II partial written test
academic year 2011/2012
January 16, 2012

Exercise 2: *Effective masses and density of levels*

Consider bulk Silicon, whose conduction band minima E_c are near the Brillouin zone boundary along $\langle 100 \rangle$ directions. Assume a parabolic conduction band with ellipsoidal constant energy surfaces around the minima, described by:

$$E(\mathbf{k}) = E_c + \frac{\hbar^2}{2}\left(\frac{k_\ell^2}{m_\ell^*} + \frac{k_t^2}{m_t^*} + \frac{k_t^2}{m_t^*}\right)$$

(t=transverse, ℓ=longitudinal, with $m_\ell^* = 0.98 m_0$ $m_t^* = 0.19 m_0$, where m_0 is the free electron mass; $\vec{k}$ is with respect to the location of the minima).

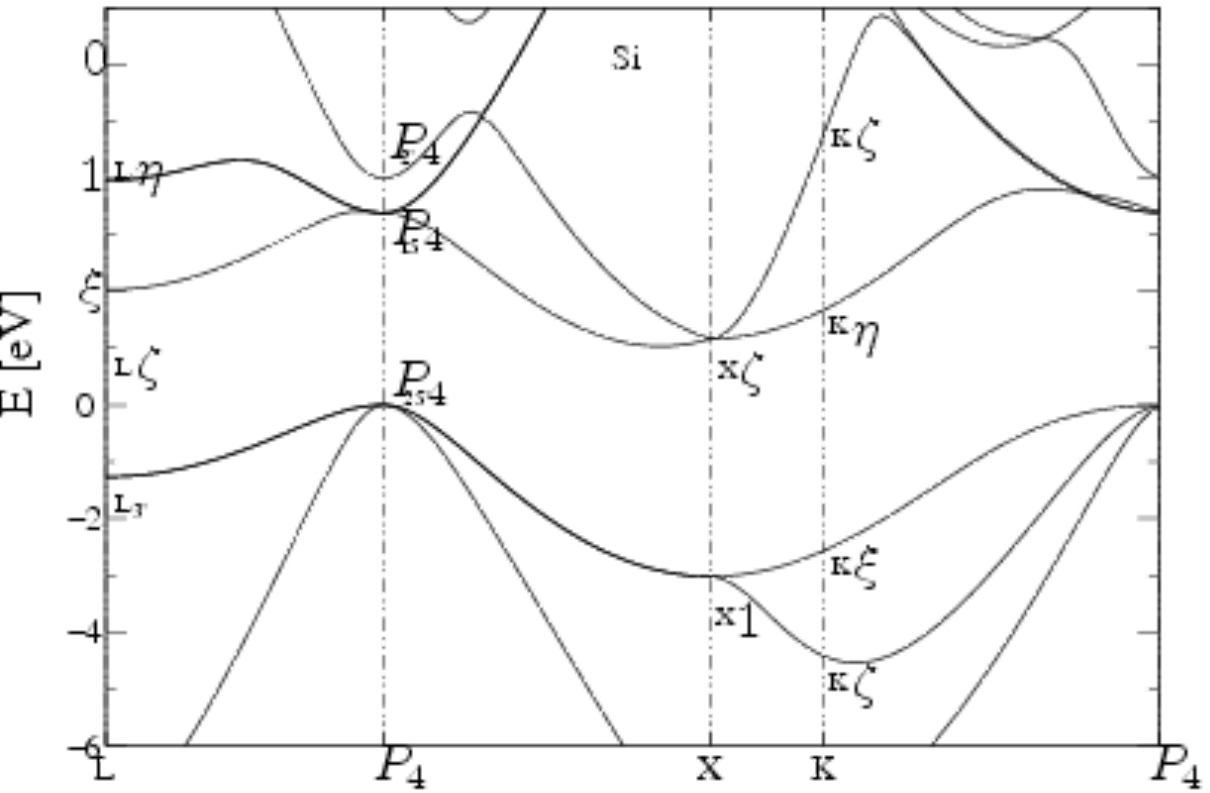
1. How many equivalent minima there are?

2. Write the expression of the density of states $g(E)$ around one of the conduction band minima, in terms of E_c, m_ℓ^*, m_t^*.

