Primer on Semiconductors

Unit 2: Quantum Mechanics

Lecture 2.6: Unit 2 Recap

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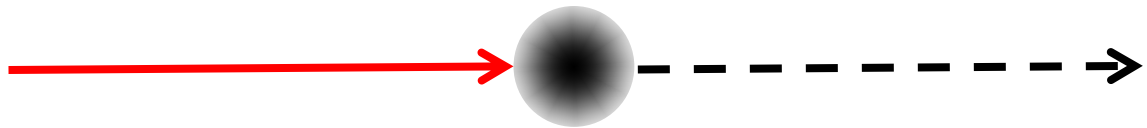
Classical particles: Newton’s Laws

$F(t)$



$p = m_0 \upsilon$

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

Equations of motion:

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

Quantum particles: Wave equation

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

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

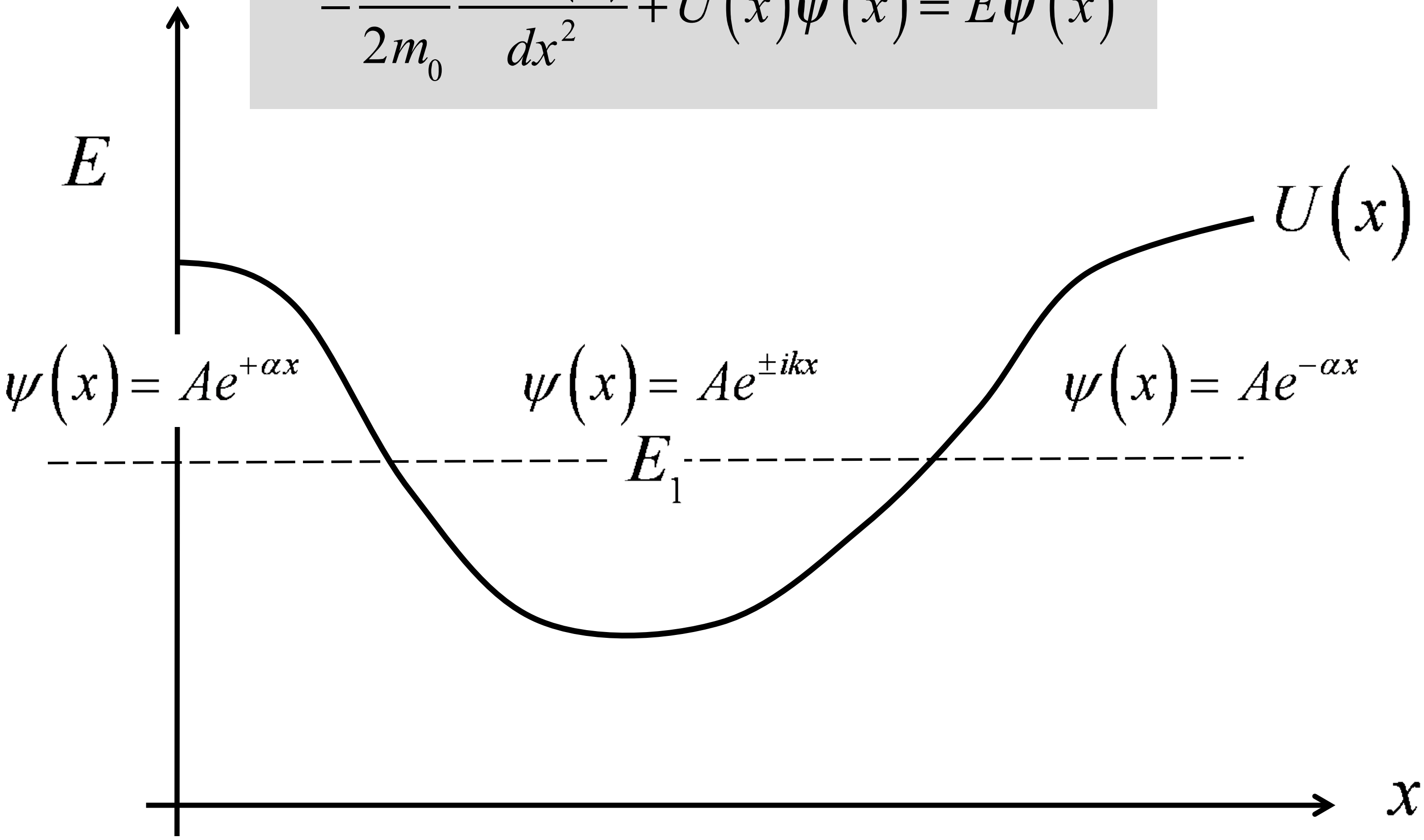
$$-\frac{\hbar^2}{2m_0}\frac{d^2\psi\left(x\right)}{dx^2}+U\left(x\right)\psi\left(x\right)=E\psi\left(x\right)$$

