Physics of Electronics:

5. Electrons in Solids - Intro to Band Theory

July – December 2008

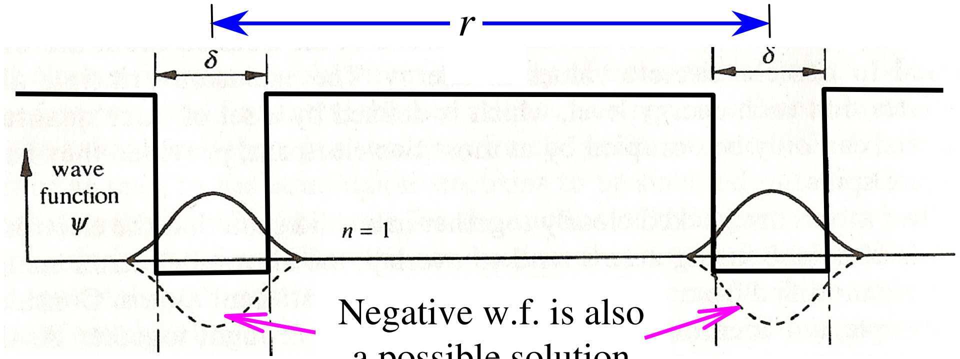
Contents overview

- Allowed energy bands.
- Velocity and effective mass of electrons in solids.
- Conductors, semiconductors, and insulators.

Allowed Energy Bands

- Energy splitting.

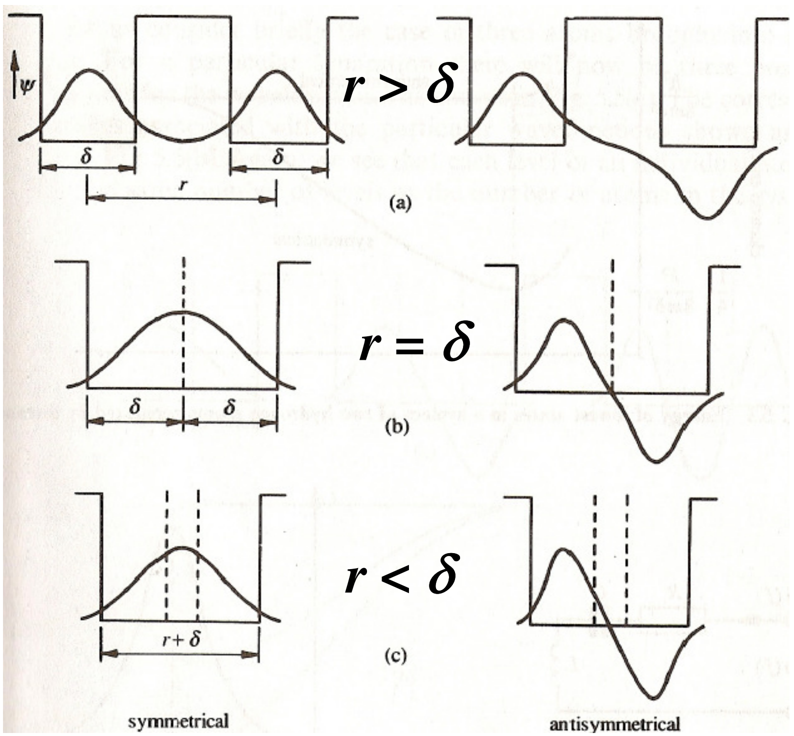
Two atoms separated a distance r modeled by potential wells. If r is large, w.f. are unperturbed.



$$E = \frac{\hbar^2 n^2 \pi^2}{2md^2} = \frac{n^2 h^2}{8md^2}$$

$$E_1 = h^2/(8m\delta^2)$$

The atoms are brought together.



$$E_{1,\text{sym}} = \frac{h^2}{8m(2\delta)^2} = \frac{1}{4}\frac{h^2}{8m\delta^2}$$

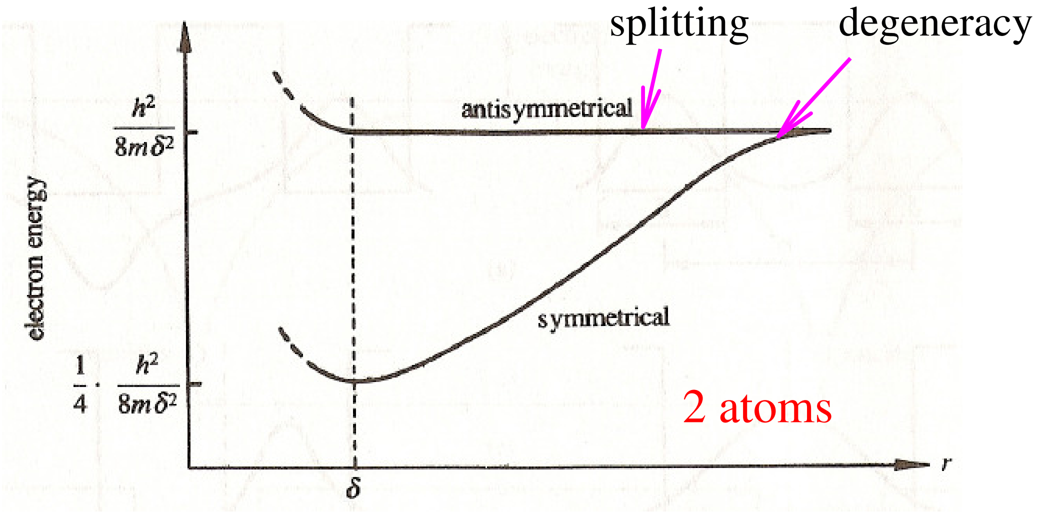
$$E_{1,\text{antisym}} = \frac{2^2 h^2}{8m(2\delta)^2} = \frac{h^2}{8m\delta^2}$$

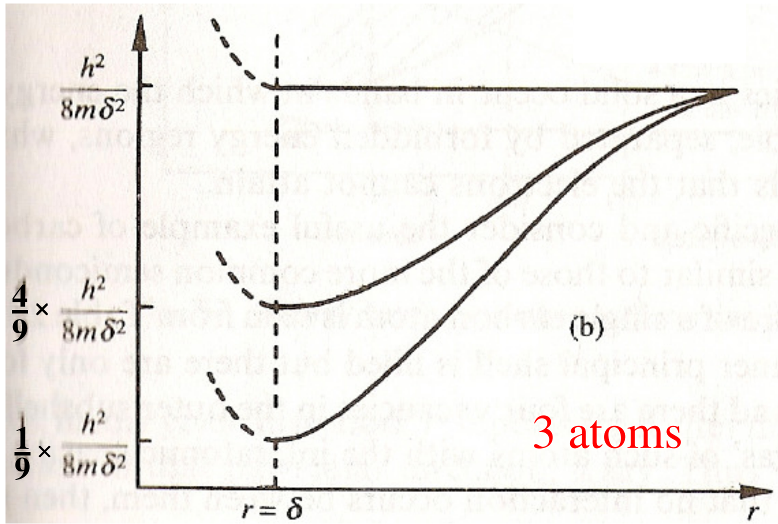
$$E_{1,\text{sym}} = \frac{h^2}{8m(r+\delta)^2}$$

