Physics of Electronics:

5. Energy Bands

July – December 2008

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  - Energy splitting
  - Bloch's theorem
  - Kronig-Penney model
- Velocity and effective mass of electrons in solids.
- Conductors, semiconductors, and insulators.
- Electrical resistance

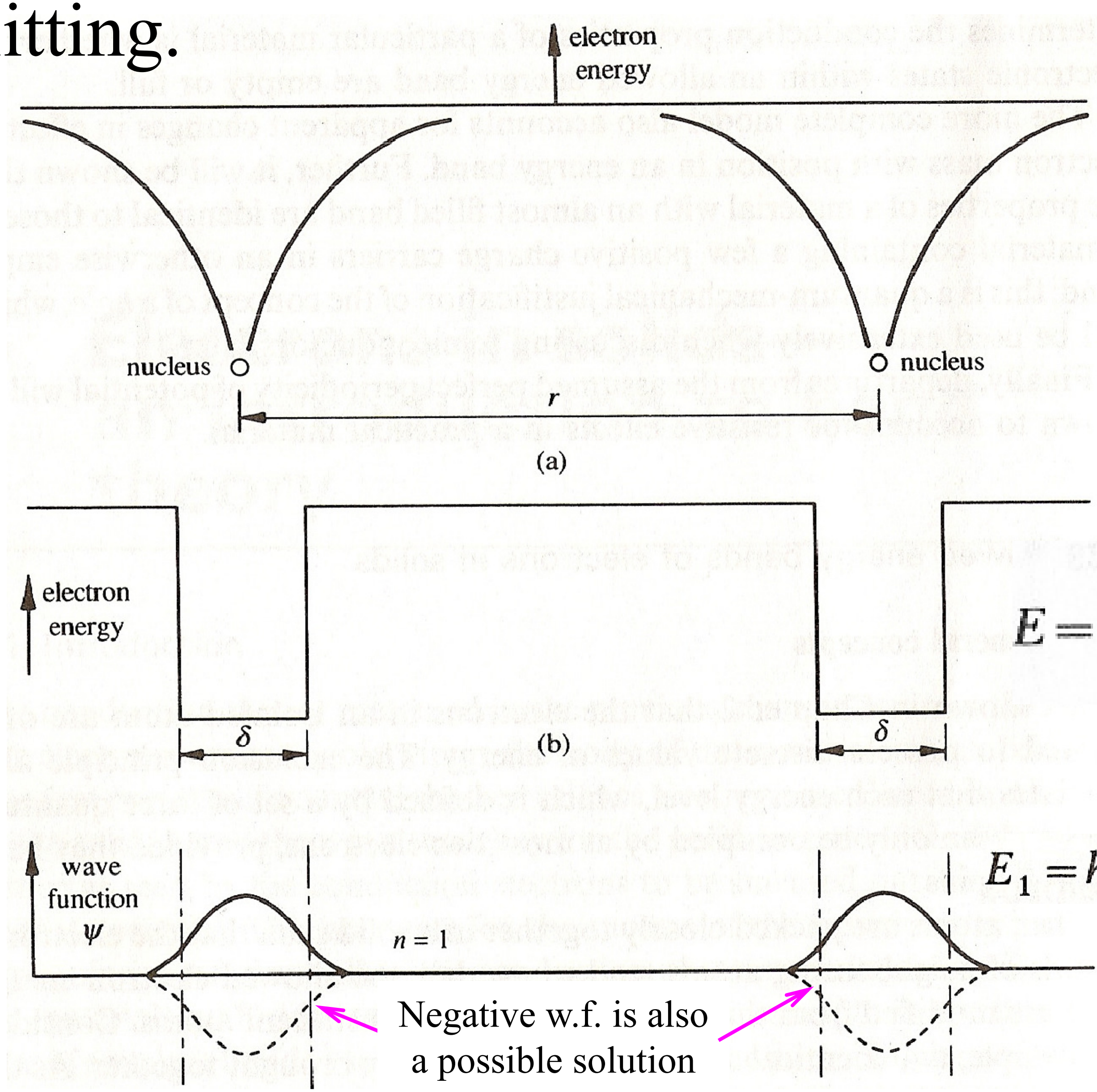
Origin of Energy Bands

- Energy splitting.

Two atoms separated a distance *r*.

Modeled by potential wells.

If *r* is large, w.f. are unperturbed.



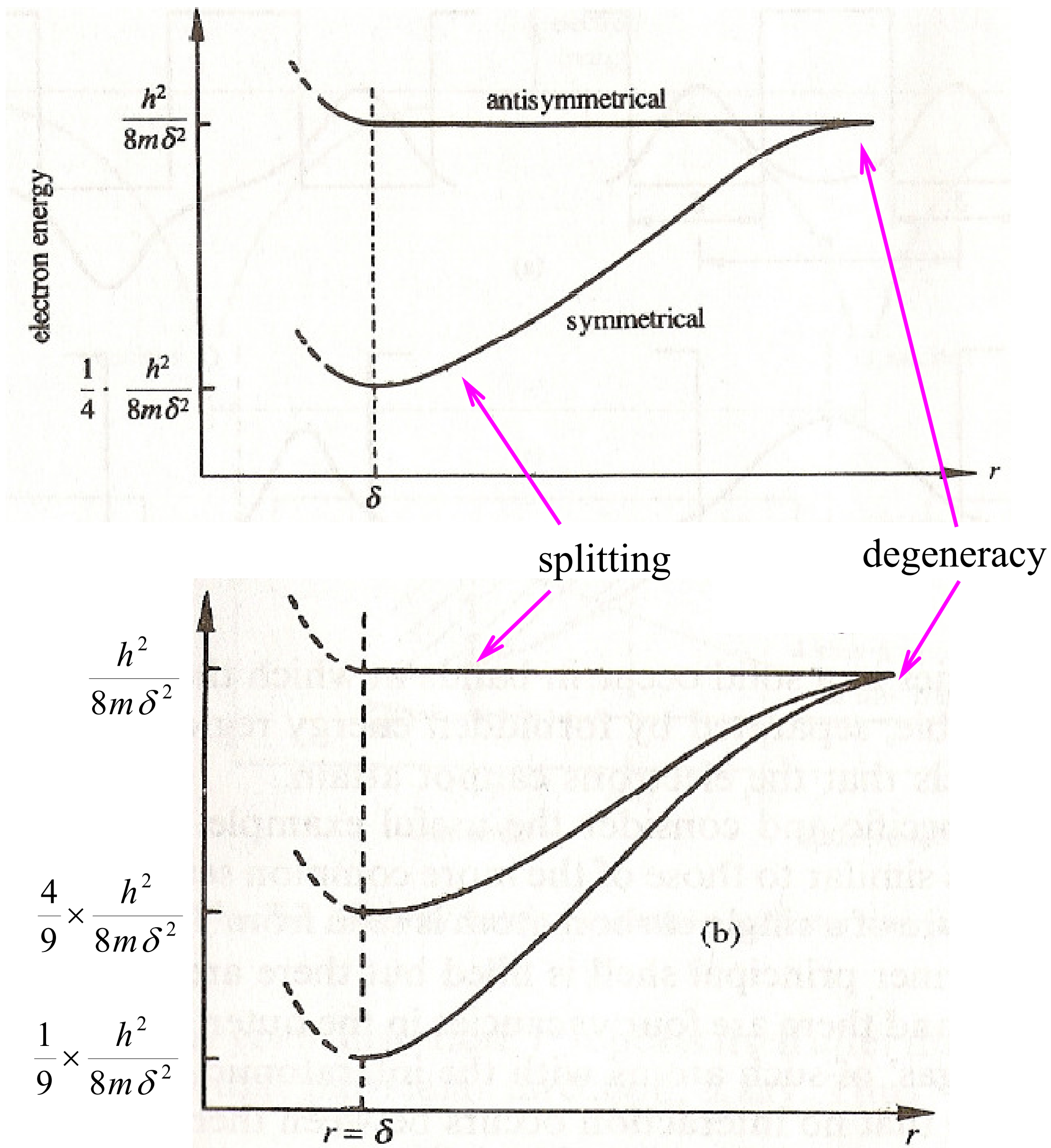
$$E = \frac{n^2 h^2}{8md^2}$$

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

Origin of Energy Bands

- Energy splitting.

