10.2 Dirac Notation

All functions of x form a vector space. our requirement that the wavefunctions be square integrable means these span a more restricted vector space called Hilbert space (by physicists) equivalent to the mathematicians L_2. mathematically, wavefunctions are abstract vectors and operators act on them via linear transformations to produce new vectors. So its all actually linear algebra.

Where we have 2 functions f, g each of which are square integrable then $\int f^* g dx$ (called an inner product) is guaranteed to exist.

We can write this inner product in shorthand notation so $\int f^* g dx =< f|g >$ called Dirac notation. i.e. that everything to the left is complex conjugate, and the whole thing is an integral. so $< f|g >=< g|f >^* = \int f^* g dx$. Its kind of all a bracket so the $< f$ bit is called a bra and the $|g >$ bit is a ket....

we showed our energy eigenfunctions are orthonormal i.e.
$\int \psi_m^* \psi_n dx =< \psi_m|\psi_m >= \delta_{mn}$

and any operator Q acting on a function returns another function which is itself square integrable. so in dirac notation, our expectation values $< Q >= \int \psi^* Q \psi dx =< \psi|Q\psi >$

10.3 Hermitian operators

we had $\int \psi^* Q \psi dx = \int (Q\psi)^* \psi dx$ as our test for a hermitian operator, as this gives $< Q >=< Q >^*$ i.e. a real value. But it turns out that this is equivalent to what looks like a slightly stronger condition which is $\int g^* Q f dx = \int (Qg)^* f dx$

let $\psi = f + cg$ where c is a constant and f, g are functions. then in dirac notation $< \psi|Q\psi >=< Q\psi|\psi >$ is equvalent to

$$< (f + cg)|Q(f + cg) >=< Q(f + cg)|(f + cg) >$$

$$< (f|Qf > +c^* < g|Qf > +c < f|Qg > +c^2 < g|Qg >=$$

$$< Qf|f > + c^* < Qg|f > + c < Qf|g > + c^2 < Qg|g >$$

$$c^* < g|Qf > + c < f|Qg >= c^* < Qg|f > + c < Qf|g >$$

let $c = 1$. Then we have

$$< Qf|f > + < Qg|f > + < Qf|g > + < Qg|g >=< Qf|f > + < Qg|f > + < Qf|g > + < Qg|g >$$

so the bits we already know about with the same wavefunctions cancel and we are left with

$$< g|Qf > + < f|Qg >=< Qg|f > + < Qf|g >$$

$c = i$

$$-i < g|Qf > + i < f|Qg >= -i < Qg|f > + i < Qf|g >$$

divide by -i and add and we get $< g|Qf >=< Qg|f >$ is equivalent to our original condition for hermitian-ness of $< \psi|Q\psi >$.

and just to show how nice the new notation is, lets look at $< \psi|xp\psi >=< \psi|xf >$ where $f = p\psi$ then $< x\psi|p\psi >=< px\psi|\psi >$ so we did in a few lines that $(px)^* = (xp)$ which took us a long and tedious derivation in lecture 8.

10.4 Time evolution of expectation values

$$\frac{d < Q >}{dt} = \frac{d}{dt} < \psi|Q\psi >=< \frac{\partial \psi}{\partial t}|Q\psi > + < \psi|\frac{\partial Q}{\partial t}\psi > + < \psi|Q\frac{\partial \psi}{\partial t} >$$

But $H\psi = i\hbar\partial\psi/\partial t$ so $\partial\psi/\partial t = -i/\hbar H$ and $\partial\psi^*/\partial t = i/\hbar H$.

$$=< -\frac{i}{\hbar}H|Q\psi > + < \psi|\frac{\partial Q}{\partial t}\psi > + < \psi|Q\frac{-i}{\hbar}H\psi >$$

$$= \frac{i}{\hbar} < H\psi|Q\psi > + < \psi|\frac{\partial Q}{\partial t}\psi > - \frac{i}{\hbar} < \psi|QH\psi >$$

$$= \frac{i}{\hbar}(< H\psi|Q\psi > - < \psi|QH\psi >) + < \psi|\frac{\partial Q}{\partial t}\psi >$$

H is hermitian so $< H\psi|f >=< \psi|Hf >$ so

$$= \frac{i}{\hbar}(< \psi|HQ\psi > - < \psi|QH\psi >) + < \psi|\frac{\partial Q}{\partial t}\psi >$$

$$= \frac{i}{\hbar} < [H, Q] > + \left\langle \frac{\partial Q}{\partial t} \right\rangle$$

10.5 Ehrenfest theorem (1st)

let $Q = x$ then

$$\frac{d < x >}{dt} = \frac{i}{\hbar} < [H, x] > + \Big\langle \frac{\partial Q}{\partial t} \Big\rangle$$

We saw that $[H, x] = -\frac{i\hbar}{m} p$, and we know that the operator (coordinate!) x has no dependence on coordinate t so $\partial x / \partial t = 0$.

$$\frac{d < x >}{dt} = \frac{i}{\hbar} < -i\hbar \frac{p}{m} >$$

$$= \frac{< p >}{m}$$

and we have indeed the link to classical physics we talked about earlier.

similarly we could prove the second one $d < p > /dt = F = - < dV/dx >$

10.6 Virial theorem

let $Q = xp$

$$\frac{d < xp >}{dt} = \frac{i}{\hbar} < [H, xp] > + \Big\langle \frac{\partial (xp)}{\partial t} \Big\rangle$$

again, we earlier showed that $[H, p] = i\hbar dV/dx$ so $[H, xp] = [H, x]p + x[H, p] = -(i\hbar/m)p.p + x.i\hbar dV/dx$.

$$= \frac{i}{\hbar} \Big\langle -(i\hbar/m)p.p + x.i\hbar dV/dx \Big\rangle + 0$$

$$=< p^2/m - xdV/dx >$$

but in steady state $d/dx < xp >= 0$ so $0 =< p^2/m - xdV/dx >$ or $< p^2/2m >=< T >= 1/2 < xdV/dx >$

so stationary states (energy eigenfunctions) should have $< T >= 1/2xdV/dx$. for the harmonic oscillartor $V = 1/2m\omega^2 x^2$ so $dV/dx = m\omega^2 x$ and $< T >= 1/2 < xm\omega^2 x >= 1/2 < m\omega^2 x^2 >=< V >$

in general calculating $< T >$ is hard as its a second order differential operator, whereas calculating $< V >$ is easier.