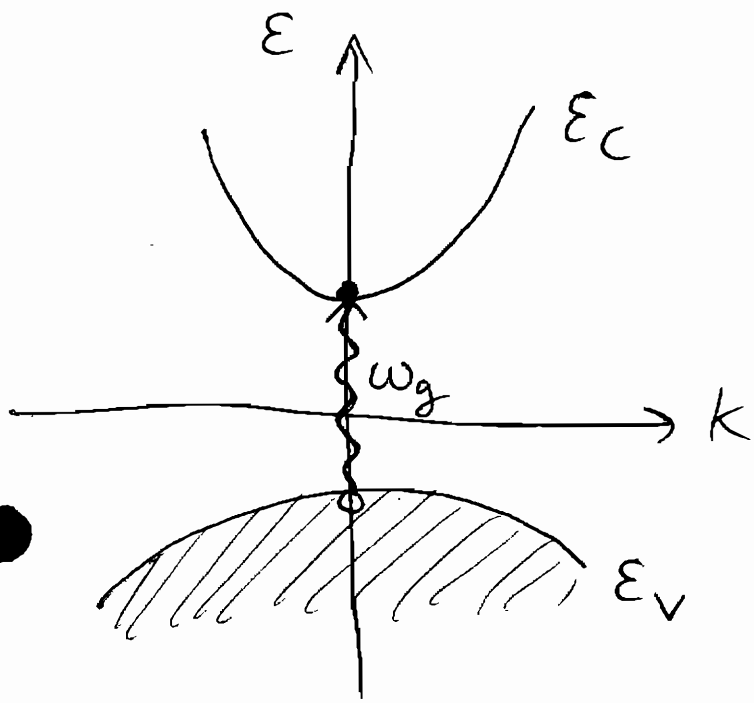
Lecture 13

Semiconductors I

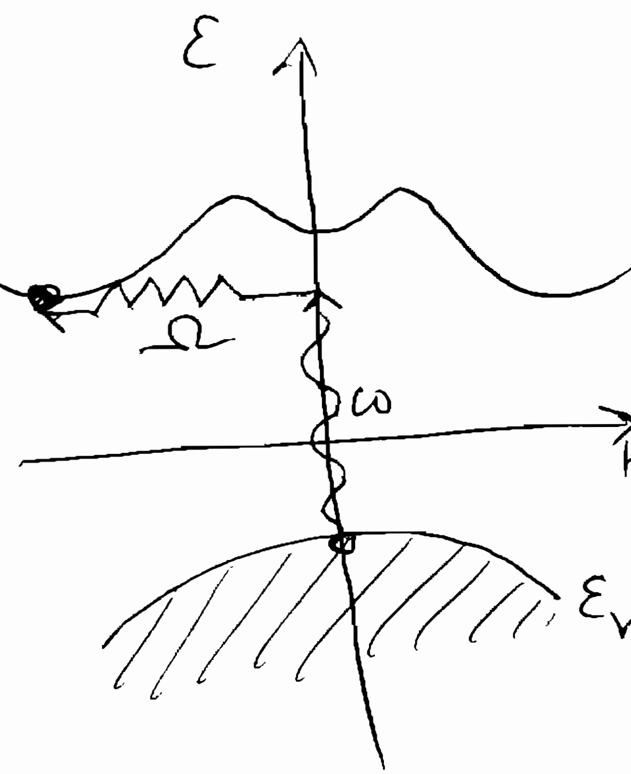
Semiconductors are materials with a band gap sufficiently small that, although they are insulators at $T = 0K$, they become conductors at room temperature due to thermally excited electrons in the conduction band and holes in the valence band. Some technologically significant examples are:

crystal	E_g energy gap [eV]	
Si	1.17	(indirect)
Ge	0.744	(indirect)
InSb	0.23	(direct)
InAs	0.43	(direct)
GaAs	1.52	(direct)
CdS	2.58	(direct)

direct gap



indirect gap



- In a <u>direct gap</u> semiconductor, the lowest point of the conduction band occurs at the same value of $\vec{k}$ as the highest point of the valence band. Absorption of a photon of energy
- $\hbar\omega_g = E_g$ excites an electron from the valence band to the conduction band.