Two atoms separated a distance r are brought together.

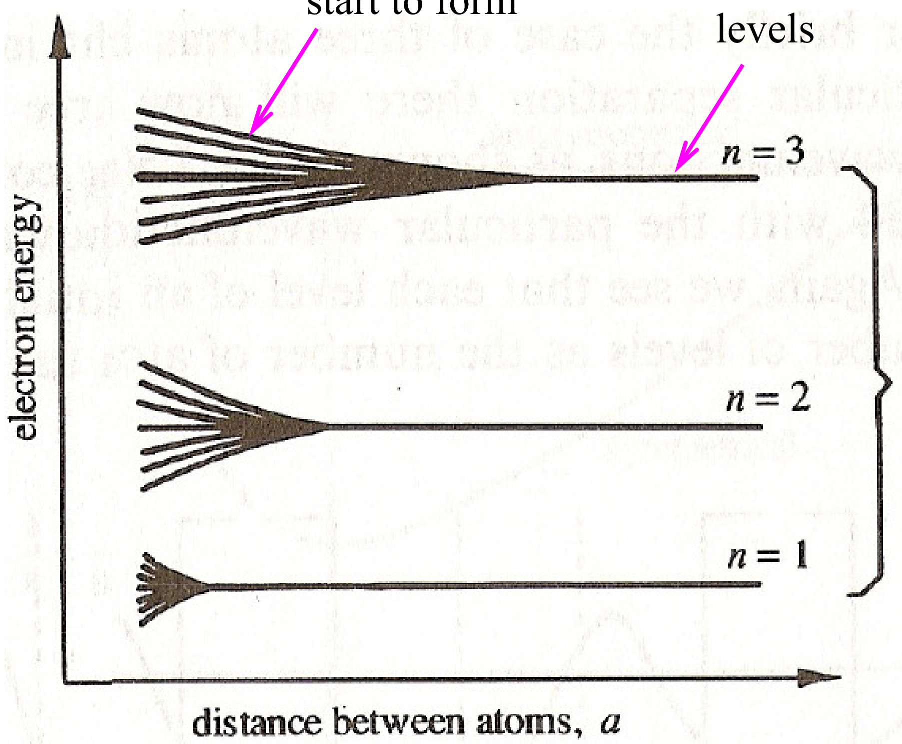


Three atoms separated a distance r are brought together.

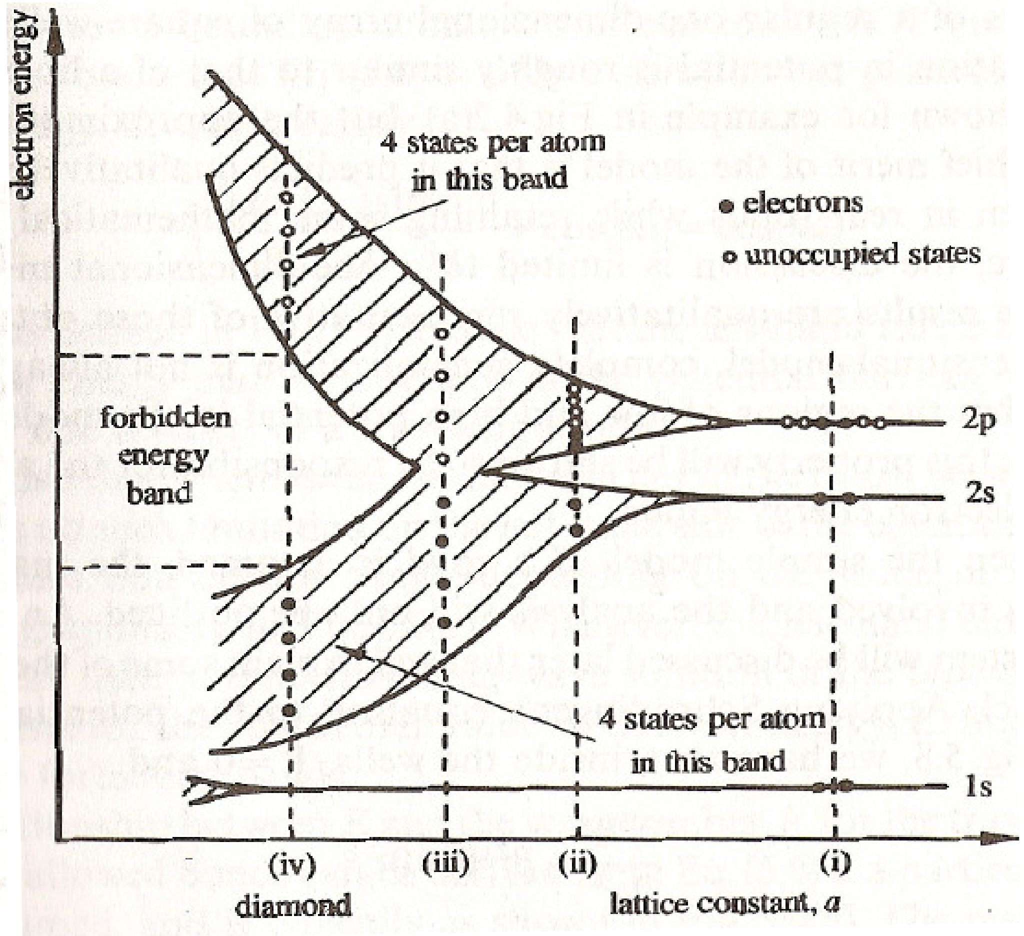
Origin of Energy Bands

- Energy splitting.

More atoms are brought together.

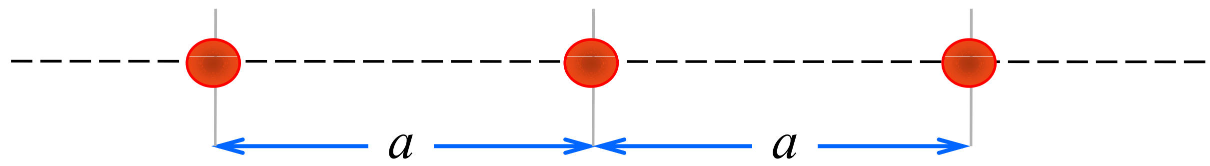


Example: Carbon.



Origin of Energy Bands

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



- The potential : $V(x) = V(x+a) = V(x+2a) = \ldots$
- Wave function: $\psi(x+a) = C\psi(x)$ with $|C|=1$
- Periodic boundary conditions: $\psi(x+Na) = \psi(x) = C^N \psi(x)$

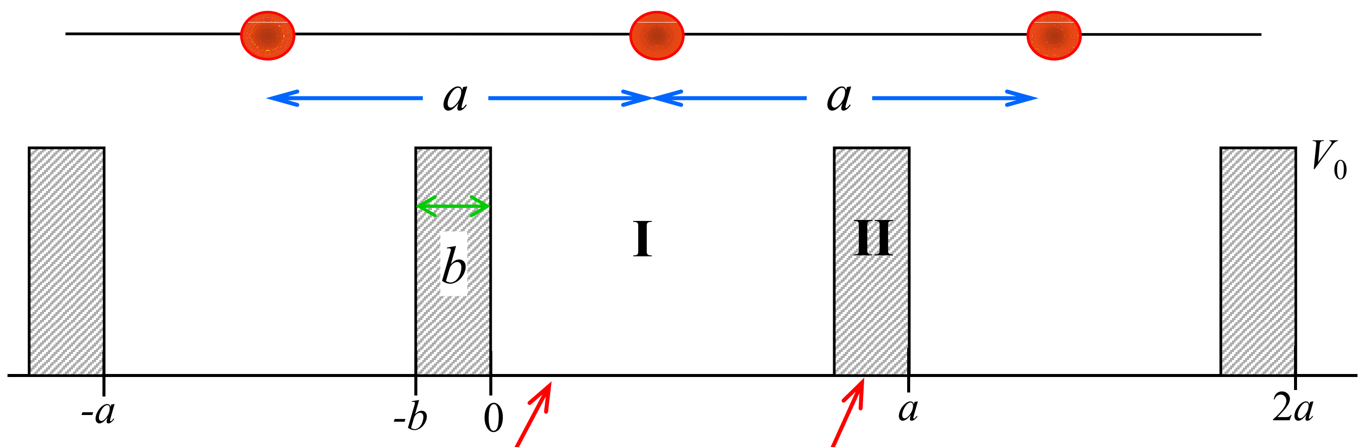
with $|C^N|=1$ ⇨ $C = \exp(i2\pi s/N)$; $s = 0, 1, 2, \ldots, N-1$.