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

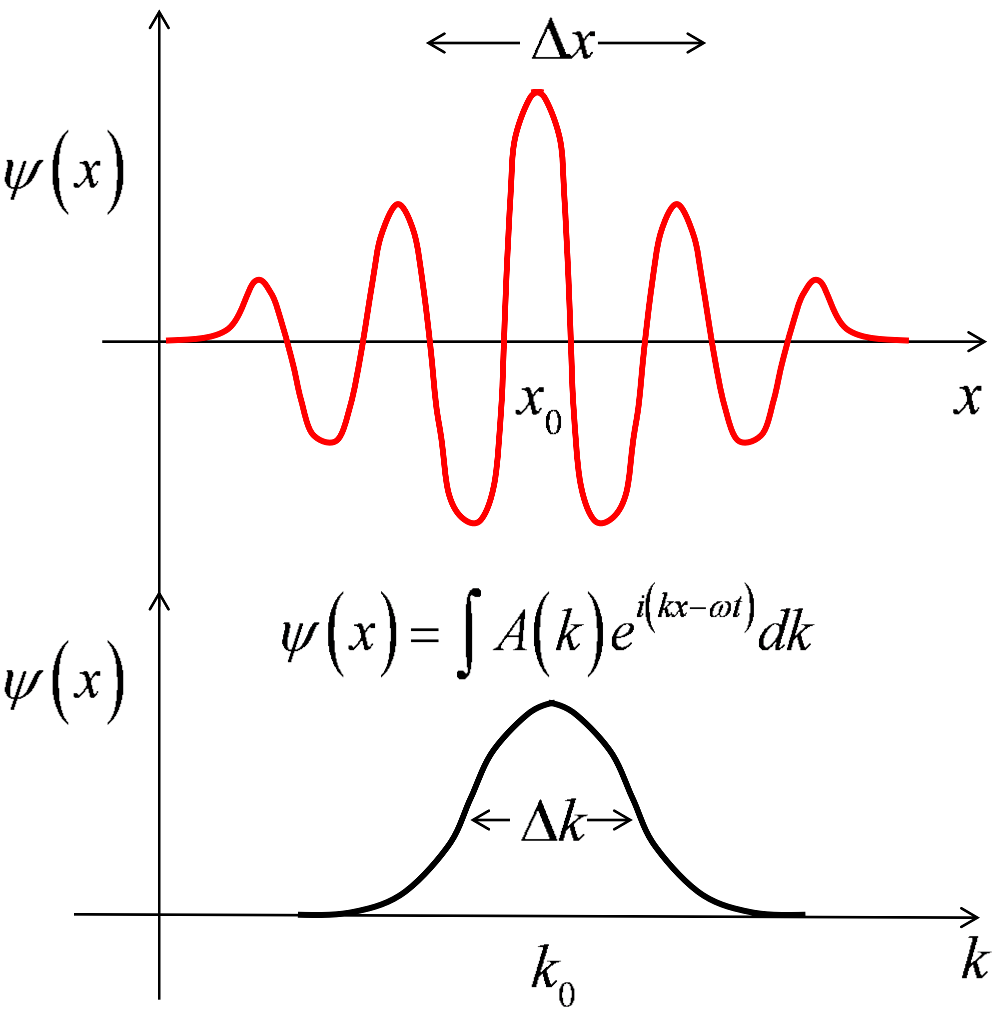
$$P\left(x,t\right)dx=\Psi^*\left(x,t\right)\Psi\left(x,t\right)dx$$