In an <u>indirect gap</u> semiconductor, the top of the valence band and the bottom of the
- conduction band occur at different

values of $\vec{k}$. It is thus not possible to excite a particle from the top of the valence band to the bottom of the conduction band by absorbing a photon

This is because a photon of energy $\hbar\omega = 1\,eV$ has a wavevector

$$k = \frac{\omega}{c} = \frac{eV}{\hbar c} = \frac{eV}{197\,eV\cdot nm} = \frac{1}{197\,nm}$$

But a typical wavevector in the 1st Brillouin zone is

- $k \sim \frac{1}{a} \sim \frac{1}{\mathring{A}}$.

It is thus necessary to absorb a photon with energy $\hbar\omega \sim E_g$ and a phonon with the appropriate wavevector and energy $\hbar\Omega \ll E_g$ in order to excite an electron from the top of the valence band to the bottom of the conduction band.

- Direct gap semiconductors,

like GaAs, are useful for optical applications, like semiconductor lasers.

Equations of motion

What are the dynamics of a wavepacket centered at $\vec{k}$ in an energy band $\varepsilon(\vec{k})$? In fact, in the semiclassical approximation, the crystal momentum $\hbar\vec{k}$ obeys Newton's second law:

$$\frac{d}{dt}\hbar\vec{k} = \vec{F} = -e\left(\vec{E} + \frac{\vec{V}_g}{c} \times \vec{B}\right)$$

where $\vec{V}_g = \frac{1}{\hbar} \frac{\partial \mathcal{E}}{\partial \vec{k}}$.

what is the group velocity of the wave packet as a function of time? Consider the ith component:

$$\frac{d V_g^{(i)}}{dt} = \sum_j \frac{1}{\hbar^2} \frac{\partial^2 \mathcal{E}}{\partial k_i \partial k_j} \frac{d}{dt} \hbar k_j$$

$$= \sum_j \frac{1}{\hbar^2} \frac{\partial^2 \mathcal{E}}{\partial k_j \partial k_j} F_j$$

$$= \sum_j \left(\frac{1}{m^*} \right)_{ij} F_j$$

By analogy with the equation

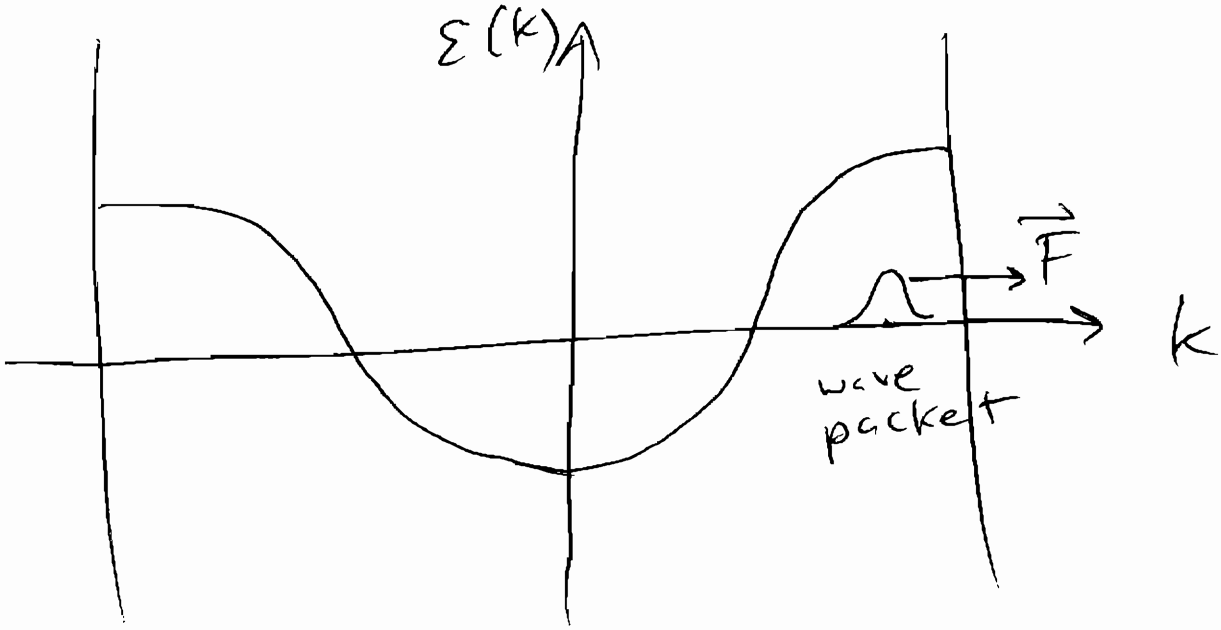
of motion of a free particle $\frac{d\vec{v}}{dt} = \frac{1}{m}\vec{F}$,

