Read 2-6 to 2-9 ; 3-2 to 3-3

Lecture 2: Quantum operators

total energy $\longleftrightarrow \hat{H}$

potential energy $\longleftrightarrow \hat{V}(x)$

position $\longleftrightarrow \hat{x}$

$\hat{V}(x)\psi(x)$

$\langle \hat{V} \rangle = \langle \psi | \hat{V}(x) | \psi \rangle$

momentum $\longleftrightarrow \hat{p}_x$ $-i\hbar\,\partial/\partial x$

3 The vector interpretation of wavefunctions

As the last equation above implied, we can think about adding together (superimposing) different eigenfunctions of the Hamiltonian. This can be thought of as the analog of addition of vectors, (albeit in a infinite-dimensional vector space!), and drove the development of a very useful notation:

ket, bra

$$\psi_i(x) \Rightarrow |i\rangle \quad \psi_i^* \Rightarrow \langle i| \quad \langle i|\, i\rangle \Rightarrow \int \psi_i^*(x)\psi_i dx \quad \text{(2-35)} \quad = 1$$

particle must somewhere

We can often learn a lot in quantum mechanics by considering the properties of these vectors, rather than expanding everything out into wavefunctions. This is the subject of sections 2-4 to 2-8 in your text, which we outline briefly next. Start with *expectation values*:

$\delta_{mn} = $ 1 if $m=n$, 0 otherwise

measurements are associated w/ operators

$$\langle \hat{A} \rangle = \frac{\langle i|\,\hat{A}\,|i\rangle}{\cancel{\langle i|\, i\rangle}} \quad \text{(2-43)}$$

$i \cdot j = |i| \cdot |j| \cos(\theta)$

Without loss of generality, we can choose functions ψ_i such that $\langle i|\, i\rangle = 1$. If we have a set of functions, $\{u_i, u_j, u_k \ldots\}$, we can generally create a linear combination of these to create a new set $\{v_i, v_j, v_k \ldots\}$ such that $\langle v_n|\, v_m\rangle = \delta_{mn}$. The the demoninator in Eq. *(2-43)* becomes unity. Please read about this in Section 2.5 of your text.

The operator $\hat{A}$ above might be the Hamitonian, or it might be some other operator. Let's learn some general things about operators. A pair of *adjoint* operators satisfy $\langle \hat{G}^\dagger \rangle = \langle \hat{G} \rangle^*$, and a *self-adjoint* or *hermitian* operator as real expectation values *(2-44),(2-45)*. A useful theorem is Theorem 2.1, which states:

$$\langle i|\,\hat{G}^\dagger\,|j\rangle = \langle \hat{G}i\,|\,j\rangle \quad \text{(2-50),(2-51)}$$

turnover rule

(Make sure you can follow the proof in the book.) Two more useful theorems are given on p. 40 of your text: the eigenvalues of a hermitian operator are real (Theorem 2-2) [and hence operators that correspond to measureable quantitites like energy or momentum must be hermitian); and the non-degenerate eigenfunctions of a hermitian operator are orthogonal (Theorem 2-3). Section 2-7 proves Theorem 2-6: if two hermitian operators *commute*, that is $\hat{A}\hat{B} - \hat{B}\hat{A} \equiv [\hat{A}, \hat{B}] = 0$, then the two operators have a common set of eigenfunctions:

$|k\rangle = \psi_k(x)$

$$\boxed{\hat{A}\,|k\rangle = a_k\,|k\rangle, \quad \hat{B}\,|k\rangle = b_k\,|k\rangle}$$

$\hat{G}$ their exist ~~its~~ its adjoint operator $\hat{G}^\dagger$

$\langle G \rangle = \langle G \rangle^* \Rightarrow$ expectation values are real numbers

suppose $G = -i\hbar\,\partial/\partial x$

$\int \psi_i^* \left[-i\hbar\,\partial/\partial x\right] \psi_j \, dx$

$\hat G \psi_i = g_i \psi_i$
$\hat G \psi_j = g_j \psi_j$ $g_i \neq g_j$ $\Rightarrow \langle \psi_i | \psi_j \rangle = 0$ $= -i\hbar \int \left[\frac{\partial}{\partial x}\psi_i^*\right] \psi_j \, dx$

