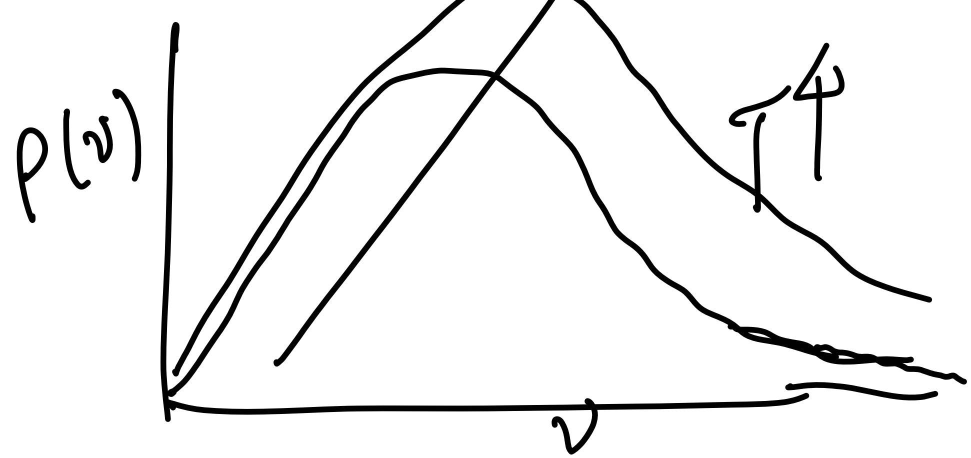
de Broglie, Heisenberg, and Schroedinger

