Week 1: Linear vector spaces and operators. Wave functions and state vectors.

- **Obtain the spectral decomposition of a state vector or wave function with respect to an arbitrary basis set: discretely and continuously labeled elements.**

  The abstract notion of a state vector or wave function can be labeled by some ket, $|\psi\rangle$. Expanding this in terms of basis sets requires getting the inner product with a complete basis, for example: in the discrete case, we label the basis set by $|n\rangle$. Then,

$$\langle n|\psi\rangle = \psi_n = \sum_n c_n |\psi_n\rangle \tag{1}$$

  while for continuous bases, such as $|\mathbf{x}\rangle$, we require the sum to be an integral:

$$\langle \mathbf{x}|\psi\rangle = \psi_\alpha(\mathbf{x}) = \int c(\alpha) w_\alpha(\mathbf{x}) d\alpha \tag{2}$$

■

- **Use inner products to perform basis transformations.**

  To perform basis transformations, we first assume that a state vector $|\psi\rangle$ can be expanded in one, such as $|m\rangle$. Then we write this expansion with the help of equation (1).

  To change basis, we insert an identity operator, which can be written in terms of some basis as an outer product of that basis, e.g. for a basis $|n\rangle$, $\hat{I}$ can be written as

$$\hat{I} = \sum_n |n\rangle\langle n| \tag{3}$$

  Then our change of basis looks like

$$|\psi\rangle = \hat{I}|\psi\rangle = \sum_m |m\rangle\langle m|\psi\rangle = \sum_m \psi_m |m\rangle \tag{4}$$

$$= \sum_n \sum_m |n\rangle\langle n|m\rangle\langle m|\psi\rangle = \sum_n \sum_m |n\rangle \delta_{nm} \langle m|\psi\rangle \tag{5}$$

$$= \sum_n |n\rangle\langle n|\psi\rangle = \sum_n \psi_n |n\rangle \tag{6}$$

■

- **Explain how commuting observables can be used to generate additional quantum numbers to label degenerate states.**

  We know that commuting observables $\hat{A}$ and $\hat{B}$ have simultaneous eigenvalues that allow us to precisely measure their outcomes simultaneously. This allows the construction of joint eigenstates, which may be complete and orthonormal when both observables have nondegenerate eigenvalues.

  If one of them, say $\hat{A}$, has degenerate eigenvalues, the joint eigenstates of both observables is not complete. We can then introduce a third operator, say $\hat{C}$, that commutes with both $\hat{A}$ and $\hat{B}$, that generates additional quantum numbers to make the joint eigenstates of all three complete. If there's still degeneracy, we can repeat the process until the CSCO is formed.

- **Establish the link between quantum states and elements of a Hilbert space; observables and Hermitian operators.**

  Quantum states, corresponding to the classical notion of a state that can be described as a single point in phase space, can now be represented by state vectors $|\psi\rangle$, a single point in the Hilbert space with unit length represented by the normalization $\langle\psi|\psi\rangle = 1$, where $\langle\psi|$ is the corresponding dual vector of the ket.

  Observables, on the other hand, can be represented by Hermitian operators; in some arbitrary basis, they can be matrix operators that would amount to having Hermitian properties, such as $A^\dagger = A$.

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Week 2: Postulates of Quantum Mechanics. Position and translation (generators). Momentum.

- **Review the core postulates of quantum mechanics.** We enumerate the postulates of quantum mechanics to complement the last bullet of **Week** 1:

  1. We associate closed systems with a Hilbert space. Then the state of the system can be described by a (normalized) state vector (or ket).
  2. The time evolution of any closed system can then be associated with a unitary operator, s.t.

  $$|\psi(t)\rangle = \hat{U}(t - t_0)\,|\psi(t_0)\rangle \tag{7}$$

  where $\hat{U}$ is defined as

  $$\hat{U}(t - t_0) \equiv \exp\left(-\frac{i}{\hbar}(t - t_0)\hat{H}\right) \tag{8}$$

  and $\hat{H}$ is the Hermitian operator. Definition (8) satifies unitarity and reduction to the identity operator when $t = t_0$. It also satisfies the composition property, for which $U(t_2 - t_1)U(t_1 - t_0) = U(t_2 - t_0)$.

3. For the observables we explained in the earlier bullet, we can only measure the eigenvalues of its operator representation. Thus, for every $\hat{A}$ operator corresponding to a physical observable A, the only results of a measurement would be its eigenvalues.

Other postulates follow from these three, such as the definition of a density operator, the expectation value of any operator, and the projection postulate.

- **Use an infinitesimal translation operator and its postulated properties to identify momentum as a generator of translations.**

  Recall the action of a translation operator on some basis $|x\rangle$ with parameter a as its displaced length:

$$T(a)\,|x\rangle = |x + a\rangle \tag{9}$$

  We then expand this in terms of small a via Taylor series:

$$T(a) = T(0) + a\frac{dT}{da}\bigg|_{a=0} + \dots \tag{10}$$

  where the first term is just the identity operator, and that $\dfrac{dT}{da}(0)$ can be classified as an operator with no parameters. We conveniently define

$$\hat{p} \equiv i\hbar\frac{dT}{da}(0) \tag{11}$$

  To prove that this operator is a Hermitian just like T, we rewrite the expansion for T as $T(a) = 1 - (i/\hbar)a\hat{p} + \dots$. Then, for Hermitian T, we get $T^\dagger = 1 + (i/\hbar)a\hat{p}^\dagger + \dots$ and $T^{-1} = T(-a) = 1 + (i/\hbar)a\hat{p} + \dots$ which should be equal, thus prompting $\hat{p}^\dagger = \hat{p}$, or that the operator $\hat{p}$ is a Hermitian one. We can then say that $\hat{p}$ is an infinitesimal translation for small a: a generator of translations.

