ECE 656: Electronic Transport in Semiconductors Fall 2017

# Semiclassical Transport


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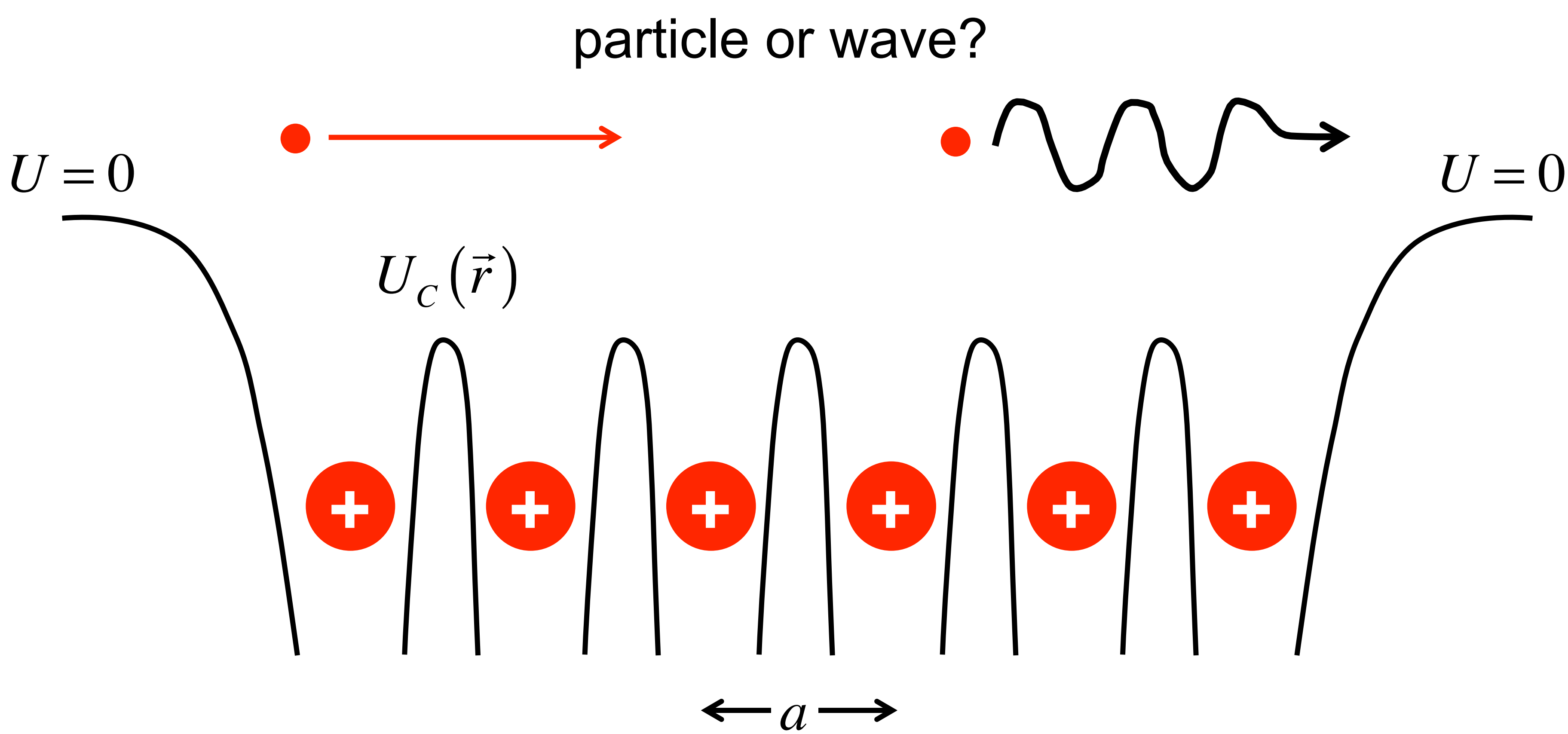
# Mobile electrons in crystals



# De Broglie Wavelength

The crystal potential varies on an atomic scale. It gives us the band structure when we solve the Schrodinger equation. Quantum mechanics is necessary.