Note Title 24-09-2009

Black body distribution

Planck's recipe $\rho(\nu) = \frac{8\pi\nu^2}{c^3} \frac{h\nu}{e^{h\nu/kT}-1}$



Wave - particle duality

1) Particles

2) Interference pattern

de Broglie

$$\lambda = \frac{h}{p}$$

Photons

$$\nu \lambda = c$$

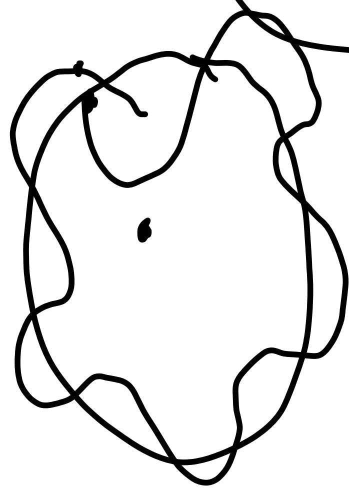
$$E = pc$$

$$\lambda = \frac{h}{p}$$

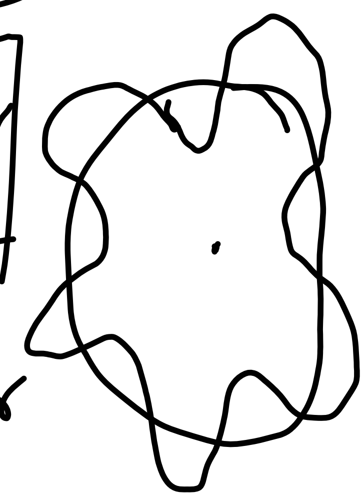
$$T = E = p^2/2m$$

Bohr atom

$$mvr = nh/2\pi$$



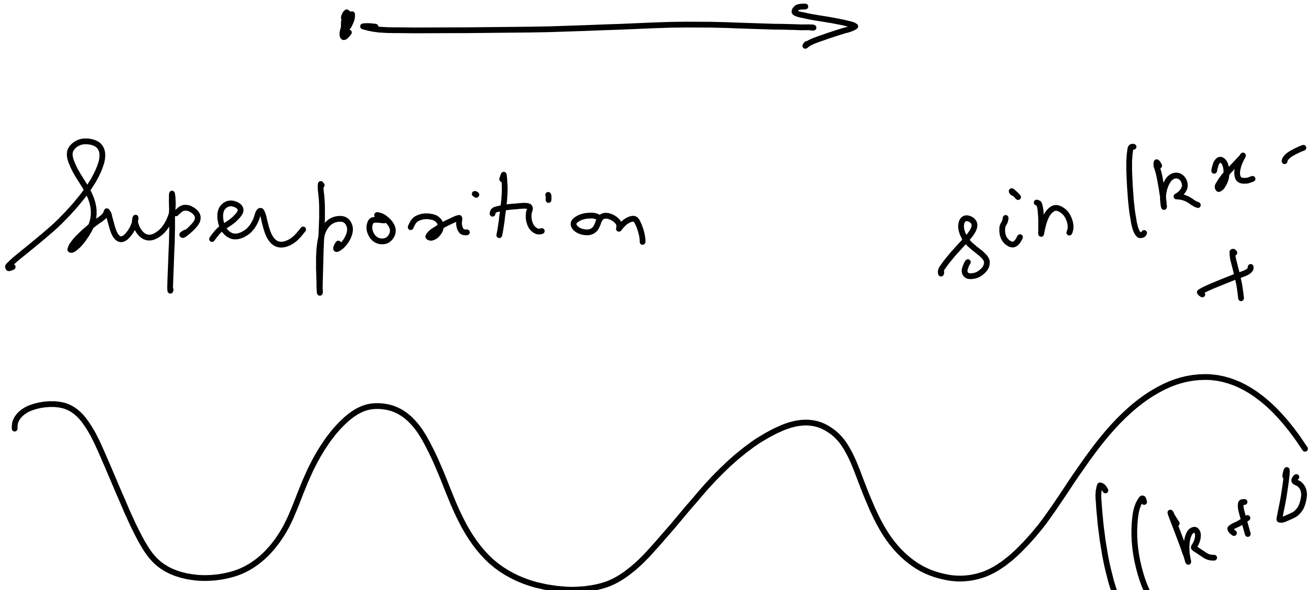
$$n\lambda = 2\pi r$$



$$n\frac{h}{p} = 2\pi r$$

$$L = pr = \frac{nh}{2\pi}$$

Superposition



$\sin(kx - \omega t)$

$+$

$\sin((k+\Delta k)x - (\omega+\Delta\omega)t)$

$\cos(\Delta k x - \Delta\omega t) \sin(k'x - \omega' t)$

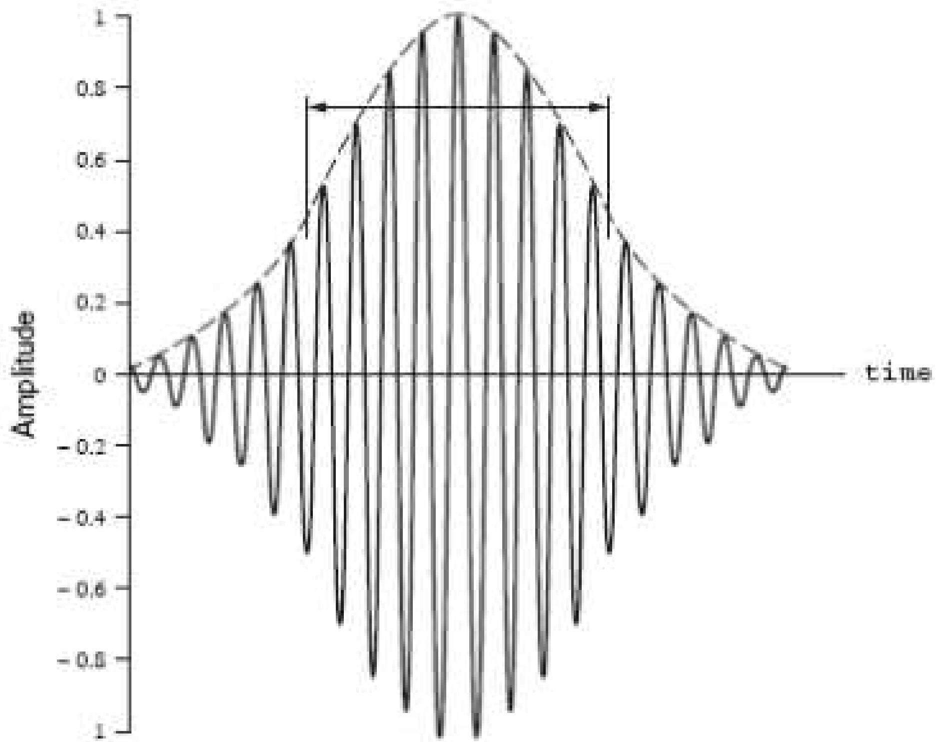
$\frac{\partial \omega}{\partial k} = v_g = v$

