Quantum Theory

Wave-particle duality
Schrödinger equation
Born interpretation: normalization, quantization

Reading: Atkins, Ch. 8 (p. 249)

Wave-particle duality

	C.M.		Exp.
electromagnetic radiation	"wave"	$\rightarrow$	also "particle" characteristics
electron	"particle"	$\rightarrow$	also "wave" characteristics

(1) Particle characteristics of electromagnetic radiation

- spectrum: electromagnetic radiation of frequency ν possesses the energies of
  0, $h\nu$, $2h\nu$ $\rightarrow$ 0, 1, 2 particles, each particle having $h\nu$ energy: "**Photon**"

e.g., yellow light (560 nm) of 100 W lamp in 0.1 s (efficiency 100 %)
$\rightarrow$ number of photons: $N = E/h\nu = Pt/h(c/\lambda) = 2.8 \times 10^{20}$
(40 min $\rightarrow$ 1 mol photons)

- photoelectric effect: light energy = $nh\nu$ $\rightarrow$ particle-like collisions of light

(2) Wave characteristics of particles

- electron diffraction (Davisson & Germer Exp. (1925)): a characteristic property of waves

→ waves interfere constructively and destructively in different directions: wave-like property of electron, molecular hydrogen

de Broglie relation

- particle $\rightarrow$ wave-like
  wave $\rightarrow$ particle-like $\Rightarrow$ "wave-particle duality"

- 1924, de Broglie (France) suggested that any particle travelling with a linear momentum p (=mv) should have a wavelength of

$$\lambda = h/p\text{: de Broglie relation}$$

- particle with high momentum $\rightarrow$ short wavelength

Macroscopic body: high momentum $\rightarrow$ wavelength are undetectably small: wave-like properties can not be observed

e.g., golf ball, 45 g, velocity 30 m/s $\rightarrow$ $\lambda = 4.9 \times 10^{-22}$ pm (no wave-like)

- wave-particle duality & quantized energy $\Rightarrow$ **new mechanics** needed

(cf. Classical mechanics treated particles abd waves as entirely separate entities)

- wave in new mechanics replaces classical concept of trajectory: rather than travelling along a definite path, a particle is distributed through space like a wave $\Rightarrow$ "wavefunction" (Ψ, psi)

Schrödinger equation

- **Schrödinger equation** (1926): Austrian physicist

- He proposed an equation for finding the wavefunction of any system
- time-independent Schrödinger equation
  particle mass m moving in 1-dimensional with energy E

V(x): potential energy of the particle at point x
E: total energy
$\hbar$ (h-cross or h-bar) = $h/2\pi$ = 1.05457×10^{-34} Js

3-D

In general case, Schrödinger equation

$$\mathbf{H\Psi = E\Psi}$$

H: hamiltonian operator

Time-dependent Schrödinger equation

cf) Derive Schrödinger equation

Born interpretation of the wavefunction

- "wavefunction" contains all the dynamic information about the system
- Max Born: interpretation of the wavefunction in terms of the location of the particle

cf: the wave theory of light: square of amplitude of electromagnetic wave = intensity: probability of finding a photon in the region

1-D

- if particle has Ψ at x, the probability of finding the particle between x and x + dx is proportional to $|\Psi|^2 dx$

$|\Psi|^2 dx = \Psi^*\Psi$ if Ψ is complex: $|\Psi|^2$ "probability density"

Ψ: probability amplitude

3-D

Ψ at r $\rightarrow$ probability of finding the particle in $d\tau = dxdydz \Rightarrow |\Psi|^2 d\tau$

(a) **Normalization**

Schrodinger equation $\rightarrow$ $N\Psi$: all probability of the particle must be 1
$\rightarrow$ possible to find "normalization constant" N

probability: $(N\Psi^*)(N\Psi)dx$
$\Rightarrow$ $N^2\int\Psi^*\Psi dx = 1 \Rightarrow N = 1/[\int\Psi^*\Psi dx]^{1/2}$

where the integral is over all the space (from $-\infty$ to $+\infty$)

We can find N and 'normalize' the wavefunction
$\rightarrow$ normalized wavefunction: $\int\Psi^*\Psi dx = 1$ or $\int\Psi^*\Psi d\tau = 1$

$d\tau = dxdydz$

in spherical polar coordinates, r, θ, ϕ

$x = r\sin\theta\cos\phi$, $y = r\sin\theta\sin\phi$, $z = r\cos\theta$

$d\tau = r^2\sin\theta\, dr\, d\theta\, d\phi$, $r: 0 \rightarrow \infty$, $\theta: 0 \rightarrow \pi$, $\phi: 0 \rightarrow 2\pi$

(b) **Quantization**

$\int\Psi^*\Psi d\tau = 1 \Rightarrow$ severe restrictions on the acceptability of wavefunctions

(i) Ψ must not be infinite anywhere

if it were $\Rightarrow N\int\Psi^*\Psi = \infty = 1 \Rightarrow N\infty = 1 \Rightarrow N = 0$ (x)

cf: acceptable: infinite Ψ over infinitesimal since $\int\Psi^*\Psi$ is finite (infinitely high x infinetely narrow = finite area) e.g., a particle at a single, precise point

(ii) $|\Psi|^2 = \Psi^*\Psi$: probability of finding the particle $\Rightarrow$ wavefunction (Ψ) must be single-valued

(iii) Ψ: 2nd-order differential equation $\Rightarrow$ 2nd derivative should exist: Ψ should be continuous

1st derivative (slope) should also be continuous

$\therefore \Psi$ must be coninuous, have a continuous slope, be single-valued, and be finite everywhere, cannot be zero everywhere (particle must be somewhere)

$\Rightarrow$ the energy of a particle is quantized (acceptable solutions of the Schrödinger equation for these severe restrictions at <u>only certain energies</u>)