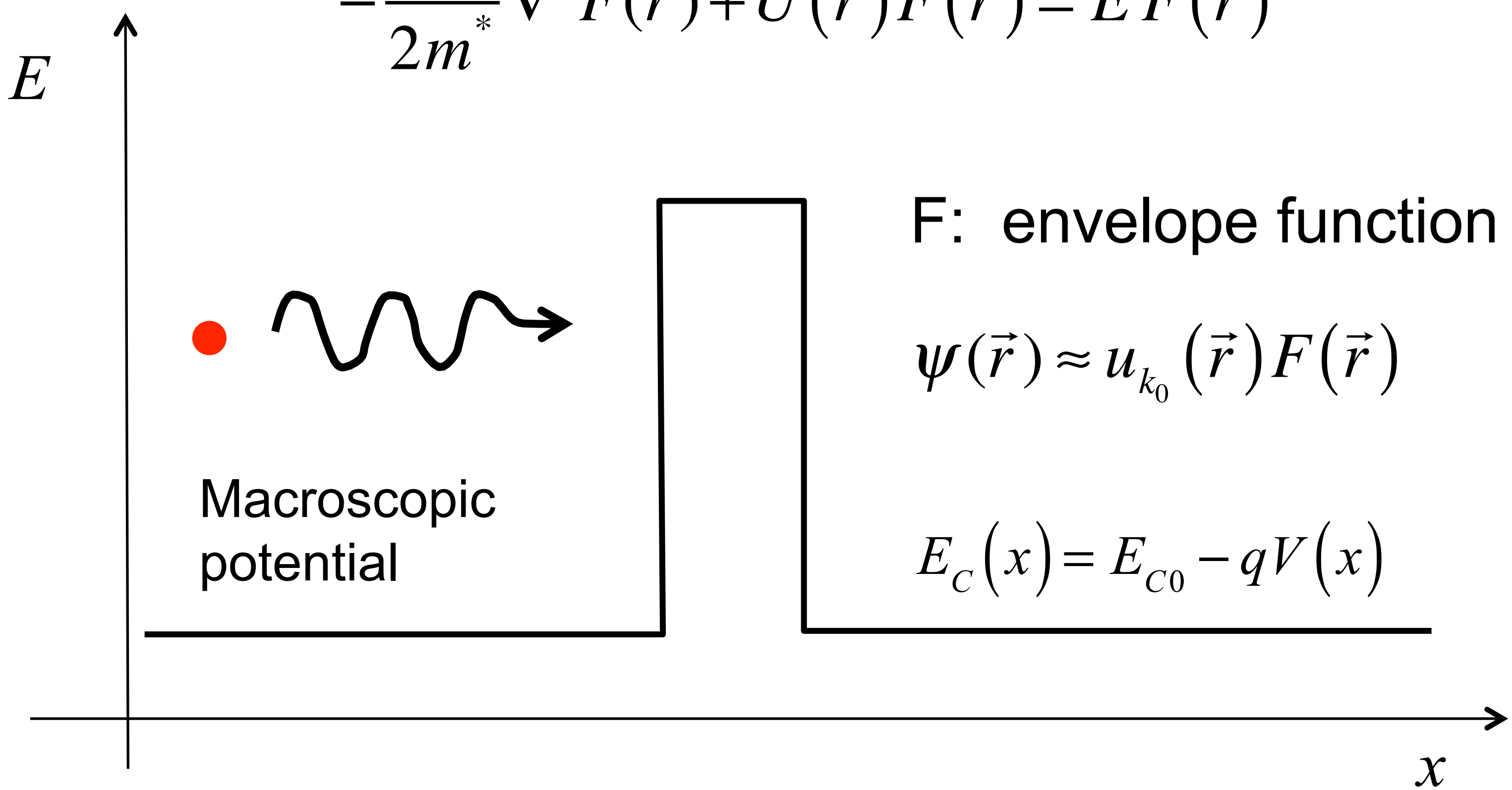
What is the wavelength of a free (mobile) electron?

$$p = \hbar k = \hbar \frac{2\pi}{\lambda_B} \qquad E = \frac{p^2}{2m^*} \approx \frac{3}{2} k_B T$$

$$\lambda_B = \sqrt{\frac{4\pi^2 \hbar^2}{3m^* k_B T}} \simeq 10\text{nm (electrons in Si at 300K)}$$

# Effective mass wave equation

$$-\frac{\hbar^2}{2m^*}\nabla^2 F(\vec{r}) + U(\vec{r})F(\vec{r}) = E\,F(\vec{r})$$



