Primer on Semiconductors

# Unit 2: Quantum Mechanics

# **Lecture 2.1: The wave equation**

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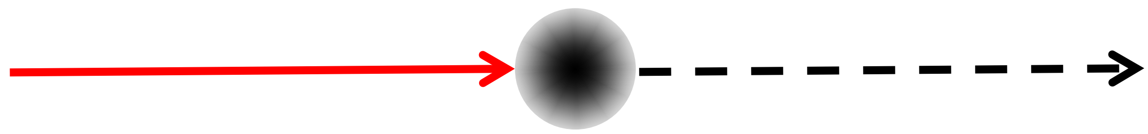
# Classical (Newtonian) mechanics

free electron

$F(t)$



$p = m_0 \upsilon$

$$F = m_0 a = m_0 \frac{d^2 x}{dt^2} = m_0 \frac{d\upsilon}{dt}$$

$$F = \frac{dp}{dt}$$

## Equations of motion:

$$p(t) = p(0) + \int_0^t F(t')\,dt' \qquad \upsilon(t) = \upsilon(0) + \frac{1}{m_0}\int_0^t F(t')\,dt' \qquad x(t) = x(0)\int_0^t \upsilon(t')\,dt'$$

# The need to go beyond classical physics

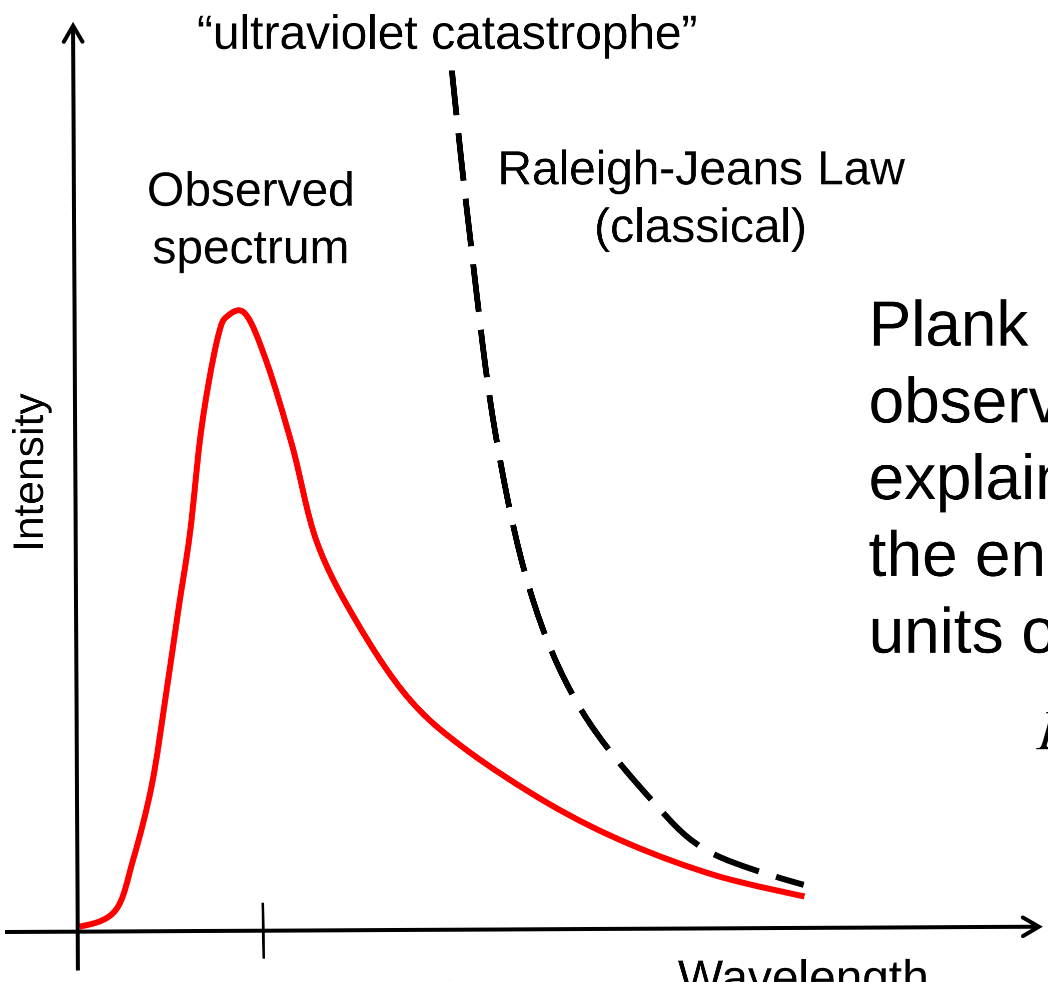
1) Black body radiation (Planck, 1901)

1) Photoelectric effect (Einstein, 1905)

2) Atomic spectra (Bohr, 1913)

1) Wave-particle duality (de Broglie, 1924)

