Quantum Mechanics

So here we are going to capitalize on your exposure to ideas in QM with a formal definition of it. We will also carefully migrate from the simple story of finite-dim. vector spaces to the ∞-dim. cases.

In the finite case a very useful idea is the "resolution of the identity in terms of projection operators".

All eigenfunctions are $\perp$

Imagine an N-dim. vector space and a Hermitian operator A acting on it. Suppose $A\phi_n = \lambda_n \phi_n$ where $\{\lambda_n, \phi_n\}$ is the set of eigens associated w/ A. Assume λ_n are non-deg.

Then: $I\phi = \sum_{n=1}^{N} \phi_n (\phi_n, \phi)$ if $\phi = c_1\phi_1 + c_2\phi_2$ then $I\phi = \phi_1(\phi_1,\phi) + \phi_2(\phi_2,\phi) = \phi_1 c_1 + \phi_2 c_2 = \phi$

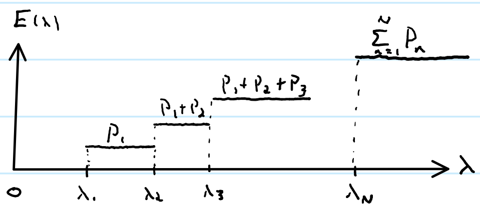
But: $P_n \phi = \phi_n(\phi_n, \phi)$ $P_n\phi = \phi_n(\phi_n,\phi) = \phi_n c_n \Rightarrow P_n^2\phi = P_n\phi_n c_n = \phi_n c_n$ $\underbrace{P_n\text{-projection}}$

Then: $I = \sum_{n=1}^{N} P_n$ Note: $P_n P_m = 0$ $n \neq m$

And: $A = \sum_{n=1}^{N} \lambda_n P_n$ since $A\phi_m = \sum_{n=1}^{N} \lambda_n P_n \phi_m = \lambda_m \phi_m$ and: $P_n\phi_m = 0$ $n \neq m$

Going to ∞ will require some rethinking. So once again, for finite-dim consider:

$$E(\lambda) = \begin{cases} 0 & \lambda < \lambda_1 \\ \sum_{n=1}^{\nu} P_n & \lambda_\nu \le \lambda < \lambda_{\nu+1} \quad \nu = 1,\dots,N-1 \\ \sum_{n=1}^{N} P_n & \lambda \ge \lambda_N \end{cases} \Rightarrow \begin{cases} E(-\infty) = 0, \; E(\infty) = I \\ \text{if } \lambda_a < \lambda_b \text{ then } E(\lambda_a)E(\lambda_b) = \sum_{n=1}^{a} P_n \sum_{n=1}^{b} P_n = \sum_{n=1}^{a} P_n \\ \text{e.g. } (P_1+P_2)(P_1+P_2+P_3) = P_1^2 + \cancel{P_1P_2} + \cancel{P_1P_3} + \cancel{P_2P_1} + P_2^2 + \cancel{P_2P_3} \\ \qquad = P_1 + P_2 \end{cases}$$



Now it turns out that by using the Stieltjes form of integrals: $\int_a^b f(x)\,dg(x) \equiv \lim_{\Delta x \to 0} \sum_{i=1}^{N} f(\bar{x}_i)[g(x_{i+1}) - g(x_i)]$

where $\bar{x}_i$ is some point between x_i and x_{i+1}, then:

$\int_{-\infty}^{\lambda} dE(\lambda) = \sum_{n=1}^{\nu} P_n$ which basically remains constant as λ increases until we hit an eigenvalue and gain a P_n.

so

$I = \int_{-\infty}^{\infty} dE(\lambda)$

$A = \int_{-\infty}^{\infty} \lambda \, dE(\lambda)$

We are now in a position to generalize to ∞-dim Hilbert space H:

For any self-adjoint A on H, there exists a unique operator valued $E(\lambda)$ s.t.

1. $E(\lambda_a)E(\lambda_b) = E(\lambda_a)$ for $\lambda_a < \lambda_b$
2. $\lim_{\lambda \to -\infty} E(\lambda) = 0$, $\lim_{\lambda \to \infty} E(\lambda) = I$
3. $I = \int_{-\infty}^{\infty} dE(\lambda)$
4. $A = \int_{-\infty}^{\infty} \lambda \, dE(\lambda)$

$E(\lambda)$ is the resolution of I for A.