Solutions of the wave equation

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



Wave packets describe particles



Particle: $x = x_0$

Momentum: $p = \hbar k_0$

Velocity: $\upsilon_g = \frac{1}{\hbar} \frac{dE}{dk}\bigg|_{k=k_0}$

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

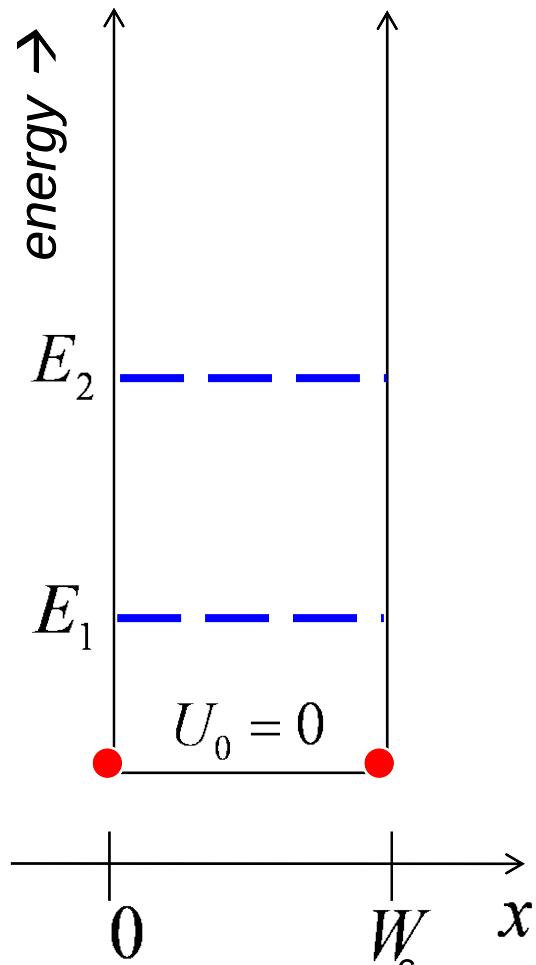
$$\Delta E \Delta t \geq \hbar/2$$

1D quantum well summary

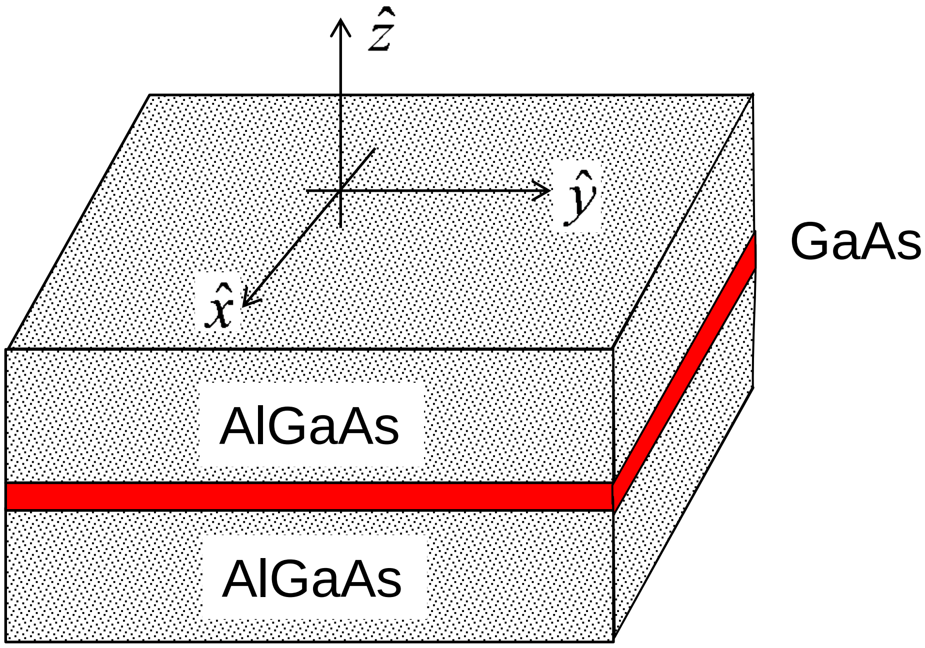
$$\psi(x) = A \sin k_j x \qquad k_j = \frac{\pi}{W} j \quad j = 1,2,3...$$