# Black body radiation



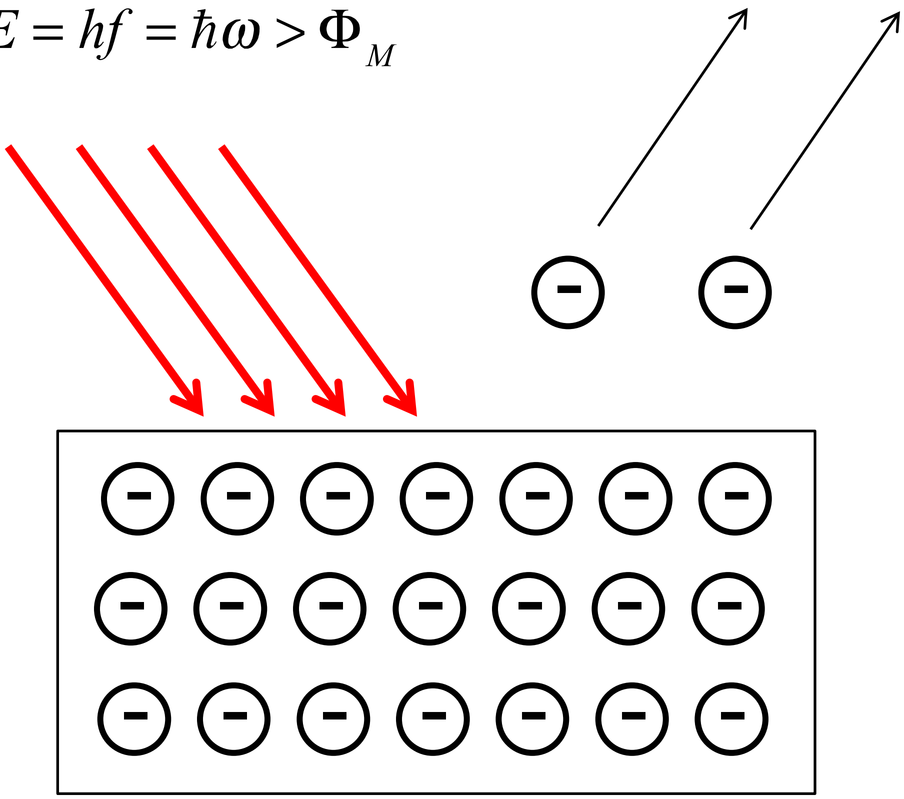

$$\lambda_{peak} = 2900\ \mu\text{m}/T$$

Plank (1901) showed that the observed spectrum could be explained by assuming that the energy was quantized in units of

$$E = hf = \frac{h}{2\pi} 2\pi f = \hbar\omega$$

# Photoelectric effect

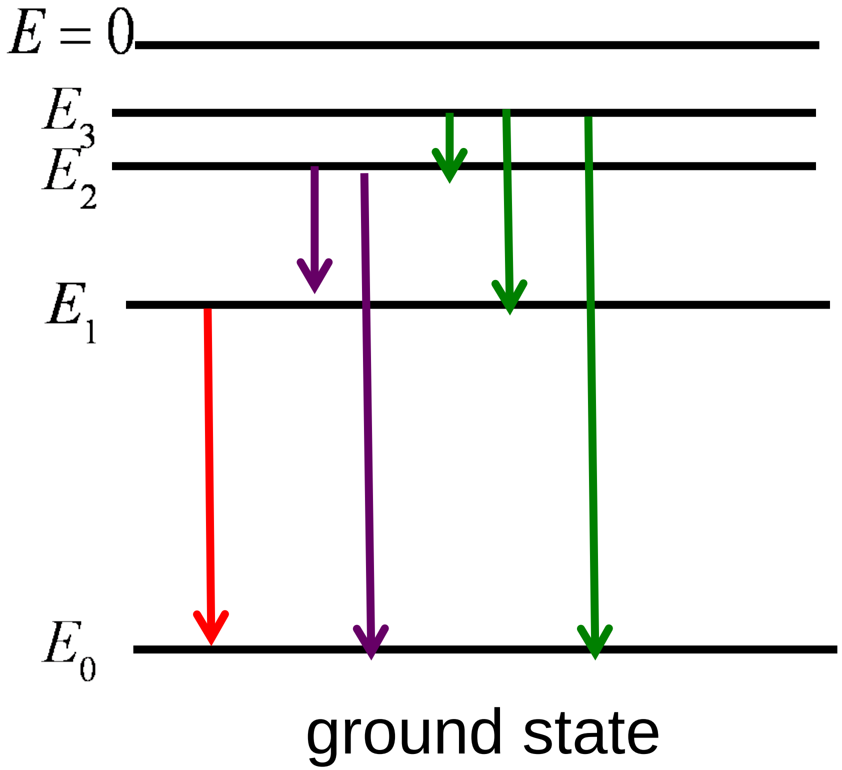
$$E = hf = \hbar\omega > \Phi_M$$



Einstein (1904) showed that light should be thought of as **particles** with an energy

