QUANTUM MECHANICS A (SPA-5319)

Time Evolution and the Expansion Theorem

Earlier in the course we found that for a time independent potential we can solve the time-independent Schrödinger equation:

$$\hat{H}\psi = E\psi$$

and obtain the set of energy eigenstates $\Psi_n(x,t) = \psi_n(x)e^{-\frac{iE_nt}{\hbar}}$, which have exactly known energies.

We have already noted the superposition principle: mathematically this is a consequence of the Schrödinger equation's linearity in Ψ. For all potentials of physical interest it can be proved that the most general solution of the TDSE can be written as a linear combination of energy eigenstates, namely:

$$\Psi(x,t) = \Sigma_n \, c_n \, \psi_n(x)e^{-\frac{iE_nt}{\hbar}}$$

We noted that these linear combinations, generally, are <u>not</u> stationary states ($|\Psi|^2 = f(t)$) nor do they have exactly defined energy ($\Delta E \neq 0$).

This is the expansion theorem and it encodes an important implication of the time-independent Schrödinger equation: even though quantum mechanics is indeterministic, the time–evolution of the wave function itself is deterministic. By indeterministic we mean that quantum mechanics can only predict the probability of a given outcome for a measurement; but the wave function is deterministic because, given the initial wavefunction, $\Psi(x,0)$ (whatever this may be at $t = 0$), the TDSE precisely determines its evolution at times $t > 0$.

The question immediately arises about how we would obtain the individual expansion coefficients, c_m, for an arbitrary wavefunction $\Psi(x,0)$ at $t = 0$. As it happens, these are simply obtained by considering the wavefunction $\Psi(x,0)$ at $t = 0$ and the individual eigenstate whose coefficient we are interested in, $\psi_m(x)$. At zero time the linear combination simplifies to $\Psi(x,0) = \Sigma_n \, c_n \, \psi_n(x)$. Multiplying by $\psi_m(x)^*$, and integrating over all space, yields

$$\int_{-\infty}^{\infty} \psi_m(x)^* \Psi(x,0) \, dx = \int_{-\infty}^{\infty} \Sigma_n \, c_n \, \psi_m(x)^* \, \psi_n(x) \; dx$$

Using the fact that the energy eigenstates are orthonormal we obtain a general expression for the expansion coefficients:

$$c_m = \int_{-\infty}^{\infty} \psi_m(x)^* \Psi(x,0) \, dx$$

Having found the expansion coefficients from this integral, we can then insert them into the expansion to find the wave function $\Psi(x,t)$ at all later times $t > 0$, given that we already know the energy eigenvalues E_n belonging to each known eigenstate $\psi_n(x)$. However, there is a proviso: the wavefunction evolves according to this prescription provided the system is left undisturbed after the initial time $t = 0$.

The complex expansion coefficients clearly play an important role in determining the wave function and its evolution. But what is their physical significance? We begin by calculating the expectation value of the energy, $\langle E \rangle$, for such a state:

$$\langle E \rangle = \int_{=\infty}^{\infty} \Psi(x,t)^* \, \hat{H}\Psi(x,t) \, dx$$

And obtain the result $\langle E \rangle = \sum_n |c_n|^2 E_n$, thus the average energy is a weighted sum over all the energies, with the weighting $|c_n|^2$ for energy E_n. This suggests that $|c_n|^2$ is the probability that the energy E_n will be the result of a measurement of energy for a particle in the state specified by the wave function $\Psi(x,t)$.

Finally we are led to the key Measurement Postulate of quantum mechanics: For a particle in the quantum state

$$\Psi(x,t) = \Sigma_n \, c_n \, \psi_n(x) e^{-\frac{iE_n t}{\hbar}}$$

the <u>only possible</u> result of a single energy measurement is one of the eigenvalues E_n, with probability $|c_n|^2$.

There is more to the Measurement Postulate: the 'Collapse of the Wave Function'. If the energy measurement yields a result E_n at time t, then immediately after the measurement the wave function 'collapses' to the corresponding eigenstate:

$$\Psi(x,t)_{after} = \psi_n(x) e^{-\frac{iE_n t}{\hbar}}$$

All future measurements then yield the same value for the energy of the state.