- **Perform a change of basis (Fourier transformation) to relate the coordinate space wavefunction $\langle\mathbf{x}|\psi\rangle$ and the momentum space wavefunctions $\langle\mathbf{p}|\psi\rangle$.**

$$\langle\mathbf{x}|\psi\rangle = \psi(\mathbf{x}) = \int d\mathbf{p}\,\langle\mathbf{x}|\mathbf{p}\rangle\langle\mathbf{p}|\psi\rangle \tag{12}$$

$$= \int d\mathbf{p}\; e^{i\mathbf{p}\cdot\mathbf{x}/\hbar}\langle\mathbf{p}|\psi\rangle = \int d\mathbf{p}\; e^{i\mathbf{p}\cdot\mathbf{x}/\hbar}\psi(\mathbf{p}) = \mathcal{F}[\psi(\mathbf{x})] \tag{13}$$

■

Week 3: Time Evolution. Heisenberg picture. Coherent states.

- **Determine the time development of states in the Schrodinger picture.**

  From equation (7), and the arguments used for equations (9)-(11), it's straightforward to derive the time development of states. We also consider an infinitesimal time operator $U(t+\epsilon, t)$ having the same properties as that of definition (8). We expand U in a similar manner as equation (10):

$$U(t+\epsilon, t) = U(t' = t, t) + \epsilon \frac{\partial U}{\partial \epsilon}(t' = t, t) + \dots \tag{14}$$

$$U(t+\epsilon, t) = 1 - \frac{i}{\hbar}\epsilon \hat{H}(t' = t, t) + \dots \tag{15}$$

  where we conveniently defined $\hat{H} \equiv i\hbar \frac{\partial U}{\partial t'}\Big|_{t'=t}$. Now we want to calculate this derivative with respect to the final time in order to obtain a differential equation that will serve as the time evolution for states.

  Using the definition of the derivative,

$$\frac{\partial U(t, t_0)}{\partial t} = \lim_{\epsilon \to 0} \frac{U(t+\epsilon, t_0) - U(t, t_0)}{\epsilon} \tag{16}$$

  Using the composition property, we can expand $U(t+\epsilon, t_0) = U(t+\epsilon, t)U(t, t_0)$ in order to get $U(t, t_0)$ out of the limits:

$$\frac{\partial U(t, t_0)}{\partial t} = U(t, t_0) \lim_{\epsilon \to 0} \frac{U(t+\epsilon, t) - 1}{\epsilon} = U(t, t_0) \lim_{\epsilon \to 0} \frac{U(t+\epsilon, t) - U(t, t)}{\epsilon} \tag{17}$$

  where we immediately recognize the derivative of U with respect to t' as evaluated at $t' = t$, which is exactly $-i\hat{H}/\hbar$. we can rewrite the previous equation as

$$\frac{\partial U(t, t_0)}{\partial t} = -\frac{i}{\hbar}\hat{H}(t)U(t, t_0) \tag{18}$$

  We then differentiate equation (7) with respect to t and apply the previous equation to obtain Schrodinger's equation:

$$i\hbar \frac{\partial U(t, t_0)}{\partial t} = \hat{H}(t)U(t, t_0) \tag{19}$$

$$\boxed{i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle = \hat{H}(t) |\psi(t)\rangle} \tag{20}$$

  We see that if the Hamiltonian is time-dependent, we can recover equation (8).

- **Determine the time development of operators in the Heisenberg picture.**

  We then contrast the previous discussion on the time evolution of states with the time evolution of operators. If $A_S(t)$ is a non-evolving operator in the Schrodinger picture, its corresponding operator in the Heisenberg picture is given by

$$A_H(t) = U(t,t_0)^\dagger A_S(t) U(t,t_0) \tag{21}$$

  where $U(t,t_0)$ and its corresponding transpose is the same U operator we've been playing with in the Schrodinger picture. We then take the time derivative of both sides to get

$$i\hbar \frac{dA_H}{dt} = i\hbar \left(\frac{\partial U^\dagger}{\partial t} A_S U + U^\dagger \frac{\partial A_S}{\partial t} U + U^\dagger A_S \frac{\partial U}{\partial t} \right) \tag{22}$$

$$= -U^\dagger H A_S U + i\hbar U^\dagger \frac{\partial A_S}{\partial t} U + U^\dagger A_S H U \tag{23}$$

  where we used the Schrodinger equation for U (equation (19)) and its adjoint, $-i\hbar \dfrac{\partial U(t,t_0)^\dagger}{\partial t} = U(t,t_0)^\dagger \hat{H}(t)$. We then insert the product of operators $UU^\dagger$ in between HA_S and $A_S H$ of the first and third terms to obtain the Heisenberg equivalents for each operator, $H_H \equiv U^\dagger H U$ and $A_H \equiv U^\dagger A_S U$. We then notice that these first and third terms can be rewritten in terms of the Poisson bracket, so that

$$\boxed{i\hbar \frac{\partial A_H}{\partial t} = [A_H, H_H] + i\hbar \left(\frac{\partial A}{\partial t} \right)_H} \tag{24}$$

  where the last term means that we differentiate A_S first before converting the differentiated term into the Heisenberg picture. This is then Heisenberg's equation of motion for operators.