The points λ for which $E(\lambda)$ is not constant is the "spectrum" of A.

$[E(\lambda), A] = 0$, and if $[A, B] = 0 \Rightarrow [E(\lambda), B] = 0$

Now we are ready: (A for Axiom)

[AI Any physical system is completely described by a normalized vector in H.

[AII To every physical observable there corresponds a self-adjoint A on H

Sometimes we can build them from classical expressions w/ $\vec{r} \to \vec{r}$, $\vec{p} \to -i\hbar\vec{\nabla}$, but sometimes (spin) not!

[AIII Physical measurement of observable A are elements of the spectrum of A

Since A is s.a. it's spectrum is real. Good for the real world we live in!

To see and appreciate the need for $E(\lambda)$, consider $A = p_x = -i\hbar \frac{d}{dx}$

We could try and say $A\phi_k = \hbar k \phi_k$ for $\phi_k = \frac{1}{\sqrt{2\pi}} e^{ikx}$ thus ϕ_k's are eigenfunctions which are normalized by $\int_{-\infty}^{\infty} \phi_k^*(x)\phi_{k'}(x)dx = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{i(k'-k)x}dx = \delta(k-k')$

Now let's define $P_k f = \phi_k(\phi_k, f)$ for $f \in H$. Sounds good right? Nope! $\underbrace{\phi_k \notin H}$

Recall elements of H are s.i.

but $\int_{-\infty}^{\infty} \phi_k^*\phi_k dx = \int_{-\infty}^{\infty} dx = \infty$

Instead let's define $E(k)f(x) = \int_{-\infty}^{k} \phi_{k'}(\phi_{k'}, f(x))dk'$

$$= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{k} e^{ik'x}\left[\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} e^{-ik'y} f(y)dy\right]dk'$$

$$= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{k} e^{ik'x}\hat{f}(k')dk'$$ where $\hat{f}(k')$ is F.T. of $f(y)$, and it exists and is s.i.

Is $E(k)$ doing what it should?

First: $E(-\infty) = 0$ since $\int_{-\infty}^{-\infty}$, $E(\infty) = I$ since $E(\infty)f(x) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} e^{ik'x}\hat{f}(k')dk' = f(x)$, $\int_{-\infty}^{\infty} dE(k) = I$

What about $E(k_1)E(k_2) = E(k_1)$ for $k_1 < k_2$?

$$E(k_1)E(k_2) = E(k_1)\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{k_2} e^{ik'x}\hat{f}(k')dk' = \frac{1}{2\pi}\int_{-\infty}^{k_1} e^{ikx}F(k)dk$$

where $F(k) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} e^{-ikx}\int_{-\infty}^{k_2} e^{ik'x}\hat{f}(k')dk'dx = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{k_2}\underbrace{\int_{-\infty}^{\infty} e^{i(k'-k)x}dx}_{2\pi\delta(k'-k)}\hat{f}(k')d\hat{k} = \begin{cases}\sqrt{2\pi}\,\hat{f}(k) & k_2 > k \\ 0 & k_2 < k\end{cases}$

Since $k_2 > k_1$ $E(k_1)E(k_2) = \frac{1}{2\pi}\int_{-\infty}^{k_1} e^{ikx}\sqrt{2\pi}\,\hat{f}(k)dk = E(k_1)$