- Therefore: $\psi(x) = u_k(x)e^{ikx}$

with $u_k(x) = u_k(x+a)$ & $k = 2\pi s/Na$

Allowed Energy Bands

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



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

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

$$\Psi_I = Ae^{j\beta x} + Be^{-j\beta x}$$

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

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

we are looking for bound states

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

Allowed Energy Bands

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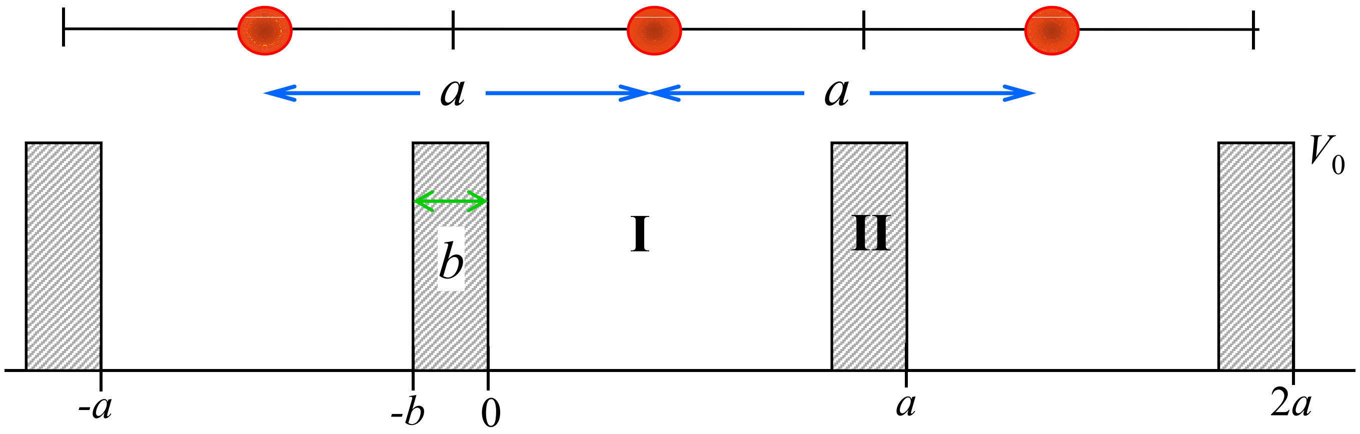


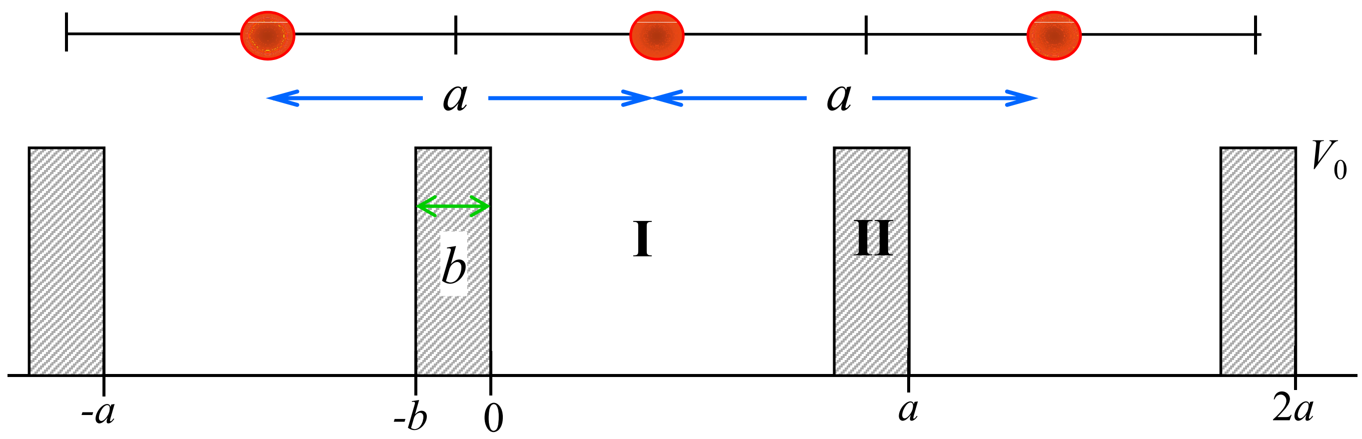
  - From continuity of ψ and dψ/dx at the boundaries:
    - At $x = 0$:

$$A + B = C + D$$

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

Allowed Energy Bands

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



  - 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.
  - Summarizing, the boundary conditions are:

$$A + B - C - D = 0$$

$$i\beta A - i\beta B - \alpha C + \alpha D = 0$$

$$Ae^{i\beta(a-b)} + Be^{-i\beta(a-b)} - Ce^{-i\alpha b - ika} - De^{i\alpha b - ika} = 0$$

$$i\beta Ae^{i\beta(a-b)} - i\beta Be^{-i\beta(a-b)} - \alpha Ce^{-i\alpha b - ika} + \alpha De^{i\alpha b - ika} = 0$$

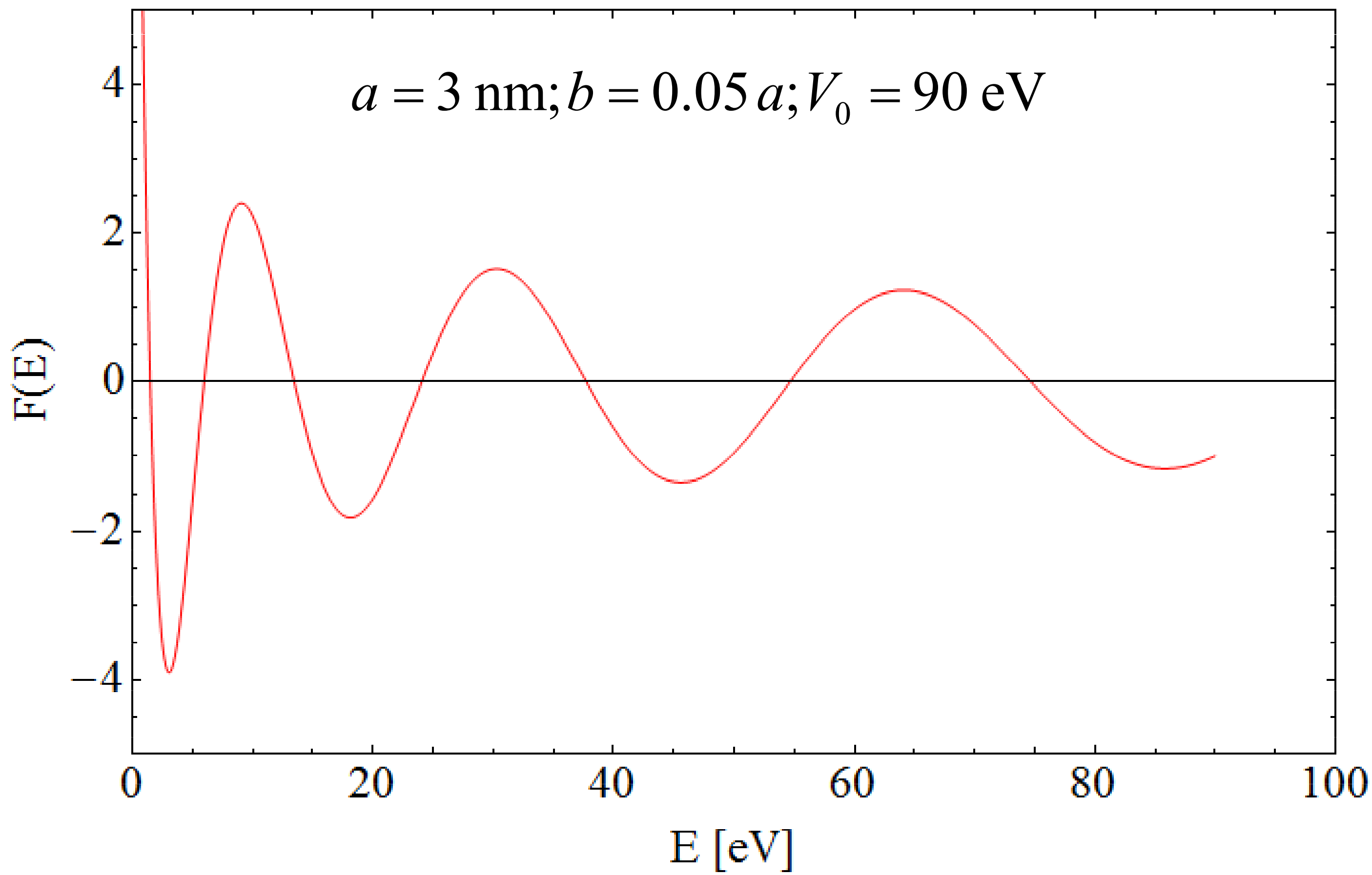
  - There is solution only if its determinant is equal to zero giving:

$$\underbrace{[(\alpha^2 - \beta^2)/2\alpha\beta] \sinh \alpha b \sin \beta(a-b) + \cosh \alpha b \cos \beta(a-b)}_{F(E)} = \cos ka$$