- **Construct coherent (Glauber) states. Calculate the expectation values of position and momentum in these states.**

  Our knowledge of the raising ($a^\dagger$) and lowering (a) operators allows us to construct coherent states. For example, we can write a coherent state $|\lambda\rangle$ in terms of the basis of harmonic oscillator energy eigenkets $|n\rangle$ by calculating $\langle n|\lambda\rangle$. We obtain the form of $|n\rangle$ and $\langle n|$ from the repeated application of $a^\dagger$, until we obtain $|0\rangle$:

$$a^\dagger |n\rangle = \sqrt{n+1}\, |n+1\rangle \tag{25}$$

$$|n\rangle = \frac{(a^\dagger)^n}{\sqrt{n!}} |0\rangle \tag{26}$$

Getting the adjoint of both sides of equation (2) yields

$$\langle n| = \langle 0| \frac{a^n}{\sqrt{n!}} \tag{27}$$

Now we are ready to calculate $\langle n|\lambda\rangle$:

$$\langle n|\lambda\rangle = \langle 0|\frac{a^n}{\sqrt{n!}}|\lambda\rangle \tag{28}$$

Then we use the fact that coherent states satisfy $a\,|\lambda\rangle = \lambda\,|\lambda\rangle$ to get rid of the operator:

$$\langle n|\lambda\rangle = \frac{\lambda^n}{\sqrt{n!}}\langle 0|\lambda\rangle \tag{29}$$

How do we solve for $\langle 0|\lambda\rangle$? We use the completeness relation for $|n\rangle$ (since the set of $|n\rangle$ is a complete set of states) to extract $|\lambda\rangle$ from (5):

$$|\lambda\rangle = \sum_{n=0}^{\infty} |n\rangle\langle n|\lambda\rangle = \langle 0|\lambda\rangle \sum_{n=0}^{\infty} \frac{\lambda^n}{\sqrt{n!}}\,|n\rangle \tag{30}$$

We normalize $|\lambda\rangle$ such that $\langle\lambda|\lambda\rangle = 1$ and $\langle n|n\rangle = 1$, so that

$$\langle z|z\rangle = |\langle 0|\lambda\rangle|^2 \sum_{n=0}^{\infty} \frac{|\lambda|^{2n}}{n!} = 1 \tag{31}$$

The summation is equivalent to $e^{|\lambda|^2}$, so that

$$\langle 0|\lambda\rangle = \exp\left(-\frac{|\lambda|^2}{2}\right) \tag{32}$$

Thus, (5) becomes

$$\boxed{\langle n|\lambda\rangle = \frac{\lambda^n}{\sqrt{n!}} \exp\left(-\frac{|\lambda|^2}{2}\right)} \tag{33}$$

Next, we can calculate the expectation values of $\hat{x}$ and $\hat{p}$ by rewriting the definitions of the raising and lowering operators as follows: take the raising and lowering operator definitions

$$a = \frac{1}{\sqrt{2m\hbar\omega}}\left(m\omega\hat{x} + i\hat{p}\right) \tag{34}$$

$$a^\dagger = \frac{1}{\sqrt{2m\hbar\omega}}\left(m\omega\hat{x} - i\hat{p}\right) \tag{35}$$

Reverting these equations to solve for $\hat{x}$ and $\hat{p}$, we get

$$\hat{x} = \left(\frac{\hbar}{2m\omega}\right)^{1/2}\left(a + a^\dagger\right) \tag{36}$$

$$\hat{p} = i\left(\frac{m\hbar\omega}{2}\right)^{1/2}\left(a^\dagger - a\right) \tag{37}$$

to get the expectation values of these operators, we let them act on $|\lambda\rangle$:

$$\langle\hat{x}\rangle = \langle\lambda|\hat{x}|\lambda\rangle = \left(\frac{\hbar}{2m\omega}\right)^{1/2}\langle\lambda|\left(a + a^\dagger\right)|\lambda\rangle \tag{38}$$

$$= \left(\frac{\hbar}{2m\omega}\right)^{1/2}\left(\lambda + \lambda^*\right) \tag{39}$$

and

$$\langle\hat{p}\rangle = \langle\lambda|\hat{p}|\lambda\rangle = i\left(\frac{m\hbar\omega}{2}\right)^{1/2}\langle\lambda|\left(a^\dagger - a\right)|\lambda\rangle \tag{40}$$

$$= i\left(\frac{m\hbar\omega}{2}\right)^{1/2}\left(\lambda^* - \lambda\right) \tag{41}$$

where we used the eigenket (and eigenbra) relationship between a and λ in trying to expand (14) and (16),

$$a\,|\lambda\rangle = \lambda\,|\lambda\rangle \tag{42}$$

$$\langle\lambda|\,a^\dagger = \langle\lambda|\,\lambda^*. \tag{43}$$

To get the time dependence of these expectation values, we first evolve equation (6) in time by adding a factor of $\exp(-iE_nt/\hbar)$ to the summation in n:

$$|\lambda, t\rangle = \exp\left(-\frac{|\lambda|^2}{2}\right) \sum_{n=0}^{\infty} \frac{\lambda^n}{\sqrt{n!}} \exp\left(\frac{-iE_n t}{\hbar}\right) |n\rangle \tag{44}$$

For the energy eigenvalues $E_n = \hbar\omega\left(n + \frac{1}{2}\right)$, we expand and simplify $|\lambda, t\rangle$:

$$|\lambda, t\rangle = e^{-|\lambda|^2/2} e^{-i\omega t/2} \sum_{n=0}^{\infty} \frac{\left(\lambda e^{-i\omega t}\right)^n}{\sqrt{n!}} |n\rangle = \exp\left(\frac{-i\omega t}{2}\right) \left|\lambda e^{-i\omega t}\right\rangle \tag{45}$$

where we used equation (6). We can then recast the calculated expectation values as follows:

$$\langle \hat{x}(t) \rangle = \left(\frac{\hbar}{2m\omega}\right)^{1/2} \left(\lambda e^{-i\omega t} + \lambda^* e^{i\omega t}\right) = \left(\frac{2\hbar}{m\omega}\right)^{1/2} \mathrm{Re}\left(\lambda e^{-i\omega t}\right) \tag{46}$$

$$\langle \hat{p}(t) \rangle = i\left(\frac{m\hbar\omega}{2}\right)^{1/2} \left(\lambda^* e^{i\omega t} - \lambda e^{-i\omega t}\right) = (2m\hbar\omega)^{1/2} \mathrm{Im}\left(\lambda e^{-i\omega t}\right). \tag{47}$$

