8.04 Final Review

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Schröedinger Equation in one dimension. Piecewise constant potentials. Boundary conditions.

In one dimension, the (time-dependent, time-independent) Schröedinger Equation is

$$-\frac{\hbar^2}{2m}\frac{\partial^2\Psi(x,t)}{\partial x^2}+V(x)\Psi(x,t)=i\hbar\frac{\partial\Psi(x,t)}{\partial t},\quad -\frac{\hbar^2}{2m}\frac{d^2\Psi(x)}{dx^2}+V(x)\Psi(x)=E\Psi(x)$$

Very generally, a wave packet moving in the positive x-direction where the constant potential is $(0, V)$ has the forms:

$$e^{ikx},\quad k=\sqrt{\frac{2mE}{\hbar^2}},\qquad e^{iqx},\quad q=\sqrt{\frac{2m(E-V)}{\hbar^2}}$$

If $V > E$, the region is classically forbidden and the wavepacket instead falls off as

$$e^{-\kappa x},\quad \kappa=\sqrt{\frac{2m(V-E)}{\hbar^2}}$$

Wavepackets are reflected (coefficient R, opposite direction) and transmitted (coefficient T, same direction) at each boundary. Furthermore, at each boundary, the solutions to $\Psi(x)$ and $\frac{d\Psi(x)}{dx}$ must match up.

We define the *probability current*, or flux:

$$J(x,t)=\frac{\hbar}{2im}\left(\psi^*\frac{\partial\psi}{\partial x}-\frac{\partial\psi^*}{\partial x}\psi\right)$$

If there is no time dependence, the flux is constant across all boundaries. In the case of negative energies (a particle is *bound*), the possible energies are quantized. Specifically, for a particle with the n^{th} bound energy level travelling along a complete path, the Wilson-Sommerfeld quantization rule gives:

$$\oint p\,dx = nh$$

Potential Step: $V(x)=0,\ x<0$ and $V(x)=V_0, x>0$.

$$\Psi(x)=\begin{cases} e^{ikx}+Re^{-ikx},\ J=\frac{\hbar k}{m}(1-|R|^2) & x<0\\ Te^{iqx},\ J=\frac{\hbar q}{m}|T|^2 & x>0\end{cases}$$

Equality of $\Psi(x)$ and $\frac{d\Psi(x)}{dx}$ from either side of $x=0$ gives us $1+R=T$ and $ik(1-R)=iqT$, respectively.

Potential Well: $V(x)=-V_0,\ -a<x<a$ and $V(x)=0$ otherwise.

$$\Psi(x) = \begin{cases} e^{ikx} + Re^{-ikx} & x < -a \\ Ae^{iqx} + Be^{-iqx} & |x| < a \\ Te^{ikx} & x > a \end{cases}$$

Potential Barrier: $V(x) = V_0, \ -a < x < a$ and $V(x) = 0$ otherwise.

$$\Psi(x) = \begin{cases} e^{ikx} + Re^{-ikx} & x < -a \\ Ae^{-\kappa x} + Be^{\kappa x} & |x| < a \\ Te^{ikx} & x > a \end{cases}$$

Attractive Delta Potential: $V(x) = -\frac{\hbar^2 \lambda}{2ma}\delta(x)$

$$\Psi(x) = \begin{cases} A_0 e^{ikx} + Ae^{-ikx} & x < 0 \\ Be^{ikx} & x > 0 \end{cases}$$

Equating $\Psi(x)$, we have $A_0 + A = B$, but because of the discontinuity of the derivative, we have $ik(A_0 - A) - ikB = \Psi(0)$.

Time evolution of the wavefunction. Decomposition into Eigenstates.

A wavefunction $\Psi(x)$ can be decomposed into some series of normalized eigenstates:

$$\Psi(x) = \sum_{n=0}^{\infty} c_n \psi_n(x), \quad c_n = \int_{-\infty}^{\infty} \psi_n(x)^* \Psi(x) dx, \quad \sum_{n=0}^{\infty} c_n^2 = 1, \quad \int_{-\infty}^{\infty} |\psi(x)|^2 dx = 1$$

If the particle is bound in a box of length a, then we can write:

$$\Psi(x) = \sum_{n=0}^{\infty} A_n u_n(x), \quad u_n(x) = \sqrt{\frac{2}{a}} sin(n\pi \frac{x}{a}), \quad E_n = \frac{\hbar^2 \pi^2}{2ma^2} n^2$$

Each eigenfunction with an associated energy E_n can be given a time evolution:

$$\psi_n(x,t) = \psi_n(x) e^{-iE_n t/\hbar}$$

If the particle is in free space, the wavefunction in momentum space may also be given a time evolution:

$$\phi(p,t) = \phi(p,0) e^{-\frac{p^2}{2m}\frac{t}{\hbar}}$$

The eigenstates of the momentum operator are simultaneous eigenstates of energy (in free space):

$$\hat{p} u_p(x) = \frac{\hbar}{i} \frac{\partial u_p(x)}{\partial x} = p u_p(x), \quad u_p(x) = \frac{1}{\sqrt{2\pi\hbar}} e^{ipx/\hbar}$$

Harmonic Oscillator (Wavefunction *and* Operator approaches).