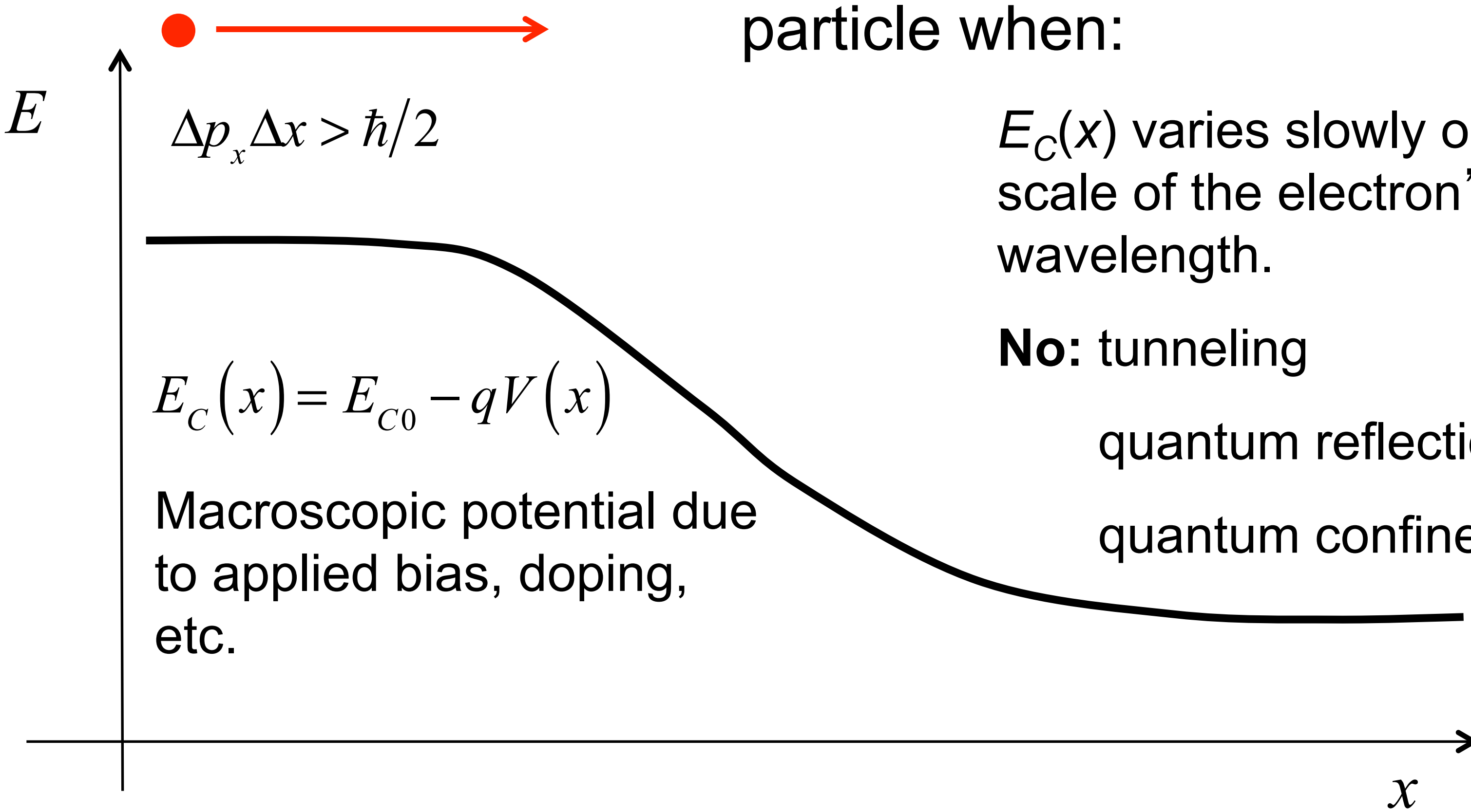

F:  envelope function

$$\psi(\vec{r}) \approx u_{k_0}(\vec{r})F(\vec{r})$$

$$E_C(x) = E_{C0} - qV(x)$$

# Semi-classical transport

particle when:




$\Delta p_x \Delta x > \hbar/2$

$E_C(x) = E_{C0} - qV(x)$

Macroscopic potential due to applied bias, doping, etc.

$E_C(x)$ varies slowly on the scale of the electron's wavelength.