Furthermore, if we substitute $\lambda = |\lambda| e^{i\delta}$, we can further recast the above equations as

$$\langle \hat{x}(t) \rangle = \left(\frac{2\hbar}{m\omega}\right)^{1/2} |\lambda| \cos(\omega t - \delta) \tag{48}$$

$$\langle \hat{p}(t) \rangle = -(2m\hbar\omega)^{1/2} |\lambda| \sin(\omega t - \delta) \tag{49}$$

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Week 4: Schrodinger's wave equation. Hamilton-Jacobi formulation. WKB approximation.

- **Identify the classical analogs of the amplitude and phase of a wavefunction in a Hamilton-Jacobi formulation.**

  In the WKB formulation, we immediately assert that the solution to the Schrodinger wave equation as

$$\psi(x) = A(x) \exp\left(\frac{i}{\hbar} S(x)\right) \tag{50}$$

  We rewrite this in order to make the amplitude unity by bringing up A to the exponential:

$$\psi(x) = \exp\left[\frac{i}{\hbar}(S(x) - i\hbar \ln A(x)\right] \tag{51}$$

$$\equiv \exp\left[\frac{i}{\hbar}W(x)\right] \tag{52}$$

where $W(x)$ is the full expansion (in $\hbar$) of the exponent, for which $W(x) = W_0(x) + \hbar W_1(x) + \hbar^2 W_2(x) + \ldots$. We can then identify that $W_0(x) = S(x)$ and $W_1(x) = -i \ln A(x)$. Substituting to the time-independent Schrodinger's equation in coonfiguration space,

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V(x)\psi(x) = E\psi(x) \tag{53}$$

$$-\frac{\hbar^2}{2m}\left[\frac{-1}{\hbar^2}\left(\frac{dW}{dx}\right)^2 e^{iW(x)/\hbar} + \frac{i}{\hbar}e^{iW(x)/\hbar}\frac{d^2W}{dx^2}\right] + Ve^{iW(x)/\hbar} = Ee^{iW(x)/\hbar} \tag{54}$$

$$\frac{1}{2m}\left(\frac{dW}{dx}\right)^2 - \frac{i\hbar}{2m}\frac{d^2W}{dx^2} + V = E \tag{55}$$

We then expand W in terms of $\hbar$, so that for $\hbar \to 0$, we recover the classical case. At order $\hbar^0$, we get

$$\frac{1}{2m}\left(\frac{dW_0}{dx}\right)^2 + V(x) = E \to \frac{1}{2m}\left(\frac{dS}{dx}\right)^2 + V(x) = E \tag{56}$$

We recall the Hamilton-Jacobi equation in one-dimension from classical mechanics

$$\frac{1}{2m}\left(\frac{dS}{dx}\right)^2 + V(x) = E \tag{57}$$

so we see that the derivative of S (the phase) is the classical momentum.

At order $\hbar^1$, we have

$$\frac{1}{2m}\left(\frac{d}{dx}(W_0 + \hbar W_1 + \ldots)\right)^2 - \frac{i\hbar}{2m}\frac{d^2}{dx}(W_0 + \hbar W_1 + \ldots) = 0$$

$$\frac{1}{2m}\left[\left(\frac{dW_0}{dx}\right)^2 + 2\hbar\frac{dW_0}{dx}\frac{dW_1}{dx} + \hbar^2\left(\frac{dW_1}{dx}\right)^2\right] - \frac{i}{2m}\frac{d^2W_0}{dx^2} = 0 \tag{58}$$

Substituting W_0 and W_1 as defined earlier, we get

$$\frac{-i}{m}\left[\frac{dS}{dx}\frac{d}{dx}\ln A\right] - \frac{i}{2m}\frac{d^2S}{dx^2} = 0 \tag{59}$$

Multiplying both sides by $2A^2$ and using $v(x) \equiv p(x)/m = 1/mdS/dx$ as well as $d\ln A/dx = 1/AdA/dx$, we get

$$v\left(2A\frac{dA}{dx}\right) + A^2\frac{dv}{dx} = 0 \tag{60}$$

$$\frac{d}{dx}\left(A^2\frac{dv}{dx}\right) = 0 \tag{61}$$

which is reminiscent of the one-dimensional version of the amplitude-transport equation

$$\frac{d}{dx}\left(A^2\frac{dS}{dx}\right) = 0 \tag{62}$$

so that we can easily identify the purpose of both A and S: $A(x)^2$ is the same as the quantum probability density $\psi^*\psi$ in the WKB approximation with form $A(x) = \text{const.}/\sqrt{p(x)}$, and the action $S(x) = \int_{x_0}^{x} p(x')\,dx'$ is the area between the x-axis and the upper part of the classical orbit in phase space.