Allowed Energy Bands

- Kronig-Penney model.
  - The solution gives the values of the allowed E:

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



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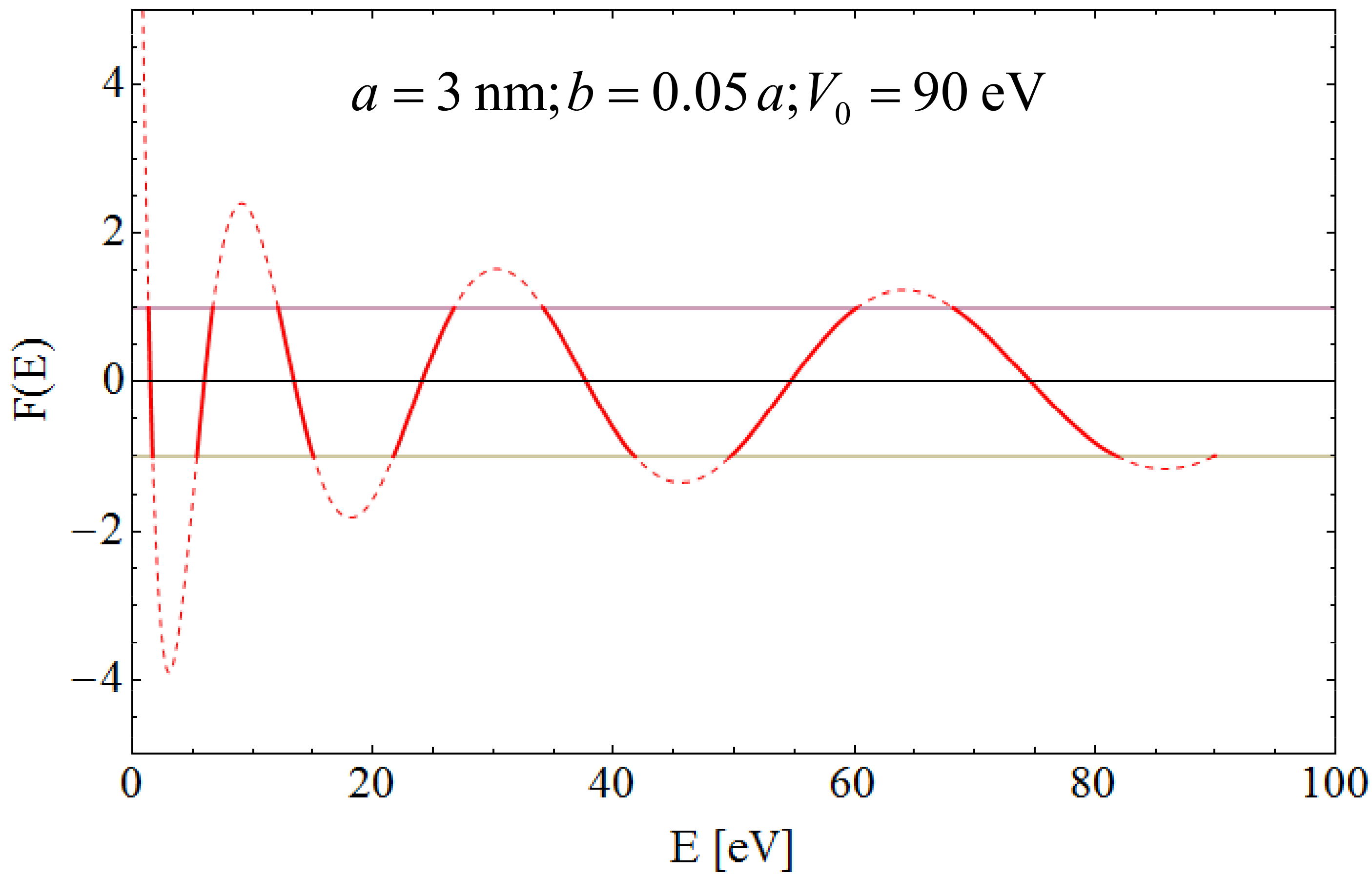

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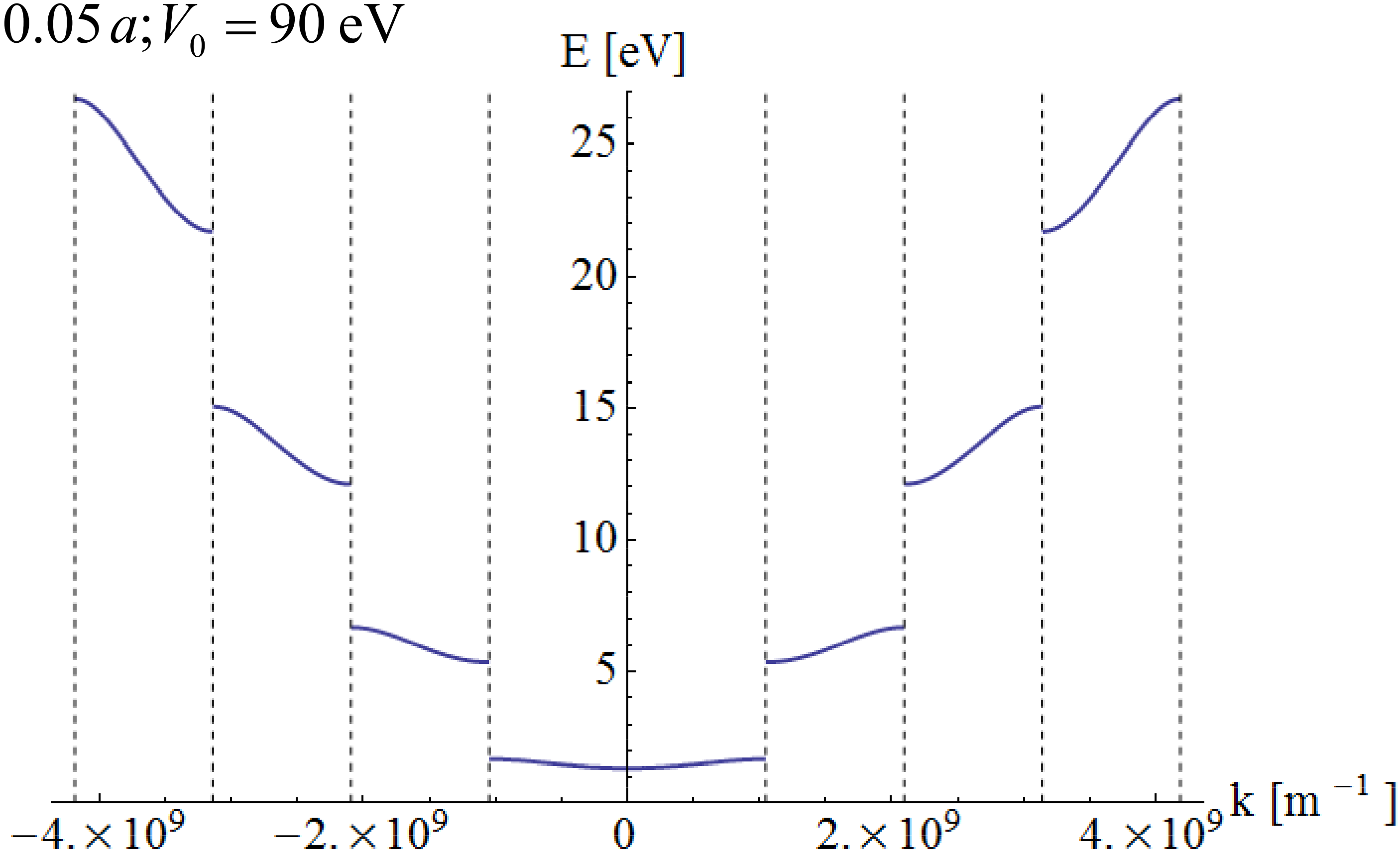
$a = 3\text{ nm}; b = 0.05\,a; V_0 = 90\text{ eV}$