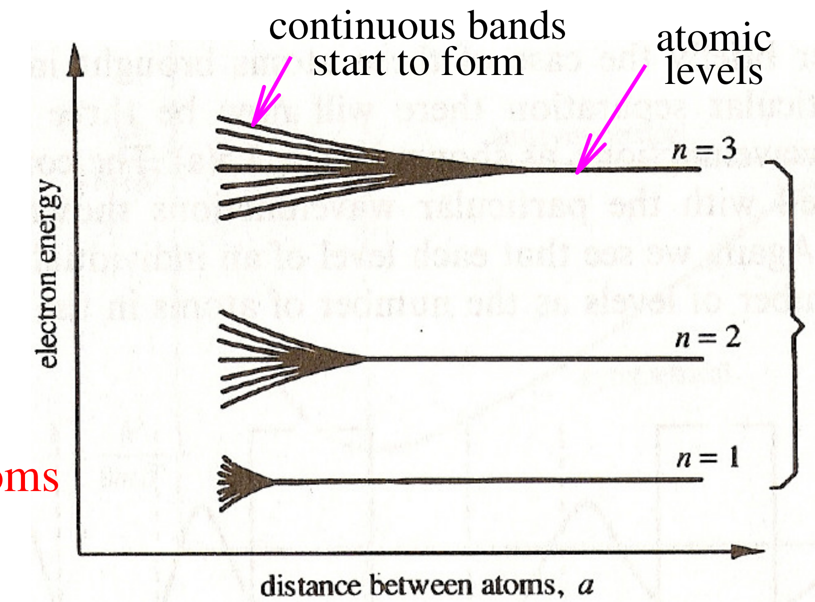
$$E_{1,\text{antisym}} = \frac{4h^2}{8m(r+\delta)^2}$$

Allowed Energy Bands

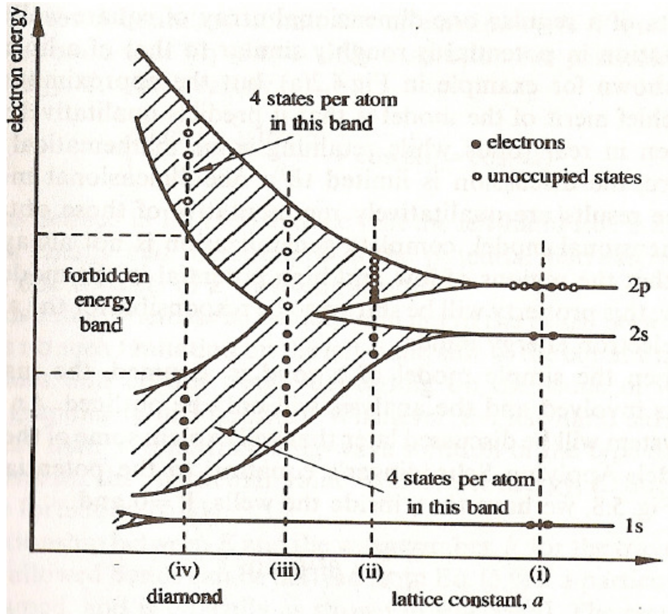
- Energy splitting.







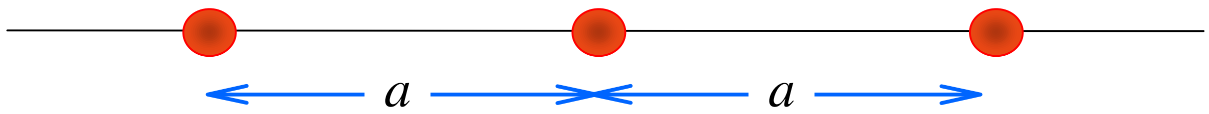
7 atoms



solid

Allowed Energy Bands

- Bloch's theorem.
  - Let's consider a 1D chain of N atoms of period a.



- The potential has the same periodicity: $V(x) = V(x+a) = V(x+2a) = \ldots$
- The w.f. has to have the same periodicity:

$$\psi(x+a) = C\psi(x)$$

- Further we consider that the chain forms a ring:

$$\psi(x+Na) = \psi(x) = C^N \psi(x)$$

$\Rightarrow$ $C^N = 1$ $\Rightarrow$ $C = \exp(i2\pi s/N)$; $s = 0, 1, 2, \ldots, N-1$.

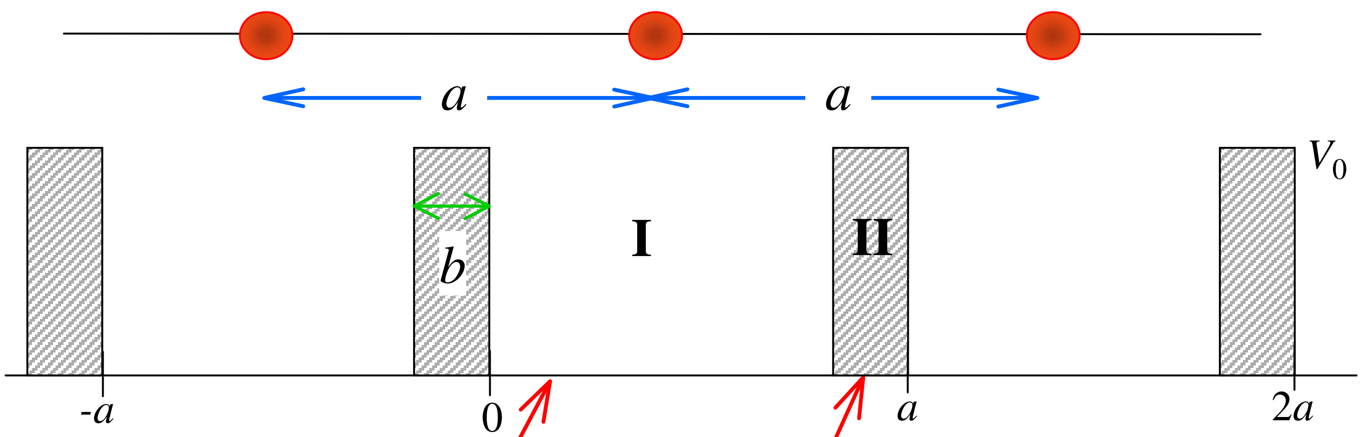
- To satisfy the previous relations, the w.f. has to be of the form:

$\boxed{\psi(x) = u_k(x)e^{ikx}}$ with: $u_k(x) = u_k(x+a)$ & $k = 2\pi s/Na$

i.e. a plane wave modulated in space

Allowed Energy Bands

- Kronig-Penney model.
  - Let's consider a 1D chain of *N* atoms of period *a*.