Beats

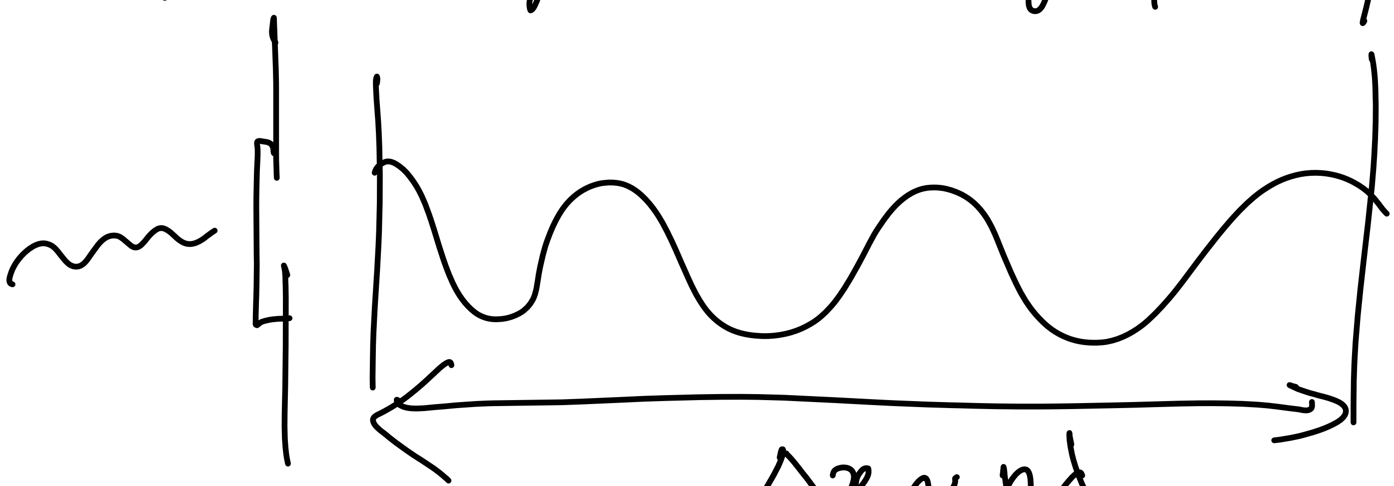
"group → velocity of the particle

velocity"

"phase velocity"