$$k^2 = \frac{2mE}{\hbar^2} \qquad E_j = \frac{\hbar^2 k_j^2}{2m} = \frac{\hbar^2 j^2 \pi^2}{2mW^2}$$

- Confined electrons have quantized energies.
- Tighter confinement (smaller *W* leads to higher energies.
- Lighter masses leads to higher energies.



Quantum confinement with heterostructures



"GaAs quantum well"

Electrons are confined in the z-direction, but free to move in the x-y plane.

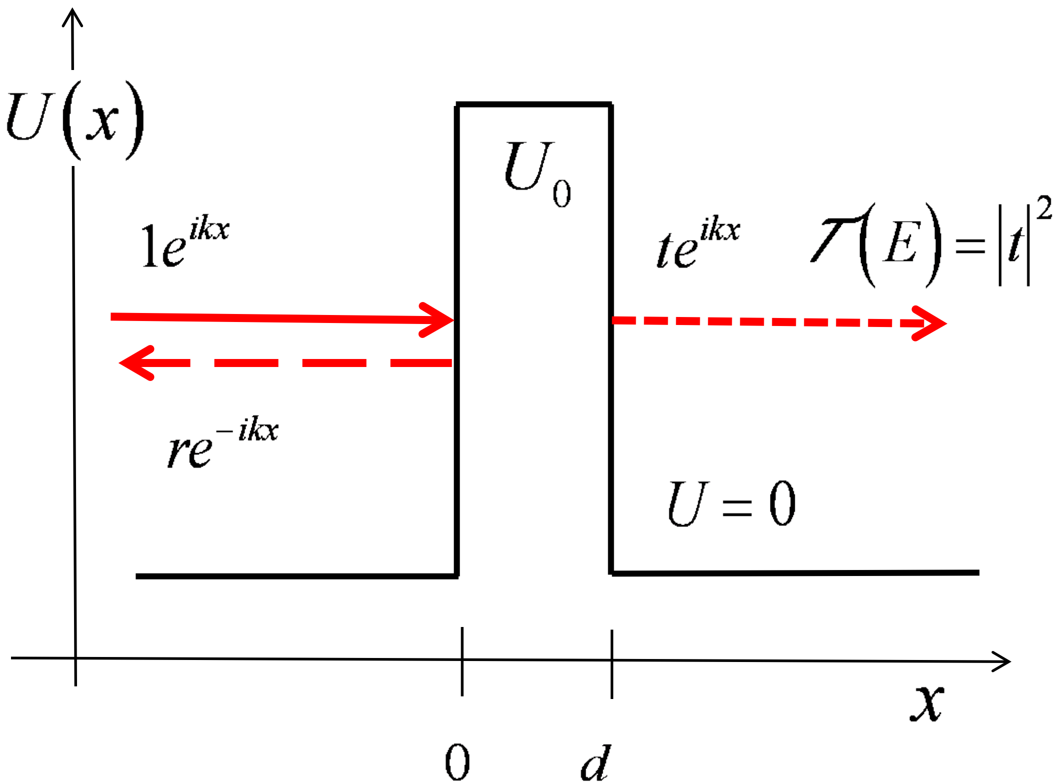
$$\psi(\vec{r}) \sim e^{i\vec{k}\bullet\vec{r}} \rightarrow \sin(k_z z) \times e^{ik_x x} \times e^{ik_y y}$$