$$\frac{\partial^2\Psi}{\partial x^2}+\beta^2\Psi=0$$

$$\frac{\partial^2\Psi}{\partial x^2}-\alpha^2\Psi=0$$

$$\beta^2=2mE/\hbar^2$$

$$\alpha^2=2m(V_0-E)/\hbar^2$$

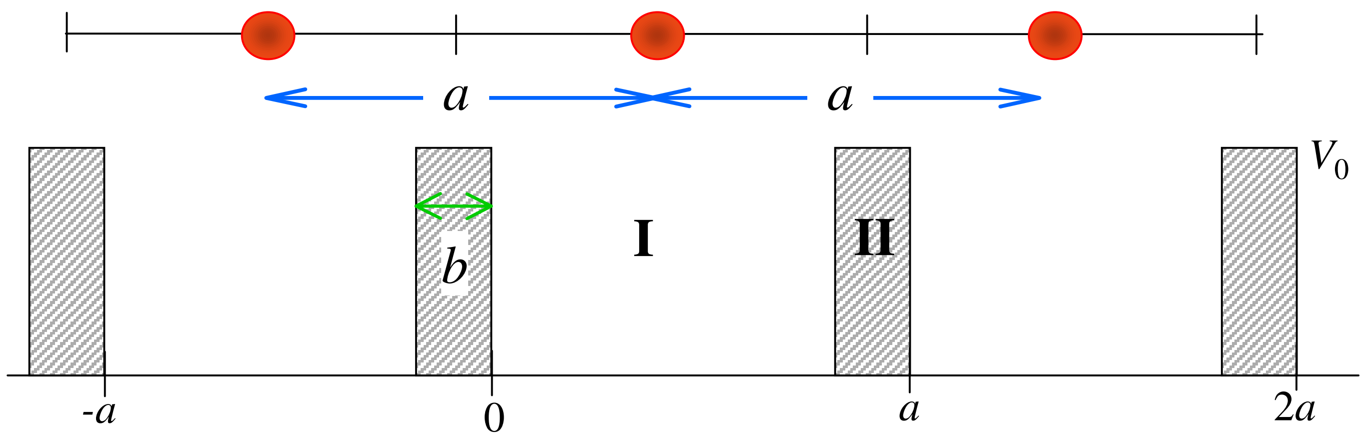
we are looking for bound states

$$\Psi_{\mathrm{I}}=Ae^{j\beta x}+Be^{-j\beta x}$$

$$\Psi_{\mathrm{II}}=C\exp(\alpha x)+D\exp(-\alpha x)$$

Allowed Energy Bands

- Kronig-Penney model.
  - Let's consider a 1D chain of N atoms of period a.



  - From continuity of ψ and **dψ/d*x*** at the boundaries:
    - At $x = 0$: $A + B = C + D$;

$$i\beta(A - B) = \alpha(C - D) .$$

  - From Bloch's theorem, $\psi(x + a) = \psi(x)e^{ika}$:
    - At $x = -b$: $Ae^{i\beta(a-b)} + Be^{-i\beta(a-b)} = (Ce^{i\alpha(-b)} + De^{-i\alpha(-b)})\, e^{-ika}$

$$i\beta(Ae^{i\beta(a-b)} - Be^{-i\beta(a-b)}) = \alpha(Ce^{i\alpha(-b)} - De^{-i\alpha(-b)})\, e^{-ika}$$

Allowed Energy Bands

- Kronig-Penney model.
  - The previous system of 4 equations have a solution only if its determinant is equal to zero giving:

$$[(\alpha^2 - \beta^2)/2\alpha\beta] \sinh \alpha b \sin \beta(a-b) + \cosh \alpha b \cos \beta(a-b) = \cos ka$$

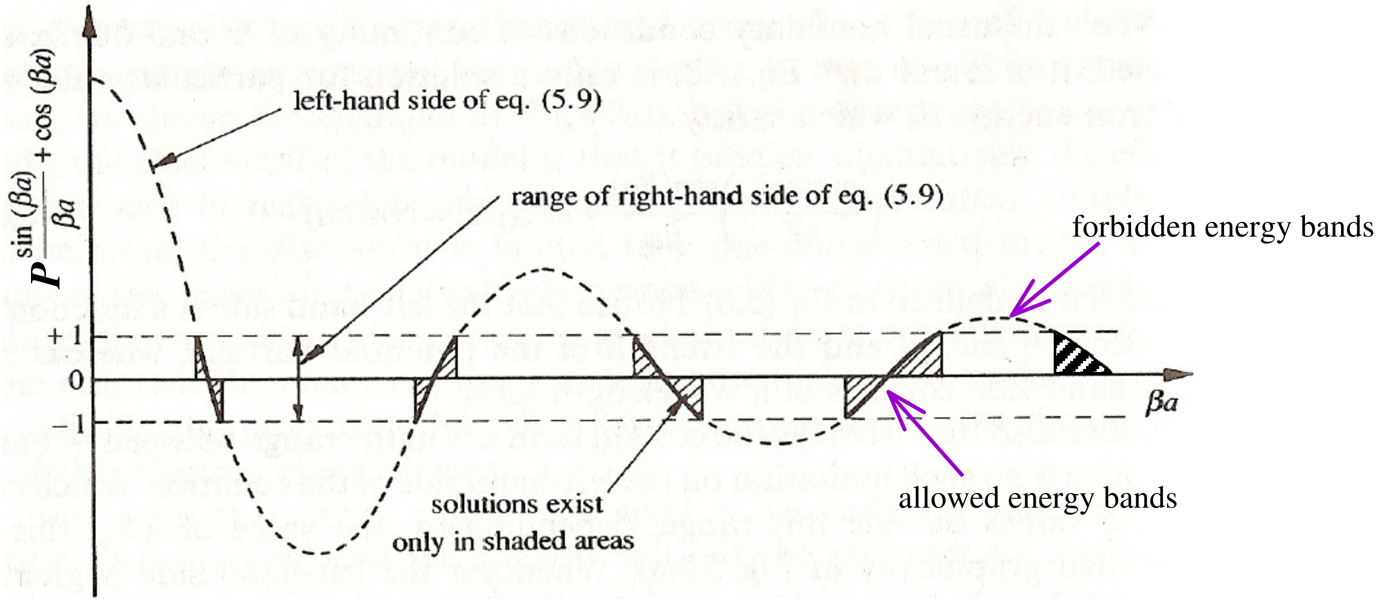
  - For simplicity, let's consider the case $\boldsymbol{b \to 0}$ & $\boldsymbol{V_0 \to \infty}$ but such that $\boldsymbol{\alpha^2 ba/2 = P}$ remains constant.

  - In this limit $\boldsymbol{\alpha \gg \beta}$ & $\boldsymbol{\alpha b \ll 1}$. Then:

$$(P/\beta a)\sin \beta a + \cos \beta a = \cos ka$$

Allowed Energy Bands

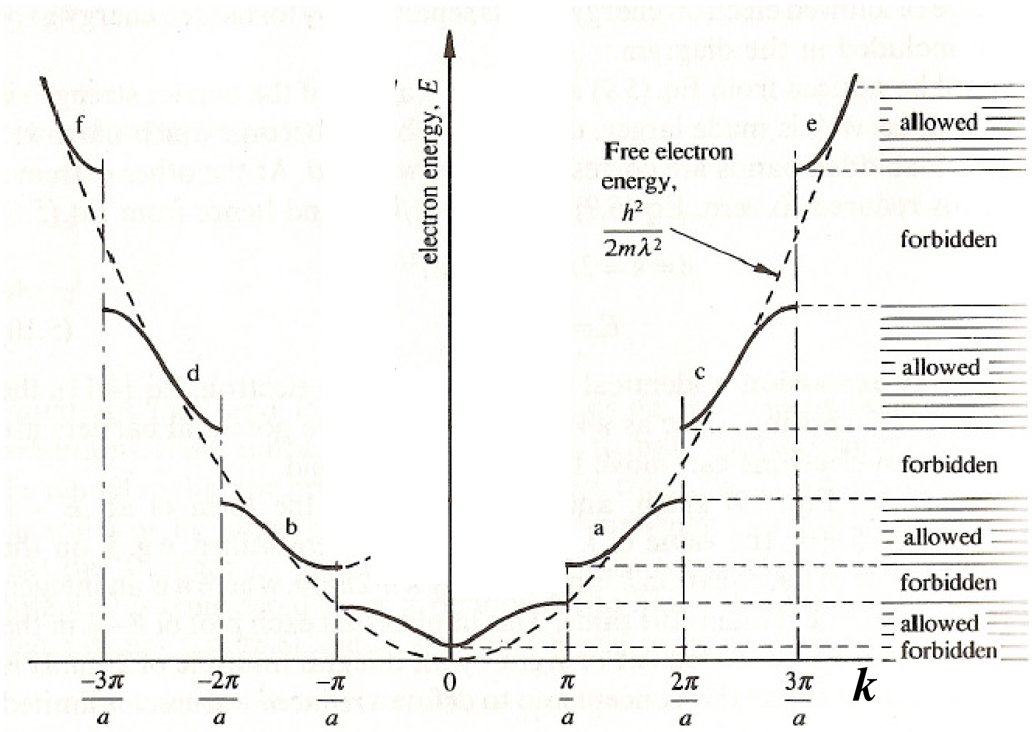
- Kronig-Penney model.
  - What are the allowed electron energies $E = \hbar\beta^2/2m$?
  - We have to solve $(P/\beta a)\sin\beta a + \cos\beta a = \cos ka$