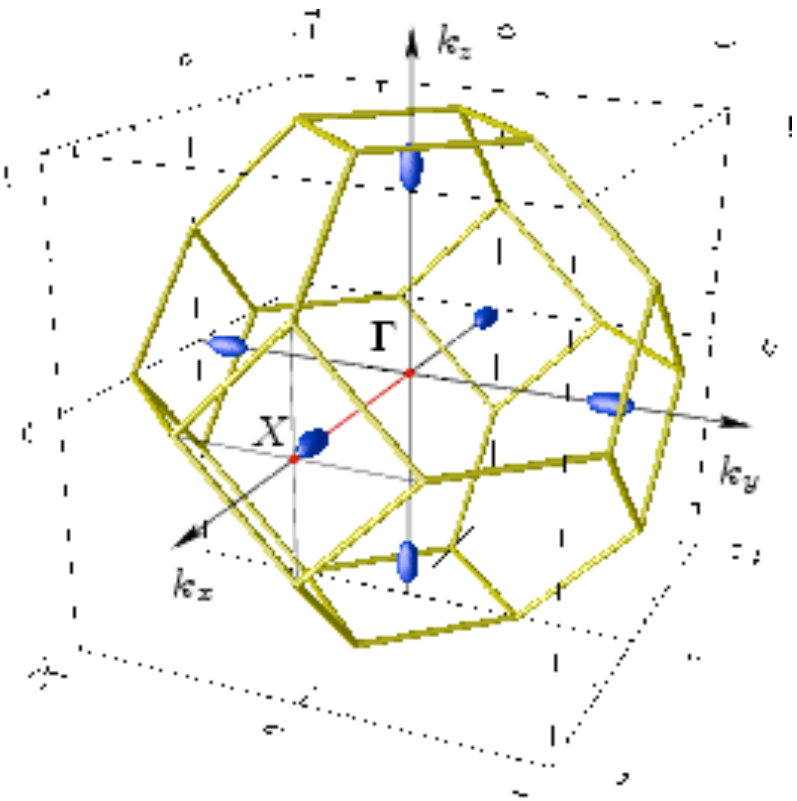
3. Calculate the number of states per unit energy for an energy 100 meV above the conduction band bottom, in a 100 × 100 × 10 nm piece of silicon. Write the result in units of eV^{-1}.

Band structure of selected semiconductors

Si



(a) Band diagram of silicon.



(b) First conduction band valleys.

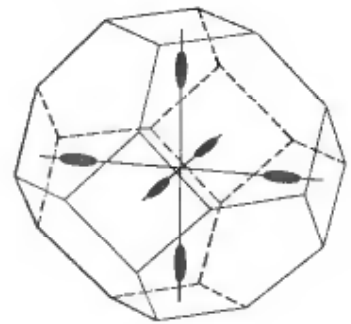
indirect gap!

Band structure of selected semiconductors

16/01/2012, II test
Ex. 2

Silicon The crystal has the diamond structure, so the first Brillouin zone is the truncated octahedron appropriate to a face-centered cubic Bravais lattice. The conduction band has six symmetry-related minima at points in the ⟨100⟩ directions, about 80 percent of the way to the zone boundary (Figure 28.5). • • •

Figure 28.5
Constant-energy surfaces near the conduction band minima in silicon. There are six symmetry-related ellipsoidal pockets. The long axes are directed along ⟨100⟩ directions.



from Ashcroft-Mermin,
Ch 28, Typical semiconductor band structure, p 569

From the Sommerfeld model:

$$g(E) = \frac{m}{\hbar^2\pi^2}\sqrt{\frac{2mE}{\hbar^2}}, \quad E > 0$$

we obtain:

$$g(E) = \frac{\sqrt{m_\ell m_t^2}}{\hbar^2\pi^2}\sqrt{\frac{2(E-E_c)}{\hbar^2}}, \quad E > 0$$

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$g(E)\cdot \mathcal{V} = ?$ where $\mathcal{V} = 10^5 mm^3 = 10^5 (10^{-7} cm)^3$

