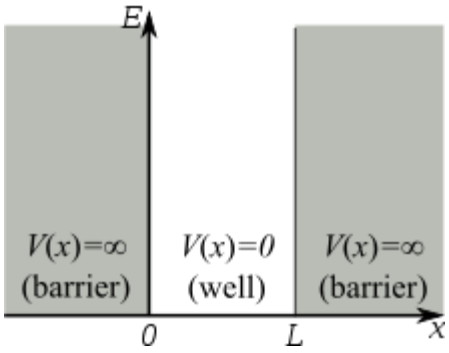
1. Calculate the first three energy levels and state functions φ(x, t) for an electron in a quantum well of width 10 Angstrom with infinite walls.



Solution:

$$V(x) = \begin{cases} 0, & 0 < x < L, \\ \infty, & \text{otherwise}, \end{cases},$$

$$i\hbar\frac{\partial}{\partial t}\psi(x,t) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x,t) + V(x)\psi(x,t),$$

16’

$\psi_n(x) = A_n \sin(k_n x)$

3’

$$\psi(x,t) = [A\sin(kx) + B\cos(kx)]\mathrm{e}^{-i\omega t},$$

$$\psi_n(x,t) = \begin{cases} A\sin(k_n x)\mathrm{e}^{-i\omega_n t}, & 0 < x < L, \\ 0, & \text{otherwise}, \end{cases}$$

$$k_n = \frac{n\pi}{L}, \quad \text{where} \quad n = \{1,2,3,4,\ldots\},$$

3’

$$E = \hbar\omega = \frac{\hbar^2 k^2}{2m}, E_n = \frac{n^2\hbar^2\pi^2}{2mL^2} = \frac{n^2h^2}{8mL^2}$$

$= \boldsymbol{0.38eV, 1.51eV, 3.39eV}$

3’

2. For metals under Sommerfeld's model, write down the wavefunction and the eigen-energies

Solutions:

For box with dimensions $L_x \times L_y \times L_z$, time independent wave function is:

$$\phi(x,y,z) = \sqrt{\frac{2}{L_x}}\sin\left(\frac{n_x\pi x}{L_x}\right)\sqrt{\frac{2}{L_y}}\sin\left(\frac{n_y\pi y}{L_y}\right)\sqrt{\frac{2}{L_z}}\sin\left(\frac{n_z\pi z}{L_z}\right), n_{x,y,z} = 1,2,\ldots$$

$$\rightarrow \phi(x,y,z) = \sqrt{\frac{8}{V}}\sin\left(\frac{n_x\pi x}{L_x}\right)\sin\left(\frac{n_y\pi y}{L_y}\right)\sin\left(\frac{n_z\pi z}{L_z}\right)$$

8'

Eigen energies:

$$E = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2\pi^2}{2m}\left(\frac{n_x^2}{L_x^2} + \frac{n_y^2}{L_y^2} + \frac{n_z^2}{L_z^2}\right)$$

5'

Describe how one calculates the density of states

The calculation for DOS starts by counting the N allowed states at a certain k that are contained within [k, k+dk] inside the volume of the system. This is done by differentiating the whole k-space volume $\Omega_{n,k}$ in n-dimensions at an arbitrary k, with respect to k. For 3-D case, the volume in k-space between two constant-k spherical surfaces is $\Delta k = 4\pi k^2 dk$. The number of states per unit volume is $\frac{2}{(2\pi)^3}(\Delta k)$. Using the parabolic band structure, we get $dk = \left\{\sqrt{\frac{m^*}{2}}\frac{1}{\hbar}\right\}\frac{1}{\sqrt{E}}dE$.

The expression for the 3D DOS is

$$N(E) = \frac{V}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\sqrt{E - E_0},$$

where V is the total volume, and $N(E - E_0)$includes the 2-fold spin degeneracy.

3. Describe qualitatively how the band structure forms from the Bloch function, with (1) the perturbation theory approach and (2) the tight-binding approach (10 points). What are the differences in the approaches (5 points)?

Two methods choose different sets of the wavefunctions as bases for expanding the approximated Hamiltonian.