  - As P becomes larger (i.e. the product bV_0), the allowed bands become narrower.
  - As $P \to 0$, $\beta \to k$ (i.e. towards the free electron model)

Allowed Energy Bands

- Kronig-Penney model.
  - Since $(P/\beta a)\sin \beta a + \cos \beta a = \cos ka$
    - The allowed energies are function of the wavenumber ***k***.
    - The solutions have the periodicity of **cos(*ka*)**.



Allowed Energy Bands

- Kronig-Penney model.
  - Since $(P/\beta a)\sin \beta a + \cos \beta a = \cos ka$
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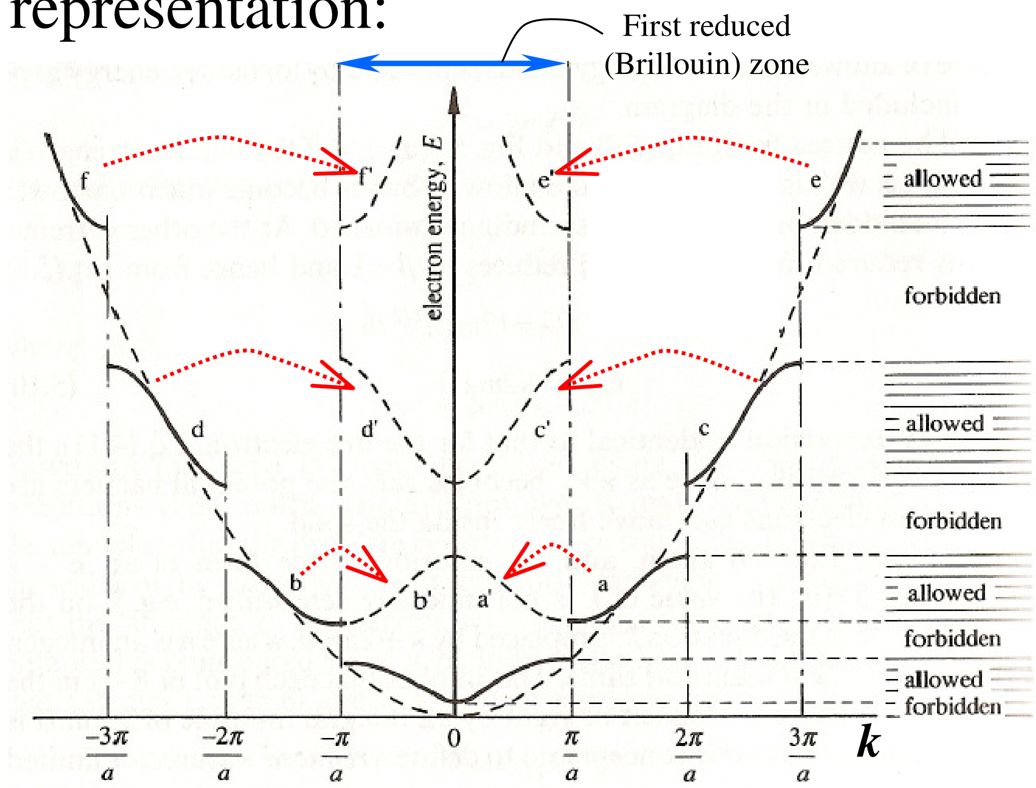
    - The solutions have the periodicity of **cos(*ka*)**.
    - To ease representation:



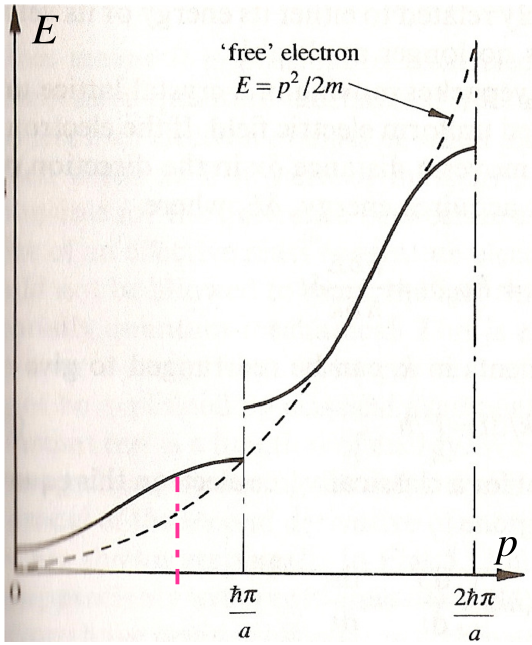
Velocity and Effective Mass

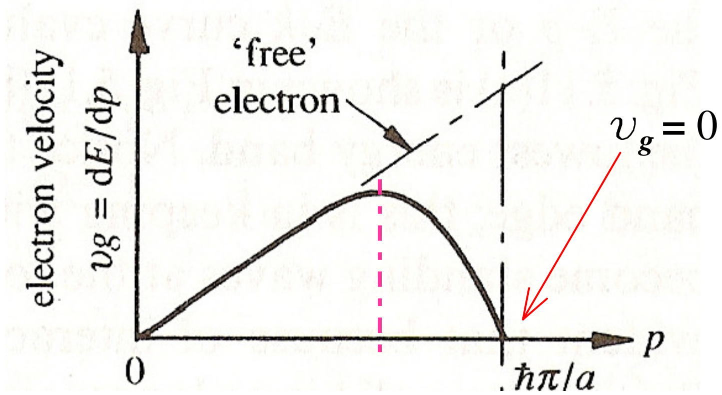
- Group velocity
  - From Bloch's theorem $\psi(x,t) = \underbrace{u_k(x)}_{\text{spatial modulation}}\ \underbrace{e^{i(kx-Et/\hbar)}}_{\text{plane wave}}$ ← wave packet
  - Therefore, the velocity of the electron is given by the group velocity

$$v_g = \frac{\partial\omega}{\partial k} = \frac{\partial(E/\hbar)}{\partial k} \Rightarrow \boxed{v_g = \frac{1}{\hbar}\frac{\partial E}{\partial k} = \frac{\partial E}{\partial p}}$$

← $p = \hbar k$

OBS. $E = f(p)$ is called dispersion relation





Velocity and Effective Mass

- Effective Mass
  - Consider an e^- in a solid moving in an external field that exerts a force F on it. The energy acquired by the e^- is:

$$\delta E = F\delta x = F v_g \delta t = \frac{F\delta E}{\hbar\,\delta k}\delta t \quad \Longrightarrow \quad \boxed{F = \hbar\,\mathrm{d}k/\mathrm{d}t = \mathrm{d}p/\mathrm{d}t}$$