Lastly, does this $E(k)$ belong to p_x? i.e. $p_x \overset{?}{=} \hbar\int_{-\infty}^{\infty} k\,dE(k)$

$$\left[\hbar\int_{-\infty}^{\infty} k\,dE(k)\right]f(x) = \frac{\hbar}{\sqrt{2\pi}}\int_{-\infty}^{\infty} k\,d\left[\int_{-\infty}^{k} e^{ik'x}\hat{f}(k')dk'\right] = \frac{\hbar}{\sqrt{2\pi}}\int_{-\infty}^{\infty} k\frac{d}{dk}\left[\int_{-\infty}^{k} e^{ik'x}\hat{f}(k')dk'\right]dk$$

$$= \frac{\hbar}{\sqrt{2\pi}}\int_{-\infty}^{\infty} ke^{ikx}\hat{f}(k)dk = -\frac{i\hbar}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\frac{d}{dx}e^{ikx}\hat{f}(k)dk$$

$$= -\frac{i\hbar}{\sqrt{2\pi}}\frac{d}{dx}\int_{-\infty}^{\infty} e^{ikx}\hat{f}(k)dk = -i\hbar\frac{df(x)}{dx} = p_x f(x)$$

And now something central:

A IV Make a measurement of observable A on a state ϕ. The probability that observed λ will lie between λ_1 and λ_2 $(\lambda_2 > \lambda_1)$ is $P(\lambda_1, \lambda_2) = \| [E(\lambda_2) - E(\lambda_1)]\phi \|^2$ w/ $E(\lambda)$ the resolution of I for A.

Two extremes:

Clearly since $\|\phi\| = 1$, $P(-\infty, \infty) = \| [E(-\infty) - E(\infty)]\phi \|^2 = \| [0-1]\phi\|^2 = 1$

and if $E(\lambda)$ is constant between λ_1 and λ_2 $P(\lambda_1, \lambda_2) = \| [E(\lambda_2) - E(\lambda_1)]\phi\|^2 = \| 0\phi\|^2 = 0$.

The in between:

If $\lambda_1 < \bar{\lambda} < \lambda_2$ and $\bar{\lambda}$ is a part of the spectrum of A, then:

$$\begin{aligned}
A[E(\lambda_2) - E(\lambda_1)]\phi &= \int_{-\infty}^{\infty} \lambda \, d\{E(\lambda)[E(\lambda_2) - E(\lambda_1)]\phi\} \\
&= \int_{-\infty}^{\infty} \lambda \, d[E(\lambda)E(\lambda_2)\phi] - \int_{-\infty}^{\infty} \lambda \, d[E(\lambda)E(\lambda_1)\phi] \\
&= \int_{-\infty}^{\lambda_2} \lambda \, d[E(\lambda)\phi] - \int_{-\infty}^{\lambda_1} \lambda \, d[E(\lambda)\phi] \\
&= \int_{\lambda_1}^{\lambda_2} \lambda \, d[E(\lambda)\phi] \\
&= \bar{\lambda}[E(\lambda_2) - E(\lambda_1)]\phi \\
&= \bar{\lambda}\phi_{\bar{\lambda}} \quad \Rightarrow \quad A\phi_{\bar{\lambda}} = \bar{\lambda}\phi_{\bar{\lambda}}
\end{aligned}$$

Now if $\psi_{\bar{\lambda}}$ is a unique normalized eigenvector associated w/ $\bar{\lambda}$, then $[E(\lambda_2) - E(\lambda_1)]\phi = \psi_{\bar{\lambda}}(\psi_{\bar{\lambda}}, \phi)$

then we can write $P(\lambda_1, \lambda_2) = |(\psi_{\bar{\lambda}}, \phi)|^2$

Note: For $A = p_x$ this gives

$$\begin{aligned}
P(k_1, k_2) &= \| [E(k_2) - E(k_1)]\phi \|^2 \\
&= \| \int_{-\infty}^{k_2} \phi_{k'}(\phi_{k'}, \phi)\, dk' - \int_{-\infty}^{k_1} \phi_{k'}(\phi_{k'}, \phi)\, dk' \|^2 \\
&= \| \int_{k_1}^{k_2} \phi_{k'}(\phi_{k'}, \phi)\, dk' \|^2 \\
&= \| \frac{1}{\sqrt{2\pi}} \int_{k_1}^{k_2} e^{ik'x} \underbrace{\left[\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-ik'y} \phi(y)\, dy\right]}_{\hat{\phi}(k') \text{ the F.T. of } \phi(y)} dk' \|^2 \\
&= \| \frac{1}{\sqrt{2\pi}} \int_{k_1}^{k_2} e^{ik'x} \hat{\phi}(k')\, dk' \|^2 \\
&= \frac{1}{2\pi} \int_{-\infty}^{\infty} \int_{k_1}^{k_2} e^{ik'x} \hat{\phi}(k')\, dk' \int_{k_1}^{k_2} e^{-ik''x} \hat{\phi}^*(k'')\, dk''\, dx \\
&= \int_{k_1}^{k_2} \int_{k_1}^{k_2} \underbrace{\left[\frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i(k'-k'')x}\, dx\right]}_{\delta(k'-k'')} \hat{\phi}(k') \hat{\phi}^*(k'')\, dk'\, dk'' \\
&= \int_{k_1}^{k_2} |\hat{\phi}(k')|^2\, dk'
\end{aligned}$$

