

Physics 200-04
Dynamics Con't.

Let us look at an example of both the Heisenberg and Schrödinger solution to a problem, that of the behaviour of an electron spin in a magnetic field.

The electron spin is related to the Pauli spin matrices by

$$\begin{aligned} S_x &= \frac{\hbar}{2} \vec{s}_x \cdot \vec{\sigma} \\ S_y &= \frac{\hbar}{2} \vec{s}_y \cdot \vec{\sigma} \\ S_z &= \frac{\hbar}{2} \vec{s}_z \cdot \vec{\sigma} \end{aligned} \tag{1}$$

where the three vectors $\vec{s}_x, \vec{s}_y, \vec{s}_z$ are chosen initially so that

$$\begin{aligned} S_x(0) &= \frac{\hbar}{2} \sigma_1 \\ S_y(0) &= \frac{\hbar}{2} \sigma_2 \\ S_z(0) &= \frac{\hbar}{2} \sigma_3 \end{aligned} \tag{2}$$

Now, we know classically that a spinning charge has a magnetic moment as well given by $\mu_x = g \frac{e}{m} S_x$ and similarly for the y and z components of the magnetic moment. Here e is the charge and m is the mass of the particle, and g is a factor which measures how the charge in the spinning object is distributed with respect to how the mass is distributed. A g greater than one means classically that the charge is distributed further from the spin axis than is the mass. The g -factor for the electron is very close to 2. There is an interaction of any magnetic moment with a magnetic field that has the form $\mu_x B_x + \mu_y B_y + \mu_z B_z$ where B is the external magnetic field. I.e., this interaction energy is trying to align the magnetic dipole with the field.

Let us assume that the external field is in the z direction, so that only B_z is non-zero. This expression for the energy of a classical spinning system is then

$$H = g \frac{e}{m} S_z = g \frac{e}{2m} \hbar B_z \vec{s}_z \cdot \vec{\sigma} \tag{3}$$

The equations of motion for the three components of the spin are now

$$i\hbar \frac{dS_x}{dt} = [S_x, H] \tag{4}$$

and similarly for S_y and S_z . The easiest equation to solve is that for S_z since H is proportional to S_z . Since any matrix always commutes with itself, we have that

$$\frac{dS_z}{dt} = 0 \quad (5)$$

and S_z will be equal to $\hbar\sigma_3/2$ for all time.

The equation of motion for S_x and S_y will be

$$i\hbar\frac{dS_x}{dt} = \frac{ge\hbar B_z}{2m}[S_x, \sigma_3] \quad (6)$$

and similarly for S_y . Writing these in terms of the 1,2,3 components, we have

$$i\hbar\frac{d\vec{s}_x}{dt} = \frac{ge\hbar B_z}{m}i\vec{s}_x \times \vec{e}_z \quad (7)$$

where \vec{e}_3 has only its 3 component equal to 1 and the other two 0. Thus we have

$$\begin{aligned} \frac{ds_{x1}}{dt} &= \frac{ge\hbar B_z}{m}s_{x2} \\ \frac{ds_{x2}}{dt} &= -\frac{ge\hbar B_z}{m}s_{x1} \\ \frac{ds_{x3}}{dt} &= 0 \end{aligned} \quad (8)$$

Thus s_{x3} which starts out as 0 remains zero. The solution for the other two components which obeys the initial condition that $s_{x1}(0) = 1$ and $s_{x2}(0) = 0$ is

$$\begin{aligned} s_{x1} &= \cos(\omega t) \\ s_{x2} &= -\sin(\omega t) \\ s_{x3} &= 0 \end{aligned} \quad (9)$$

where

$$\omega = \left| \frac{ge\hbar B_z}{m} \right| \quad (10)$$

Similarly solving the equations for S_y gives

$$s_{y2} = \cos(\omega t)$$

$$\begin{aligned} s_{y1} &= \sin(\omega t) \\ s_{y3} &= 0 \end{aligned} \tag{11}$$

The Spin components thus are

$$\begin{aligned} S_x &= \frac{\hbar}{2} \begin{pmatrix} 0 & (\cos(\omega t) + i \sin(\omega t)) \\ (\cos(\omega t) - i \sin(\omega t)) & 0 \end{pmatrix} \\ S_y &= \frac{\hbar}{2} \begin{pmatrix} 0 & (-i \cos(\omega t) + \sin(\omega t)) \\ (i \cos(\omega t) + \sin(\omega t)) & 0 \end{pmatrix} \end{aligned} \tag{12}$$

The expectation value – the average value of the measured components of the spin components are given by $\langle \psi | S_w | \psi \rangle$, where $|\psi\rangle$ is the state. One has many options for the state. However, let us say that the state is

$$|\psi\rangle = \frac{1}{5} \begin{pmatrix} 3 \\ 4 \end{pmatrix} \tag{13}$$

(note this is purely an example– this state has no special significance)

Then we have

$$\begin{aligned} \langle \psi | S_x(t) | \psi \rangle &= \frac{\hbar}{50} \begin{pmatrix} 3 & 4 \end{pmatrix} \begin{pmatrix} 0 & (\cos(\omega t) + i \sin(\omega t)) \\ (\cos(\omega t) - i \sin(\omega t)) & 0 \end{pmatrix} \begin{pmatrix} 3 \\ 4 \end{pmatrix} \\ &= \frac{\hbar}{50} (12e^{i\omega t} + 12e^{-i\omega t}) = \frac{24}{50} \cos(\omega t) \end{aligned} \tag{14}$$

Similarly we find that

$$\langle \psi | S_y(t) | \psi \rangle = \frac{24}{50} \hbar \sin(\omega t) \tag{15}$$

and

$$\langle \psi | S_z(t) | \psi \rangle = \frac{7}{50} \hbar \tag{16}$$

Ie, the average vector moves so that its z component stays constant, while its x and y components rotate about the z axis with frequency ω .