- **Set up the WKB connection formulas to be able to approximate the energy eigenvalues in (spatially) slowly-varying potentials.**

  Therefore, from the previous bullet we are able to show that the Schrodinger equation follows the classical Hamilton-Jacobi equation for small $\hbar$. We now use this for the case of a spatially slowly-varying potential, as seen in figure 1

  Together with the appropriate substitutions for $S(x)$ and $A(x)$, there will be three distinct solutions to the general WKB solution for the Hamilton-Jacboi equation. In region I of figure 1, the classically permitted region allows for wave functions that oscillate classically, such that

$$\psi_{\text{I}}(x) = c_r\frac{\exp(iS(x)/\hbar)}{\sqrt{p(x)}} + c_\ell\frac{\exp(-iS(x)/\hbar)}{\sqrt{-p(x)}} \tag{63}$$

  and for the classically forbidden region II, we want the wave function to behave as an exponentially decaying one (cf. tunneling), such that if we define $K(x) \equiv -iS(x) = \int_{x_r}^{x}\sqrt{2m[V(x') - E]}dx'$, we get

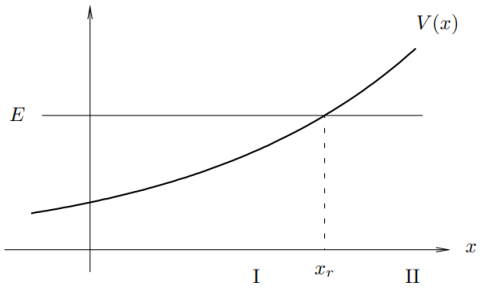

Figure 1: A spatially slowly-varying potential $V(x)$. Here we designate x_r as the turning point for particles with energy E.

$$\psi_{\text{II}}(x) = c_g \frac{\exp(K(x)/\hbar)}{\sqrt{|p(x)|}} + c_d \frac{\exp(-K(x)/\hbar)}{\sqrt{|-p(x)|}} \tag{64}$$

therefore we have for constants, c_r (wave going to the right), c_ℓ (wave going to the left), c_g (exponentially growing to the right), and c_d (exponentially decaying to the right). Recalling that the Schrodinger equation is a 2nd order DE only, we suspect that there must be some dependence between the coefficients. We determine these so-called connection rules in order to show the dependence.

We also show the third distinct solution: the connection that would make the two solutions valid near the turning point. We then show this solution by linearly approximating the potential near the turning point using Taylor series, which would turn the Schrodinger equation into an Airy differential equation:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V'(x_r)(x - x_r)\psi = 0 \tag{65}$$

where, if we let $x = x_r + az$, $a = \left(\dfrac{\hbar^2}{2mV'(x_r)}\right)^{1/3}$, we can convert the equation into a nice-looking one:

$$\frac{d^2\psi}{dz^2} - z\psi = 0 \tag{66}$$

with a general solution

$$\psi_{\text{tp}}(z) = c_a\ \text{Ai}(z) + c_b\ \text{Bi}(z) \tag{67}$$

We proceed to connect by using the asymptotic forms of Ai and Bi functions for $z << 0$,

$$\begin{aligned}\mathrm{Ai}(z) &= \frac{1}{\sqrt{\pi}(-z)^{1/4}}\cos\alpha(z)\\ \mathrm{Bi}(z) &= \frac{1}{\sqrt{\pi}(-z)^{1/4}}\sin\alpha(z)\end{aligned} \tag{68}$$

where $\alpha(z) = -\frac{2}{3}(-z)^{3/2} + \frac{\pi}{4}$ which would allow us to recast ψ_{tp} in the same form as ψ_{I}. Using algebra, we end up proving that the phases must be equal (albeit a shift of $\pi/4$ s.t. $\alpha(z) = S(x)/\hbar + \pi/4$), and that the connection formulas only relate the amplitudes, as given by

$$\begin{aligned}\frac{1}{2\sqrt{\pi}}(c_a - ic_b) &= \sqrt{\frac{a}{\hbar}}c_r, \qquad a = \left(\frac{\hbar^2}{2mV'(x_r)}\right)^{1/3}\\ \frac{1}{2\sqrt{\pi}}(c_a + ic_b) &= \sqrt{\frac{a}{\hbar}}c_\ell\end{aligned} \tag{69}$$

while in the other end, for $z >> 0$, we have an exponential asymptote for the Airy functions,

$$\begin{aligned}\mathrm{Ai}(z) &= \frac{1}{2\sqrt{\pi}z^{1/4}}\exp(-\beta(z)), \qquad \beta(z) = \frac{2}{3}z^{3/2}\\ \mathrm{Bi}(z) &= \frac{1}{\sqrt{\pi}z^{1/4}}\exp(\beta(z))\end{aligned} \tag{70}$$

so that we could connect it to ψ_{II}:

$$\begin{aligned}\frac{1}{2\sqrt{\pi}}c_a &= \sqrt{\frac{a}{\hbar}}c_d\\ \frac{1}{\sqrt{\pi}}c_b &= \sqrt{\frac{a}{\hbar}}c_g\end{aligned} \tag{71}$$

By eliminating c_a and c_b in equations (71) and (73), we get the connection between c_r, c_ℓ and c_d, c_g.

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Week 6: Propagators, Feynman path integrals.

- **Recognize the propagator as a Green's function and integral kernel.**

  We define the propagator as a function of two space-time points s.t.

$$K(x,t;x',t') \equiv \langle x|U(t,t')|x'\rangle \tag{72}$$

  where we used the time evolution operator $U(t,t')$ with properties $U(t',t') = 1$ and $U(t,t')^{-1} = U(t,t')^\dagger$. We see then that if we set $t = t'$,

$$K(x,t';x',t') = \langle x|x'\rangle = \delta(x-x') \tag{73}$$

  We also recall that time evolution operator has a differential equation (19). We then use this to evolve the propagator in time:

$$\begin{aligned} i\hbar\frac{\partial K(x,t;x',t')}{\partial t} \rightarrow \langle x|i\hbar\frac{\partial U(t,t')}{\partial t}|x'\rangle &= \langle x|\hat{H}(t)U(t,t')|x'\rangle = \hat{H}(t)\langle x|U(t,t')|x'\rangle \\ &= \left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x,t)\right]K(x,t;x',t') \end{aligned} \tag{74}$$

  so that K is also a solution of the time-dependent Schrodinger equation, for initial conditions $\psi(x,t') = \delta(x-x')$, which makes it a Green's function.