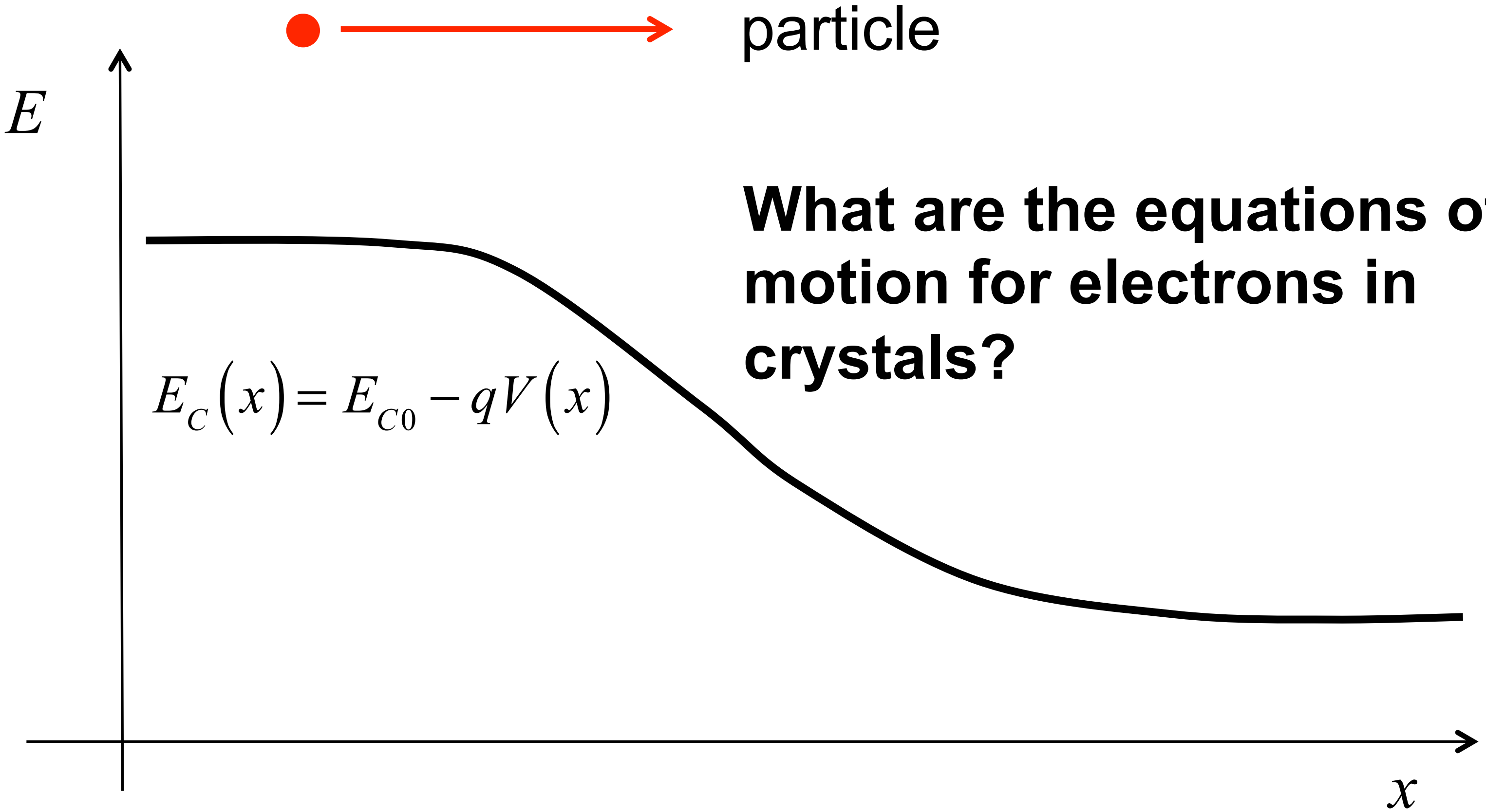
**No:** tunneling

quantum reflections

quantum confinement

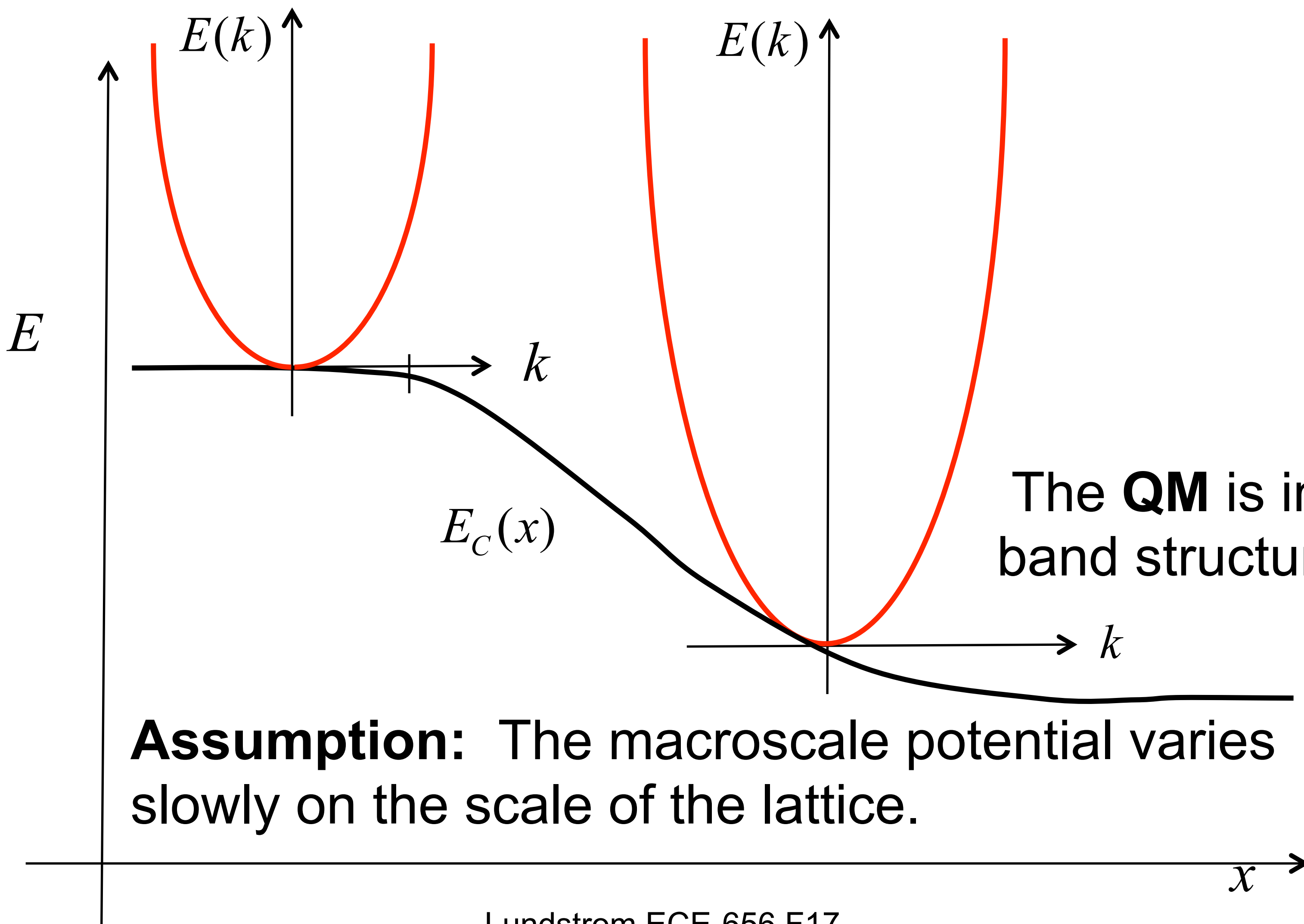
**But**: Quantum mechanics determines the band structure (e.g. effective mass)