Heisenberg uncertainty principle



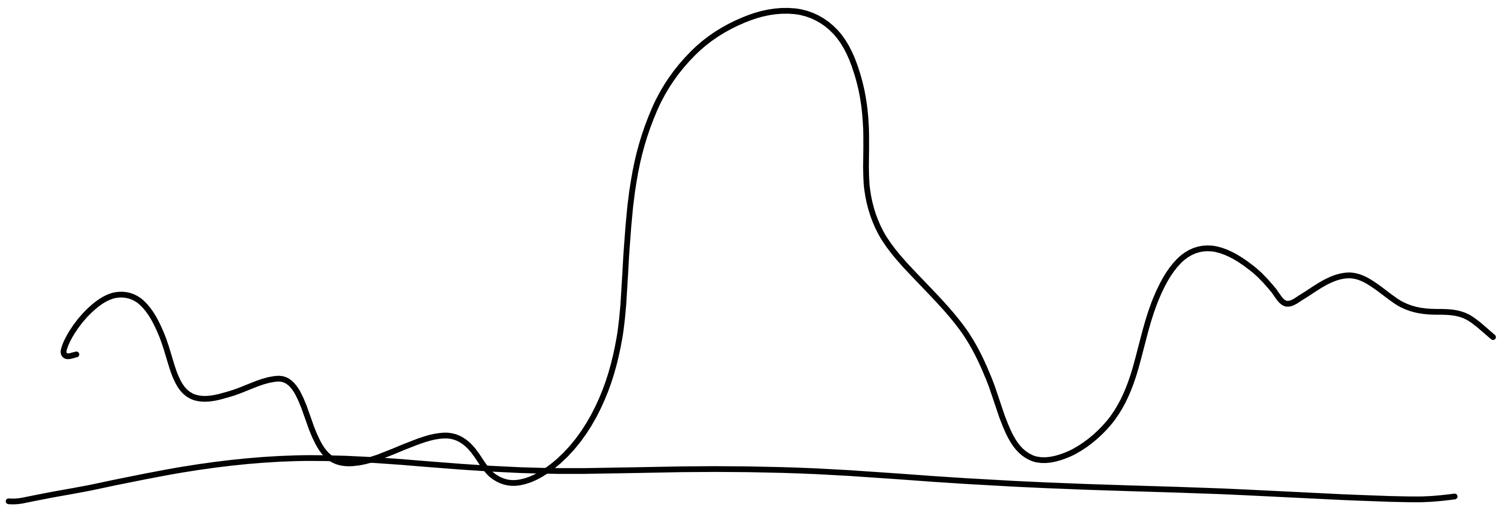
$$\Delta x \sim n\lambda$$

$$\frac{\Delta\lambda}{\lambda} \sim \frac{1}{n}$$

$$\frac{\Delta\lambda}{\lambda} = \frac{\Delta p}{p}$$

$$\Delta x \Delta p = h$$

$$\boxed{\Delta x \Delta p \geq \hbar/2}$$



$$\Delta x \, \Delta p \geq \hbar/2$$

"complementary"

The more precisely the position is determined, the less precisely the momentum is known in this instant, and vice versa.

--Werner Heisenberg, 1927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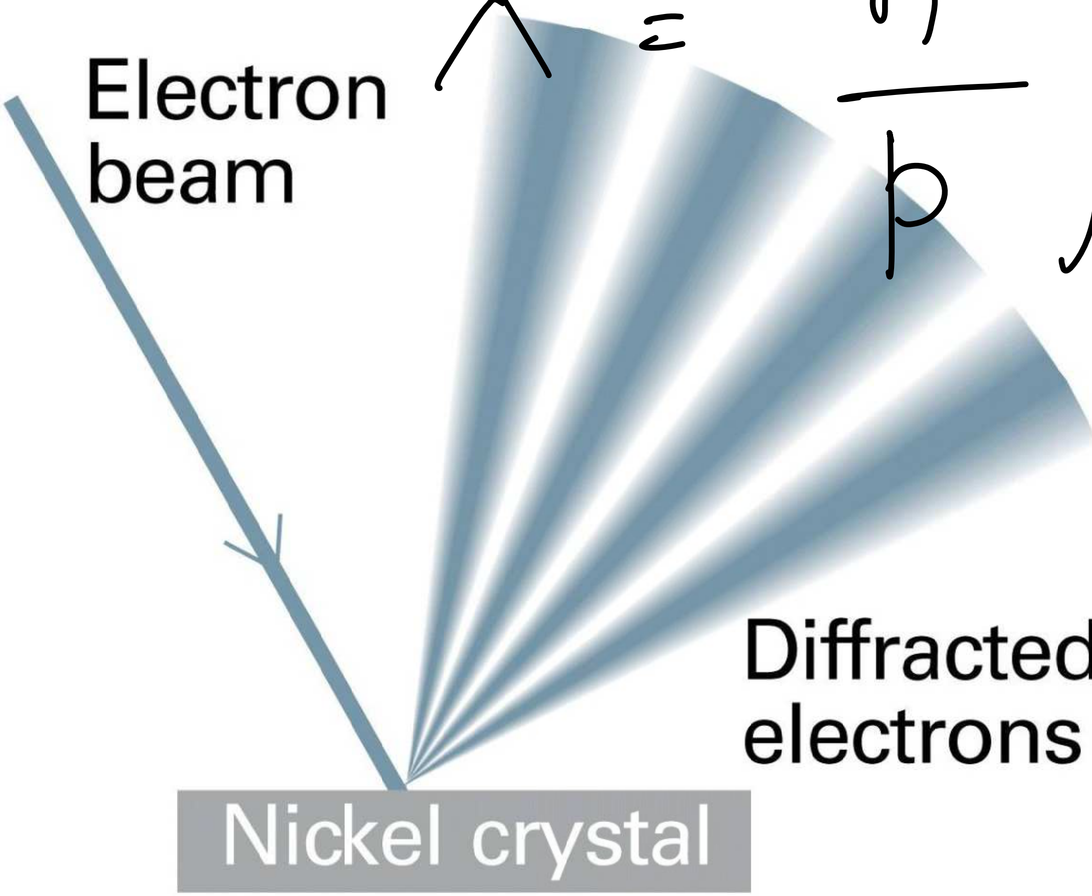