  We also see that the propagator can show the general solution of the time-dependent Schrodinger equation. It can be easily deduced that the propagator can be an integral kernel due to being a Green's function, but we can also show it by evolving $\psi(x,t)$ from $\psi(x,t')$ and using equation (7):

$$\begin{aligned} \psi(x,t) \rightarrow \langle x|\psi(t)\rangle = \langle x|U(t,t')|\psi(t')\rangle &= \int dx'\ \langle x|U(t,t')|x'\rangle\langle x'|\psi(t')\rangle \\ &= \int dx'\ K(x,t;x',t')\psi(x',t') \end{aligned} \tag{75}$$

- **Write down the propagator as a Feynman path integral.** To write the propagator as a path integral, we need to derive the path integral for a one-dimensional problem with Hamiltonian $H = T + V = \dfrac{p^2}{2m} + V(x)$. This is a time-independent one, so that we can simplify the propagator such that $t' = 0$ and t becomes the elapsed time: $K(x,t;x') = \langle x|U(t)|x'\rangle$. The key to path integration relies on breaking down the time evolution operator into little pieces in time. We break the time interval $[0,t]$ into N intervals with duration ϵ so that $U(t) = [U(\epsilon)]^N$. Then, the time evolution operator for time ϵ is

$$U(\epsilon) = \exp\left(-\frac{i}{\hbar}(T+V)\right) \tag{76}$$

But the kinetic and potential energies do not commute, so that in general, $\exp(T+V) \neq \exp T \ \exp V$. We then proceed to expand $U(\epsilon)$ in a Taylor series manner:

$$U(\epsilon) = 1 - \frac{i}{\hbar}(T+V)\epsilon + \mathcal{O}(\epsilon^2) \tag{77}$$

which is approximately equal to $e^{-i\epsilon T/\hbar}e^{-i\epsilon V/\hbar} + \mathcal{O}(\epsilon^2)$. We raise both sides to N to obtain

$$U(t) = \left[\exp\left(-\frac{i\epsilon}{\hbar}T\right)\exp\left(-\frac{i\epsilon}{\hbar}V\right)\right]^N + \mathcal{O}(1/N) \tag{78}$$

since $\mathcal{O}(\epsilon^2)^N = \mathcal{O}(1/N^2)^N$. Substituting this to the propagator definition, we get

$$K(x,t;x') = \lim_{N\to\infty} \langle x|[e^{-i\epsilon T/\hbar}e^{-i\epsilon V/\hbar}]^N|x'\rangle \tag{79}$$

since there are N factors, we can put $N-1$ identity resolutions $1 = \int dx_i \, |x_i\rangle\langle x_i|$, so that with $x = x_N$,

$$\begin{aligned} K(x,t;x') = \lim_{N\to\infty} &\int dx_1 \ldots dx_{N-1} \\ &\times \langle x_N|e^{-i\epsilon T/\hbar}e^{-i\epsilon V/\hbar}|x_{N-1}\rangle \langle x_{N-1}|\ldots|x_1\rangle \langle x_1|e^{-i\epsilon T/\hbar}e^{-i\epsilon V/\hbar}|x'\rangle \end{aligned} \tag{80}$$

We can then evaluate one of these factors to give a (slightly) closed expression for the integrand. For that specific integrand, we insert an identity resolution in momentum space such that

$$\langle x_{j+1}|e^{-i\epsilon T/\hbar}e^{-i\epsilon V/\hbar}|x_j\rangle = \int dp \langle x_{j+1}|e^{-i\epsilon\hat{p}^2/2m\hbar}|p\rangle \langle p|e^{-i\epsilon V(\hat{x})/\hbar}|x_j\rangle \tag{81}$$

We let the operators act on the eigenstates, where we recall $\hat{p}\,|p\rangle = p\,|p\rangle$, and $\langle x_{j+1}|p\rangle\langle p|x_j\rangle = \frac{1}{2\pi\hbar}\exp\left(\frac{i}{\hbar}p(x_{j+1}-x_j\right)$. Then the integral becomes

$$\langle x_{j+1}|e^{-i\epsilon T/\hbar}e^{-i\epsilon V/\hbar}|x_j\rangle = \frac{1}{2\pi\hbar}\int dp \exp\left[-\frac{i\epsilon}{2m\hbar}p^2 + \frac{i(x_{j+1}-x_j)}{\hbar}p - \frac{i\epsilon}{\hbar}V(x_j)\right] \tag{82}$$

$$= \sqrt{\frac{m}{2\pi i\epsilon\hbar}}\exp\left[\frac{i}{\hbar}\left[\frac{1}{2}m\left(\frac{(x_{j+1}-x_j)}{\epsilon}\right)^2 - V(x_j)\right]\right] \tag{83}$$

which we can insert back into the fray of a product of exponentials, for which the product becomes a sum upon multiplying:

$$\boxed{K(x,t;x') = \lim_{N\to\infty}\left(\frac{m}{2\pi i\epsilon\hbar}\right)^{N/2}\int dx_1\ldots dx_{N-1}\exp\left[\frac{i}{\hbar}\left[\frac{1}{2}m\left(\frac{(x_{j+1}-x_j)}{\epsilon}\right)^2 - V(x_j)\right]\right]} \tag{84}$$