» External forces and effects of the lattice are included

  - Applied for the case of a free electron (i.e. $p = mv$):

$$F = \frac{\mathrm{d}}{\mathrm{d}t}(\hbar k) = \frac{\mathrm{d}p}{\mathrm{d}t} = m\frac{\mathrm{d}v}{\mathrm{d}t}$$

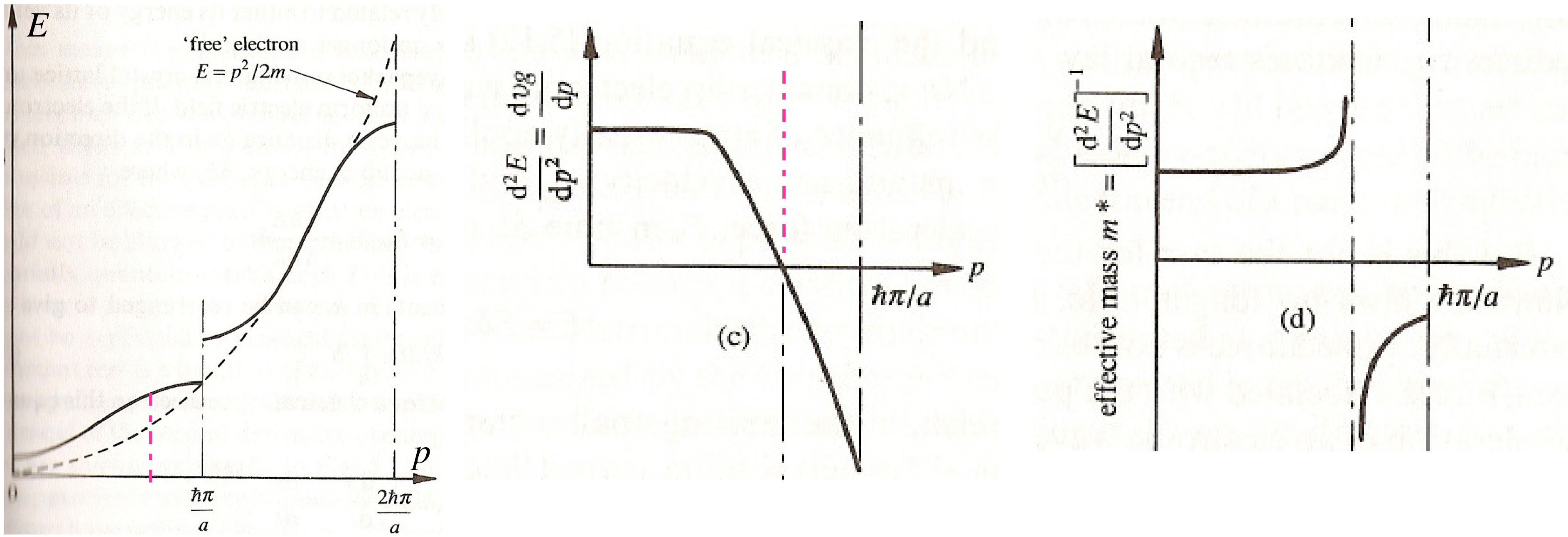
  - Now, in general, differentiating v_g:

$$\frac{\mathrm{d}v_g}{\mathrm{d}t} = \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\mathrm{d}E}{\mathrm{d}p}\right) = \frac{\mathrm{d}^2E}{\mathrm{d}t\,\mathrm{d}p} = \frac{\mathrm{d}p}{\mathrm{d}t}\frac{\mathrm{d}^2E}{\mathrm{d}p^2} = F\frac{\mathrm{d}^2E}{\mathrm{d}p^2} \quad \Longrightarrow \quad F = \left(\frac{\mathrm{d}^2E}{\mathrm{d}p^2}\right)^{-1}\frac{\mathrm{d}v_g}{\mathrm{d}t}$$

Velocity and Effective Mass

- Effective Mass
  - Comparing both we define:

$$\boxed{m^* = \left(\frac{d^2E}{dp^2}\right)^{-1} = \hbar^2\left(\frac{d^2E}{dk^2}\right)^{-1}} \quad \Rightarrow \quad F = m^* dv_g/dt$$



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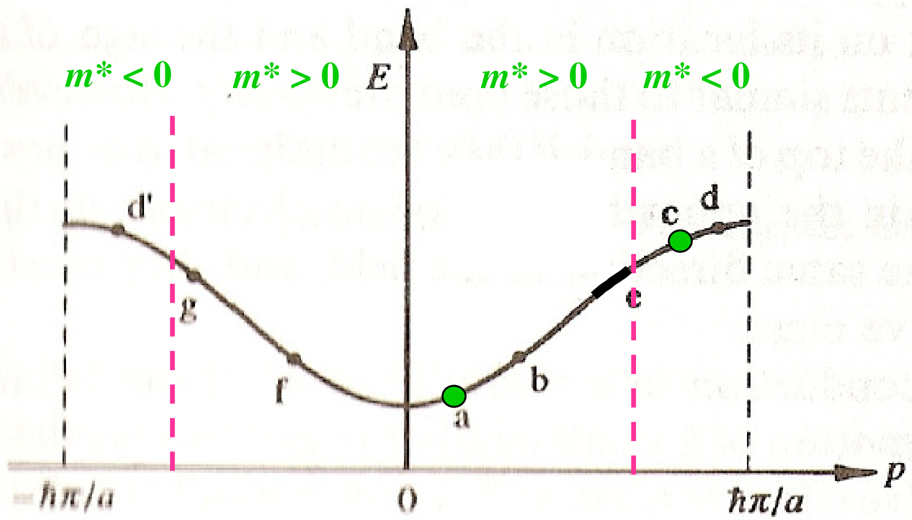

