Quantum Cook Book April 14.

The basic ideas of quantum mechanics are very simple and sometimes get hidden in the use of differential equations and complex functions that arise when we do the real thing, as in class. Here is a bare bone version that illustrates all the ideas of quantum mechanics.

In the real world, even in one space dimension, whether on a ring or a box of size L), x has a continuous infinity of values, p and E have a discrete infinity of values labeled by some integer n.

Imagine a simpler world in which each variable can have only three values: the position can be $x = x_1, x_2, x_3$, momentum can be $p = p_1, p_2, p_3$ and the energy can be $E = E_1, E_2, E_3$.
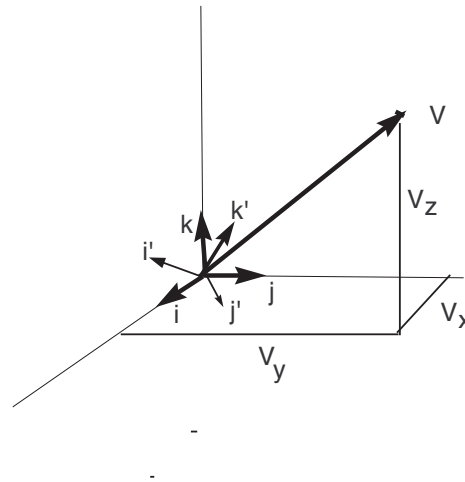
See Figure 1

Figure 1: The state of the particle in a general situation is given by $\mathbf{V}$. The vectors $\mathbf{i}$, $\mathbf{j}$ and $\mathbf{k}$ are special in that a particle in $\mathbf{i}$ has a definite position x_1 and likewise for $\mathbf{j}$ and $\mathbf{k}$. The vectors $\mathbf{i}'$, $\mathbf{j}'$ and $\mathbf{k}'$ are special in that a particle in $\mathbf{i}'$ has a definite momentum p_1 and likewise for $\mathbf{j}'$ and $\mathbf{k}'$

Postulate 1: The state of the particle in a general situation is given by $\mathbf{V}$. The length does not matter, so we assume that from this family of parallel vectors we have chosen one which has length 1, i.e., is normalized. The vectors $\mathbf{i}$, $\mathbf{j}$ and $\mathbf{k}$ are also vectors, but special in that a particle in $\mathbf{i}$ has a definite position x_1 and likewise for $\mathbf{j}$ and $\mathbf{k}$

Mathematical result We can write for any $\mathbf{V}$,

$$\mathbf{V} = \mathbf{i}V_x + \mathbf{j}V_y + \mathbf{k}V_z \tag{1}$$

Math The basis vectors are orthonormal: $\mathbf{i}\cdot\mathbf{i} = 1, \mathbf{i}\cdot\mathbf{j} = 0$ and so on. Using this $V_x = \mathbf{i}\cdot\mathbf{V}$ etc follow.

Postulate 2: If the position is measured the only possible answers are x_1, x_2, x_3 and these will occur with probability $P(x_1) = V_x^2 = (\mathbf{i} \cdot \mathbf{V})^2$, $P(x_2) = V_y^2 = (\mathbf{j} \cdot \mathbf{V})^2$ and $P(x_3) = V_z^2 = (\mathbf{k} \cdot \mathbf{V})^2$.

Postulate 3: Right after the measurement, the state will collapse to the corresponding basis vector. Thus if x_2 was the result, $\mathbf{V} \to \mathbf{j}$.

Suppose we now ask about another variable like momentum. States of definite momentum are given by another triplet of orthonormal vectors $\mathbf{i}', \mathbf{j}', \mathbf{k}'$, as shown in the figure. To find the odds we need to express the SAME $\mathbf{V}$ in terms of $\mathbf{i}', \mathbf{j}', \mathbf{k}'$:

$$\mathbf{V} = \mathbf{i}'V_x' + \mathbf{j}'V_y' + \mathbf{k}'V_z' \tag{2}$$

Then as before $P(p = p_1) = |V_x'|^2 = |\mathbf{V} \cdot \mathbf{i}'|^2$ and so on and the state will collapse following the momentum measurement to one of $\mathbf{i}', \mathbf{j}', \mathbf{k}'$.

A similar orthonormal set of vectors $\mathbf{i}", \mathbf{j}", \mathbf{k}"$ define states of definite energy. In general these do not have a simple relation to the x-basis or p-basis with one exception: if it happens that $E = p^2/2m$, then a state of definite p is also a state of definite $E = p^2/2m$.

Note that if we first measure x and got x_1 (and $\mathbf{v} \to \mathbf{i}$), and then measured p and got p_1 ($\mathbf{V} \to \mathbf{i}'$) we have no assurance a measurement of x will still yield x_1: it can be any of the three values in our example since $\mathbf{i}'$ has projections along $\mathbf{i}, \mathbf{j}, \mathbf{k}$.

Where do these basis vectors corresponding to states of definite x or states of definite p come from? We need a postulate for that. You may not follow this if you do not know what a matrix is, but give it a shot.