$= 10^5 \cdot 10^{-21} cm^3 = 10^{-16} cm^3$

and $\bar{E} = E_c + 100\ meV$

and $m_l = 0.98 m_0$, $m_t = 0.19 m_0$

$$g(E) = \frac{\sqrt{0.98 \cdot 0.19^2}}{\hbar^2 \pi^2} m_0^{3/2} \sqrt{\frac{2 \cdot 0.1\ eV}{\hbar^2}} =$$

$$= \frac{\sqrt{0.98 \cdot 0.19^2}}{\pi^2 (1.05 \cdot 10^{-27} erg \cdot s)^3} (9.11 \cdot 10^{-28} g)^{3/2} \left(2 \cdot 0.1 \cdot 1.6 \cdot 10^{-12} erg\right)^{1/2}$$

$$= \frac{0.188}{\pi^2 1.05^3} (9.11)^{3/2} (.32)^{1/2} \frac{10^{-\frac{14}{8}\cdot 3} \cdot 10^{-\frac{12}{2}\cdot 1}}{10^{-27\cdot 3}} = 10^{33}$$

-42, -6, -81

$= 0.256 \cdot 10^{33}\ cm^{-3} erg^{-1} \Rightarrow g(E)\cdot \mathcal{V} = 0.256 \cdot 10^{17}\ erg^{-1}$

$= 0.256 \cdot 1.6 \cdot 10^5\ eV^{-1}$

$= 0.4 \cdot 10^5\ eV^{-1}$

$[1\ eV = 1.6 \cdot 10^{-12} erg] \rightarrow \frac{1}{erg} = \frac{1.6 \cdot 10^{-12}}{eV}$

$[\hbar] = [g][t]$

$$\frac{[m]^{3/2}}{[g]^2 [t]^2} \frac{[g]^{1/2}}{[g][t]} \stackrel{?}{=} \frac{1}{[g]} \frac{1}{[L]^3}$$

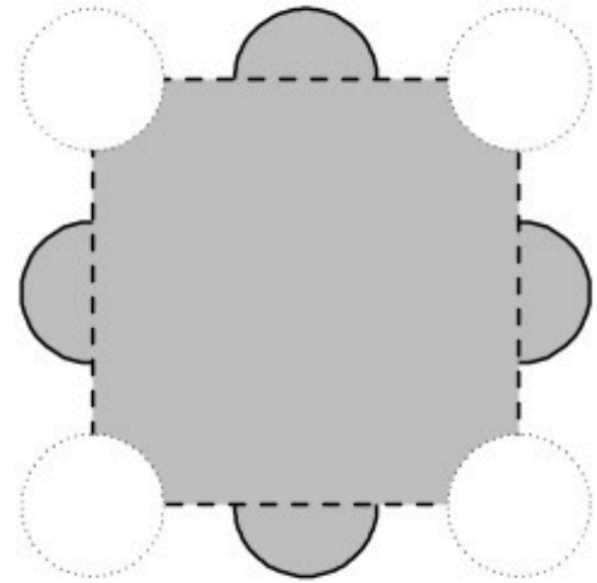
$[g] = [F \cdot l] = [m a \cdot l] = [m][L]^2 [t]^{-2}$

$$\frac{[m]^{3/2}}{[g]^{3/2}[t]^3} = \frac{[m]^{3/2}}{[m]^{3/2}[L]^{2\cdot\frac{3}{2}}[t]^{-2\cdot\frac{3}{2}}[t]^3}$$

Ok!