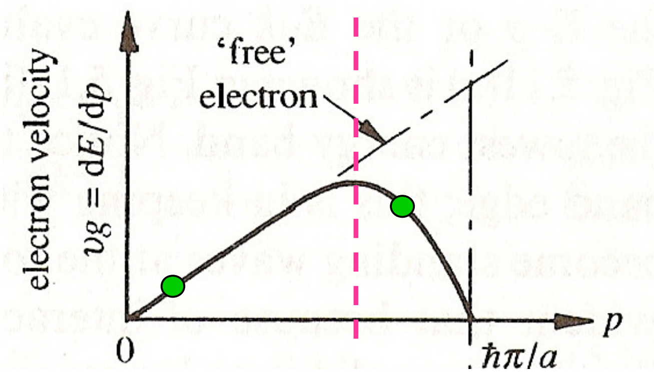

$\mathscr{E} = 0$

Velocity and Effective Mass

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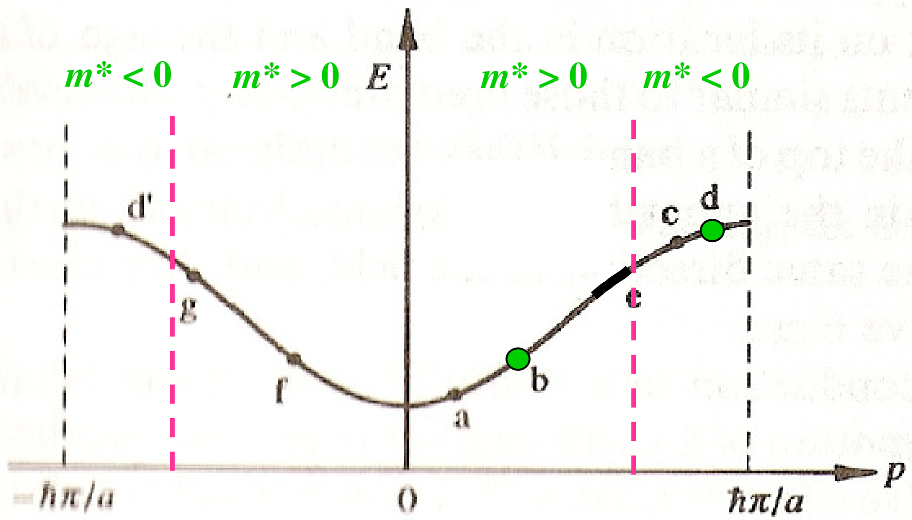
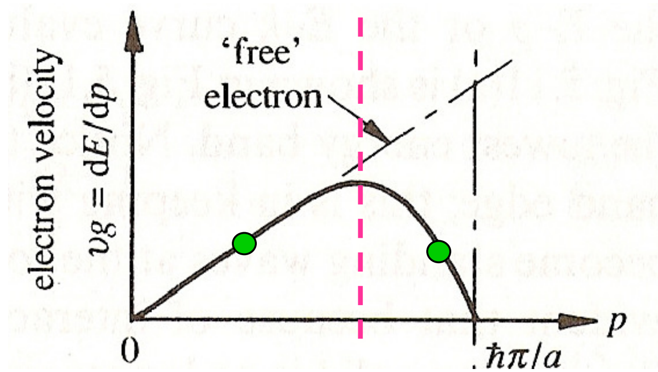


$\mathscr{E} \neq 0$



an electron with negative mass
≡
an "electron" with positive charge

Velocity and Effective Mass

- Effective Mass
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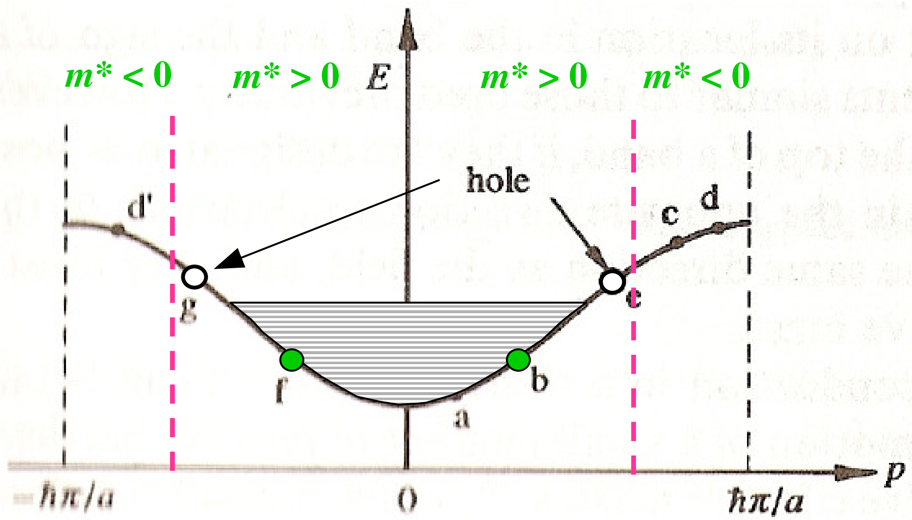