$$E = hf = \hbar\omega$$

# Atomic spectra



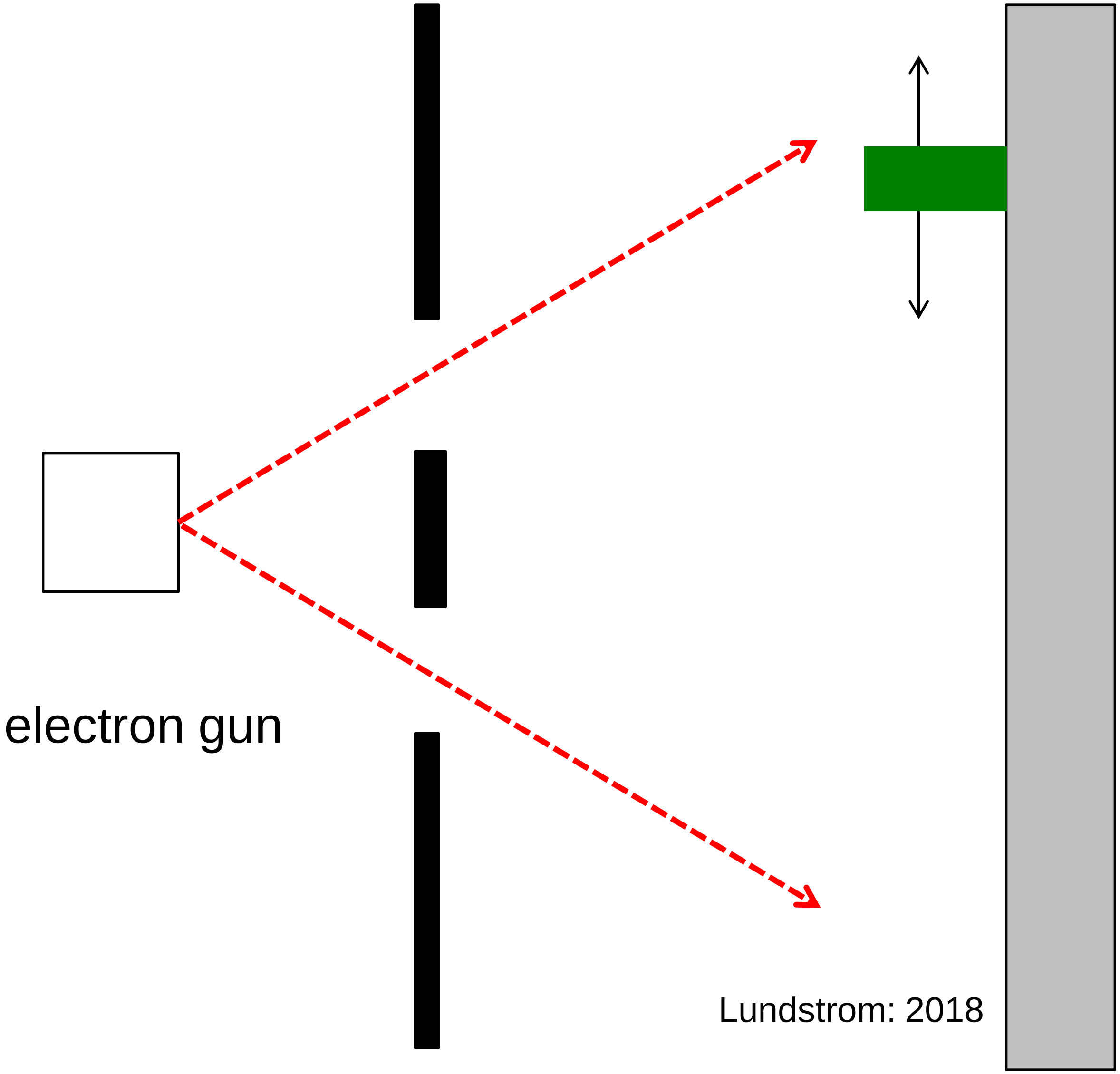

The light emitted by excited atoms comes in discrete colors.

Bohr (1913) showed that the light was produced by transitions between discrete energies:

$$\omega_{if} = \frac{E_i - E_f}{\hbar}$$

Discrete energies can be explained if electrons are treated as **waves**.

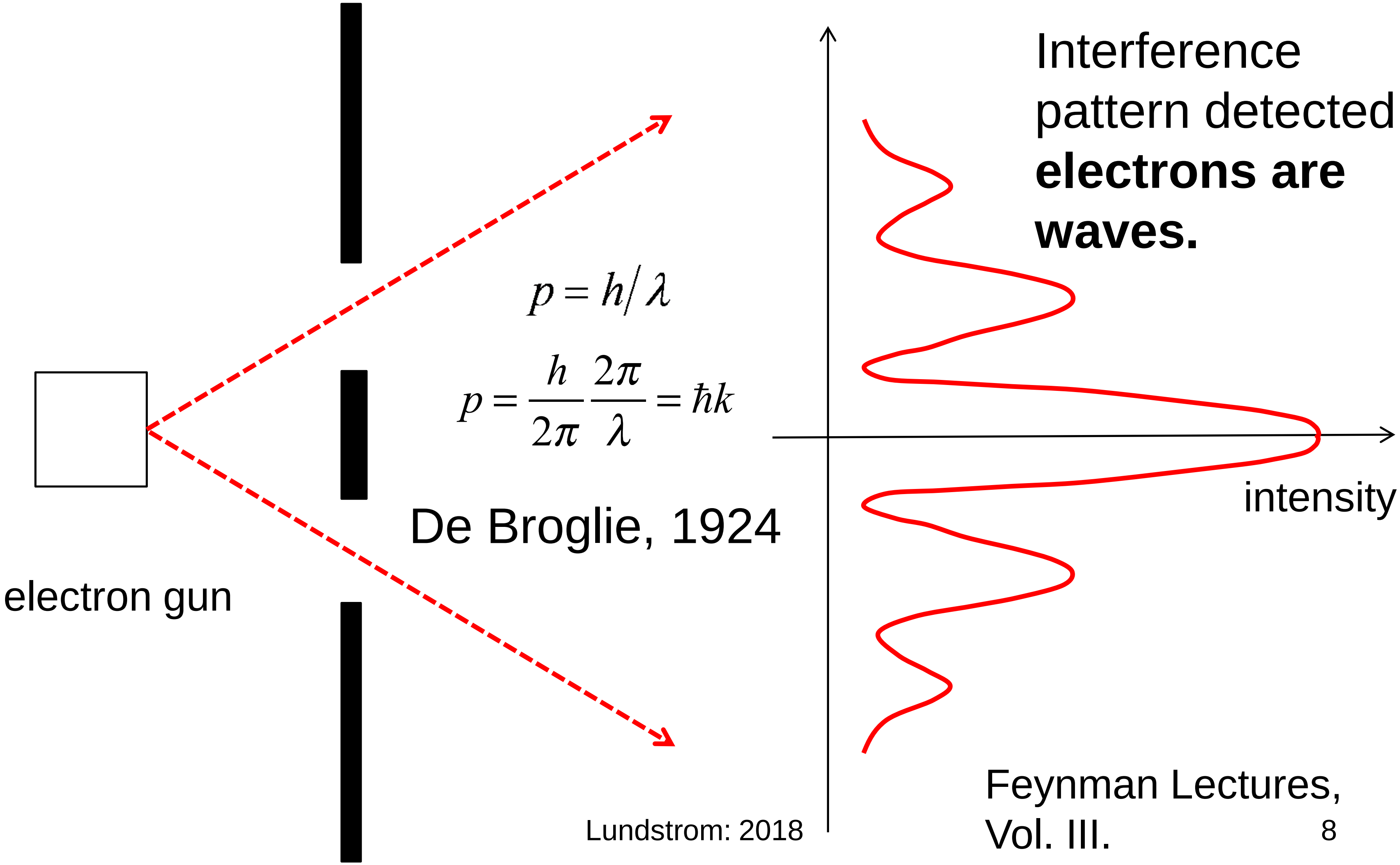
# Wave particle duality




Only particles are detected – **electrons are particles.**

Feynman Lectures, Vol. III.

# Wave particle duality




$$p = h/\lambda$$

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

De Broglie, 1924

Interference pattern detected – **electrons are waves.**

Feynman Lectures, Vol. III.

# Experimental summary

1) Experimental evidence shows that energy is quantized (blackbody radiation, emission spectra of atoms).

2) Experimental evidence shows that waves can behave like particles (photoelectric effect) and particles like waves.

# Waves and particles

1) Waves show the effects of quantization when boundary conditions are applied.