Moving along:

$$\langle A\rangle \equiv \lim_{\Delta\to 0}\sum_i \bar{\lambda}_i \,\|[E(\lambda_i+\Delta)-E(\lambda_i)]\phi\|^2$$ is the "expectation value" of A for state ϕ.

That is, the average outcome of many measurements of A on a large collection of systems in ϕ.

Each $\bar{\lambda}_i$ is weighted by its probability.

Going back to our simple model, the only contributions will come from $\lambda_1, \lambda_2, \lambda_3, \lambda_4, \lambda_5$ so

$$\langle A\rangle = \lambda_1|c_1|^2 + \lambda_2|c_2|^2 + \lambda_3|c_3|^2 + \lambda_4|c_4|^2 + \lambda_5|c_5|^2$$

But:

$$\langle A\rangle = (\phi, A\phi)$$

Proof: $(\phi, A\phi) = (\phi, \int_{-\infty}^{\infty}\lambda\, dE(\lambda)\phi)$

$$= \int_{-\infty}^{\infty}\lambda\, d[(\phi, E(\lambda)\phi)]$$

$$= \lim_{\Delta\to 0}\sum_i \bar{\lambda}_i\,(\phi, [E(\lambda_i+\Delta)-E(\lambda_i)]\phi)$$

But since $E(\lambda)$ is composed of projections, $[E(\lambda_i+\Delta)-E(\lambda_i)] = [E(\lambda_i+\Delta)-E(\lambda_i)]^2$

and since the $E(\lambda)$'s are self-adjoint:

$$(\phi, A\phi) = \lim_{\Delta\to 0}\sum_i \bar{\lambda}_i\,([E(\lambda_i+\Delta)-E(\lambda_i)]\phi, [E(\lambda_i+\Delta)-E(\lambda_i)]\phi)$$

$$= \lim_{\Delta\to 0}\sum_i \bar{\lambda}_i\,\|[E(\lambda_i+\Delta)-E(\lambda_i)]\phi\|^2$$

$$= \langle A\rangle$$

Once again: $(\phi, A\phi) = (\sum_{i=1}^{5} c_i\phi_i, \sum_{i=1}^{5}\lambda_i c_i\phi_i) = \sum_{i=1}^{5}\lambda_i|c_i|^2 = \langle A\rangle$

Furthermore we can define the mean square deviation which measures deviation from the mean $\langle A \rangle$:

[$(\Delta A)^2$ is the expectation value of $[A - \langle A \rangle]^2$ in the state ϕ for which $\langle A \rangle$ is computed.

which leads to:

[$(\Delta A)^2 = \langle A^2 \rangle - \langle A \rangle^2$

Proof: $(\Delta A)^2 = \langle [A - \langle A \rangle]^2 \rangle = (\phi, [A - \langle A \rangle]^2 \phi)$

$$= (\phi, [A^2 - 2A\langle A \rangle + \langle A \rangle^2]\phi)$$
$$= (\phi, A^2\phi) - 2(\phi, A\phi)\langle A \rangle + \langle A \rangle^2$$
$$= \langle A^2 \rangle - \langle A \rangle^2$$

Now $(\Delta A)^2 = (\phi, [A - \langle A \rangle]^2 \phi) = ([A - \langle A \rangle]\phi, [A - \langle A \rangle]\phi)$ since A is s.a. and $\langle A \rangle$ is real

$$= \| [A - \langle A \rangle]\phi \|^2$$

But this means $\Delta A = 0 \Rightarrow [A - \langle A \rangle]\phi = 0 \Rightarrow A\phi = \langle A \rangle \phi$ so $\Delta A = 0$ only for ϕ to be a single eigenstate.