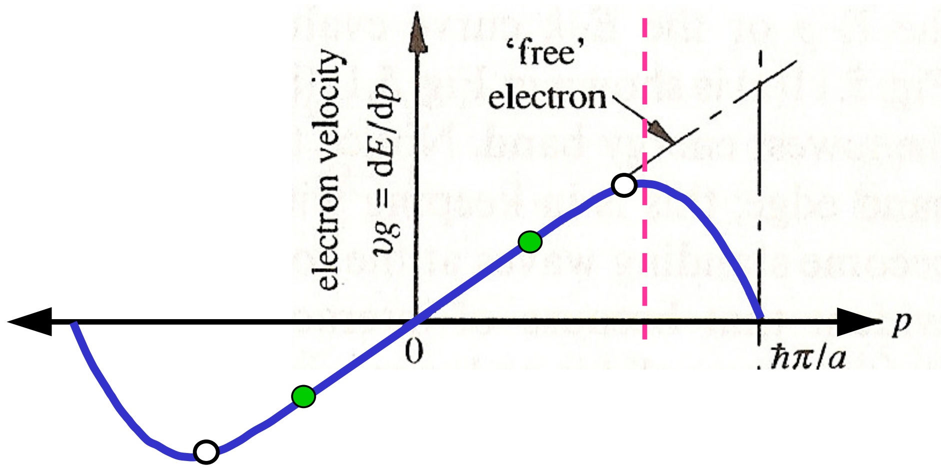

Opposite velocities. No net current,

Velocity and Effective Mass

- Effective Mass
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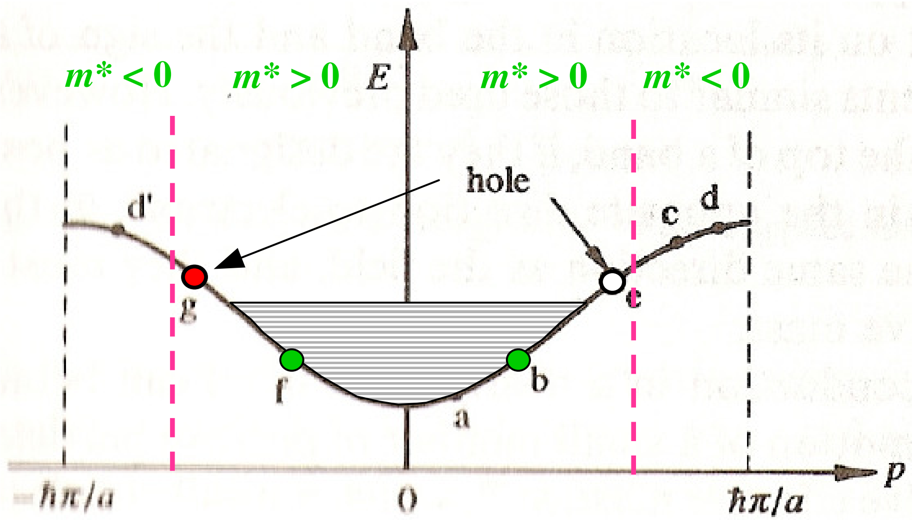
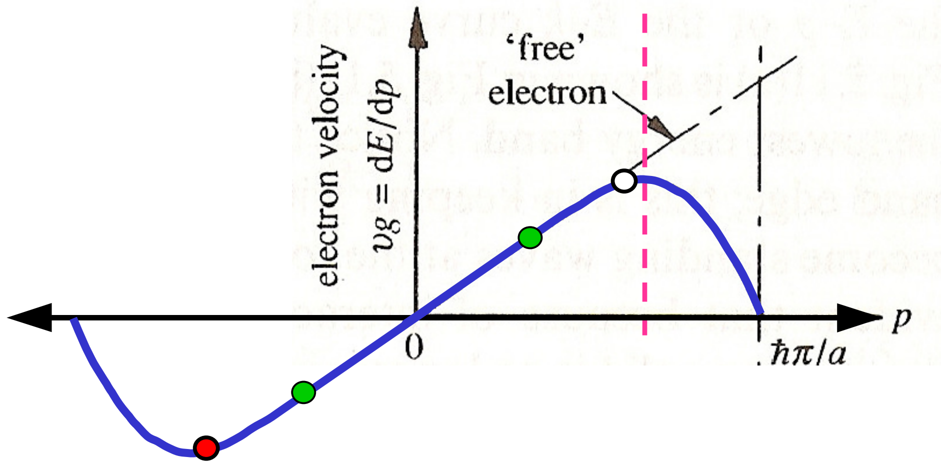
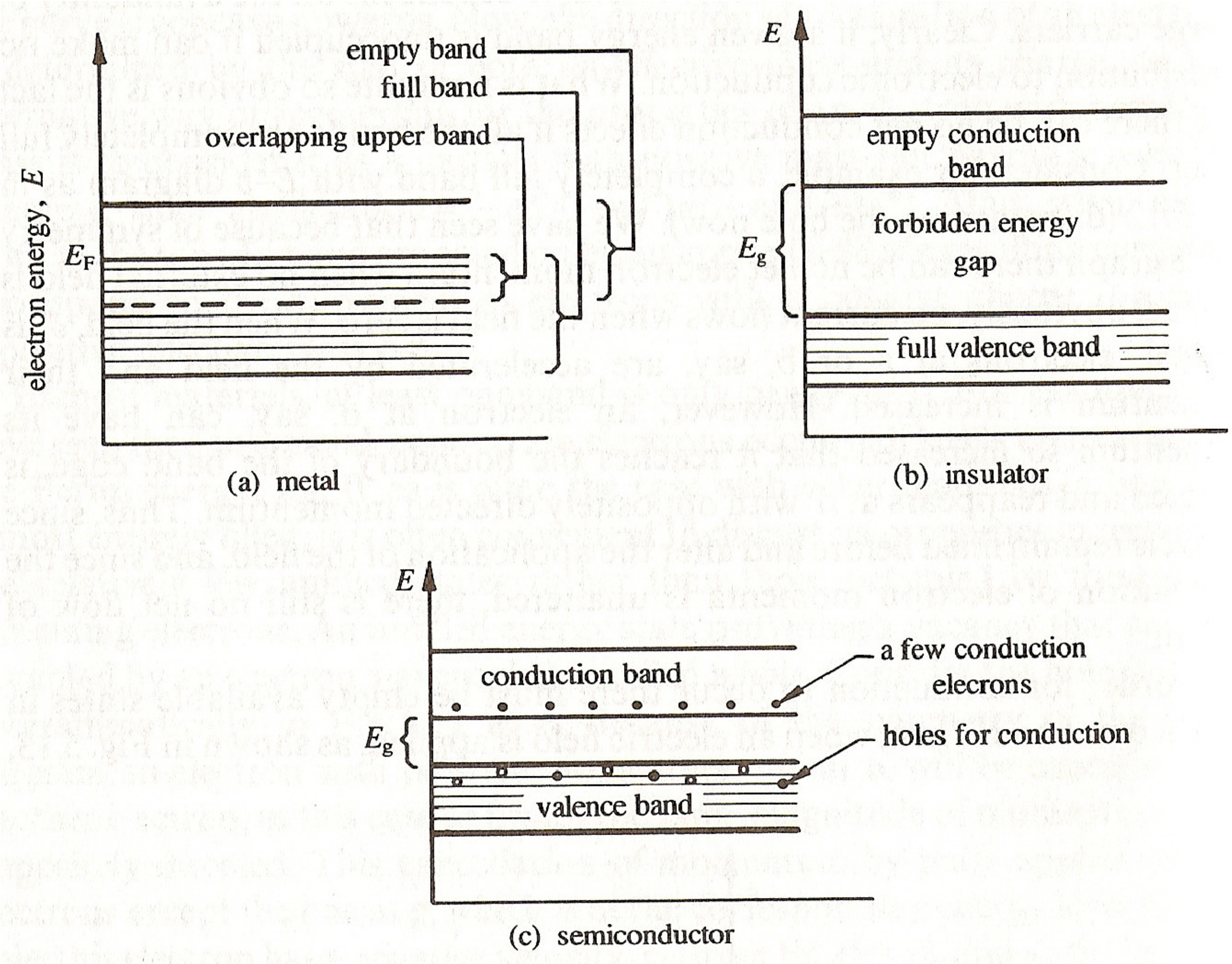




- Opposite velocities. No net current,
- Not cancelled. Net current.