2) Waves can be localized by adding up different wavelengths (wave packets)

**We need a wave equation for electrons!**

# Schrodinger wave equation

$$-\frac{\hbar}{i}\frac{\partial}{\partial t}\Psi(x,t) = -\frac{\hbar^2}{2m_0}\frac{\partial^2}{\partial x^2}\Psi(x,t) + U(x)\Psi(x,t)$$

To solve this equation, use "separation of variables"

$$\Psi(x,t) = \psi(x)\phi(t)$$

$$\phi(t) = e^{-i\omega t}$$

$$E = \hbar\omega$$

$$\phi(t) = e^{iE/\hbar}$$

$$\psi(x) = ?$$

# Time-independent wave equation

$$\boxed{-\frac{\hbar^2}{2m_0}\frac{d^2\psi(x)}{dx^2}+U(x)\psi(x)=E\psi(x)}$$

$$\Psi(x,t)=\psi(x)\phi(t)=\psi(x)e^{-i\omega t} \qquad \omega = E/\hbar$$

The probability of finding an electron between *x* and *x*+*dx*, is:

$$P(x,t)dx=\Psi^*(x,t)\Psi(x,t)dx$$

# Solving the time independent wave equation

$$-\frac{\hbar^2}{2m_0}\frac{d^2\psi(x)}{dx^2}+U(x)\psi(x)=E\psi(x)$$

$$\frac{\partial^2\psi(x)}{\partial x^2}+\underbrace{\frac{2m_0}{\hbar^2}\left[E-U(x)\right]}\psi(x)=0$$

Solutions depend on whether *E* > *U*(*x*) or *E* < *U*(*x*)

# Electron energy > potential energy

$$\frac{d^2\psi(x)}{dx^2} + \frac{2m_0}{\hbar^2}\left[E - U(x)\right]\psi(x) = 0$$

$$E > U(x) \qquad k^2 = \frac{2m_0}{\hbar^2}\left[E - U(x)\right] \qquad \frac{d^2\psi(x)}{dx^2} + k^2\psi(x) = 0$$

Solution: $\psi(x) = Ae^{\pm ikx}$

$$\Psi(x,t) = \psi(x)\phi(t)$$

This is a wave travelling in the +/- x direction.

$$\Psi(x,t) = Ae^{\pm i(kx - \omega t)}$$

# Waves: phase velocity

$$\Psi(x,t) = Ae^{i(kx-\omega t)} = Ae^{i\theta} \qquad U(x) = U_0 \qquad k(x) \text{ is constant}$$

Follow a point of constant phase:

$$\frac{d\theta}{dt} = 0 \qquad \frac{d(kx - \omega t)}{dt} = 0 = k\frac{dx}{dt} - \omega$$

Phase velocity of the wave: $\upsilon_p = \dfrac{\omega}{k}$

# Waves: wavelength

$$\Psi(x,t) = Ae^{i(kx-\omega t)} = Ae^{i\theta}$$

$$k = \frac{\sqrt{2m_0(E-U_0)}}{\hbar}$$

At a given time, the phase at a given x + 1 wavelength must be 2π plus the phase at x.

$$\theta(x+\lambda,t) = \theta(x,t) + 2\pi \qquad k(x+\lambda) - \omega t = kx - \omega t + 2\pi \qquad k\lambda = 2\pi$$

Wavelength: $\lambda = \dfrac{2\pi}{k}$

Wavevector: $k = \dfrac{2\pi}{\lambda}$

# Waves: momentum

$$\frac{d^2\psi(x)}{dx^2}+\frac{2m_0}{\hbar^2}\left[E-U(x)\right]\psi(x)=0$$

$$U(x)=U_0$$

$$\frac{d^2\psi(x)}{dx^2}+\frac{2m_0}{\hbar^2}\left(E-U_0\right)\psi(x)=0$$

$$\psi(x)=Ae^{ikx}$$

$$k^2=\frac{2m_0}{\hbar^2}\left(E-U_0\right)$$

$$E=U_0+\frac{\hbar^2k^2}{2m_0}=U_0+\frac{p^2}{2m_0}\rightarrow$$

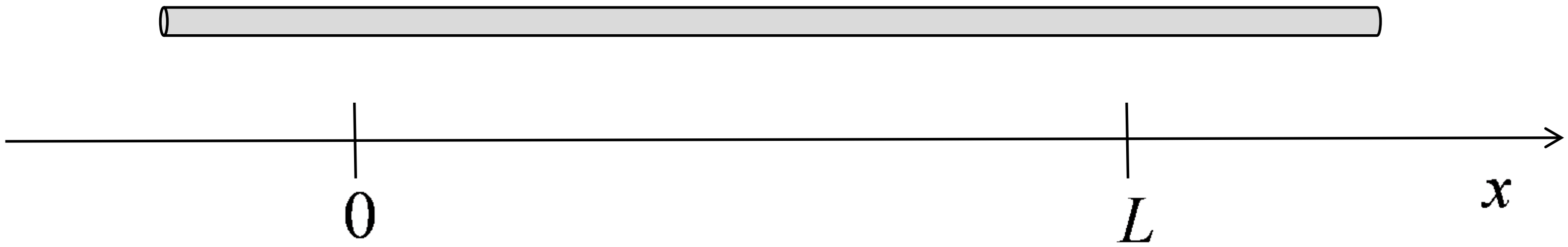
$$\boxed{p=\hbar k}$$

de Broglie (1924)