the matrix

$$\left(\frac{1}{m^*}\right)_{ij} = \frac{1}{\hbar^2}\frac{\partial^2 \varepsilon}{\partial k_i \partial k_j}$$

is known as the (inverse) effective mass tensor.

1D example $\quad \varepsilon(k) = -2t\cos ka$



- What happens to a wave packet near the Brillouin zone boundary when an external force F in the direction shown is applied?

Near $k = \frac{\pi}{a}$,

- $$\varepsilon(k) \simeq 2t\left(1 - \frac{k^2a^2}{2} + \cdots\right)$$

$$= 2t - ta^2k^2 + \cdots$$

$$\frac{1}{m^*} = -\frac{2ta^2}{\hbar^2} \qquad (t > 0)$$

- $$\frac{dv_g}{dt} = \frac{1}{m^*} F$$

$\Rightarrow$ The particle accelerates in the opposite direction to the applied force!

Bloch oscillations

Under a constant applied force F, the equation of motion is

$$\hbar \frac{dk}{dt} = F$$

$$k(t) = k(0) + \frac{Ft}{\hbar}$$

$$V_g = \frac{1}{\hbar} \frac{\partial \mathcal{E}}{\partial k} = \frac{1}{\hbar} \frac{\partial}{\partial k} \left[-2 + \cos ka \right]$$

- $v_g = \frac{2ta}{\hbar} \sin ka$

$$v_g(t) = \frac{2ta}{\hbar} \sin\left(k(0)a + \frac{Fat}{\hbar}\right)$$

- The wavepacket thus undergoes simple harmonic motion with frequency

$$\omega = \frac{Fa}{\hbar} \quad \text{(Bloch oscillations)}.$$

$$\boxed{\text{Proof of} \quad \hbar \frac{d\vec{k}}{dt} = \vec{F}}$$

- In quantum mechanics, the

- time derivative of an observable $\hat{A}$ is determined by

$$\frac{d\langle \hat{A} \rangle}{dt} = \frac{i}{\hbar}\langle [\hat{H}, \hat{A}] \rangle,$$

where $\hat{H}$ is the Hamiltonian.

- Consider the translation operator $\hat{T}$ defined by

$$\hat{T}\psi(x) = \psi(x+a).$$

For a Bloch wavefunction,

$$\hat{T}\psi_k(x) = e^{ika}\psi_k(x)$$

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The crystal Hamiltonian H_0 commutes with T, $[H_0, T] = 0$.

If we add a uniform external force F, then $H = H_0 - Fx$.

i) $[H, T] = Fa\,T$

Proof: $[H, T]\psi(x) = -F[x, T]\psi(x)$

$$= -F\left\{x T\psi(x) - T\{x\psi(x)\}\right\}$$

$$= -F\left[x\psi(x+a) - (x+a)\psi(x+a)\right]$$

$$= Fa\,\psi(x+a) = Fa\,T\psi(x)$$

Since this is true for any $\psi(x)$, it follows that $[H, T] = Fa\,T$.