# Semi-classical transport




**What are the equations of motion for electrons in crystals?**

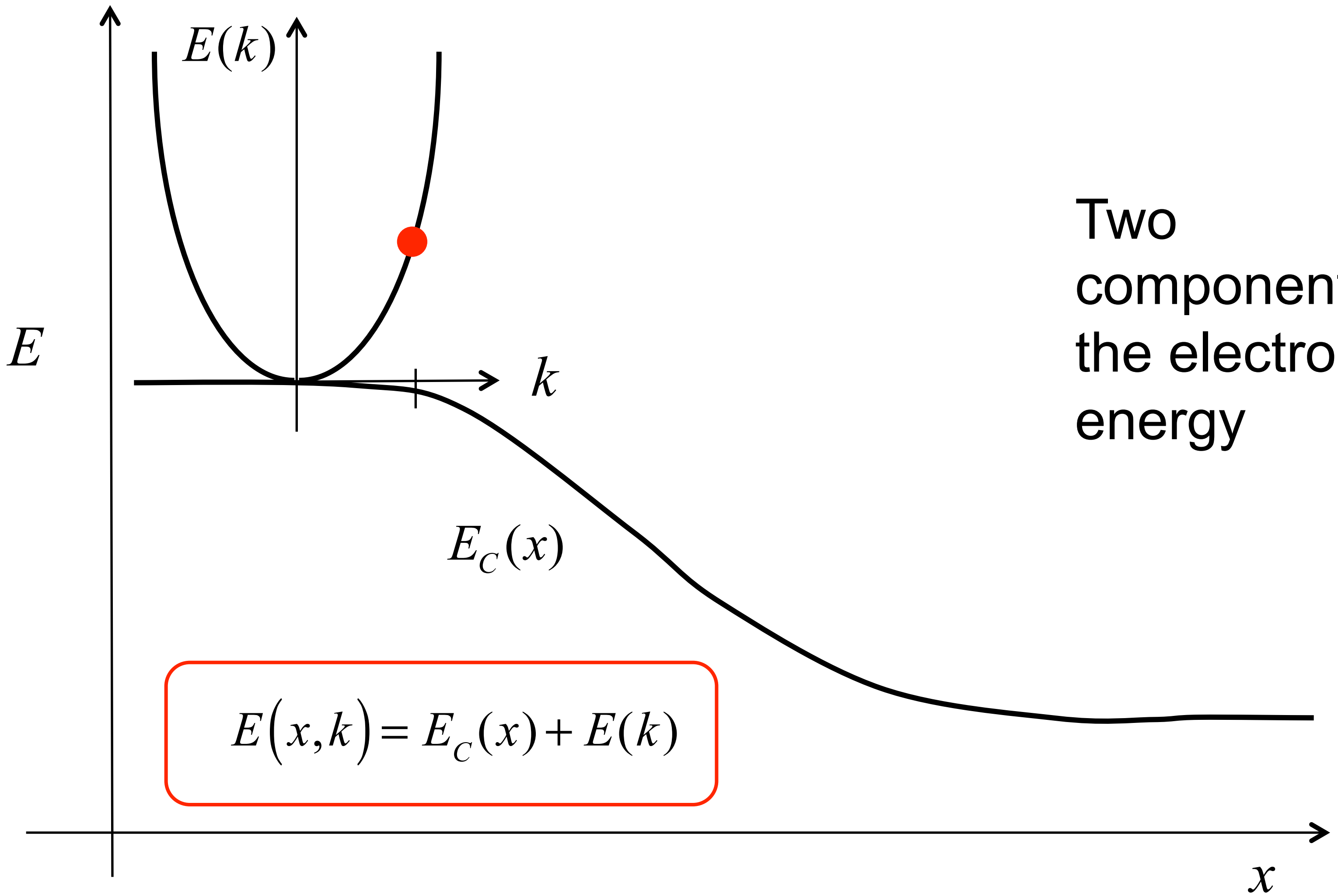
# Semi-classical transport




The **QM** is in the band structure.