# Electron waves in 1D

nanowire

$$U(x) = U_0$$

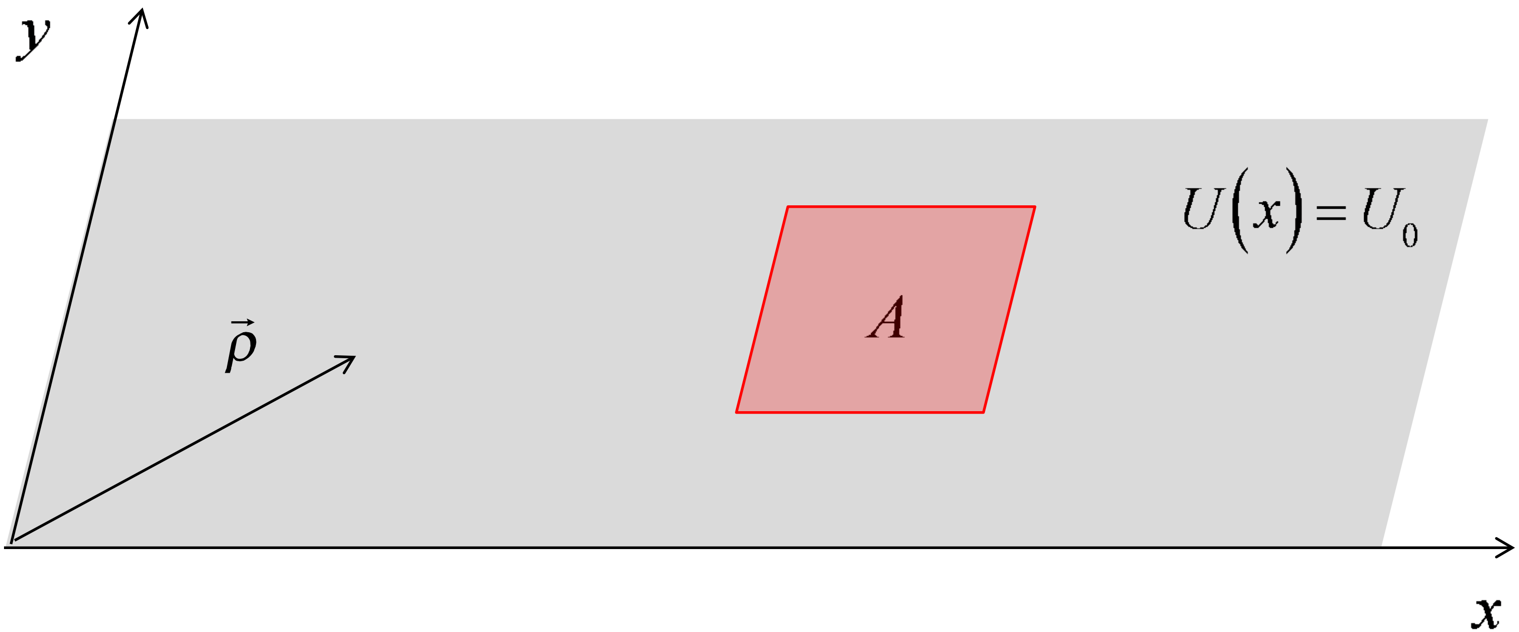



$$\psi(x) = Ae^{\pm ikx}$$

$$\int_0^L \psi^*(x)\psi(x)dx = 1$$

$$\psi(x) = \frac{1}{\sqrt{L}}e^{ikx}$$ (normalized in 1D)

# Electron waves in 2D

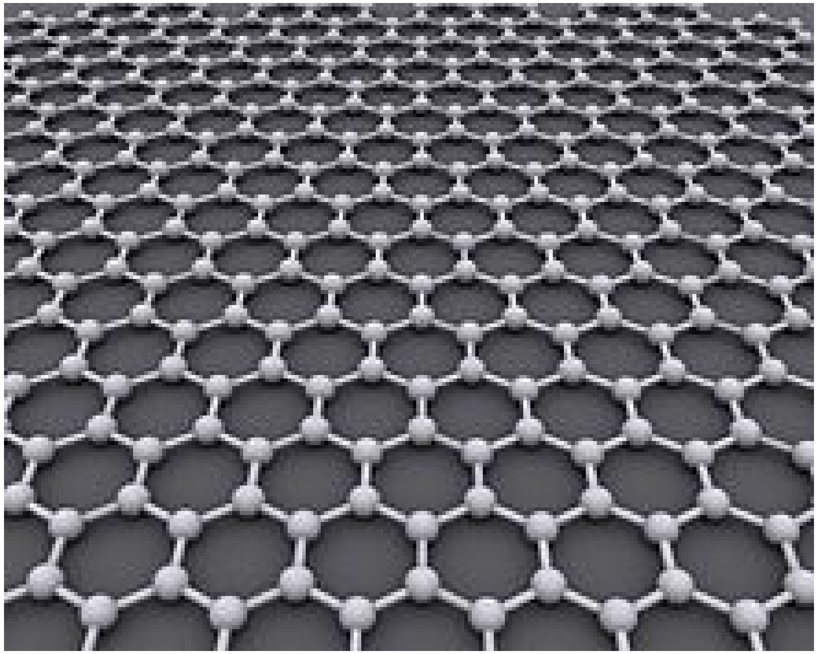



$$\psi(x,y) = Ae^{\pm i(k_x x + k_y y)} = Ae^{i\vec{k}\bullet\vec{\rho}}$$

e.g. graphene

$$\psi(\vec{\rho}) = \frac{1}{\sqrt{A}} e^{i\vec{k}\bullet\vec{\rho}}$$ (normalized in 2D)