$$\lambda = \frac{h}{p}$$ } de Broglie

Davisson-
Germer
G. P. Thomson

Figure 8-15
Atkins Physical Chemistry, Eighth Edition

Heisenberg.

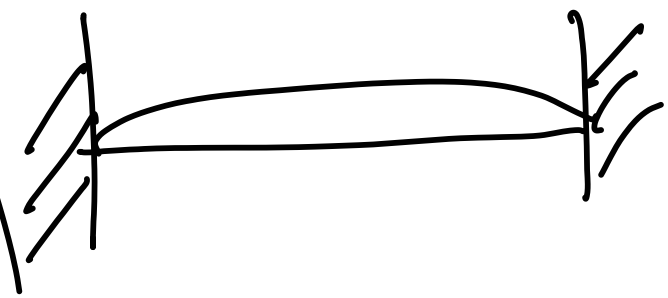
$$\begin{cases} \Delta x \, \Delta p_x \geq \hbar/2 \\ \Delta y \, \Delta p_y \geq \hbar/2 \\ \Delta x \, \Delta p_y \geq 0 \end{cases}$$

$$-\frac{\partial V}{\partial x} = F = ma$$

$x(t)$

classical wave equation

$$\frac{\partial^2 u}{\partial x^2} = \frac{1}{v^2}\frac{\partial^2 u}{\partial t^2}$$



