Physics 501-22

Heisenberg and Schroedinger

Heisenberg first came up with what we now know as QM in 1925 while a post doc with Neils Bohr. Exactly how he did so is still a mystery to me.

His idea was to replace teh dynamic variables of ordinary classical Hamiltonian mechanics by ,what he later learned were matricees. Given a particle travelling in 1-dimension, with dynamical variables x, p, the position and momentum (which are represented in the mathematics by real functions of time) with square complex matrices, X, P. These matrices were Hermitian ($X^\dagger = (X^*)^T = X$, $P^\dagger = P$). These matrices were defined as operators on a complex vector space $\mathcal{H}$, with vectors which we will anachronistically designate by $|\psi\rangle$ (That notation was invented by dirac about 5 years later). Matrix multiplication is famously non-commutative such that if one defines the multiplication in the usual way

$$AB_{ij} = \sum_k A_{ik}B_{kj} \tag{1}$$

then, in general $AB \neq BA$. Defining the commutator $[A,B] = AB - BA$ he required that $[XP - PX] = iI$ where I is the identity matrix ($AI = IA = A$ for all A). This might well have been motivated by the classical Poisson bracket

$$\{f(p,x), g(p,x)\} = \partial_x f \partial_p g - \partial_p f \partial_x g \tag{2}$$

Then classically, given some function of p, q which is the Hamiltonian one has from classical Hamiltonian mechanics

$$\frac{d}{dt}f(p,x) = \{f(p,x), H(p,x)\} \tag{3}$$

He made this be

$$i\frac{d}{dt}F(P,X) = [F(P,X), H(P,X)] \tag{4}$$

as the equation of motion for the matrices. Since measurements of dynamic variables gave numbers rather than matrices, one had to come up with a rule as to how one would transcribe outcomes of measurements on matrices into numbers.

He solved the quantum mechanics of the simple harmonic oscillator and Pauli solved the Heisenberg equations for the Hydrogen atom.

Given the classical Hamiltonian for an electron around a nucleus (the model for an atomdeveloped by Rutherford in the early 1900), he wrote the classical Hamiltonian

$$\frac{(p_x^2 + p_y^2 + p_z^2)}{2m} - \frac{e^2}{\sqrt{x^2 + y^2 + z^2}} \tag{5}$$

as an matrix function

$$\frac{P_x^2 + P_y^2 + P_z^2}{2m} - \frac{e^2}{\sqrt{X^2 + Y^2 + Z^2}} \tag{6}$$

1

Classically, this equation has six constants of motion The energy E, given here by H, the three components of the angular momentum vector $\vec{L} = \vec{X} \times \vec{P}$, and the Runge Lens vector $\vec{A} = \vec{P} \times \vec{L} - me^2 \frac{\vec{X}}{R}$. Each of these quantum objects commuted with H, given the commutation relations of $\vec{X}$ and $\vec{P}$. Via an algebraic tour-de-force, Heisenberg was able to solve the equations for the eigenvectors H, $\vec{L} \cdot \vec{L}$ L_z and A^2 and obtained essentially what Bohr had hypothesised to explain the spectum of Hydrogen.

Shortly thereafter, without knowing what Heisenberg did, Schroedinger was deeply impressed with the thesis work of deBroglie, who hypothesised that, just as Einstein, 20 years earlier, had argued that electromagnetism, that prototypical field theory, was, under certain circumstances behaved as if it were made up of particles, so matter (like electrons) could under certain circumstances behave like waves. If so, what would the equation of those waves be? On his honeymoon in the Austrian alps, Schroedinger wrote a series of papers, in which he "guessed" at an equation.

$$i\partial_t(\psi(t,x,y,z)) = \frac{1}{2m}\vec{\nabla} \cdot \vec{\nabla}\psi(t,x,y,z) - \frac{e^2}{\sqrt{x^2+y^2+z^2}}\psi(t,x,y,z) \qquad (7)$$

Again, he was able to solve this wave type equation. under the assumption that $\partial_t\psi(t,x,y,z) = -iE\psi(t,x,y,z)$, and found that the energies were exactly the same as what Pauli, using Heisenberg's formalism, had found. This was of course supremely confusing, since one seemed to have two totally different theories which gave the same answers. Once Schroedinger became aware of Heisenberg's work, he, (and Dirac) quickly figured out that in fact the two theories were equivalent. Instead of regarding X and P as matrices, one could regard them as more general linear operators. Heisenberg's matrices were operators which acted on the vectors in the space $\mathcal{H}$, while Schroedinger's were operators acting on the vector space of functions of x. In Schroedinger's formalism, taking X to be multiplication of the function by x and P to be complex differentiation

$$P_x\psi(t,x,y,z) = -i\partial_x\psi(t,x,y,z) \qquad (8)$$

one sees immediately that

$$
\begin{aligned}
XP_x\psi - P_xX\psi &= x(-i\partial_x\psi(t,x,y,z)) - (-i\partial_x(x\psi(t,x,y.z))) &(9)\\
&= x(-i\partial_x\psi(t,x,y,z)) + i\psi(t,x,y,z) + x(i\partial_x\psi(t,x,y,z)) &(10)\\
&= i\psi(t,x,y,z) = iI\psi(t,x,y,z) &(11)
\end{aligned}
$$

where $I\psi(t,x,y,z) = \psi(t,x,y,z)$.