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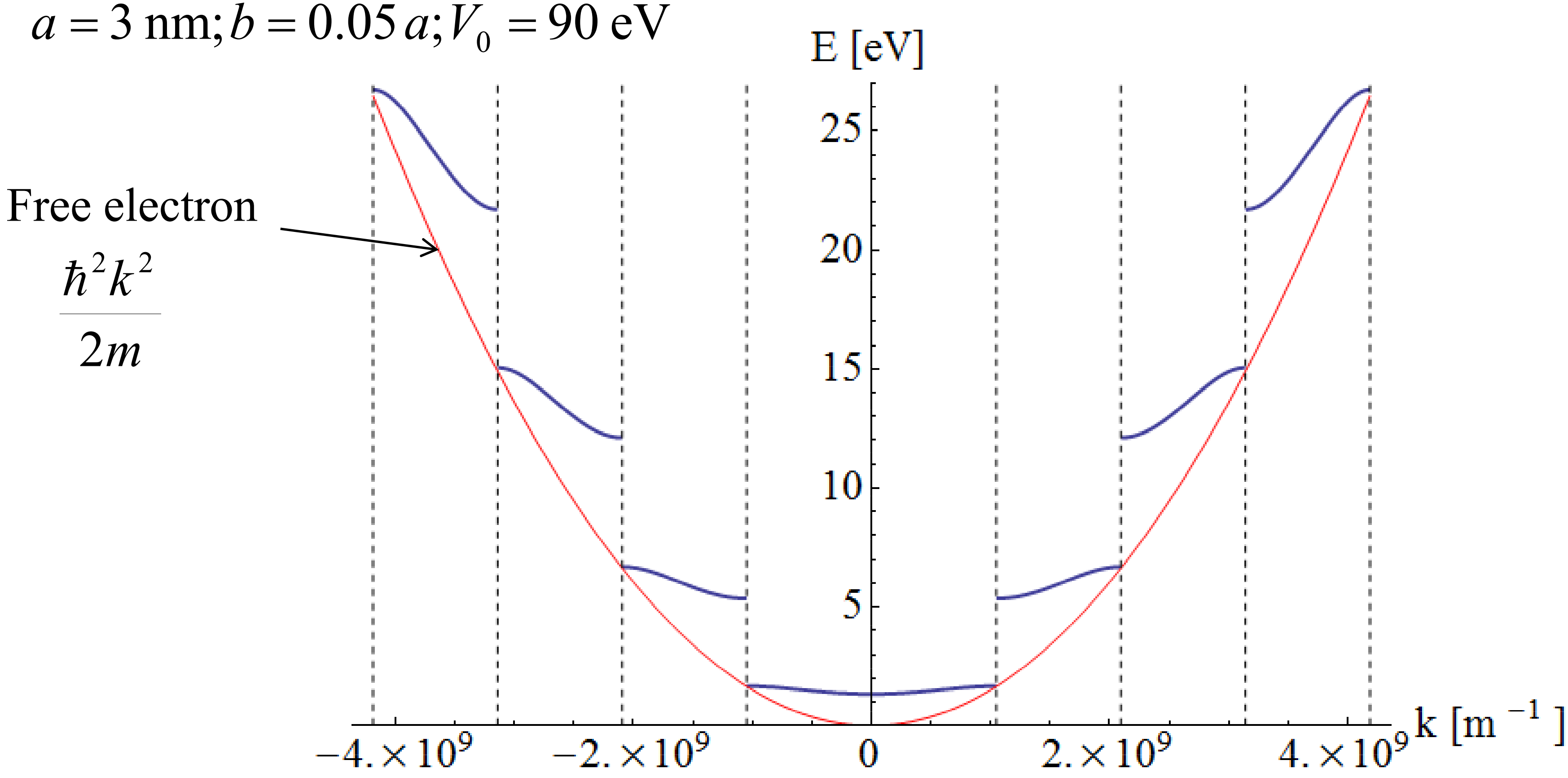


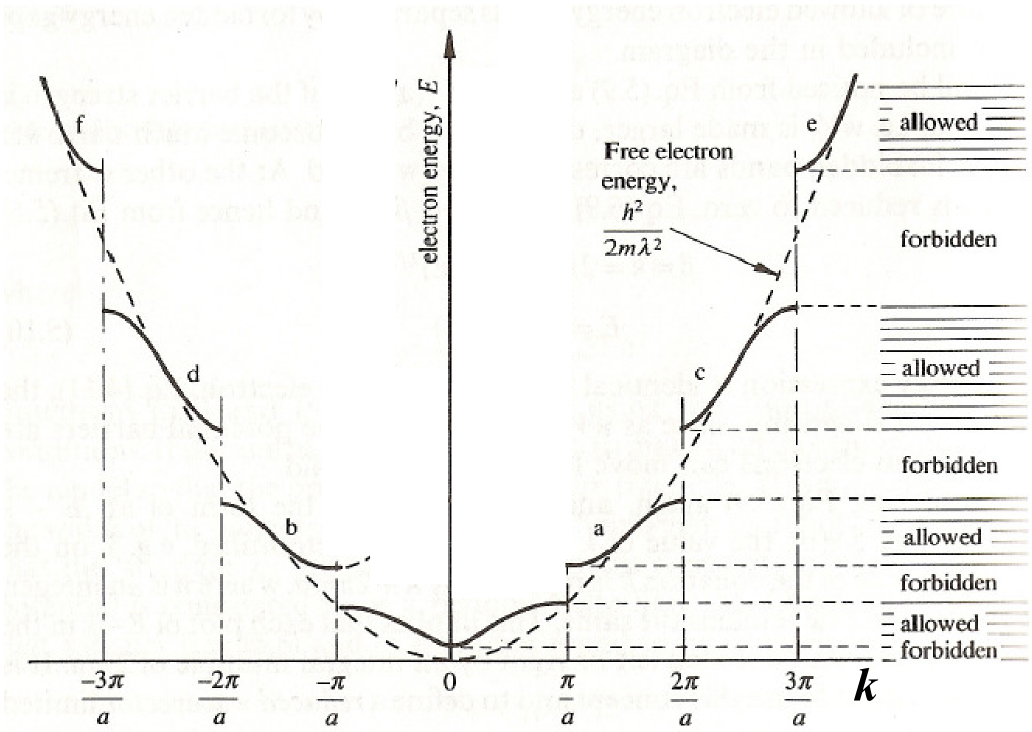
Allowed Energy Bands

- Kronig-Penney model.
  - EXERCISE: Consider the case $b \to 0$ & $V_0 \to \infty$ but such that $\alpha^2 ba/2 = P$ remains constant.

    Hint: In this limit, what are the relations between α and β, and the product αb and 1?.