**Assumption:** The macroscale potential varies slowly on the scale of the lattice.

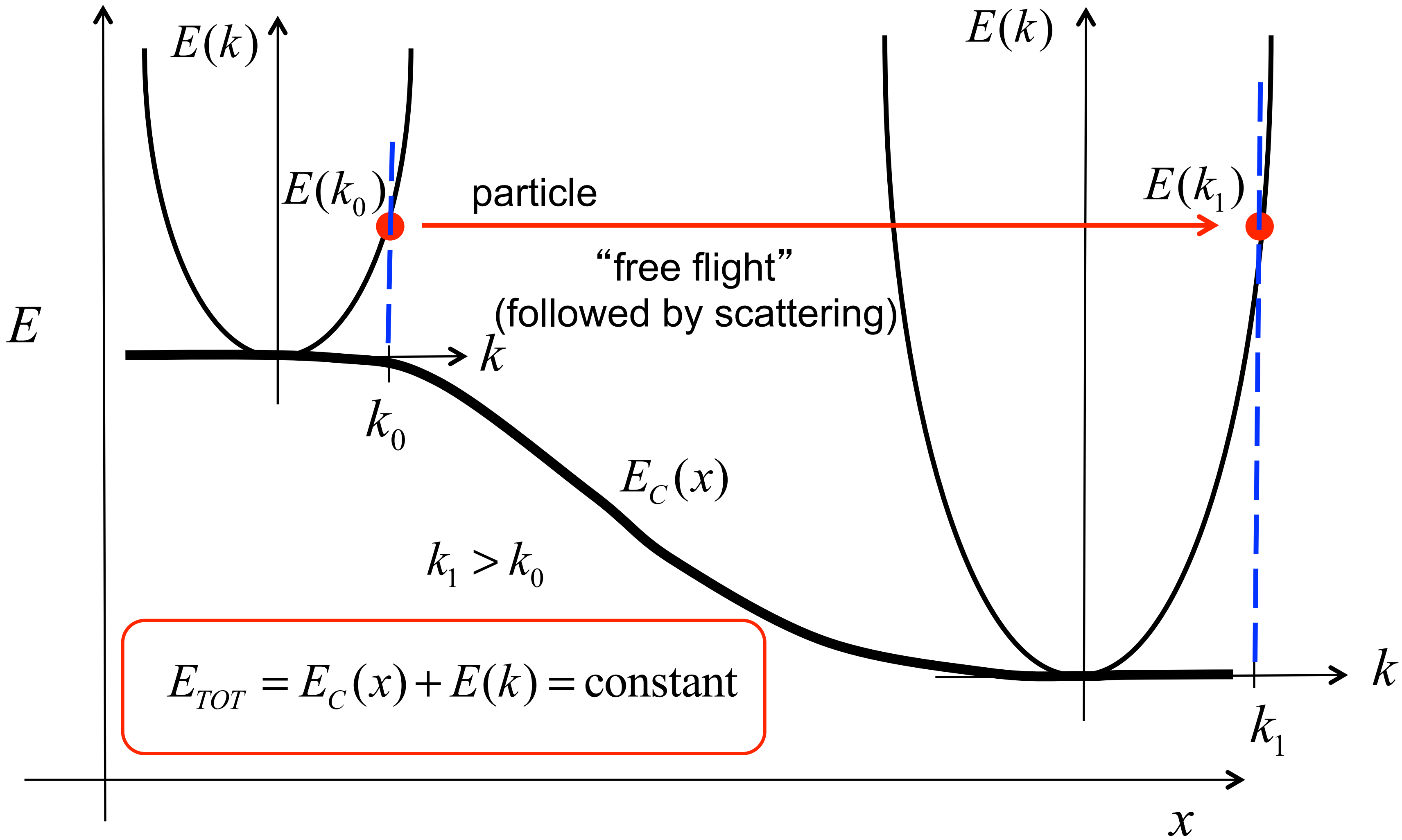
# Semi-classical transport




$$E(x,k) = E_C(x) + E(k)$$

Two components of the electron energy

# Semi-classical transport




$$E_{TOT} = E_C(x) + E(k) = \text{constant}$$

# Semi-classical transport

$$E_{TOT} = E_C(x) + E(k)$$

$$\frac{dE_{TOT}\left(x,k\right)}{dt} = 0 = \frac{dE_C(x)}{dx}\frac{dx}{dt} + \frac{dE(k)}{dk_x}\frac{dk_x}{dt}$$

$$0 = \frac{dE_C(x)}{dx}\upsilon_x + \frac{1}{\hbar}\frac{dE}{dk_x}\frac{d\left(\hbar k_x\right)}{dt}$$

$$0 = \frac{dE_C(x)}{dx}\upsilon_x + \upsilon_x\frac{d\left(\hbar k_x\right)}{dt}$$

$$\boxed{\frac{d\left(\hbar k_x\right)}{dt} = F_e = -\frac{dE_C(x)}{dx}}$$

$$p_x = \hbar k_x$$

$$\frac{dp_x}{dt} = F_e$$

"Newton's Law"