We can generalize to multiple measurements of different things.

[A IV' Let A, B, C be observables s.t. $[A,B] = [A,C] = [B,C] = 0$.

Then $P(a_1, a_2 ; b_1, b_2 ; c_1, c_2) = \| [E_A(a_2) - E_A(a_1)][E_B(b_2) - E_B(b_1)][E_C(c_2) - E_C(c_1)]\phi \|^2$

where $E_J(j)$ are resolutions of I w.r.t. J. order doesn't matter due to

Everything so far is at an instant of time. The question then is "how does the story evolve w/ time?"

[A V For every system there exists a Hermitian operator H (the Hamiltonian) from which:

$H\Psi(x,t) = i\hbar \frac{\partial \Psi(x,t)}{\partial t}$ T.D.S.E. provided no measurements are made!

Now this leads to: [$\frac{\partial}{\partial t}(\Psi, \Psi) = 0$

since H is Hermitian

Proof: $\frac{\partial}{\partial t}(\Psi, \Psi) = (\frac{\partial \Psi}{\partial t}, \Psi) + (\Psi, \frac{\partial \Psi}{\partial t}) = (\frac{1}{i\hbar} H\Psi, \Psi) + (\Psi, \frac{1}{i\hbar} H \Psi) = -\frac{1}{i\hbar}(\Psi, H\Psi) + \frac{1}{i\hbar}(\Psi, H\Psi) = 0$

This implies that A I is compatible w/ A V.

Furthermore, if H does <u>not</u> depend on t, then $\Psi(x,t) = e^{-i\frac{Ht}{\hbar}}\Psi(x,0)$, from which one can show that if $[A, H] = 0$ w/ H time ind. then measurement results of A will be time ind. as well.

And we finish w/ a means of gaining all the information needed to determine Ψ.

A VI If at $t=0$ one measures commuting A, B, C and finds w/ certainty $a \in [a_1, a_2]$, $b \in [b_1, b_2]$, $c \in [c_1, c_2]$ then $[E_A(a_2) - E_A(a_1)][E_B(b_2) - E_B(b_1)][E_C(c_2) - E_C(c_1)]\Psi = \Psi$

That is the measurements project the original wavefunction onto a subspace of Hilbert associated w/ the projector $[E_A(a_2) - E_A(a_1)][E_B(b_2) - E_B(b_1)][E_C(c_2) - E_C(c_1)]$.

Start w/ a single measurement of A. If there is only one value between a_1 and a_2 then $\Psi = e^{i\alpha}\Phi_a$ (a is non-deg) where Φ_a is a normalized eigenvector of A belonging to a, and $e^{i\alpha}$ is an indeterminate phase factor.

Now if a is degenerate, then the measurement has projected us into a subspace of Hilbert space which is spanned by the orthonormal eigenvectors associated w/ a, i.e. $\Psi = \sum_{\nu=1}^{n_a} c_\nu \Phi_a^{(\nu)}$ where $n_a > 1$ is the degeneracy of a. So Ψ is not well defined. But we can solve this by measuring B where $[A, B] = 0$. If this doesn't resolve it, then measure C where $[A, C] = [B, C] = 0$ and so on.

Returning to our simple example: If $A\phi = \lambda\phi_1 + \lambda\phi_2 + \beta\phi_3 + \beta\phi_4 + \beta\phi_5$ then measuring A is not enough since λ could mean ϕ_1 or ϕ_2, and β could mean ϕ_3, ϕ_4 or ϕ_5. But imagine B where $[A, B] = 0$. If $B\phi = \gamma\phi_1 + \delta\phi_2 + \gamma\phi_3 + \delta\phi_4 + \eta\phi_5$, then knowing the eigenvalues of A and B (or measuring both) is enough to specify the state.

In the end, to fully specify Ψ, we need the results of a complete set of commuting observables.