What this ψ was was straightened out by Max Born (the same person who had pointed out to Heisenberg that what he was doing was manipulting matrices), who, in probably the most famous footnote in science, suggested that $\psi^*(t,x,y,z)\psi(t,x,y,z)$ should be interpreted as the probability density for finding the particle at the location x,y,z at time t. It was easy to prove that the total probability

$$\mathcal{P} = \partial_t \int\int\int |\psi(t,x,y,z)|^2 dxdydz = 0 \qquad (12)$$

2

by the Schroedinger equation satisfied by ψ. If we interpret $\mathcal{P}$ as the probability that that the particle should be somewhere at time t, it is natural to scale ψ by a constant, so that $\mathcal{P} = 1$, ie the probability is unity that the particle be somewhere. This also implies that the probabilities are independent– ie, there is zero probability that the particle is at more than one place at time t (the probability that it be both at x and x' is zero since otherwise the total probability would not equal the sum on the individual probabilities. A fundmental theorem of probabilities is

$$Prob(x \; or \; x') = Prob(x) + Prob(x') - Prob(x \; and \; x') \tag{13}$$

It was rapidly realised that Heisenberg's formulation should also have something equivalent to ψ. However, since in the Heisenberg representation, it is the dynamic variables which are time dependent, the "state" should not be.

Thus in the Schroedinger representation, it is the state (ψ) which is dynamic, and the operators which represent the dynamic attributes of the particle are not time dependent. In the Heisenberg representation, it is the dynamic operators which are time dependent while the state is not.

Let us look at a simple situation. Consider a free particle, with unit mass, and Hamiltonian

$$H = \frac{1}{2}P^2 \tag{14}$$

In the Heisenberg representation, the equations of motion are

$$\partial_t X = P \tag{15}$$
$$\partial_t P = 0 \tag{16}$$

with solution

$$X(t) = X(0) + P(0)t \tag{17}$$
$$P(t) = P(0) \tag{18}$$

Let us now assume that we have (somehow) determined that at t=0, or rather in terms of $X(0) and P(0)$ the Heisenberg state is $\psi(x_0) = Ne^{-\frac{x_0^2}{4\Delta^2}}$. where N is a normalisation constant. Then we have

$$\int (\psi(x_0)^* \psi(x_0) dx = 1 \tag{19}$$

or

$$\int N^2 e^{-\frac{x_0^2}{2\Delta}} dx_0 = \sqrt{2\pi} N^2 \Delta \tag{20}$$

or $N = \frac{1}{\sqrt{\sqrt{2\pi}\Delta}}$.

On the other hand the Schroedinger equation is

$$i\partial_t \psi(t,x) = -\frac{1}{2}\partial_x^2 \psi(t,x) \tag{21}$$

3

While this is certainly solvable it is not trivial.

However, let us look at the Heisenberg representation again. The state ψ obeys the equation

$$(iP(0) + \frac{X(0)}{2\Delta^2})\psi(x_0) = 0 \tag{22}$$

$$(\partial_{x_0} + \frac{x_0}{2\Delta^2})\psi = 0 \tag{23}$$

Writing $P(0)$ and $X(0)$ in terms of $P(t)$ and $X(T)$ we get

$$P(0) = P(t) \tag{24}$$

$$X(0) = X(t) - P(t)t \tag{25}$$

and the state $\psi(x_0)$ becomes

$$iP(t) + \frac{(X(t) - P(t)t)}{2\Delta^2})\psi = 0 \tag{26}$$

Using $X(t) \to x_t$, $P(t) = -i\partial_{x_t}$, we get

$$(\partial_{x_t} + \frac{x_t}{2\Delta^2 + it})\psi(x_t) = 0 \tag{27}$$

or

$$\psi(t, x_t) = N_t e^{-\frac{x^2}{4\Delta^2 + 2it}} \tag{28}$$

with

$$N_t^2 = \sqrt{\frac{4\Delta^2}{2\pi(4\Delta^4 + t^2)}} \tag{29}$$

This is precisely the solution of the Schroedinger equation, where we take $x_t \to x$ as can be seen by substituting it into the Schroedinger equation.