Exercise 3: *Semi metals*

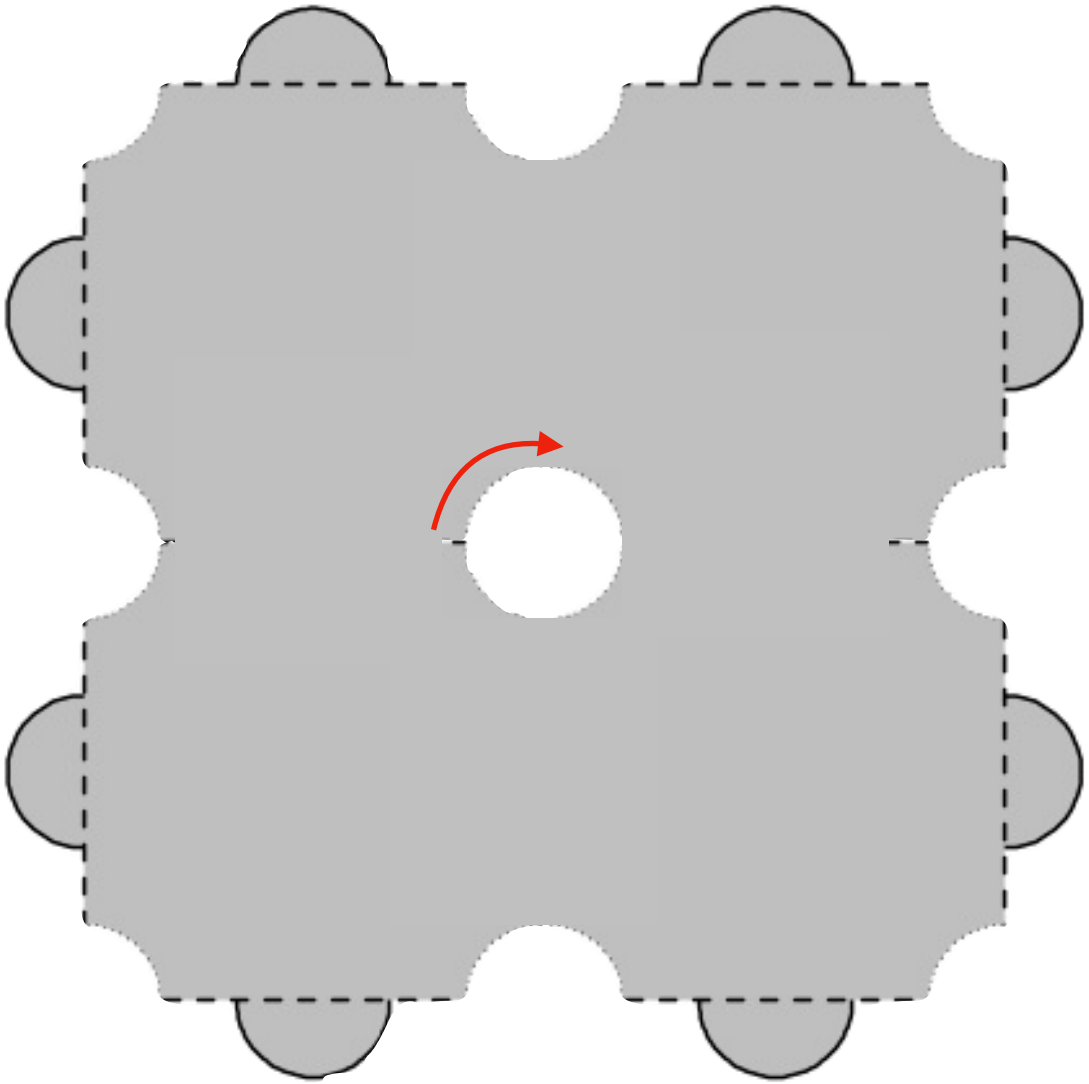
Bismuth is a "semi metal"; it has the second lowest thermal conductivity (after mercury) and the highest Hall coefficient, a high electrical resistance (or low electrical conductivity) (look for instance at Tab 1.2 and 1.6 of A&M book!).
The unit cell is rhombohedral with two atoms (see Tab 7.5 A&M book), so it *could* be an insulator. However, there is a little band overlap that makes the situation similar to the case of a divalent metal with simple cubic lattice, whose Fermi-surfaces in (k_x, k_y) plane is shown in the figure. We refer therefore for simplicity to this case.