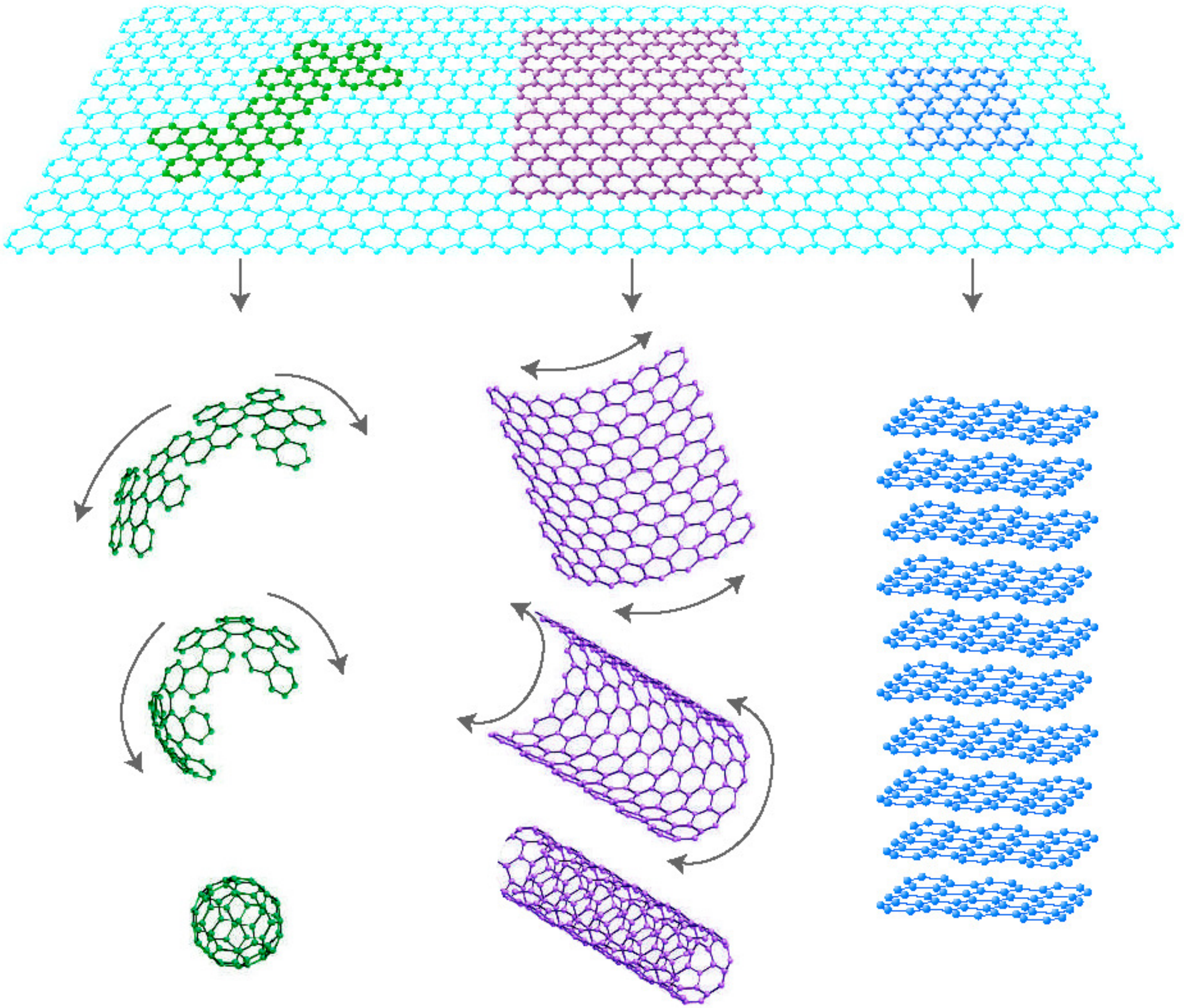
Conductors, Semiconductors & Insulators

- Classification according to the filling of the gaps



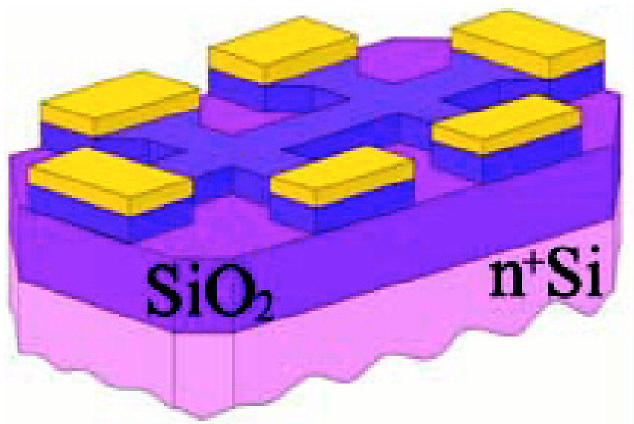
Energy Bands in Graphene

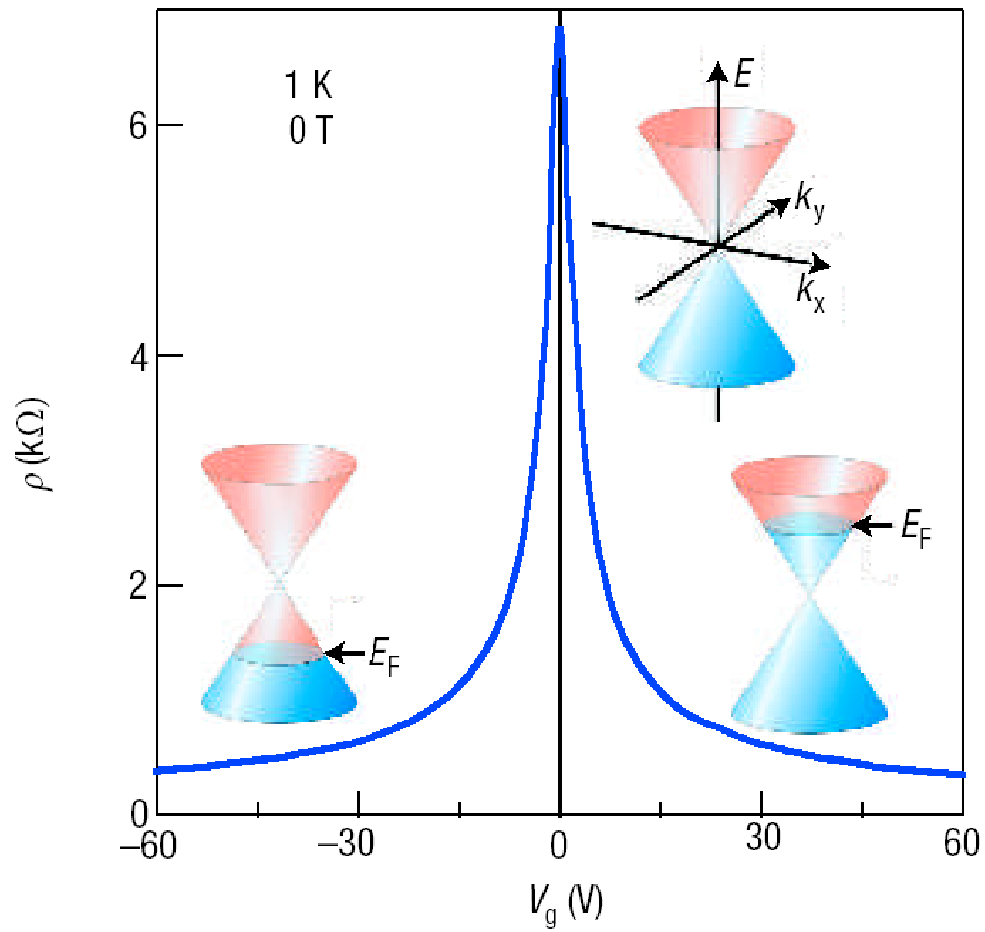
- Graphene and other related structures



Energy Bands in Graphene

- Ideal band structure

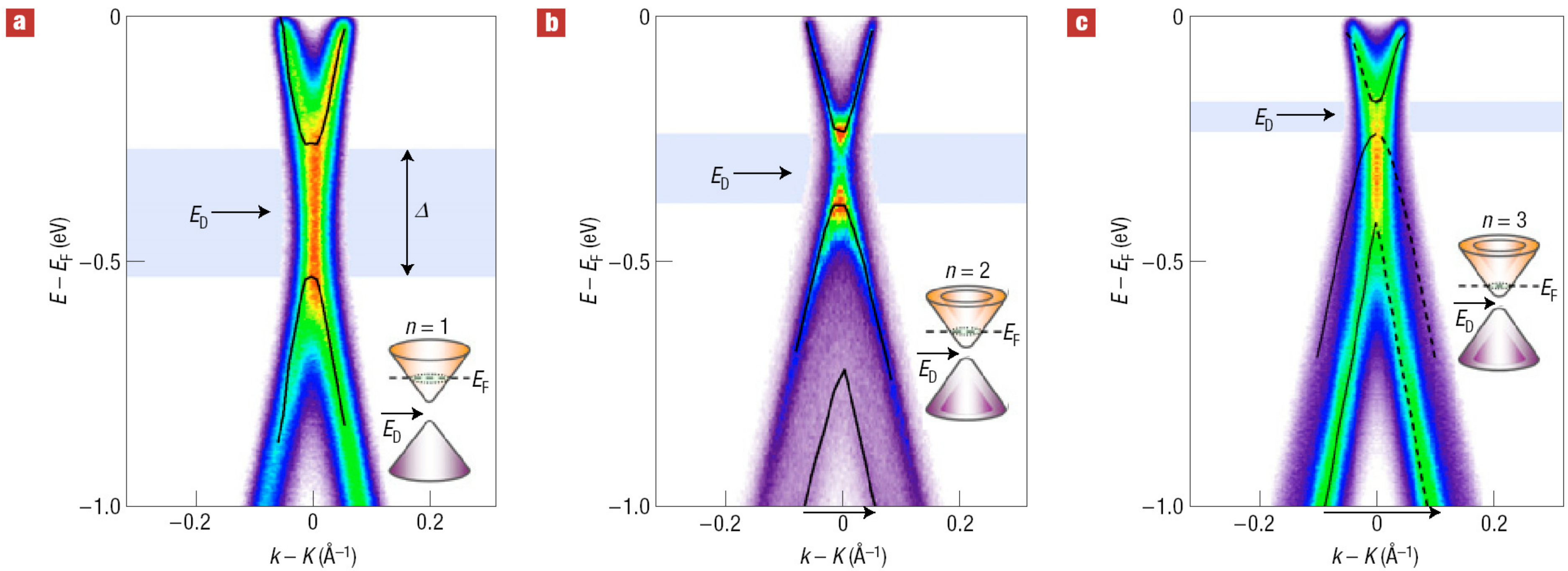




http://www.nature.com/nmat/journal/v6/n3/full/nmat1849.html

Energy Bands in Graphene

- Measured band structure



http://www.nature.com/nmat/journal/v6/n10/pdf/nmat2003.pdf