Ie, in this case solving the Heisenberg equation and then deriving the Schroedinger solution is far easier than solving the Schroeding equation directly. This will often be the case especially if the equations of motion are linear.

We see that the dynamic variables in the Schroedinger picture at time t are the dynamic variables in the Heisenberg representation at time t. And the state at time t is the initial state expressed in terms of these dynamic variables.

Formally, One can define a unitary operator $U(t, t')$ which obeys the equation

$$i\frac{d}{dt}U(t, t') = HU(t, t') \tag{30}$$

$$U(t', t') = 1 \tag{31}$$

Then the Schroedinger picture,

$$|\psi(t)\rangle = U(t, t')\,|\psi(t')\rangle \tag{32}$$

4

or in the postition basis where $ket\psi = \int \psi(t,x)\,|x\rangle$

$$\psi(t,x) = \int \langle x|\, U(t,t')\, |x'\rangle\, \psi(t',x')dx' \tag{33}$$

$U(t,x,t',x')$ is often called the Green's function for the Hamiltonian.

If the Hamiltonian is time independent, then we can formaly solve the equation by

$$U(t,t') = e^{-i(t-t')H} \tag{34}$$

where the exponential is defined via its taylor expansion

$$e^{S} = \sum_{0}^{\infty} \frac{S^n}{n!} \tag{35}$$

If H is explicitly time dependent however, this does not work One might expect to do something like

$$\hat{U}(t,t') = e^{-i\int_{t'}^{t} H(t'')dt''} \tag{36}$$

But if $[H(t'), H(t'')]$ is not equal to zero, this will not work $i\frac{d}{dt}(\sum_n \frac{(-i\int_{t'}^{t} H(t'')dt'')^n}{n!})$ is not equal to $H(t)U$ because $\frac{dH}{dt}(t)$ does not in general commute with $H(t'')$. Consider the second term in that expansion

$$\frac{d}{dt}(\int_{t'}^{t} H(t'')dt'')^2 = (H(t)\int_{t'}^{t} H(t'')dt'' + \int_{t'}^{t} H(t'')dt'' H(t). \tag{37}$$

Unless$H(t)$ commutes with all $H(t'')$ for t'' between t' and t, this is not the same as $2H(t)\int_{t'}^{t} H(t'')$. One often sees the solution written as $U = \mathbf{T}e^{-i\int_{t'}^{t} H(t'')dt''}$ which would seem to say that the solution is just what I hypothesised. But the $\mathbf{T}$ stands for "time ordered", which means that in each term $\int_{t'}^{t} H(t'')^n$, the H(t") are reordered so that if $t'' > \tilde{t}''$ where t'' is from one of those n terms in the product, and $\tilde{t}''$ is from another, then the product of the H's are taken such that $H(t'')$ is to the left of $H(\tilde{t}'')$ in that product. If the commutator of $H(t'')$ and $H(\tilde{t}'')$ are all small, (and the commutators of those commutators are evensmaller, etc) one can approximate the unitary operator by means of the Magnus expansion.

If we have

$$\partial_t U(t,t') = A(t)U(t,t') \tag{38}$$

with $U(t',t') = I$, then Magnus showed that one can write the solution in terms of a sequence of operators. In particular write

$$U = e^{\Omega(t,t')} \tag{39}$$

5

Then one has

$$\Omega \;=\; \sum_n \Omega_n \qquad\qquad\qquad (40)$$

$$\Omega_0 \;=\; \int_{t'}^{t} A(t_1)dt'_1$$

$$\Omega_1 \;=\; \frac{1}{2}\int_{t'}^{t}\int_{t'}^{\tilde{t}_1} [A(t_1),A(t_2)]dt_2dt_1$$

$$\Omega_2 \;=\; 1/6\int_{}^{t}\int_{t'}^{t_1}\int_{t'}^{t_2} ([A(t_1),[A(t_2),A(t_3)]]+[A(t_3),[A(t_2),A(t_1)]]dt_3dt_2dt_1$$

$$...$$

For our situation, $A=-iH(t)$, and each Ω_n is anti-Hermitian ($\Omega_n^{\dagger}=-\Omega_n$. Thus, if one truncates the Magnus expansion at some value of n, then the operator U is Unitary. $U^{\dagger}=U^{-1}$.

Each term Ω_n has more commutators in it than lower values of n. In particular $\Omega_n = \sum [A,[A,....[A,A]]...]\overbrace{n}$ where each A has a different time argument . If those commutators are all small, then this is an expansion which converges rapidly. If they are not, then this may still be an assymptotic expansion. Thus of the great advantage of the Magnus expansion is that if one truncates the series in Ω at some order, the operator U is still a Unitary operator. Most other expansions do not share this feature. Most truncated series does not give a unitary operator, and the evolution is non-unitary to that order.