# Semi-classical transport: k-space

$$\frac{d\left(\hbar\vec{k}\right)}{dt}=-\nabla_r E_C(\vec{r})=-q\vec{\mathcal{E}}(\vec{r})$$

$$\left\{\ \frac{d\vec{p}}{dt}=\vec{F}_e\ \right\}$$

$$\hbar\vec{k}\left(t\right)=\hbar\vec{k}\left(0\right)+\int_0^t -q\vec{\mathcal{E}}(t')dt'$$

equation of motion for "semi-classical transport" in k-space.

*No band structure (or effective mass) is involved)!*

# Semi-classical transport: real-space

$$\frac{d\left(\hbar\vec{k}\right)}{dt} = -\nabla_r E_C(\vec{r}) = -q\vec{\mathcal{E}}(\vec{r})$$

$$\hbar\vec{k}\left(t\right) = \hbar\vec{k}\left(0\right) + \int_0^t -q\vec{\mathcal{E}}(t')dt'$$

$$\left.\begin{aligned}\vec{\upsilon}_g(t) &= \frac{1}{\hbar}\nabla_k E\left[\vec{k}\left(t\right)\right] \\ \vec{r}\left(t\right) &= \vec{r}\left(0\right) + \int_0^t \vec{\upsilon}_g(t')dt'\end{aligned}\right\}$$

equations of motion for semi-classical transport in real-space.

*Motion in real space brings in the band structure!*

# Semi-classical transport: parabolic bands

Equations of motion for semi-classical transport.

$$\frac{d\left(\hbar\vec{k}\right)}{dt} = -\nabla_r E_C(\vec{r}) = -q\vec{\mathcal{E}}(\vec{r})$$

$$\hbar\vec{k}\left(t\right) = \hbar\vec{k}\left(0\right) + \int_0^t -q\vec{\mathcal{E}}(t')dt'$$

$$\vec{\upsilon}_g(t) = \frac{1}{\hbar}\nabla_k E\left[\vec{k}\left(t\right)\right]$$

$$\vec{r}\left(t\right) = \vec{r}\left(0\right) + \int_0^t \vec{\upsilon}_g(t')dt'$$

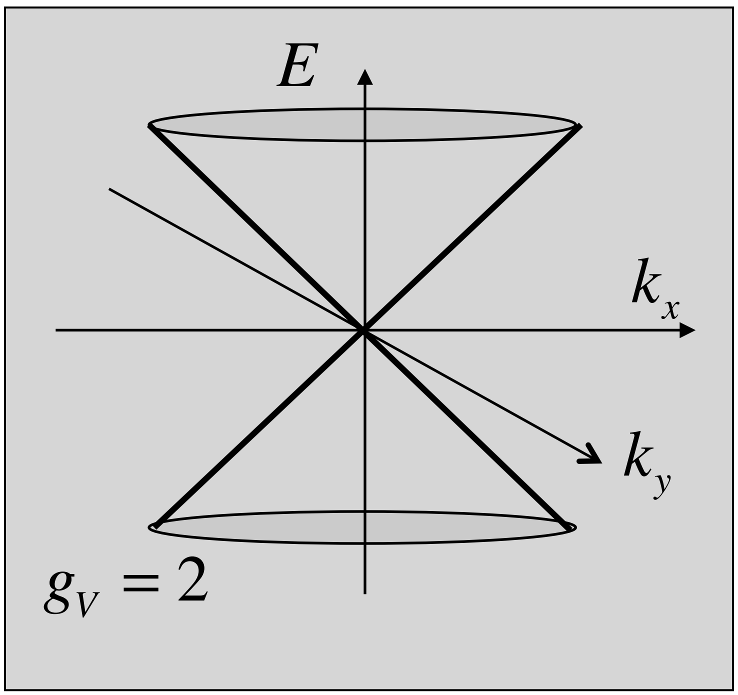
Parabolic energy bands:

$$E\left(k\right) = \frac{\hbar^2 k^2}{2m^*}$$

$$\vec{\upsilon}_g(t) = \frac{\hbar\vec{k}}{m^*}$$

# Exercise 1: graphene

What are the equations of motion for electrons in graphene?