4 Expectation values and superpositions

$\hat H \phi = E \phi$

The real point of all of this abstract algebra about operators comes in Section 2-8, which is only one page long, but is key to understanding quantum mechanics. Let the eigenfunctions of $\hat A$ be called $\{\psi_1, \psi_2, \ldots\}$, and the wavefunction of the system be ϕ, an eigenfunction of $\hat H$. The performing a measurement that corresponds to operator $\hat A$ will yield the *expectation value* $\langle \phi | \hat A | \phi \rangle$. We can expand the wavefunction in eigenvalues of $\hat A$:

system wavefn.

$$\phi = \sum_i c_i |i\rangle \;\Rightarrow\; \langle \phi | \phi \rangle = \sum_i \sum_j c_i^* c_j \langle i | j \rangle = \sum_i c_i^* c_i = 1$$

probability comes in expectation value is the mean of many measurements

which will be 1 if ϕ is normalized. Now there are two cases:

- $\hat A$ and $\hat H$ commute: then ϕ will simply be one of the eigenfunctions of $\hat A$, say $|m\rangle$, and $\langle \hat A \rangle = a_m$.

each individual measurement yields a_m sharp distribution

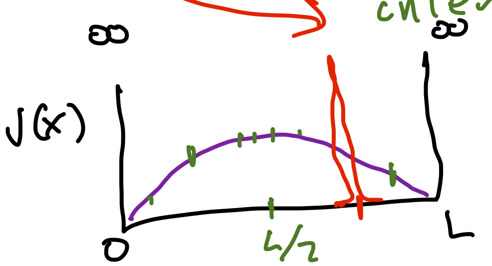
- $\hat A$ and $\hat H$ do not commute: then $\langle \hat A \rangle = \sum_i c_i^* c_i a_i$.

Brief dicussion of state preparation, measurement, and "collapse"

$\phi = \sum_i c_i |i\rangle$ pick out one $c_i = \delta_{mi}$

$\langle m | \hat A | m \rangle = a_m \langle m | m \rangle = a_m$

interpretation : each individual measurement will give a different result only the average is given by the expectation value



$\langle \hat x \rangle = \frac{L}{2}$

$\langle \hat v \rangle = 0$

notion : act of measurement collapses $\phi \Rightarrow |x\rangle$ particle is localized at x

position operator $\hat x$
momentum operator $-i\hbar\, \partial/\partial x = \hat p$

$\hat x \hat p \neq \hat p \hat x$

$[\hat x, \hat p] = \hat x \hat p - \hat p \hat x \neq 0$

$\hat x \hat p \psi(x) = \hat x(-i\hbar\, \partial\psi/\partial x)$
$= -i\hbar\, x\, \partial\psi/\partial x$

$\hat p \hat x \psi(x) = -i\hbar\, \partial/\partial x\, [x \psi(x)]$
$= -i\hbar [\psi(x) + x\, \partial\psi/\partial x]$

extra

5 The particle in a box

(Note: skip Section 3-1 for now). Suppose we have a system where $V(x) = 0$ inside a box from $x = 0$ to $x = L$, and infinite elsewhere.

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) = E\psi(x) \quad k^2 = \frac{2mE}{\hbar^2} \Rightarrow \frac{d^2\psi}{dx^2} + k^2\psi = 0 \quad \textit{(3-27)}$$

This leads to $\psi(x) = C\sin(kx)$, and to satisfy the boundary conditions, $kL = n\pi$, $n = 1,2,3,\ldots$ *(3-37)*. The energy of state n is

$$E_n = n^2\frac{h^2}{8mL^2} \text{ or, in two dimensions, } E_n = (n^2 + m^2)\frac{h^2}{8mL^2} \quad \textit{(3-42),(3-46)}$$

Study Figs 3-6 to 3-8 to see results for a particle in a two-dimensional box. Pay careful attention to the discussion of *degeneracy*.