# Graphene and 2D materials

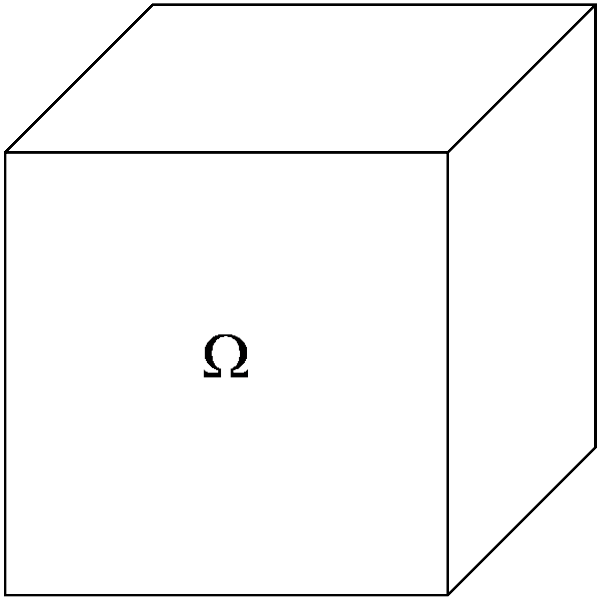


A 2D hexagonal lattice of carbon atoms

https://en.wikipedia.org/wiki/Graphene

# Electron waves in 3D

$$U(x) = U_0$$

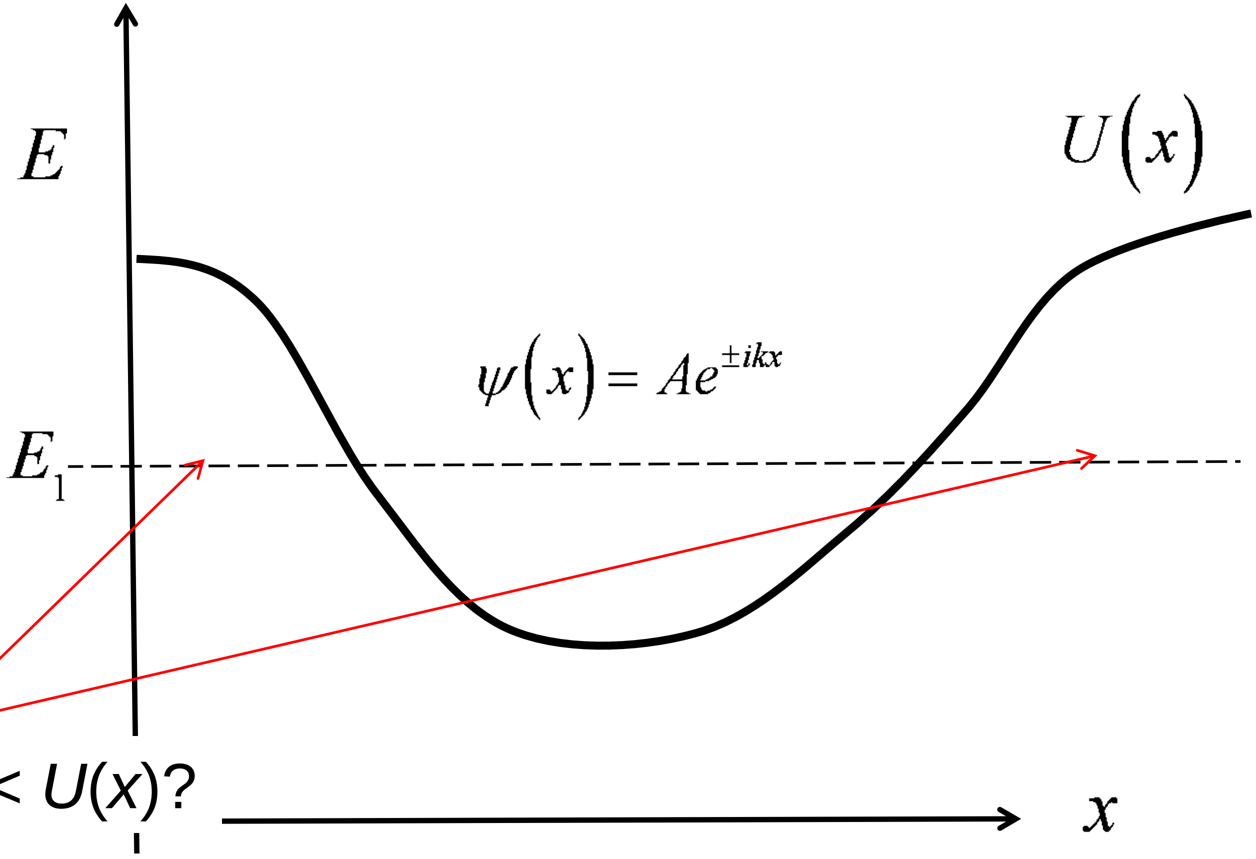



bulk solid

$$\psi(\vec{r}) = \frac{1}{\sqrt{\Omega}} e^{i\left(k_x x + k_y y + k_z z\right)} = \frac{1}{\sqrt{\Omega}} e^{i\vec{k}\bullet\vec{r}}$$

(normalized in 3D)

# Solutions of the wave equation




What if $E < U(x)$?

# Electron energy < potential energy

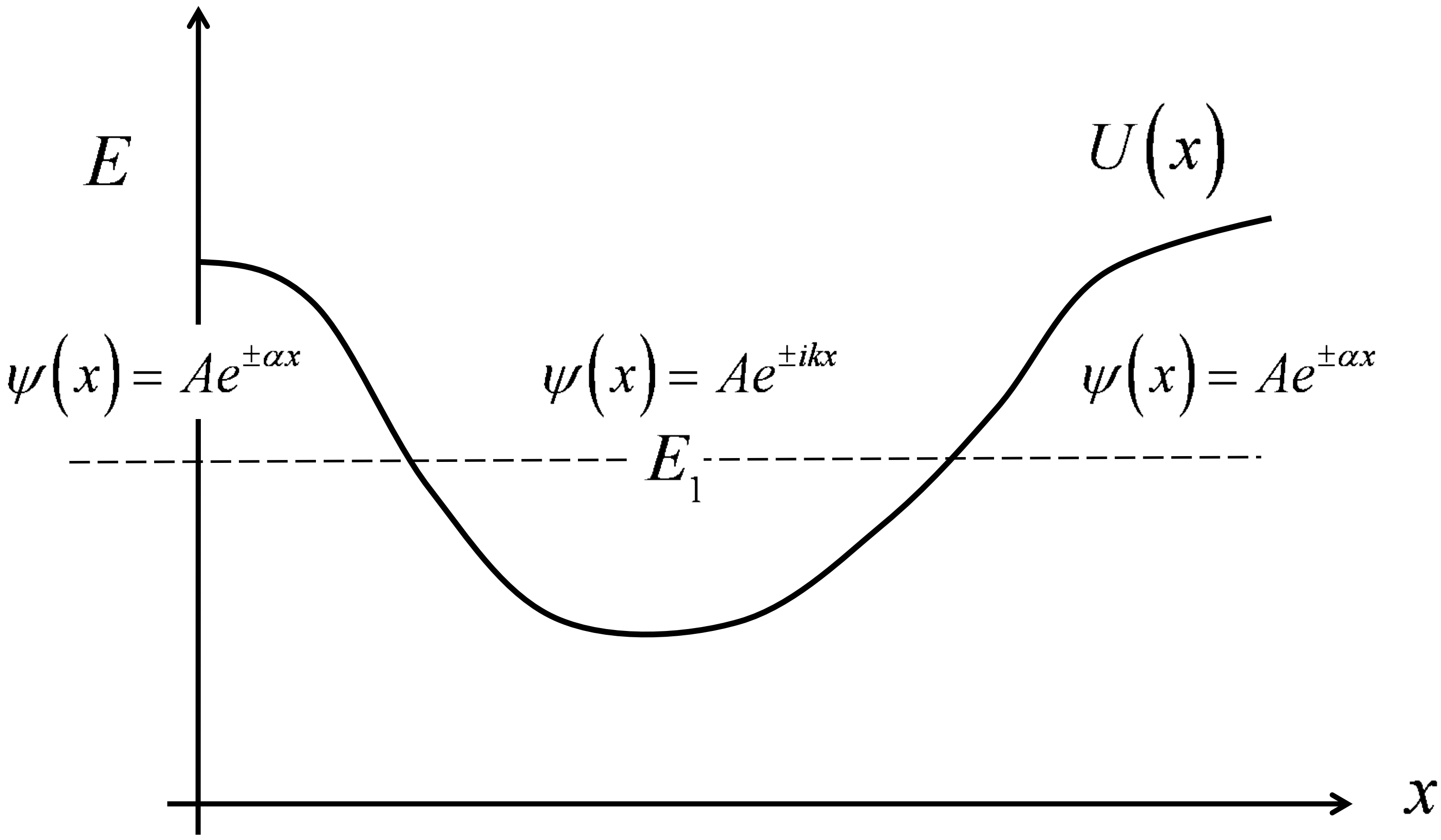
$$\frac{\partial^2 \psi(x)}{\partial x^2} + \frac{2m_0}{\hbar^2}\left[E - U(x)\right]\psi(x) = 0$$