Example: Electron in hydrogen can use H, L^2, L_z, S^2, S_z to fully specify the state.
Alternatively H, L^2, S^2, J^2, J_z w/ $J = L + S$ works.

Okay, so let's go back to the finite dimensional version of this for a clearer picture.

Say the system being studied is described by a vector in 5D, call it ϕ. Now we can express the vector in terms of components along an orthonormal basis, but which one?

Well it depends on what we want to measure about our system. Suppose we want to measure "A" which has a corresponding self adjoint operator A in the 5D vector space. Furthermore, suppose that A has 5 distinct eigenvalues $\{\lambda_i\} \Rightarrow$ it must have 5 orthogonal eigenvectors $\{\phi_i\}$ because its s.a.. So we can express $\phi = \sum c_i \phi_i = c_1\phi_1 + c_2\phi_2 + c_3\phi_3 + c_4\phi_4 + c_5\phi_5$

Now to obtain this, we could have used the resolution of the identity affiliated w/ A, i.e. $I = \sum_{i=1}^{5} \phi_i(\phi_i, \phi)$

or $I\phi = \phi_1(\phi_1,\phi) + \phi_2(\phi_2,\phi) + \phi_3(\phi_3,\phi) + \phi_4(\phi_4,\phi) + \phi_5(\phi_5,\phi) = \phi_1 c_1 + \phi_2 c_2 + \phi_3 c_3 + \phi_4 c_4 + \phi_5 c_5$.

Now realize that I is just a sum of projection operators $P_i\phi = \phi_i(\phi_i,\phi) = \phi_i c_i$ which gives the component of ϕ along ϕ_i, i.e. $\phi_i c_i$ or $c_i\phi_i$.

But $A\phi = \lambda_1 c_1\phi_1 + \lambda_2 c_2\phi_2 + \lambda_3 c_3\phi_3 + \lambda_4 c_4\phi_4 + \lambda_5 c_5\phi_5 = \lambda_1 P_1\phi + \lambda_2 P_2\phi + \lambda_3 P_3\phi + \lambda_4 P_4\phi + \lambda_5 P_5\phi = \sum_{i=1}^{5}\lambda_i P_i\phi$

Now is there anything important about the labelling 1,2,3,4,5? No, but we $\underline{\underline{\text{can}}}$ label it in terms of increasing eigenvalues, i.e. $A\phi_i = \lambda_i\phi_i$ and $\lambda_1 < \lambda_2 < \lambda_3 < \lambda_4 < \lambda_5$.

Having done so we can now build $E(\lambda) = \begin{cases} 0 & \lambda < \lambda_1 \\ \sum_{i=1}^{\nu} P_i & \lambda_\nu < \lambda \leq \lambda_{\nu+1} \\ \sum_{i=1}^{5} P_i & \lambda_5 < \lambda \end{cases}$ where λ is a continuous dial from $-\infty$ to ∞.

Notice that $E(\lambda)$ is intimately affiliated w/ A!

Turning the λ-dial, $E(-\infty) = 0$, $E(\infty) = I$.

Now to interpret A IV we need one more piece of the story. First of all $(\phi,\phi) = 1 \Rightarrow \sum_{i=1}^{5}|c_i|^2 = 1$ which means that we can interpret $|c_i|^2$ as the probability that the vector would be realized in state ϕ_i upon measurement.

In other words $|c_i|^2$ is the probability that measuring A on ϕ would give λ_i, that is $|c_2|^2$ is the probability of getting λ_2.

What about the probability of getting λ_2 or λ_3? Obviously its $|c_2|^2 + |c_3|^2$ but we can write this as $\|[E(\lambda_{3.5}) - E(\lambda_{1.5})]\phi\|^2 = \|[P_1 + P_2 + P_3 - P_1]\phi\|^2 = \|c_2\phi_2 + c_3\phi_3\|^2 = (c_2\phi_2 + c_3\phi_3, c_2\phi_2 + c_3\phi_3)$

$= (c_2\phi_2, c_2\phi_2) + (c_2\phi_2, c_3\phi_3) + (c_3\phi_3, c_2\phi_2) + (c_3\phi_3, c_3\phi_3)$

$= |c_2|^2 + |c_3|^2$