$u(x,t)$

$$\lambda = \frac{h}{p}$$

p

$$\psi = A e^{i(kx - \omega t)}$$

$$\frac{h}{\lambda} = p = \hbar k$$

x

$$E = \hbar\omega$$

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

$$\frac{\partial \psi}{\partial x} = ik\psi$$

$$\frac{\partial^2 \psi}{\partial x^2} = -k^2 \psi$$

$$\frac{\partial \psi}{\partial t} = -i\omega\psi$$

Schrödinger equation

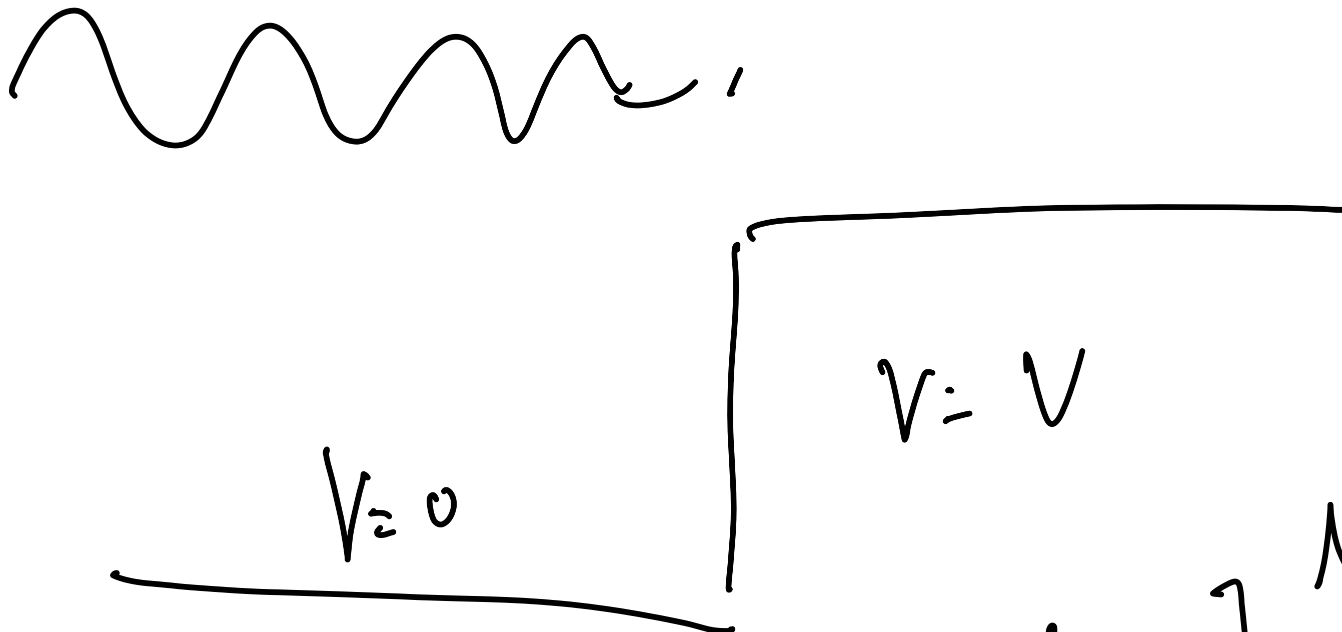
$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2}$$

$$i\hbar \frac{\partial \psi}{\partial t} = (T + V)\psi$$

Time dependent Schrödinger equation

$$E = T + V(x)$$

$$i\hbar \frac{\partial \psi}{\partial t} = \left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V \right) \psi$$



$$\frac{\partial^2 u}{\partial x^2} = \frac{1}{v^2} \frac{\partial^2 u}{\partial t^2}$$

$$i\hbar \frac{\partial u}{\partial t} = \frac{-\hbar^2}{2m} \frac{\partial^2 u}{\partial x^2}$$

] linear "superposition"

$\Psi(x, t)$ = wave function

probability amplitude $e^{i(kx - \omega t)}$

$\Psi^* \Psi$ → "Born" probability density of finding the particle at (x, t)