$$k_{zj} = j\frac{\pi}{W} \qquad E_j = \frac{\hbar^2 j^2 \pi^2}{2mW^2}$$

"subbands" $\quad E = E_j + \dfrac{\hbar^2 k_{\parallel}^2}{2m}$

Quantum tunneling

$$\mathcal{T}(E) \approx \exp\left(-2d\sqrt{2m(U_0 - E)/\hbar^2}\right)$$

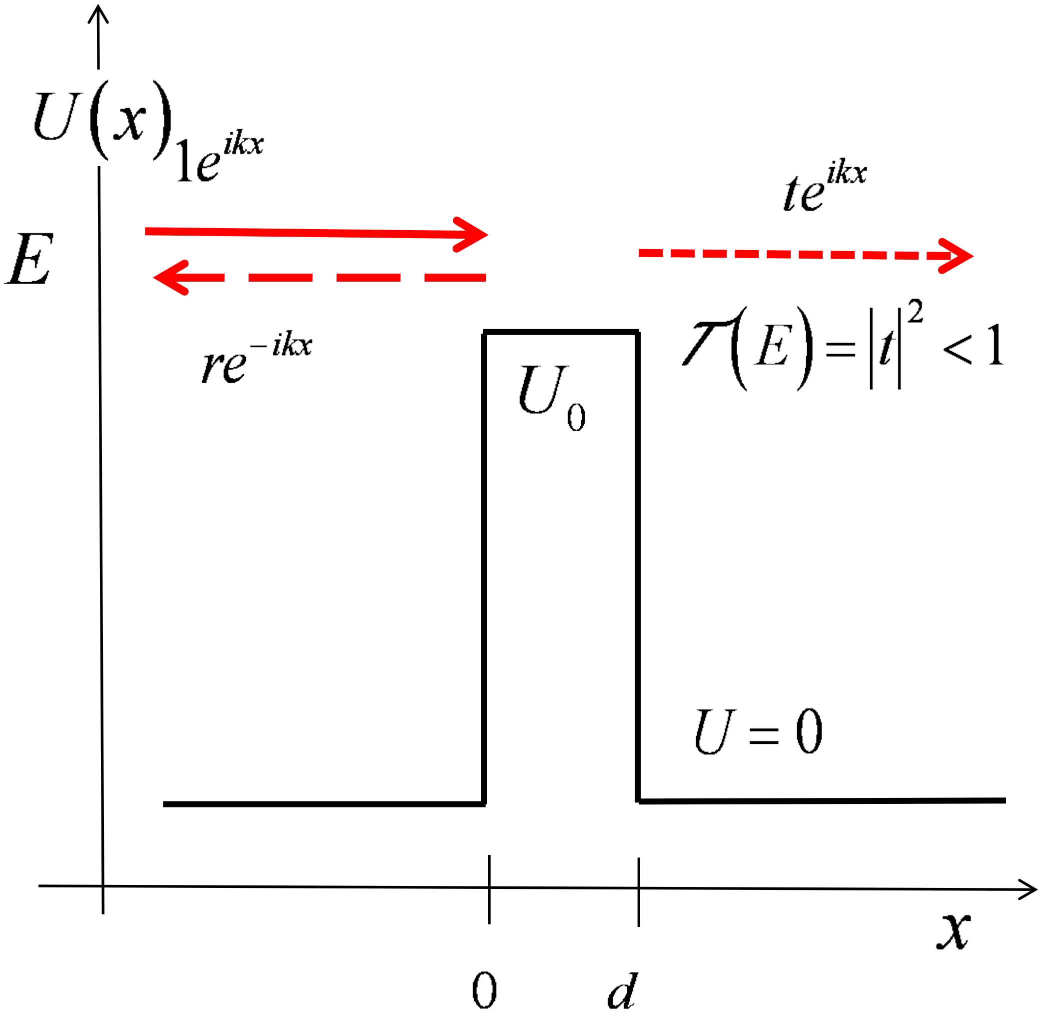


1) Tunneling decreases exponentially with increasing barrier thickness.

2) Tunneling decreases exponentially with increasing barrier height.