- **Provide examples where a path integral formulation is convenient.**

  (a) Time-dependent potentials

  (b) Electromagnetic fields

  (c) Quantization of gauge fields

  (d) Perturbation expansions in field theory

■

Week 7: Potentials and gauge transformations

- **Describe how the scalar and vector potentials enter the Schrodinger equation for quantum systems in the presence of electromagnetic fields.**

  In order for the effects of the gauge potentials to appear in the context of quantum mechanics, we need to set up an experiment in which a charged particle traverses a constant magnetic field. We recall how the scalar Φ and vector $\mathbf{A}$ potentials are defined from the fields they represent:

$$\mathbf{E} \equiv -\boldsymbol{\nabla}\Phi \tag{85}$$
$$\mathbf{B} \equiv \boldsymbol{\nabla}\times\mathbf{A} \tag{86}$$

  Then, the classical equations of motion happen to be

$$m\ddot{\mathbf{x}} = q\mathbf{E}(\mathbf{x},t) + \frac{q}{c}\dot{\mathbf{x}}\times\mathbf{B}(\mathbf{x},t) \tag{87}$$

  In terms of the Hamiltonian $H = T+V$, we replace these fields with their corresponding potentials by using the Lagrangian that can reproduce the classical equations of motion and then using Legendre transformation to arrive at the Hamiltonian:

$$H = \frac{1}{2m}\left[\mathbf{p} - \frac{q}{c}\mathbf{A}(\mathbf{x},t)\right]^2 + q\Phi(\mathbf{x},t) \tag{88}$$

where $\mathbf{p}$ here is the canonical momentum which we replace by $-i\hbar\nabla$ when converting the Hamiltonian into its corresponding operator form.

We can then insert the operator form of H in the Schrodinger equation freely because of gauge invariance for the Hamiltonian itself.

- **Explain how the Aharanov-Bohm effect can distinguish situations in which a quantum particle confined to an annular cylinder is subject to the vector potential of a magnetic field within the hollow or not.**

  Consider a charged quantum particle inside an annular cylinder. We have shown in the problem set that the Aharonov-Bohm effect ensures that a charged quantum particle will experience a phase shift in its wave function when it's subjected to a solenoid with a nonzero vector potential inside, even if there's no field outside the solenoid.

  Thus, to determine if there's a vector potential inside, we measure the relative phase shift due to the Aharonov-Bohm effect with magnitude $2\pi\varphi/\varphi_0$, where $\varphi_0 \equiv hc/e$ is called the *flux quantum*.

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Week 8: Angular momentum and tensor operators.

- **Identify advanced experimental situations that utilize angular momentum eigenstates.**

  (a) Spectroscopy

  (b) Precession measurements

  (c) Neutron interferometry

- **Construct angular momentum operators as generators of rotations.**

  In order to construct angular momentum operators $U(\mathsf{R})$, we first postulate the properties of these operators:

  (a) Unitary in order to preserve probabilities such that $U(\mathsf{R})^{-1} = U(\mathsf{R})^\dagger$

  (b) Goes back to the identity when the amount of rotation R is just I: $U(\mathsf{I}) = 1$

  (c) The product of two rotations can be written as a product of unitary operators, so that $U(\mathsf{R}_1\mathsf{R}_2) = U(\mathsf{R}_1)U(\mathsf{R}_2)$. This also implies that $U(\mathsf{R}^{-1}) = U(\mathsf{R})^{-1} = U(\mathsf{R})^\dagger$.

  Then, we define the near-identity rotation as one having a small change in the angle so that $\mathsf{R} = \mathsf{I} + \epsilon\mathsf{A}$. Parametrizing R so that $\boldsymbol{\theta} = \theta\hat{\mathbf{n}}$ is a vector of angles that can define the rotation, we get

$$\mathsf{R}(\boldsymbol{\theta}) = \mathsf{I} + \boldsymbol{\theta}\cdot\mathbf{J} + \dots \tag{89}$$

where we have $J_k = \left.\dfrac{\partial \mathsf{R}(\boldsymbol{\theta})}{\partial \theta_k}\right|_{\boldsymbol{\theta}=0}$, for $k = 1, 2, 3$. We then parametrize the unitary operator by the same $\boldsymbol{\theta}$,

$$U(\boldsymbol{\theta}) = 1 + \sum_k \left.\frac{\partial U(\boldsymbol{\theta})}{\partial \theta_k}\right|_{\boldsymbol{\theta}=0} \theta_k + \dots \tag{90}$$

We then define the angular momentum of the quantum system as the vector operator $\mathbf{J}$ with components given by $J_k = i\hbar \left.\dfrac{\partial U(\boldsymbol{\theta})}{\partial \theta_k}\right|_{\boldsymbol{\theta}=0}$ so that we can rewrite the infinitesimal rotation operator as

$$U(\boldsymbol{\theta}) = 1 - \frac{i}{\hbar}\boldsymbol{\theta} \cdot \mathbf{J} \tag{91}$$

we then obtain the finite rotation operator by using the same procedure as that of the linear momentum operator: get the limit of products of infinitesimal operators as the factors increase infinitely:

$$U(\mathsf{R}(\boldsymbol{\theta})) = \lim_{N\to\infty} \left(1 - \frac{i}{\hbar}\frac{\theta}{N} \cdot \mathbf{J}\right)^N = \exp\left(-\frac{i}{\hbar}\theta \mathbf{J}\right) \tag{92}$$

so that the angular momentum can be considered a generator of rotations.

