Quantum Mechanics 3 2001/2002

Solution set 4

(1) The given states are eigenstates with given energy. This means they must satisfy the eigen-equation

$$Hu_n(x) = E_n u_n(x),$$

where H is the Hamiltonian operator. This is just a short way of writing the time-independent Schrödinger equation. Sets of eigenstates are *complete*: this term means that we can expand any general wavefunction:

$$\psi(x) = \sum_j a_j u_j(x) \quad \Rightarrow \quad \psi(x)^* = \sum_j a_j^* u_j(x)^*.$$

The expectation value $\langle\psi|H|\psi\rangle$ means

$$\langle\psi|H|\psi\rangle = \int \psi^* \, H \, \psi \, dV.$$

Using the expansion of ψ,

$$H\psi = H \sum_j a_j u_j(x) = \sum_j a_j H u_j(x) = \sum_j a_j E_j u_j(x).$$

Now put the expansions for ψ and $H\psi$ in the integral, using a different dummy index for each sum, to avoid confusion:

$$\langle\psi|H|\psi\rangle = \int \left(\sum_i a_i^* u_i(x)^*\right) \left(\sum_j a_j E_j u_j(x)\right) \, dV = \sum_i \sum_j a_i^* a_j E_j \int u_i(x)^* u_j(x) \, dV.$$

Using orthonormality of the u's, the last integral is just δ_{ij}, so that

$$\langle\psi|H|\psi\rangle = \sum_i |a_i|^2 \, E_i.$$

In other words, the expectation of H is just the sum of the eigenvalues, weighted by the probability of being in each state, $|a_i|^2$. Since $E_i \geq E_0$, by definition of the ground state as the state of lowest energy, we see that

$$\langle\psi|H|\psi\rangle \geq \sum_i |a_i|^2 \, E_0 = E_0,$$

where the last step follows becuase the probabilities add up to unity: $\sum_i |a_i|^2 = 1$.

(2) The Fourier transform is a specific example of the expansion in eigenstates. The state $u = \exp(ikx)$ is an eigenstate of momentum:

$$p_x u(x) = \frac{\hbar}{i}\frac{\partial}{\partial x} u(x) = \hbar k u(x),$$

and the momentum eigenvalue is $\hbar k$, as expected. Thus, when we write

$$\psi(x) \propto \int \tilde{\psi}(k) \, \exp(ikx) \, dk,$$

this is just like writing $\psi = \sum_i a_i u_i(x)$. The Fourier coefficients $\tilde{\psi}(k)$ are analogous to a_i. Therefore, just as $|a_i|^2$ is the probability of being in the ith state, so $|\tilde{\psi}(k)|^2$ is proportional to the probability of getting momentum $\hbar k$.

The wavefunction is correctly normalized, so its Fourier transform is

$$\tilde{\psi} = \frac{1}{\sqrt{4\pi a}} \int_{-a}^{a} \exp(ikx) \, dx = \frac{1}{\sqrt{\pi a}} \frac{\sin ka}{ka}.$$

Putting $p = \hbar k$ gives the probability distribution of momentum, which is proportional to $|\tilde{\psi}|^2$. The mean value of momentum is clearly zero, because the distribution is symmetric, but the variance is

$$\langle p^2 \rangle \propto \int_{-\infty}^{\infty} \left(\frac{\sin pa/\hbar}{pa/\hbar} \right)^2 \, p^2 \, dp.$$

The integrand is thus just proportional to $\sin^2(pa/\hbar)$, which has an average value of 0.5. The integral diverges. The uncertainty principle is an inequality, and defines a minimum uncertainty for a Gaussian wavefunction. In general, the uncertainty will be larger than the minimal value, as in this example. If we take a different definition of the spread in momentum (e.g. the range enclosing 50% of the values), then something closer to $\delta p \simeq \hbar/a$ will be found.

(3) Differentiate $\langle O \rangle = \int \psi^* O \psi \, dV$ inside the integral to get two terms. Now use $H\psi = i\hbar\dot{\psi}$ and the complex conjugate relation $(H\psi)^* = -i\hbar\dot{\psi}^*$, plus the Hermitian property of H ($\int (H\psi)^* \phi \, dV = \int \psi^* H \phi \, dV$, where $\phi = O\psi$ in this case). Remember the meaning of the commutator symbol: $[H, O] = HO - OH$.

For the second part, use the general relation with $O = x$ or $O = p_x$. This just requires the operator form of momentum and the ability to differentiate a product. For example, $(d/dx)(x)\psi = (x)(d/dx)\psi + \psi$, so $(d^2/dx^2)(x)\psi = (x)(d^2/dx^2)\psi + (d/dx)\psi + (d/dx)\psi$. Now use the fact that, in 1D,

$$H = \frac{p_x^2}{2m} + V(x) = \frac{-\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)$$

so $[H, x] = -(\hbar^2/m)(d/dx) = (\hbar/i)p_x/m$ (we have cancelled out a factor of ψ on either side, since this operator equation applies for any ψ).

The reasoning for $[H, p_x]$ is similar. Notice that it's only the terms involving derivatives that cause trouble: commutators like $[V(x), x]$ always vanish.

The final Ehrenfest equations are very satisfying: classical mechanics is obeyed by the average properties of quantum particles – which explains why we can get sensible results on laboratory scales using classical laws.