A matrix is an array of numbers, which will by $3X3$ in our problem. For example

$$M = \begin{pmatrix} 1 & 2 & 3 \\ 4 & 13 & 9 \\ 0 & 7 & 11 \end{pmatrix} \tag{3}$$

is a matrix. Given any vector with components V_x, V_y, V_z we can get a new one by acting with M as follows:

$$\begin{pmatrix} V_x' \\ V_y' \\ V_z' \end{pmatrix} = \begin{pmatrix} 1 & 3 & 2 \\ 4 & 13 & 9 \\ 8 & 7 & 11 \end{pmatrix} \begin{pmatrix} V_x \\ V_y \\ V_z \end{pmatrix} = \begin{pmatrix} V_x + 3V_y + 2V_z \\ 4V_x + 13V_y + 9V_z \\ 8V_x + 7V_y + 11V_z \end{pmatrix} \tag{4}$$

We write this schematically as

$$V' = MV \tag{5}$$

Thus M turns any given vector with components V_x, V_y, V_z into another with components V_x', V_y', V_z'.

The resulting vector in general points in some new direction.

Suppose however that for a given M there is a vector V_v such that

$$MV_v = vV_v \tag{6}$$

where v is just a number. This means that M simply rescales V. I do not mean a trivial case like

$$M = \begin{pmatrix} 3 & 0 & 0 \\ 0 & 3 & 0 \\ 0 & 0 & 3 \end{pmatrix} \tag{7}$$

which rescales every vector by 3. I mean something that only rescales a few special vectors.

When this happens we say V_v is an eigenvector of M with eigenvalue v. How many such vectors can we find for a certain matrix M?

Math If M is a real symmetric matrix, it will have three eigenvectors which will be orthogonal and the corresponding eigenvalues v will be real. The vectors can be rescaled to be of unit length since a multiple of an eigenvector is also an eigenvector with the same eigenvalue.

This means that every symmetric matrix can be used to find an orthonormal basis.

Postulate 4: In our problem the matrix corresponding to x is

$$X = \begin{pmatrix} x_1 & 0 & 0 \\ 0 & x_2 & 0 \\ 0 & 0 & x_3 \end{pmatrix} \tag{8}$$

and the three eigenvectors are just $\mathbf{i}$, $\mathbf{j}$ and $\mathbf{k}$ and the three eigenvalues are x_1, x_2, x_3. You should verify this explicitly using

$$\mathbf{i} = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \tag{9}$$

and so on.

Postulate 5 There is similarly a nondiagonal matrix P whose eigenvectors are $\mathbf{i}', \mathbf{j}', \mathbf{k}'$. Since this is just an illustrative example, let me make something up:

$$P = \begin{pmatrix} 1 & 3 & 0 \\ 3 & 5 & 7 \\ 0 & 7 & 4 \end{pmatrix} \tag{10}$$

Its eigenvalues will give p_1, p_2, p_3 and its eigenvectors will be $\mathbf{i}', \mathbf{j}', \mathbf{k}'$. The math department tells us how to find the eigenvectors and eigenvalues.

What is the matrix for energy $E = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2$? This matrix, denoted by the symbol H (for Hamiltonian) is determined by the matrices X and P as follows

$$H = \frac{P^2}{2m} + \frac{1}{2}m\omega^2 X^2 \tag{11}$$

the eigenvectors for H will not be simply related to those of X or P unless $E = p^2/2m$ in which case $H = P^2/2m$ and any eigenvector of P will be an eigenvector of $P^2/2m$ with eigenvalue $p^2/2m$ (Check this.) .

Postulate 6: The state vector evolves according to the equation

$$i\hbar \frac{dV}{dt} = HV \tag{12}$$

Coming back to the real quantum problem here is the dictionary:

$$\mathbf{V} \Leftrightarrow \psi(x) \tag{13}$$

$$\mathbf{i}, \mathbf{j}, \mathbf{k} \Leftrightarrow \psi_{x_0}(x)\text{spike at } x = x_0 \tag{14}$$

$$\mathbf{i}', \mathbf{j}', \mathbf{k}' \Leftrightarrow \psi_p(x) = \frac{e^{\frac{ipx}{\hbar}}}{\sqrt{L}} \tag{15}$$

Eigenvalue equation for momentum $\quad\Leftrightarrow\quad -i\hbar\dfrac{d\psi_p(x)}{dx} = p\psi_p(x)$ $\hfill(16)$

Eigenvalue equation for position $\quad\Leftrightarrow\quad x\psi_{x_0} = x_0\psi_{x_0}(x)$ $\hfill(17)$

Eigenvalue equation for energy $\quad\Leftrightarrow\quad \dfrac{1}{2m}(-i\hbar\dfrac{d}{dx})(-i\hbar\dfrac{d}{dx})\psi_E(x) + V(x)\psi_E(x) = E\psi_E(x)$

Dynamics: $i\hbar\frac{dV}{dt} = HV$ $\quad\Leftrightarrow\quad i\hbar\dfrac{\partial\psi(x,t)}{\partial t} = \dfrac{1}{2m}(-i\hbar\dfrac{d}{dx})(-i\hbar\dfrac{d}{dx})\psi_(x,t) + V(x)\psi_(x,t)$