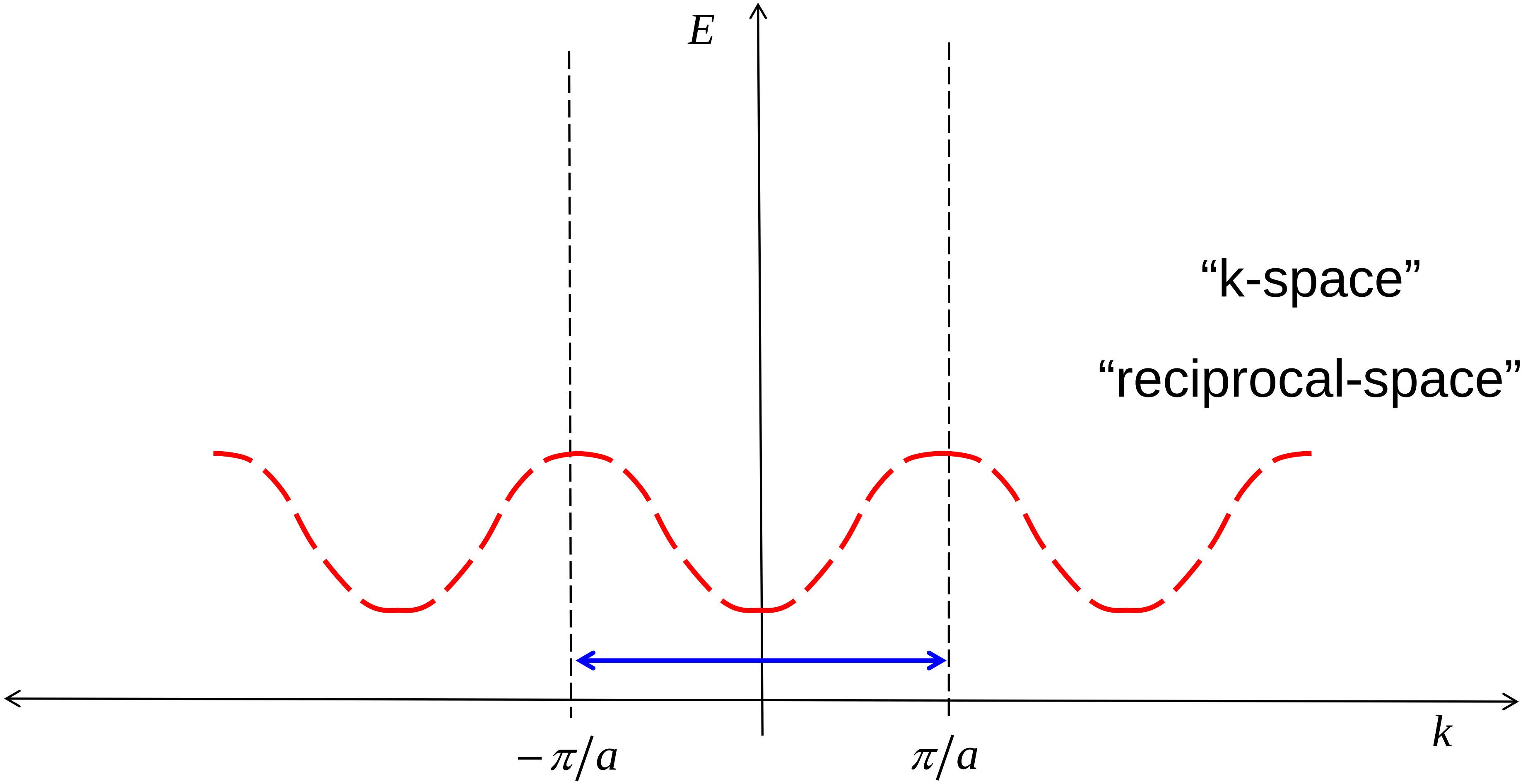
3) Tunneling decreases exponentially with increasing mass.

Quantum reflection



The potential must change slowly (on the scale of the electron's wavelength) to treat the electron as a classical particle.