- **Familiarize oneself with the notation used for vector and tensor operators. Use the formalism to write angular momentum operators as spherical tensor operators.**

  Recall that tensors are classically defined as objects that follow the same transformation rules as that of a tensor. One basic transformation rule is that of rotation. Reducible tensors are those whose components can be combined and arranged so that the rotations only act on these combinations. For rank 2 tensors, it is not just some coincidence that these so called irreducible subgroups are the numbers of elements of angular momenta representations for $j = 0, 1, 2$.

  To write angular momentum operators as spherical tensor operators, we consider the matrix elements of the rotation operator. We then define a spherical tensor as a set of operators such that under transformation they transform among themselves with exactly the same matrix of coefficients as that of the angular momentum eigenkets $|m\rangle$, with the eigenvalue j as the rank:

$$U(\mathsf{R}) T_k^q U^\dagger(\mathsf{R}) = \sum_{q'} D^{(k)}_{q'q} T_k^{q'} \tag{93}$$

We then use the infinitesimal representation of the rotation operator to exploit the angular momentum operator, and using the definition above, to obtain commutation relations between $J_\pm$ and T^q_k as well as J_z and T^q_k, which allows us to define spherical tensors from angular momentum operators.

- **Illustrate use cases for the projection formula.**

  The projection formula is a special case of the Wigner-Eckart theorem for $j' = j$. We could use it to derive the Landé g-factor from scratch. We know that the g-factor is a factor that allows us to rewrite the magnetic moment vector as the angular momentum **J**. Then, we can use first-order perturbation theory to derive the change in energy brought about by the extra potential from the external magnetic field, $V = -\boldsymbol{\mu} cdot \mathbf{B}$. The **B** goes out of the matrix element calculation since it's a constant, then we use the projection theorem to calculate the matrix elements of μ.

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Week 9: Eigenvalues and eigenstates (of AM operators).

- **Construct AM eigenkets and derive the corresponding eigenvalues using ladder operators.**

  Just as is pointed in bullet 3 in week 1, we can only create simultaneous eigenkets from commuting observables. However, the angular momentum operators in each direction J_x, J_y, and J_z only commute with the magnitude operator, J^2. So that's what we're going to solve.

  We can do this by defining the ladder operators $J_\pm \equiv J_x \pm iJ_y$, which have commutation relations with J_z: $[J_z, J_\pm] = \pm\hbar J_\pm$. They must then commute with J^2 and the directional angular momentum operators. We then define the eigenkets by two numbers, $|a, b\rangle$, where a is the eigenvalue of J^2 while b is the eigenvalue for J_z. We then solve for both eigenvalues by applying $J_z J_\pm$ to the eigenket, noting that $J_\pm |a, b\rangle$ is another eigenvalue of J_z due to the properties of the operators and b being an eigenvalue of J_z. Next we calculate the inner product of $J_\pm |a, b\rangle$ with itself, and noting that a must be nonnegative due to being an eigenvalue of J^2 and that b is real, we conclude that b must be bounded. By establishing the relationships between a and b, we get the eigenvalues for which $j = b_{\max}$, and $b = m\hbar$, so that $a = j(j+1)\hbar^2$ and the simultaneous eigenkets are $|j, m\rangle$.

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Week 10: Pure and mixed states.

- **Use the density operator formulation to distinguish pure from mixed states.**

  The most direct answer is to write the corresponding density operator $\rho = |\psi\rangle\langle\psi|$ and diagonalize it for some normalized ket $|\psi\rangle$. If all the eigenvalues are zero except one

that is 1, and if the eigenvalue 1 is nondegenerate, then the state is pure, and it is represented by the eigenket of ρ with eigenvalue 1. In that case ρ is a projection operator onto the one-dimensional eigenspace of eigenvalue 1.

For a pure state $|\psi\rangle$, we can write this in terms of an eigenbasis $|n\rangle$ so that

$$|\psi\rangle = \sum_n a_n |n\rangle \tag{94}$$

We can then write its corresponding density operator (which we denote by ρ_{pure} by $\rho_{\text{pure}} \equiv |\psi\rangle\langle\psi| = \sum_n |a_n|^2 |n\rangle\langle n|$.

For mixed states, we can recast this formulation by recasting the sum as a weighted sum of each of the pure states, so that

$$\rho_{\text{mixed}} = \sum_n p_n |\psi_n\rangle\langle\psi_n| \tag{95}$$

for which both p_n and a_n are both normalized. Getting the expectation value for both density operators,

$$\langle\rho_{\text{pure}}\rangle \equiv \langle n|\rho_{\text{pure}}|n\rangle = \sum_n |a_n|^2 \langle n|\psi\rangle\langle\psi|n\rangle = \sum_n |a_n|^2 |\psi_n|^2 \tag{96}$$

$$\langle\rho_{\text{mixed}}\rangle \equiv \langle n|\rho_{\text{mixed}}|n\rangle = \sum_n |p_n|^2 \langle n|\psi_n\rangle\langle\psi_n|n\rangle = \sum_n |p_n|^2 |a_n|^2 |\psi_n|^2 \tag{97}$$

$$= \sum_n p_n \langle\rho_{\text{pure}n}\rangle \tag{98}$$

which satisfies the definition that mixed states are just mixtures of pure states.

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Week 12: Quantum correlations.

- **Explain how quantum correlations are measured in simple entangled systems.**

  Consider a two-electron system with a spin singlet given by $\frac{1}{\sqrt{2}}|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle$. Then, when a measurement dictates that electron 1's spin state is up, we should be sure that electron 2's spin state must be down. This correlation persists even if the system is disintegrated into its separate subsystems, and this process is called quantum entanglement. This correlation then asserts that we can measure ANY correlated two-level eigenvalue in one subsystem and find out the opposite value in the other, such as measuring S_z which then leads to an immediate answer for the value of S_x.

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