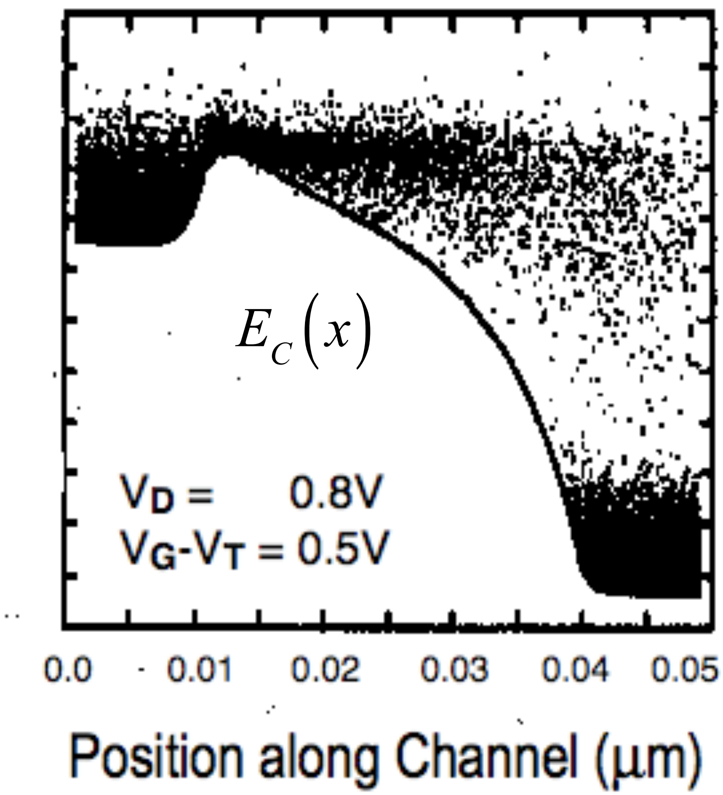

$$E(k) = \pm\hbar\upsilon_F\sqrt{k_x^2 + k_y^2} = \pm\hbar\upsilon_F k$$

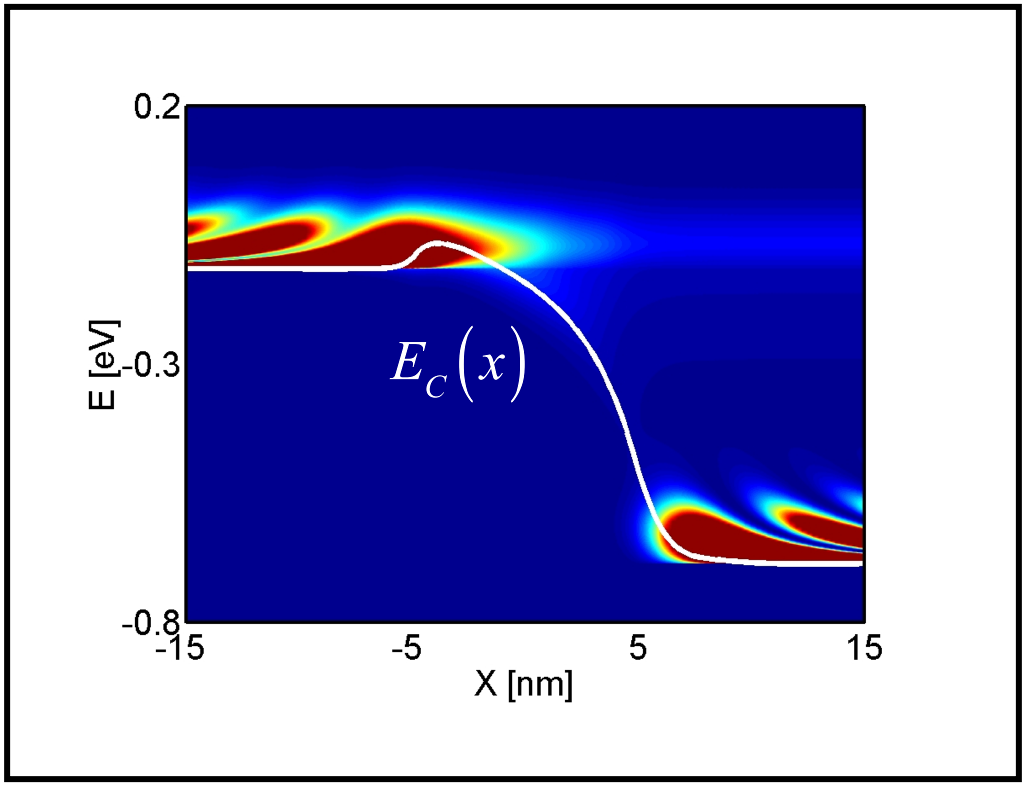
# Exercise 2: equations of motion for m*(x)

What are the equations of motion for electrons in a parabolic band semiconductor with a position dependent effective mass?

$$E\left(k,\vec{r}\right) \approx \frac{\hbar^2 k^2}{2m^*(\vec{r})}$$

# Semiclassical vs. Quantum Transport




Frank, Laux, and Fischetti, IEDM Tech. Dig., p. 553, 1992.

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# Summary

1) Semiclassical transport means that the potential changes slowly – and that the uncertainty in position and energy is small enough.

2) Motion in k-space is simple.

3) Motion in real space involves the bandstructure.