Has a potential of the form $V(x) = \frac{1}{2}kx^2$, and we let $\omega = \sqrt{\frac{k}{m}}$. Has energy of the form

$$E_n = \left(n + \frac{1}{2}\right)\omega\hbar, \quad n = 0, 1, 2, \ldots$$

And eigensolutions of the form (here $f_n(x)$ is an n^{th} degree polynomial):

$$\psi_n(x) = f_n(x)e^{-\frac{x^2}{2a^2}}, \quad \text{valid for all } x$$

See below for some treatment of the Operator Method. Note that the $|0>$ state is such that $\hat{A}|0> = 0$, and $H|0> = \frac{1}{2}\hbar\omega|0>$. A properly normalized eigenket is

$$|n> = \frac{1}{\sqrt{n!}}\left(A^+\right)^n|0>$$

If our eigenkets are properly normalized, then $<n|m> = \delta_{n,m}$. If they are not, then $<n|n>$ $= n!$. To return back to the wavefunction, we have (for $n = 0$, for example):

$$<x|0> = \hat{A}\psi_0(x) = \left(m\omega x + \hbar\frac{d}{dx}\right)\psi_0(x) = 0 \Rightarrow \psi_0(x) = Ce^{-\frac{m\omega x^2}{2\hbar}}, \; C = \left(\frac{m\omega}{\hbar\pi}\right)^{\frac{1}{4}}$$

Operator Algebra and Commutators. Dirac notation.

Some common operators:

$$\hat{x} = \hbar i\frac{d}{dp}, \quad \hat{p} = \frac{\hbar}{i}\frac{d}{dx}, \quad \hat{H} = \frac{\hat{p}^2}{2m} + V(x) = -\frac{\hbar^2}{2m}\frac{\partial}{\partial x} + V(x)$$

We also have an energy lowering operator $\hat{A}$ and an energy raising operator $\hat{A^+}$, such that:

$$\hat{H} = \hbar\omega\left(\hat{A^+}\hat{A} + \frac{1}{2}\right), \quad (\hat{A}, \hat{A^+}) = \sqrt{\frac{m\omega}{2\hbar}}x \pm i\frac{p}{\sqrt{2m\omega\hbar}}$$

With properties that are, in the case of the Harmonic Oscillator:

$$\hat{A}|n> = \sqrt{n}|n-1>, \quad \hat{A^+}|n> = \sqrt{n+1}|n+1>$$

The commutator of $\hat{A}$ and $\hat{B}$ is:

$$[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$$

$\hat{A}$ and $\hat{B}$ are said to *commute* if $[\hat{A}, \hat{B}] = 0$. Commutators have all sorts of intuitive properties. Some important commutator results are $[\hat{x}, \hat{p}] = i\hbar$, and $[\hat{A}, \hat{A^+}] = 1$.

TODO: (need more here about Hermitians, conjugate adjoints and how they work backwards on dirac notation etc.)

TODO: Dirac notation

Expected Values and Uncertainty.

The Heisenberg Uncertainty relation is

$$\Delta x \Delta k > \frac{1}{2}, \quad \Delta x \Delta p \geq \frac{\hbar}{2}$$

The expected value of an operator $\hat{A}$ over a function $\psi(x)$ is

$$< A >=< A|\psi|A >= \int_{-\infty}^{\infty} \psi(x)^* A \psi(x) dx$$

In general,

$$(\Delta A)^2_\psi (\Delta B)^2_\psi \geq \frac{1}{4} < i[\hat{A}, \hat{B}] >^2_\psi$$

Angular Momentum Formalism and Operators

We can express the Schrӧedinger Equation in spherical coordinates,

$$\left(-\frac{\hbar^2}{2M}\frac{\partial^2}{\partial r^2} + \frac{\hat{L}^2}{2Mr^2} + V(r)\right)(r\psi) = E(r\psi)$$

We also have angular momentum operators in each direction $\hat{L_x}$, $\hat{L_y}$, $\hat{L_z}$. We can define

$$\hat{L}^2 = \hat{L_x}^2 + \hat{L_y}^2 + \hat{L_z}^2$$

However, only one of the momentum operators and $\hat{L}^2$ can have simultaneous eigenfunctions. Let this be $\hat{L_z}$. (Then, by rotational symmetry, $< L_x >=< L_y >= 0$.) We also introduce a lowering $\hat{L_+}$ and raising $\hat{L_-}$ operators that act to change m such that

$$L_\pm = L_x \pm iL_y, \quad L_\pm|l, m > = \hbar\sqrt{(l \mp m)(l \pm m + 1)}|l, m \pm 1 >$$

Note the following commutator properties:

$$[L_i, L_j] = i\hbar\epsilon_{ijk}L_k, \quad [L^2, L_i] = 0, \quad [L^2, L_\pm] = 0$$

Let l be the angular momentum quantum number, and m the magnetic quantum number. If we let our eigenkets be $|l, m >$, then

$$\hat{L}^2|l, m > = \hbar^2 l(l + 1)|l, m >, \quad \hat{L_z}|l, m > = \hbar m|l, m >$$

For a spherically symmetrical $V(\rho)$, the solutions look like $\Psi(\rho, \theta, \phi) = R(\rho)Y(\theta, \phi)$. For a given energy level n, $0 \geq l \geq n - 1$, and $-l \geq m \geq l$. $Y(\theta, \phi)$ typically has terms of order $sin^{|m|}(\theta)$, $cos^{(l-|m|)}(\theta)$ and $e^{i\phi m}$.

See the formula sheet for some $Y_{ml}(\theta, \phi)$.

Hydrogen Atom, Quantum Numbers, Energy Levels

This problem is characterized by $V(r) = -\frac{Ze^2}{4\pi\epsilon_0 r}$.
(needs to be populated)