$I \propto |E|^2$

$P \propto |\Psi|^2$

$\Psi^* \Psi \, dx$

$\Psi^* \Psi_2$

$$\int \psi^* \psi \, dx = 1$$

wave function – square integrable

1) Finite
2) single valued
3) continuous

(1–2 bracketed:) ψ & $\frac{d\psi}{dx}$

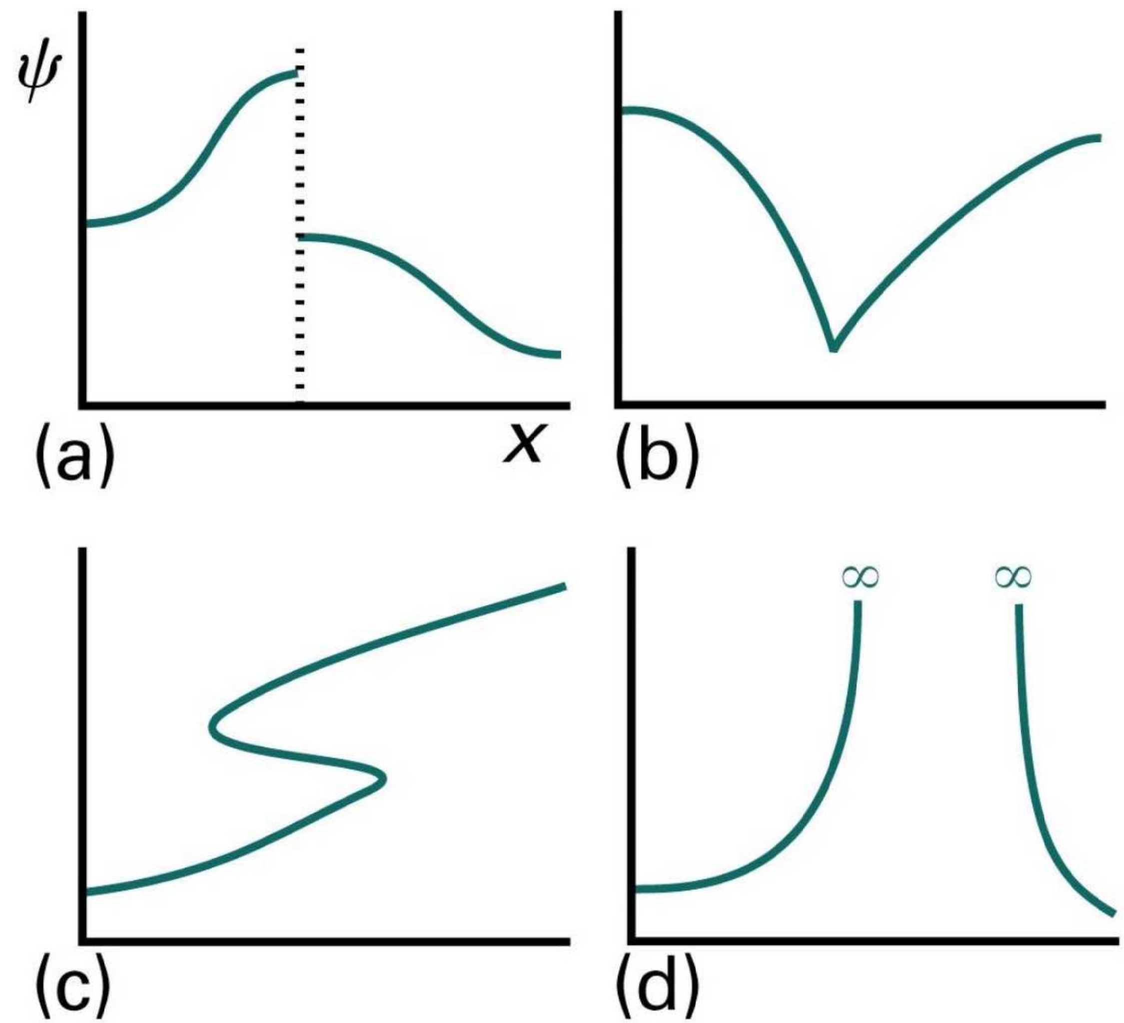


Figure 8-24
Atkins Physical Chemistry, Eighth Edition

$$i\hbar \frac{\partial \psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2}$$

$$\psi(x,t) = u(x)\, v(t)$$

$$i\hbar \frac{\partial}{\partial t} \left(u(x)\, v(t) \right) = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \left(u(x)\, v(t) \right)$$

$$\frac{1}{u(x)v(t)}\, i\hbar\, u(x) \frac{\partial}{\partial t} v(t) = -\frac{\hbar^2}{2m} v(t) \frac{\partial^2}{\partial x^2} u(x)$$

$$\underbrace{i\hbar \frac{1}{v}\frac{\partial v}{\partial t}}_{\text{fn of } t} = \underbrace{-\frac{\hbar^2}{2m}\frac{1}{u}\frac{\partial^2 u}{\partial x^2}}_{\text{fn of } x} = E$$

Time Independent S E

$$-\frac{\hbar^2}{2m}\frac{d^2 u}{dx^2} = E u$$

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\right)u = E\psi$$

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

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V\right)\psi = E\psi$$

$$\frac{d^2\psi}{dx^2} + \frac{2m(E-V)}{\hbar^2}\psi = 0$$

$$\Psi(x,t)$$

$$\lambda = \frac{h}{p}$$

$$-\frac{\hbar^2}{2m}\nabla^2\psi = i\hbar\frac{\partial\psi}{\partial t}$$

$$\Delta x\,\Delta p \geq \hbar/2$$

$$-\frac{\hbar^2}{2m}\frac{d^2\Psi(x,t)}{dx^2} = i\hbar\frac{\partial\Psi(x,t)}{\partial t}$$

$$\mathcal{H}\psi(x) = E\,\psi(x)$$