 of Griffiths. (You can also get this expression by plugging the ansatz $\psi(x) = e^{\frac{i}{\hbar} S(x)}$ into the Schrödinger equation and solving order-by-order in $\hbar$.)

[End of Lecture 16]