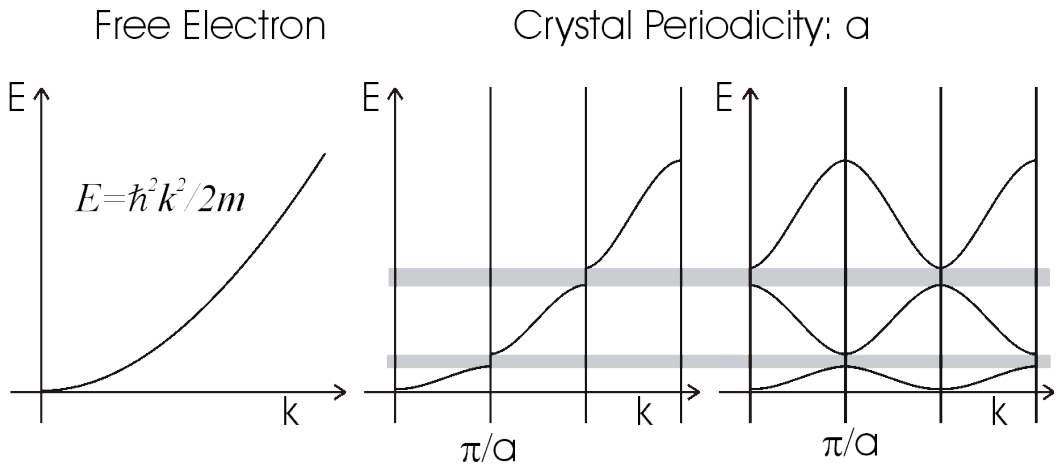
Perturbation theory: Treat electrons as nearly free electrons, where the lattice potential adds perturbation.

$$H = H_0 + H'_{\mathbf{k}}, \quad H_0 = \frac{p^2}{2m} + V, \quad H'_{\mathbf{k}} = \frac{\hbar^2 k^2}{2m} + \frac{\hbar \mathbf{k} \cdot \mathbf{p}}{m}$$

The "unperturbed Hamiltonian" is H_0, which in fact equals the exact Hamiltonian at k=0 (i.e., at the Gamma point). The "perturbation" is the term H'_k.

Tight-binding approach: Treat electrons as closed bond with nucleus. The band splitting is solved by considering the interaction between neighboring atoms.

Please draw a band structure for a 1D semiconductor lattice



How do we compute the electron effective mass from the E-k relation, or how do we understand the electron effective mass?

The effective mass is a quantity that is used to simplify band structures by constructing an analogy to the behavior of a free particle with that mass. It is calculated as $m^* = \frac{\hbar^2}{\frac{d^2E}{dm^2}}$ *for 1D case. And it is inversely proportional to the curvature of E-K curve.*

4. A new 2 dimensional material called graphene has attracted extensive interest of the researchers due to its excellent properties. It has been found that *E-k* relation in this novel material is given as

$$E = \hbar v_F |k| = \hbar v_F \sqrt{k_x^2 + k_y^2} \text{ for } E > 0$$

where constant $v_F = 10^6\, m/s$. Assume the Fermi level is given by $E_F = 0.2eV$ for T=0K

a) Please calculate the density of the states for this new material as a function of E
b) Calculate the electron density at 0K (you can assume L=1 (unit length) if you need).

c) Estimate Fermi velocity (Fermi velocity is the velocity of the electron at Fermi level. Hint: the group velocity of the wavefunction is given by $v_g \approx \partial\omega/\partial k$ for $e^{i(\vec{k}\vec{r}-\omega t)}U(\vec{r})$)

Sol:

a) Given a 2-dimensional material, we have

$$D(E)\Delta E = \frac{1}{(2\pi)^2} \cdot 2\pi k \cdot \Delta k \cdot 2 \text{ (for spin)}$$

3'

i.e.,

$$D(E) = \frac{k}{\pi}\left(\frac{dE}{dk}\right)^{-1} = \frac{E}{\pi(\hbar v_F)^2}$$

4'

b) *The electron density is given by*

$$n = \int_0^\infty D(E) f_{E_F}(E) dE$$

2'

At T=0K, $n = \int_0^{E_F} D(E)dE$ *2'*

$$n = \int_0^{E_F} D(E)dE = \frac{E_F^2}{2\pi(\hbar v_F)^2} \approx 1.47 \times 10^{15}/m^2$$

3'

c) *The magnitude of the velocity of any electron is given by*

$$v = v_g = \frac{\partial\omega}{\partial k} = \frac{1}{\hbar}\frac{\partial E}{\partial k} = v_F$$

3'

So the Fermi velocity is given by

$$v_F = 10^6\, m/s$$

3'