Note that this is exactly the same as the motion of a spinning top classically. Ie, the equations of motion of the expectation value of the components is the same as classical equations of motion.

This is a generic feature of quantum systems. The expectation values tend to obey equations that are very similar to the classical equations of motion

of the system. Note that if we do successive measurements on a system we will not see this kind of motion. Instead we will see random jumping around. However if we make measurements on a huge number of particles, all starting in the same initial state and then average over the measured values, we do tend to get something that looks classical.

Classical physics seems to be something which is an approximation to the quantum physics if we only look at averages.

Schrödinger.

Let us look at the same problem from the Schrödinger point of view. Here the operators corresponding to the physical attributes (ie the spin components) do not change in time. Instead it is the state $|\psi\rangle$ which changes in time. In particular we have

$$i\hbar \frac{d|\psi\rangle}{dt} = H|\psi\rangle \quad (17)$$

Just as above

$$H = \frac{geB_z\hbar}{2m}\sigma_z \quad (18)$$

Thus we have writing

$$|\psi\rangle = \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} \quad (19)$$

we have

$$\begin{pmatrix} i\hbar \frac{d\psi_1}{dt} \\ i\hbar \frac{d\psi_2}{dt} \end{pmatrix} = \frac{\omega}{2}\hbar \begin{pmatrix} \psi_1 \\ -\psi_2 \end{pmatrix} \quad (20)$$

Thus

$$\begin{aligned} \psi_1 &= \psi_1(0)e^{-i\omega t/2} \\ \psi_2 &= \psi_2(0)e^{i\omega t/2} \end{aligned} \quad (21)$$

Note that this expression is not terribly transparent. In our example $\psi_1(0) = 3$ and $\psi_2(0) = 4$

We note that in many ways, solving the Schrödinger equation is much simpler than solving the Heisenberg equation. For one thing we do not have

to solve for our three separate matrices, just the one column vector $|\psi\rangle$. This is true in general. The Heisenberg representation is almost never used to actually solve problems. The Schrödinger representation is almost always used. This does not mean that the Heisenberg is not important– it is very important theoretically.

Just to give a very very very brief taste of the quantum mechanics of say a single particle moving in the x direction. The usual attribute is the position matrix X , together with the momentum P . As hinted, these two operators are related by

$$[X, P] = i\hbar I \quad (22)$$

We can write a general ket vector in terms of the amplitudes in the x basis– ie in terms of the eigenvalues of the X matrix, which we will call $|x\rangle$. Thus, a general state is

$$|\psi\rangle = \int \langle x|\psi\rangle |x\rangle dx \quad (23)$$

where we have replaced the sum over the eigenvectors by this integral. Yes, I know I said that the eigenvectors of X do not really exist, but let us ignore this for now.

We will define the $\psi(x) = \langle x|\psi\rangle$ as the amplitudes for the state $|\psi\rangle$ to have eigenvalue x . The probability to have the value x between x_1 and x_2 is given by $\int_{x_1}^{x_2} |\psi(x)|^2 dx$.

Now we have to figure out what P is. P is supposed to be a matrix such that $XP - PX = i\hbar I$. Let me not prove it but just state that

$$P \int \psi(x) |x\rangle = \int -i\hbar \frac{\partial \psi(x)}{\partial x} |x\rangle dx \quad (24)$$

Since P This definition of P acting on any vector expanded out in terms of the X eigenvectors certainly obeys the required commutation relations.

From classical physics, we know that the energy of the harmonic oscillator for example is

$$H = \frac{1}{2} \left(\frac{P^2}{m} + kX^2 \right) \quad (25)$$

. We can use exactly this same expression for the Quantum harmonic oscillator.

Just plugging in for what X and P are we find

$$H|\psi\rangle = \int \left(-\frac{\hbar^2}{2m} \frac{\partial^2 \psi(x)}{\partial x^2} + \frac{k}{2} x^2 \psi(x) \right) |x\rangle dx \quad (26)$$

and the eigenvalue equation for H , namely $H|\psi_E\rangle = E|\psi_E\rangle$ becomes

$$\int \left(-\frac{\hbar^2}{2m} \frac{\partial^2 \psi_E(x)}{\partial x^2} + \frac{k}{2} x^2 \psi_E(x) - E \psi_E(x) \right) |x\rangle dx = 0 \quad (27)$$

In order that the left hand side be a zero ket vector, each coefficient of the $|x\rangle$ must be zero. Thus one finally finds the differential equation

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \psi_E(x)}{\partial x^2} + \frac{k}{2} x^2 \psi_E(x) - E \psi_E(x) = 0 \quad (28)$$

If we solve this equation, we find that this energy is NOT continuous. It comes in discrete lumps, as

$$E = \left(n + \frac{1}{2} \right) \hbar \omega \quad (29)$$

where $\omega = \sqrt{\frac{k}{m}}$ the classical angular frequency of the oscillator. This discrete energy is NOT fed in from the beginning. Instead it is derived from the definition of P and X and the energy as defined in terms of these quantities.

Note that there is no classical physics here, except maybe in defining the energy in terms of P and X . There is no imposing some funny quantization conditions onto the classical solutions ($\int p \dot{q} dt = nh$). One simply defines the dynamic variables X and P , demands the commutation relation between them, writes down the Hamiltonian and derives the fact that the energy comes in discrete lumps.

Furthermore, if one looks at the Heisenberg equations of motion, P and X obey exactly the same equation in this quantum system as the classical equations do.