Solutions are periodic in k-space



"k-space"

"reciprocal-space"

Brillouin zone

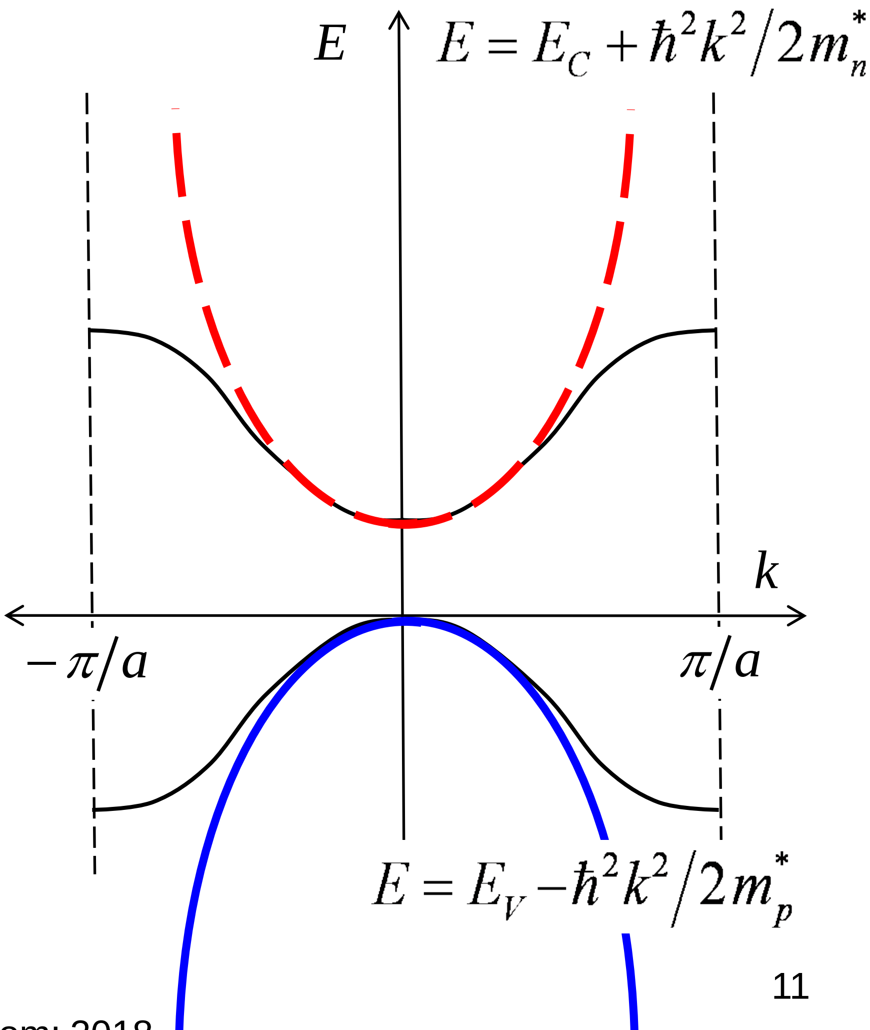
Reduced zone and effective mass

Near a band minimum or maximum, $E(k)$ is a parabola.

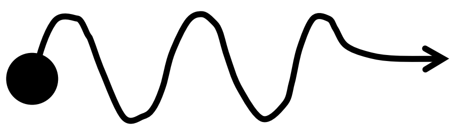
$$E \approx E_C + \hbar^2 k^2 / 2m_n^*$$

The curvature of the parabola is the **effective mass**.