- ii) $\frac{d}{dt}\langle T\rangle = \frac{i}{\hbar} Fa \langle T\rangle$

$$d\ln\langle T\rangle = \frac{iFa}{\hbar}\, dt$$

$$\langle T(t)\rangle = \langle T(0)\rangle\, e^{\frac{iFa}{\hbar}t}$$

- But for a Bloch wavefunction, we have $\langle T\rangle = e^{ika}$:

$$\Rightarrow \quad e^{ik(t)a} = e^{i\left[k(0)a + \frac{Fa}{\hbar}t\right]}$$

$$\hbar k(t) = \hbar k(0) + Ft$$

- $\boxed{\hbar \frac{dk}{dt} = F \qquad \text{Q.E.D.}}$

It is straightforward to generalize this result to 3-dimensional systems.

Holes

A wavepacket near the top of the valence band accelerates in the opposite direction to a free electron in an applied electric field. It is conventional to ascribe this to a positive effective charge rather than to a negative effective mass.

A full valence band has total wavevector zero. If one electron of wavevector $\vec{k}_e$ is removed, the total wavevector of the system is

$$\boxed{\vec{k}_h = -\vec{k}_e.}$$

This can be interpreted as the <u>wavevector</u> of the the hole left behind. The <u>energy</u> necessary to create the hole (up to an additive constant) is

$$\boxed{\begin{aligned} \varepsilon_h(\vec{k}_h) &= -\varepsilon_e(\vec{k}_e) \\ &= -\varepsilon_e(\vec{k}_h) \end{aligned}}$$

since $\varepsilon(-\vec{k}) = \varepsilon(\vec{k})$.

The group velocity of the hole is

$$\boxed{\vec{V}_h = \frac{1}{\hbar}\frac{\partial \varepsilon_h}{\partial \vec{k}_h} = \frac{1}{\hbar}\frac{\partial \varepsilon_e}{\partial \vec{k}_e} = \vec{V}_e}$$

The effective mass of the hole is

$$\left(\frac{1}{m_h^*}\right)_{ij} = \frac{1}{\hbar^2}\frac{\partial^2 \varepsilon_h}{\partial k_h^{(i)} \partial k_h^{(j)}}$$

$$= -\left(\frac{1}{m_e^*}\right)_{ij}$$

- The <u>equation of motion</u> is

$$\boxed{\hbar \frac{d\vec{k}_h}{dt} = e\left(\vec{E} + \frac{\vec{v}_h}{c} \times \vec{B}\right)}$$

The hole behaves as a particle of positive effective mass and positive charge. It is the solid state analogue of a positron, which was originally described by Dirac as a hole in a Fermi sea of negative energy states.

Cyclotron resonance

The effective mass tensor can be messured by the technique of cyclotron resonance in a constant magnetic field $\vec{B}$

$$\frac{d\vec{V}_h}{dt} = \left(\frac{1}{m^*}\right)\frac{e}{c}\vec{V}_h \times \vec{B}.$$

For simplicity, let m^* be a scalar.

$$\frac{d\vec{V}_h}{dt} = -\frac{e\vec{B}}{m^* c} \times \vec{V}_h$$

Ansatz: $\vec{B} = B\hat{z}$ 30

$V_x(t) = V_0 \cos \Omega t$

$V_y(t) = -V_0 \sin \Omega t$

$$-\Omega V_0 \sin \Omega t = -\frac{eB}{m^*c} V_0 \sin \Omega t$$

$$-\Omega V_0 \cos \Omega t = -\frac{eB}{m^*c} V_0 \cos \Omega t$$

$$\boxed{\Omega = \frac{eB}{m^*c}}$$

$$x(t) = x(0) + \int_0^t V_x(t')\,dt'$$

$$= x(0) + \frac{V_0}{\Omega} \sin \Omega t$$

$$y(t) = y(0) + \frac{V_0}{\Omega} \cos \Omega t$$

$$(x(t) - x_0)^2 + (y(t) - y_0)^2$$
$$= \frac{v_0^2}{\Omega^2}$$

Cyclotron radius

$$R_c = \frac{m^* v_0}{\frac{e}{c} B}$$

The frequency is independent of the radius of the orbit.

By applying an AC electric field of frequency Ω, one can make the particle spiral outward, absorbing energy.