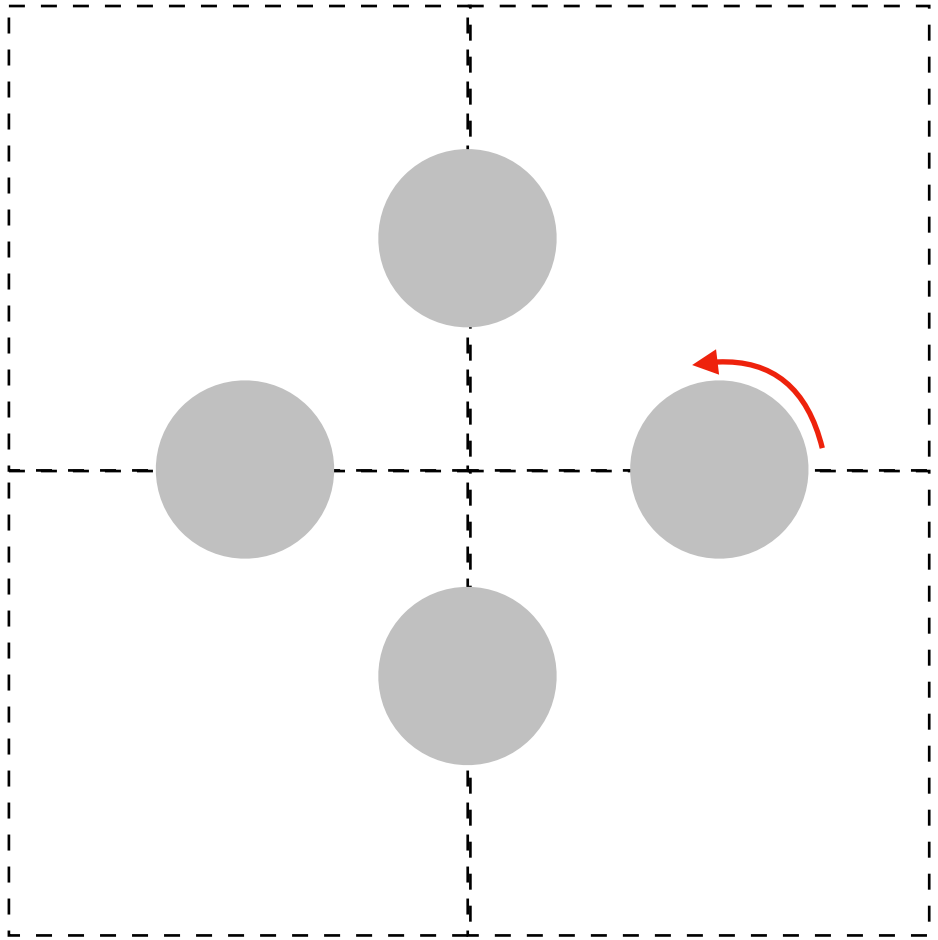
1. Make the same picture using the repeated zone scheme. Which part of the Fermi-surface can be described as electron-like and which as hole-like?

2. By which factor is the specific heat of the electrons at low temperatures ($k_B T << E_F$) smaller than the electronic specific heat in the model of free electrons? For numerical estimations use the following data: the radius of the electronic Fermi-sphere is $k_e = 0.1 G_0$, where G_0 is the shortest reciprocal lattice vector; the bands in the vicinity of E_F are parabolic with effective masses $m_e = m_h = 0.1 m_0$.

3. Why is the conductivity of such metals smaller than in the model of free electrons?



h-like



e-like

Es. 3.2 - 16.1.2012

Specific heat of free e^- :

$$c_v = \frac{\pi^2}{2}\left(\frac{k_B T}{\varepsilon_F}\right) n k_B \qquad (2.81)$$

here $\varepsilon_F = \frac{\hbar^2 k_F^2}{2m^*}$ with $k_e = 0.1\ G_0$, $m^* = 0.1\ m_0$

$$G_0 = \frac{2\pi}{a}\ ; \quad n_0 = \frac{2}{a^3} \quad \text{but} \quad k_F^3 = 3\pi^2 n_0 = \frac{6\pi^2}{a^3}$$

$$\left(\frac{n}{\varepsilon_F}\right)^{3D} \propto \frac{k_F^3 m_0}{k_F^2} = m_0 k_F$$

$$\boxed{\frac{c_v^*}{c_v^{free}} = \frac{k_F m^*}{k_F^{free} m_0} = 0.1 \cdot \frac{0.1\ 2\pi/a}{(6\pi^2)^{1/3}/a} = 0.1 \cdot \frac{0.628}{3.9} \simeq 0.016}$$