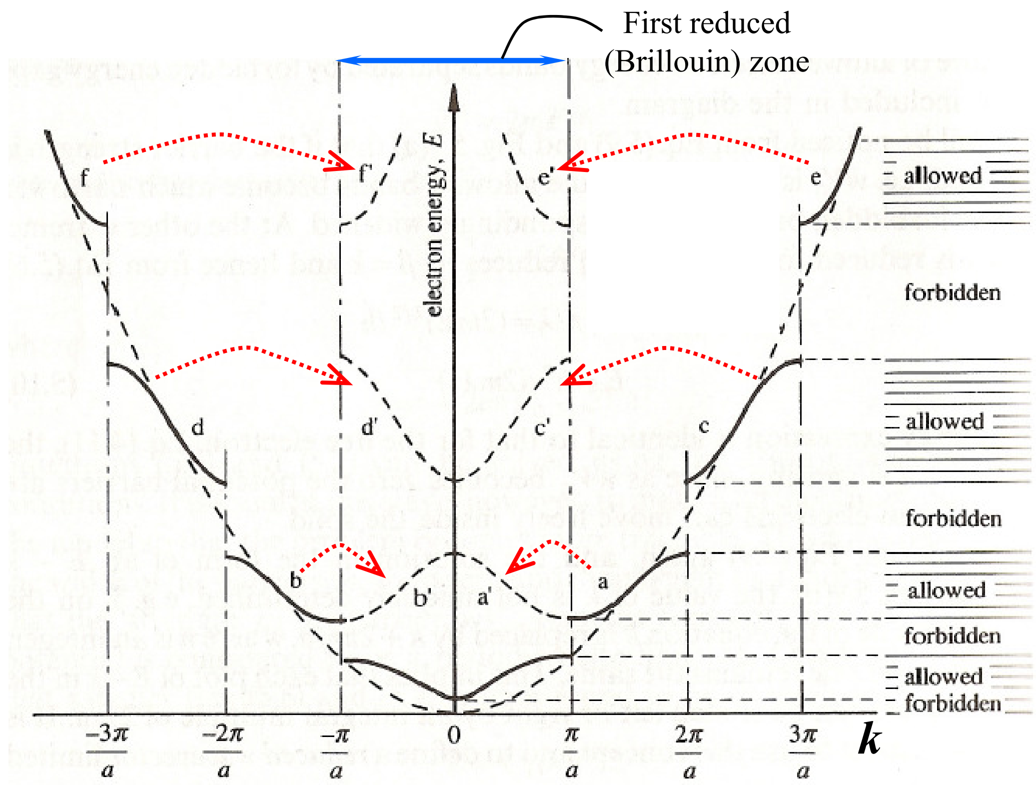
Allowed Energy Bands

- Kronig-Penney model.
  - The allowed energies are function of the wavenumber ***k***.
  - The solutions have the periodicity of **cos(*ka*)**.



Allowed Energy Bands

- Kronig-Penney model.
  - The allowed energies are function of the wavenumber $\boldsymbol{k}$.
  - The solutions have the periodicity of **cos(*ka*)**.
  - To ease representation:



Velocity and Effective Mass

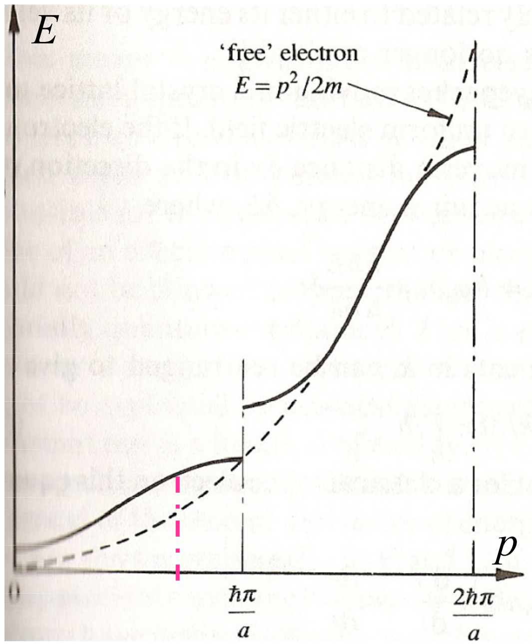
- Group velocity
  - From Bloch's theorem $\psi(x, t) = u_k(x)\, e^{i(kx - Et/\hbar)}$ ← wave packet

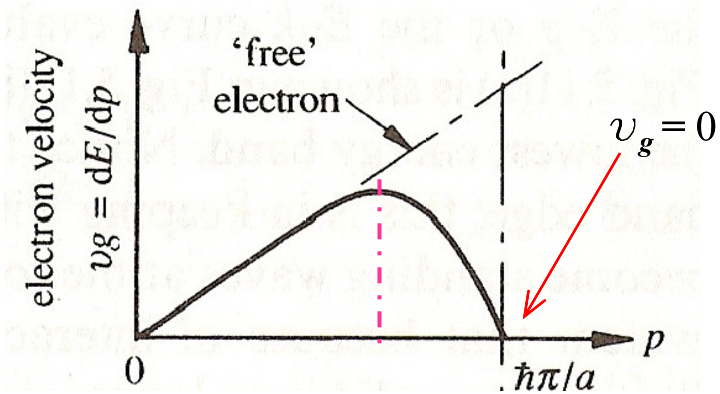
    ($u_k(x)$: spatial modulation; $e^{i(kx - Et/\hbar)}$: plane wave)

  - Therefore, the velocity of the electron is given by the group velocity

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

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:

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

    » External forces and effects of the lattice are included

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

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

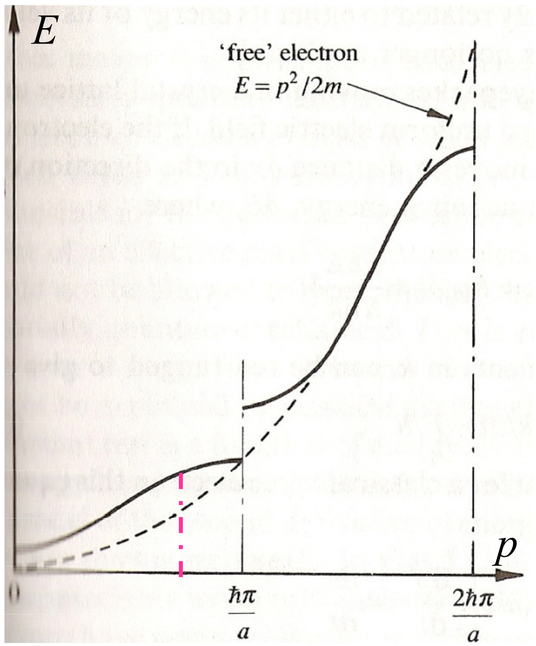
  - Now, in general, differentiating υ_g:

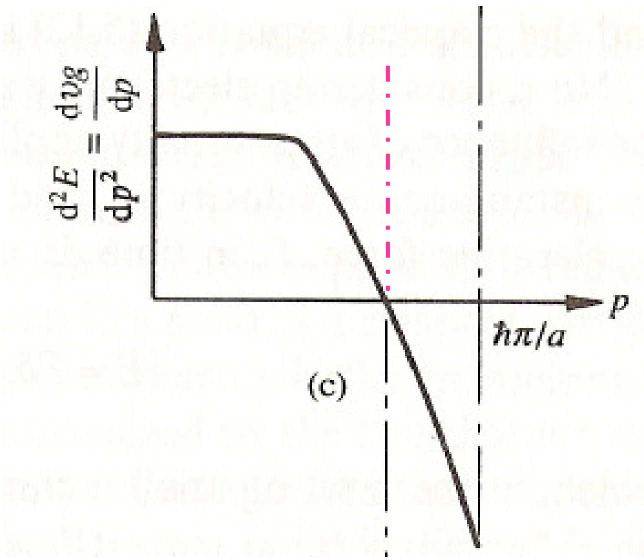
$$\frac{\mathrm{d}v_g}{\mathrm{d}t} = \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\mathrm{d}E}{\mathrm{d}p}\right) = \frac{\mathrm{d}^2 E}{\mathrm{d}t\mathrm{d}p} = \frac{\mathrm{d}p}{\mathrm{d}t}\frac{\mathrm{d}^2 E}{\mathrm{d}p^2} = F\frac{\mathrm{d}^2 E}{\mathrm{d}p^2} \;\Rightarrow\; F = \left(\frac{\mathrm{d}^2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

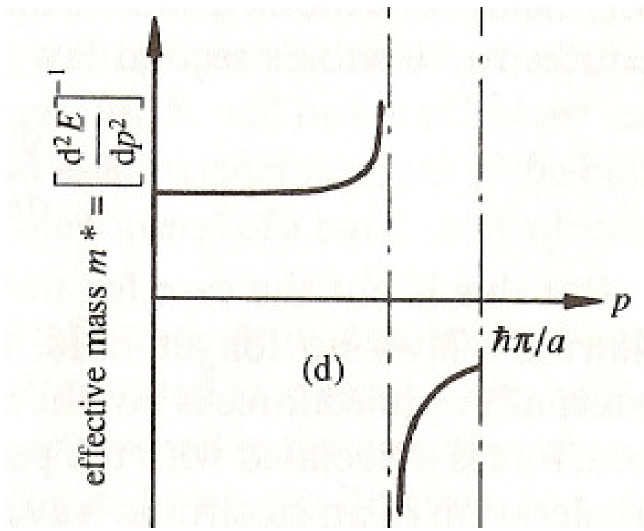
Velocity and Effective Mass

- Effective Mass
  - Comparing both we define:

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







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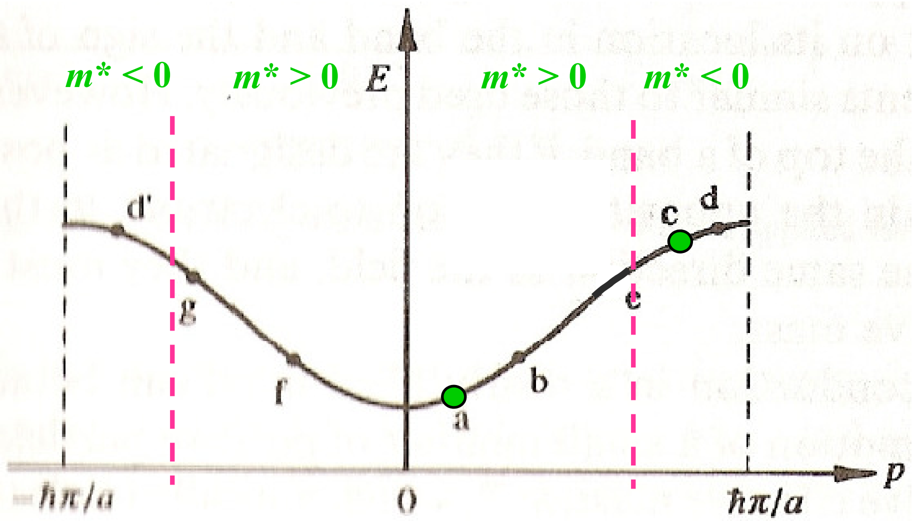

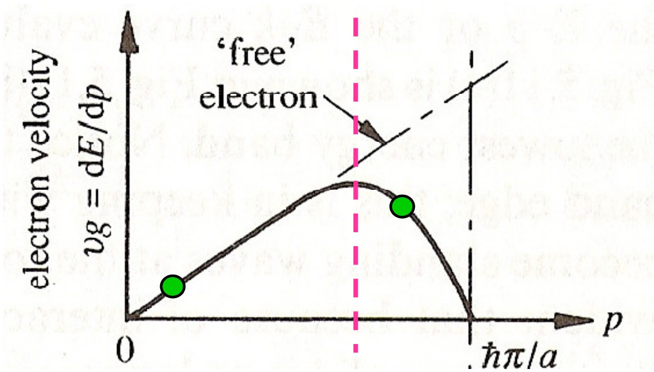

$\mathscr{E} = 0$

Velocity and Effective Mass

- Effective Mass
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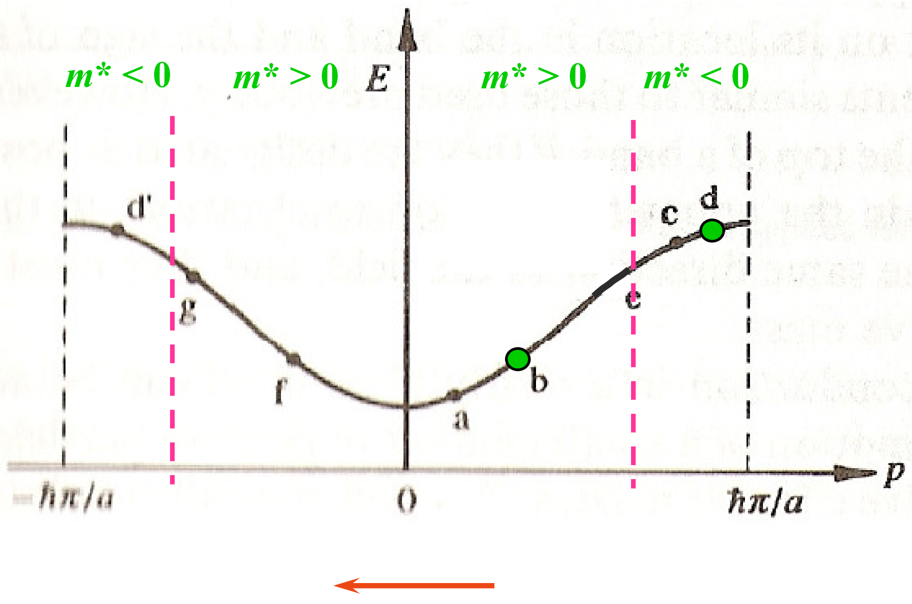
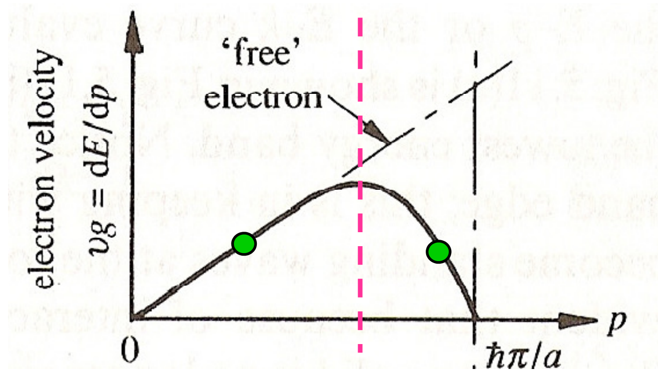


$\mathscr{E} \neq 0$



an electron with negative mass

≡

an "electron" with positive charge

Velocity and Effective Mass

- Effective Mass
  – Comparing both we define:

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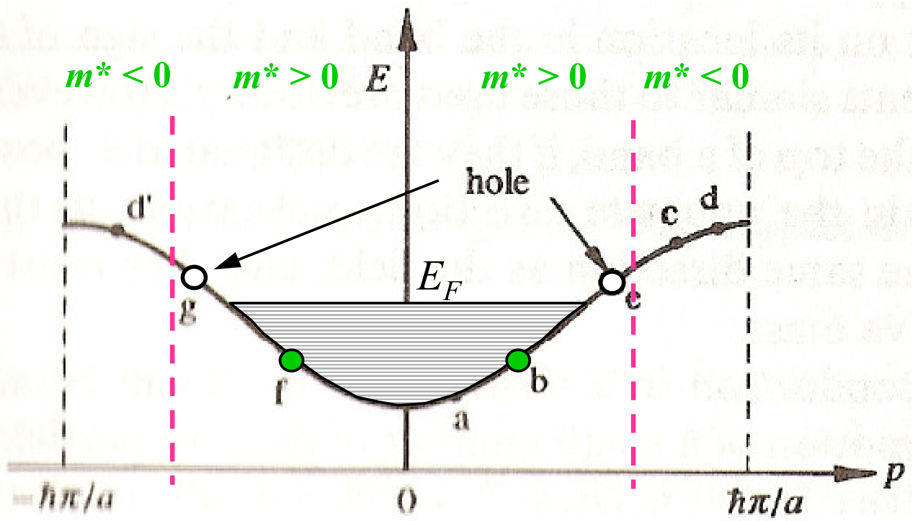

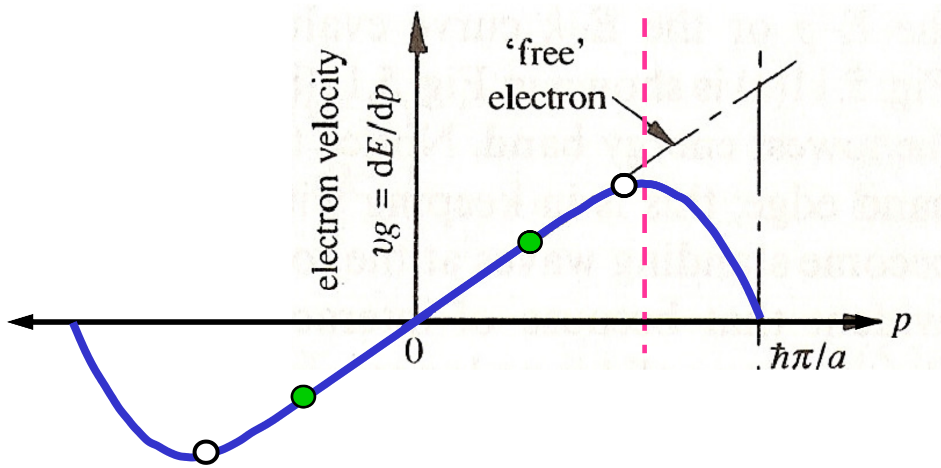

● Opposite velocities. No net current,

Velocity and Effective Mass

- Effective Mass
  - Comparing both we define:

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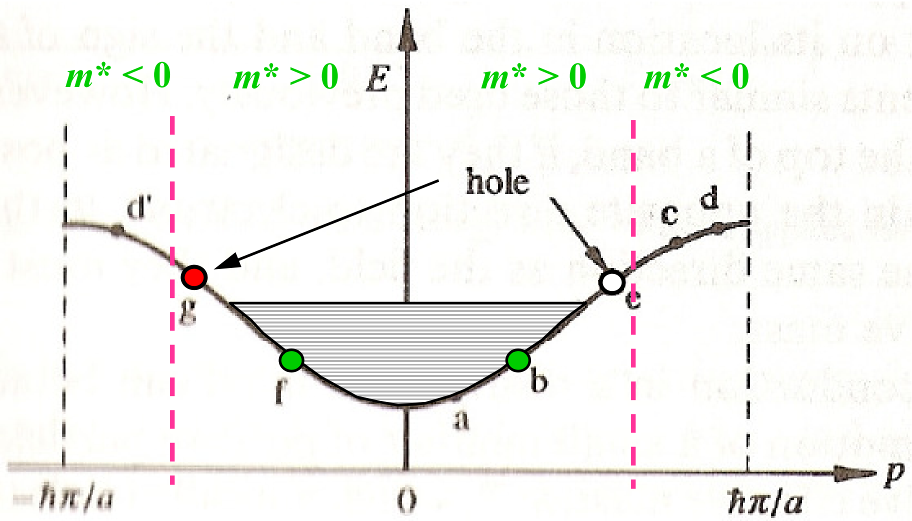
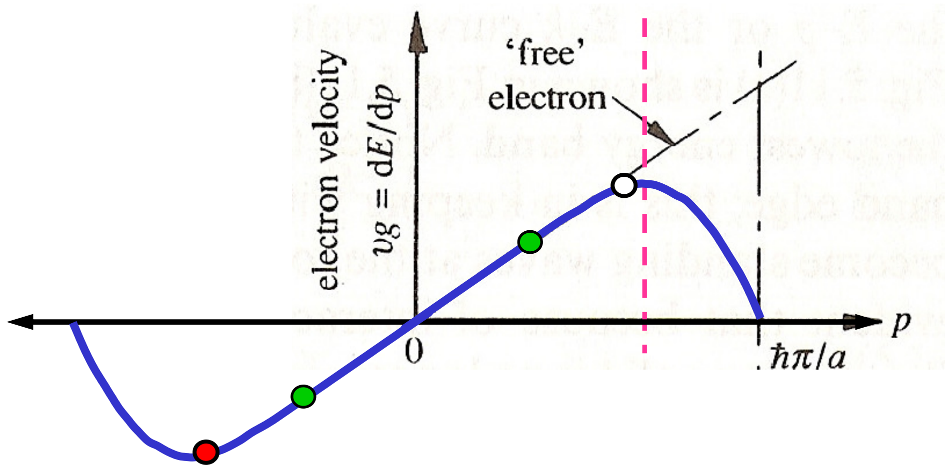
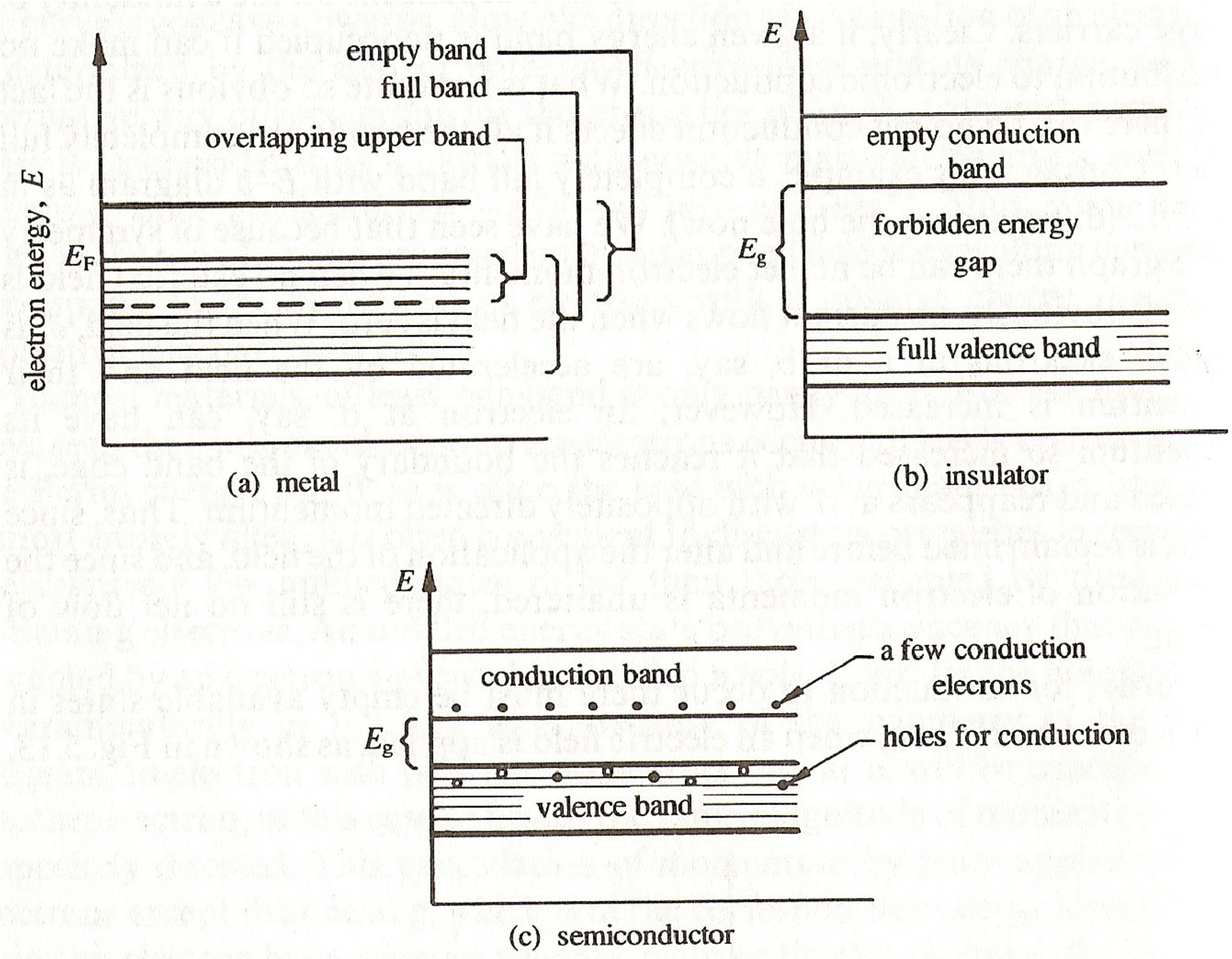




- Opposite velocities. No net current,
- Not cancelled. Net current.

Conductors, Semiconductors & Insulators

- Classification according to the filling of the gaps



Electrical Resistance

- Relations in previous chapter still valid BUT with m^*.

- Collision (or scatter) centers:
  - Thermal lattice vibrations (phonons)
  - Impurity atoms
  - Lattice defects
  - Boundaries

} Aperiodic potential fields

Conclusions

- When going from isolated atoms to an assembly of them, energy bands start to form.
- Electrons can only exist in those bands. Not all energies are permitted.
- Bands are defined by a dispersion function.
- From a dispersion function we define an effective mass and an effective velocity (group velocity).
- Metals, semiconductors and isolators are defined trough their filling of energy bands.