$$E < U(x) \qquad \alpha^2 = \frac{2m_0}{\hbar^2}\left[U(x) - E\right] \qquad \frac{\partial^2 \psi(x)}{\partial x^2} - \alpha^2 \psi(x) = 0$$

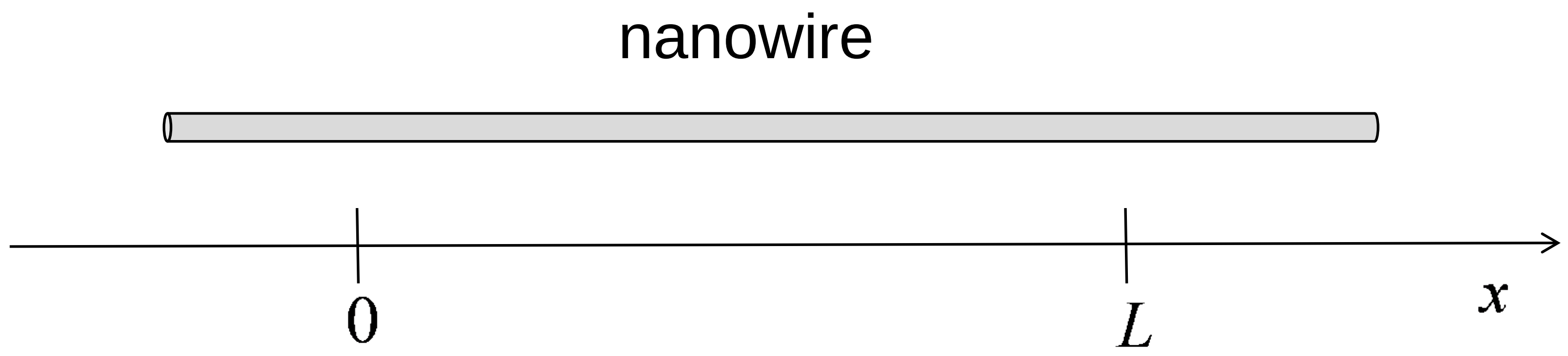
Solution: $\psi(x) = Ae^{\pm\alpha x}$

This is an exponentially decaying or growing solution.

# Solutions of the wave equation



# Electrons are waves **and** particles

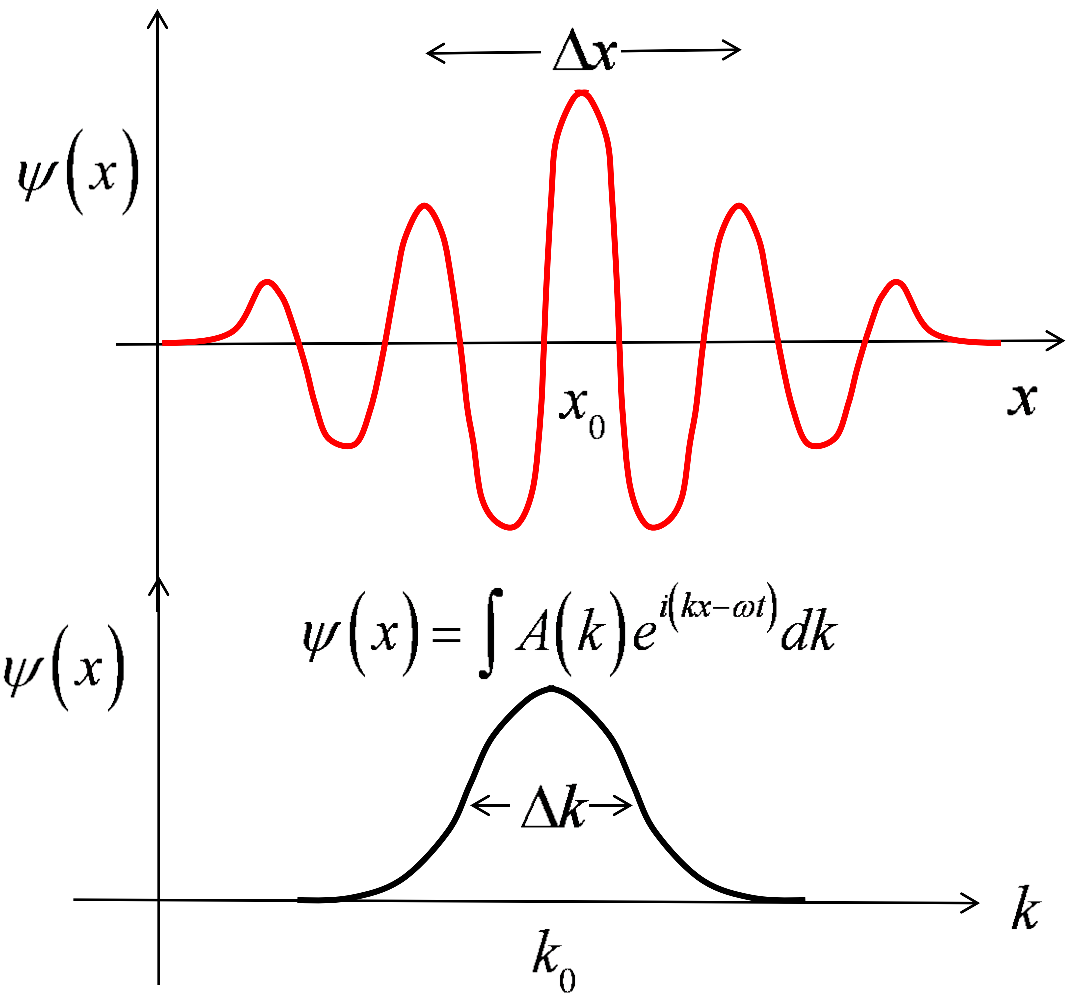



$$\psi(x) = \frac{1}{\sqrt{L}} e^{ikx}$$

$$P(x)dx = \psi^*(x)\psi(x)dx = \frac{dx}{L}$$

**Waves are everywhere!**

# Wave packets




Particle: $x = x_0$

Momentum: $p = \hbar k_0$

$\Delta k \Delta x = 1/2$

# Uncertainty relations

A wave packet that is localized in space is spread out in k-space.

