QM
Phys 651

Lecture #2

Wave aspects of matter

As we discussed last time, light exhibits wave-particle duality. What about material particles? Do they have a wave aspect? $\Rightarrow$ yes!

De Broglie: wave picture $\Rightarrow$ a particle is described by a frequency ν and a wave vector $\vec{k}$

$$E = h\nu = \hbar\omega$$

energy

$$\vec{p} = \hbar\vec{k} = \hbar \cdot \frac{2\pi}{\lambda}\frac{\vec{k}}{|\vec{k}|} = \frac{h}{\lambda}\frac{\vec{k}}{|\vec{k}|}$$

momentum

wavelength

unit vector $\parallel \vec{k}$

postulated to be valid for <u>all</u> particles

Then, to every free particle, a plane wave determined up to an amplitude factor A is assigned:

$$\Psi(\vec{r},t) = A e^{i(\omega t - \vec{k}\cdot\vec{r})} = A e^{i(Et - \vec{p}\cdot\vec{r})/\hbar}$$

The plane wave associated with the particle has wavelength $\lambda = \frac{2\pi}{k} = \frac{h}{p} \underset{\uparrow}{=} \frac{h}{mv}$

valid if rest mass $\neq 0$

Let's make an estimate of λ for non-relativistic electron with energy $E = 10\,keV$ $\Rightarrow$ $\lambda_e = \frac{h}{m_e v} \underset{\uparrow}{=} \frac{h}{\sqrt{2m_e E}}$

$E = \frac{mv^2}{2} = \frac{p^2}{2m}$

$h = 6.63 \cdot 10^{-34}\,J.s$

$E = 10\,keV = 10^4 \cdot 1.6 \cdot 10^{-19}\,J$

$m_e = 9.1 \cdot 10^{-31}\,kg$

$\Downarrow$

$$\lambda = \frac{6.63 \cdot 10^{-34}}{\sqrt{2 \cdot 9.31 \cdot 10^{-31} \cdot 1.6 \cdot 10^{-15}}} = 1.23 \cdot 10^{-11}\,m =$$

$$= \underline{0.123\,\mathring{A}}$$

Note:

If you have a choice between optical microscopy ($\lambda \sim 400-700\,nm$) and electron microscopy ($\lambda \sim 0.1\,\mathring{A}$)

$\Downarrow$

electron microscopy provides a much better resolution and is a powerful tool for research in nanoscience and nanotechnology

Chronology of experiments on wave aspect of particles:

1927 Davisson & Germer ⇒ diffraction of accelerated electrons from a crystal surface

1928 Thomson ⇒ diffraction of electrons on polycrystalline thin films

⇓

nowadays utilized in SEM (scanning electron microscopy) and TEM (transmission electron microscopy)

1932 Stern ⇒ crystal-diffraction experiments are repeated with helium atoms and hydrogen molecules

. . . .

1999 (see articles in Nature, HW#1) diffraction of C_{60} (60 atoms; $m = 720$ amu) particles (almost classical objects!!)

2011 (—"—) 430-atom molecules! $m = 6910$ amu, $\lambda = 1$ pm

Bottom line: Wave-like behavior is a very general property of material objects

How do we interpret a wave describing a particle? $\Rightarrow$ introduce statistical interpretation of matter waves $\Rightarrow$

Wave function

(i) replace classical concept of a trajectory with a concept of time-varying state

(ii) quantum state of a particle is characterized by a wave function $\Psi(\vec{r}, t, \ldots)$

e.g. spin variables

(iii) $\Psi(\vec{r}, t)$ is interpreted as a probability amplitude

(iv) probability to find a particle at time t in a volume element $d^3r = dx\,dy\,dz$ around $\vec{r}$ is $d\mathcal{P}(\vec{r}, t) = C\, |\Psi(\vec{r}, t)|^2 d^3r$

normalization constant

probab density

(v) principle of spectral decomposition

(recall Lecture #1) applies to the measurement of an arbitrary physical quantity:

- the result of measurement must belong to a set of eigen-results $\{a\}$
- with each eigenvalue a there is an associated eigenstate $\Rightarrow$ a function $\varphi_a(\vec{r})$

This function is such that if $\psi(\vec{r}, t_0) = \varphi_a(\vec{r})$ (where t_0 is the time at which the measurement is performed), the measurement will always yield a

- for any $\psi(\vec{r}, t)$, the probability $\mathcal{P}_a$ of finding the eigenvalue a for a measurement at time t_0 is found by decomposing $\psi(\vec{r}, t_0)$ in terms of $\varphi_a(\vec{r})$:

$$\psi(\vec{r}, t_0) = \sum_a c_a \varphi_a(\vec{r})$$

Then, $\mathcal{P}_a = \dfrac{|c_a|^2}{\sum_a |c_a|^2}$ (total probability $\sum_a \mathcal{P}_a = 1$)

- if the measurement indeed yields a, the wavefunction of the particle immediately after the measurement is:

$$\Psi_{after}(\vec{r}, t_0) = \Psi_a(\vec{r})$$

(vi) Equation describing time evolution of $\Psi(\vec{r}, t)$ is the Schrödinger equation:

$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \Delta \Psi(\vec{r}, t) + V(\vec{r}, t)\Psi(\vec{r}, t)$$

$\Delta = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$ – Laplacian operator

V – potential

Important constraints on $\Psi(\vec{r}, t)$:

- must be square-integrable, i.e. $\int |\Psi(\vec{r}, t)|^2 d^3r$ is <u>finite</u>
- in most cases (but not always!) $\Rightarrow$ $\int |\Psi(\vec{r}, t)|^2 d^3r = 1$ ← normalization