$$\upsilon_g(k) = \frac{1}{\hbar}\frac{dE(k)}{dk} = \frac{\hbar k}{m_n^*}$$



Mobile electrons in crystals

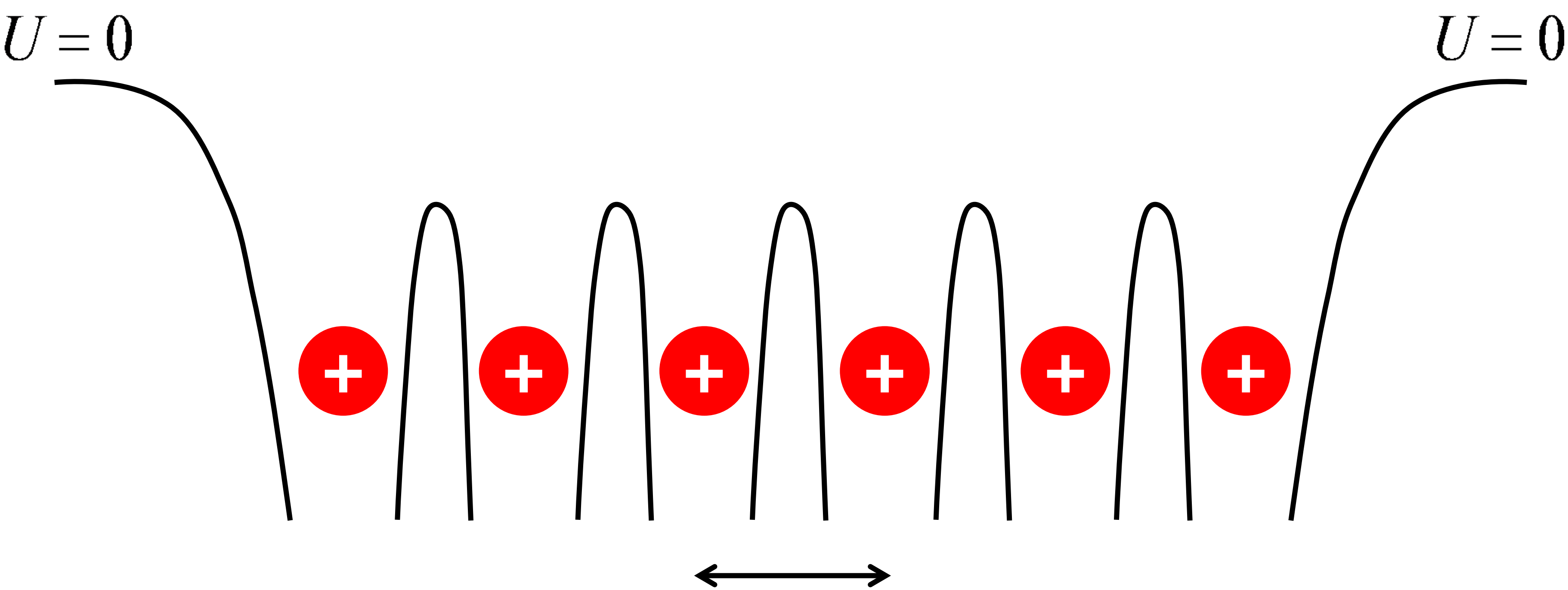


$$E(k) = \hbar^2 k^2 / 2m^*$$

$$p = \hbar k$$

$$\upsilon_g = (1/\hbar) dE/dk = \hbar k / m^*$$

$$F = dp/dt$$



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Summary

1) The crystal potential varies rapidly on an atomic scale. It determines the effective mass.

2) If the applied potential varies rapidly on the scale of the electron's wavelength, then we must solve a wave equation (e.g. semiconductor quantum wells)

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

3) If the applied potential varies slowly on the scale of the electron's wavelength, then we can treats electrons as classical particles with an effective mass.

$$E(k)=\hbar^2k^2/2m^* \qquad p=\hbar k \qquad \upsilon_g=\hbar k/m^* \qquad F=dp/dt$$

Vocabulary

1) Black body radiation
2) Photoelectric effect
3) De Broglie wavelength
4) Wave equation
5) Phase velocity
6) Group velocity
7) Wavevector
8) Uncertainty relations
9) Tunneling
10) Quantum reflection
11) Crystal potential
12) Bloch wave
13) Brillouin zone
14) Crystal momentum
15) Band structure
16) Effective mass
17) Kane bands
18) Spherical energy bands
19) Ellipsoidal energy bands
20) Density of states (DOS)
21) Valley degeneracy
22) DOS effective mass