$$\Delta k \Delta x \geq 1/2 \rightarrow \Delta p \Delta x \geq \hbar/2 \qquad \left( p = \hbar k \right)$$

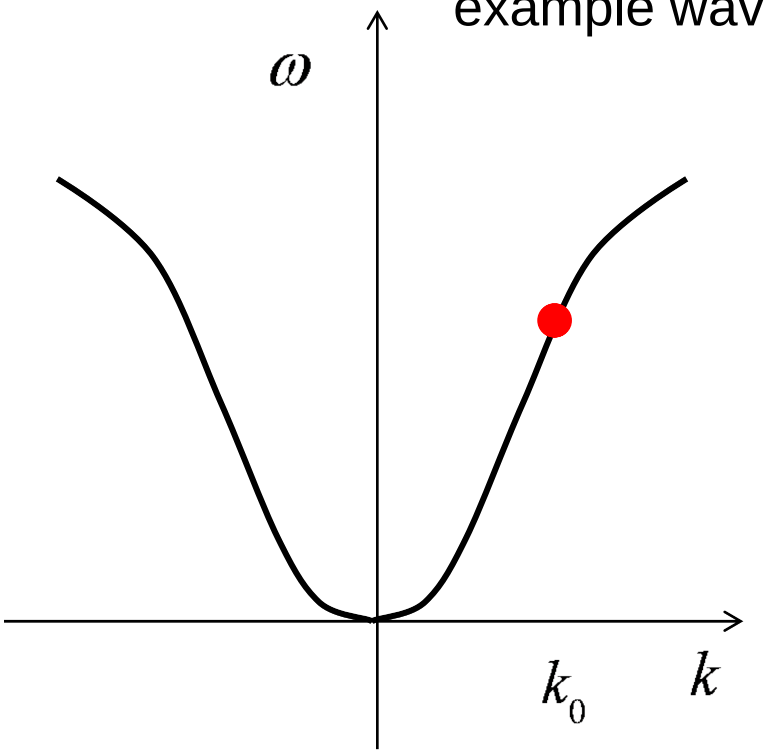
Similarly, a wave packet that is sharply defined in time, is spread out in frequency.

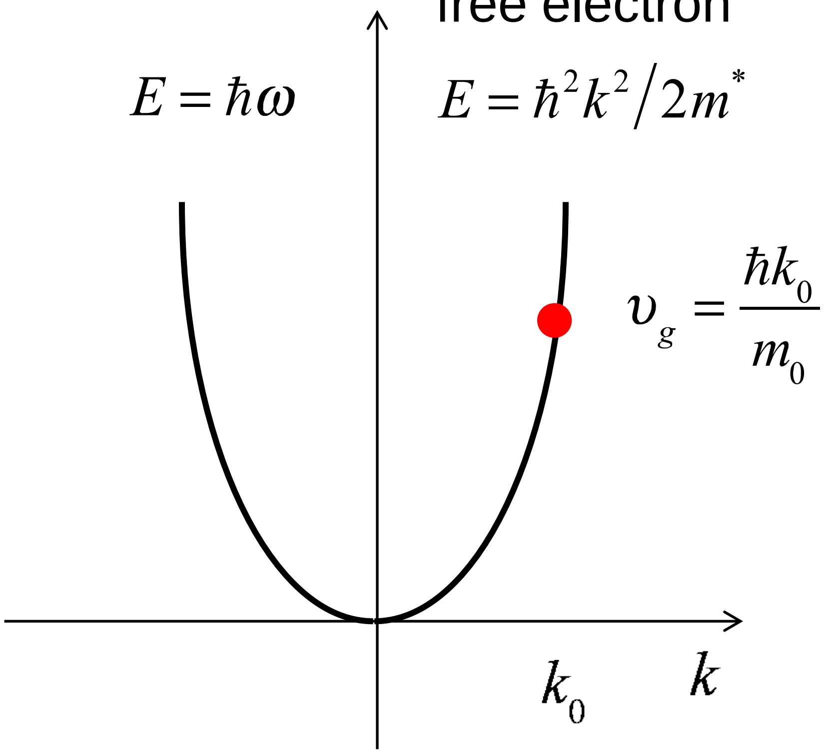
$$\Delta \omega \, \Delta t \geq 1/2 \rightarrow \Delta E \Delta t \geq \hbar/2 \qquad \left( E = \hbar \omega \right)$$

# Uncertainty relations

$$\boxed{\begin{gathered}\Delta p \Delta x \geq \hbar/2 \\[2em] \Delta E \Delta t \geq \hbar/2\end{gathered}}$$

# Wave packets: group velocity




For any wave: $\omega(k)$ (dispersion)

$$\upsilon_g = d\omega/dk = (1/\hbar)\, dE/dk$$

Group velocity: $\upsilon_g = d\omega/dk$

$$\upsilon_p = \omega/k$$

# Summary

## Classical Mechanics

$$F = m_0 a$$

## Quantum Mechanics

$$\Psi(x,t) = \psi(x) e^{-i\omega t}$$

$$E = \hbar\omega = hf$$

$$-\frac{\hbar^2}{2m_0}\frac{d^2\psi(x)}{dx^2} + U(x)\psi(x) = E\psi(x)$$

$$P(x)dx = \psi^*(x)\psi(x)dx$$

$$\Delta p \Delta x \geq \hbar/2 \qquad \Delta E \Delta t \geq \hbar/2$$