Department of Physics and Astronomy
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Home assignment # 1 Physics 570

1.

(a)

According to the free electron model, the valence electrons in a crystalline metal are considered to be detached from the atoms and able to move throughout the material with infrequent deflections from their paths. Yet the electrostatic potential due to a lattice of ionised atoms has strong gradients and ought to deflect electrons easily. Why does an individual electron not see a potential with strong spatial variation? Briefly discuss why an electron in a crystalline metal is only rarely deflected by the weakly varying potential it actually does see.

(b)

A quantum mechanical treatment of valence electrons moving in a constant potential in a three dimensional volume V leads to the density of states

$$D(E) = D_0 E^{1/2}$$

where E is the electron energy, $D_0 = (2m)^{1/2} mV/(\pi^2\hbar^3)$, and m is the electron mass. Show that the energy of the highest occupied state at a temperature T=0 K is

$$E_F = \frac{\hbar^2(3\pi^2 n)^{2/3}}{2m}$$

where n is the number of valence electrons per unit volume.

If $n = 5.86 \times 10^{28}$ m^{-3} for silver, calculate E_F for this metal.

i. Show that the Fermi velocity is given by

$$v_F = \frac{\hbar}{m}\left(3\pi^2 n\right)^{1/3}$$

where n is the free electron density in the material.

ii. Calculate the Fermi velocity for electrons in aluminium if the free electron density is 1.81×10^{29} m^{-3}.

(c)

The response of a set of free electrons in a material to an external force F in the x direction can be modelled using the following transport equation:

$$\frac{dv_D}{dt} + \frac{v_D}{\tau} = \frac{F}{m}$$

where v_D is the drift velocity in the x direction, t is time, τ is the relaxation time and m is the electron mass.

i. Solve this equation in the steady state for a constant applied electric field to show that the electrical conductivity of the material, according to the model, is given by

$$\sigma = ne^2\tau/m$$

where n is the free electron density and e is the electronic charge.

ii. If the electrical conductivity of aluminum at room temperature is 3.8×10^7 $\Omega^{-1}m^{-1}$, and using the free electron density given above, calculate the relaxation time and drift velocity of a free electron in an electric field of 100 Vm^{-1}.

iii. If the temperature of the metal is raised above room temperature, would you expect the electrical conductivity of aluminum to increase, decrease, or stay the same? Why?

2. (a) Quantum mechanics tells us that the energy of an electron of mass m in a cubic box of side L is given by:

$$E(n_x, n_y, n_z) = \frac{h^2}{8mL^2}[n_x^2 + n_y^2 + n_z^2]$$

where n_x, n_y, n_z are quantum numbers that are allowed to take only integer values.

Consider an 8 atom metal in which each atom is confined in a cubic box of side a, with the whole system itself being confined in a (obviously larger) cubic box. One valence electron can be detached from its parent atom. If each *electron* is confined

within the box occupied by its parent atom, show that the total energy of the 8 atom system is

$$E_1 = 3h^2/ma^2$$

By now allowing each electron to move freely throughout the whole 8-atom metal, show that the total energy of the system is now

$$E_2 = 0.44E_1$$

b. Suggest how your calculation is relevant to the free electron theory of metals.

(c)

Each quantum state occupies a volume $\Delta\Omega = 4\pi^3/V$ in k space, where V is the volume of the metal. Show that the number of quantum states with k values in the range k, $k+dk$, is

$$dN = \frac{Vk^2}{\pi^2}dk$$

Hence, knowing the relationship between E and k for an electron, show that the density of states

$$g(E) = dN/dE = \frac{V\sqrt{2m^3E}}{\pi^2\hbar^3}$$

Consider a piece of metal of volume $1cm^3$. How many quantum states are there with energy in the range 1 to $1.001eV$?

3.

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(a)

It is believed that the energy spectrum of electrons in materials is divided into bands separated by gaps. Describe with the aid of diagrams how experimental evidence for band structure and band gaps can be obtained using photons

(b)

The materials copper, silicon and diamond have electrical conductivities at room temperature of 6×10^7, 10^3, and 10^{-11} respectively, in units of $\Omega^{-1}m^{-1}$.What can you deduce about the way electrons occupy the band structure for each material? Illustrate your answer with sketches of the energy spectrum in each case.

If small quantities of boron (valence 3) were added to pure silicon (valence 4), would you expect the room temperature electrical conductivity of the resulting material to be greater than, less than, or the same as that of pure silicon? Explain why.

(c)

The energy of an electron in a linear chain of atoms with uniform spacing a is characterised by the function $E(k)$ where k is the wavevector of the electron. The velocity of the electron is given by $v = \hbar^{-1} dE/dk$ and the momentum is mv where m is the free electron mass. If the wavevector of the electron responds to an external force F according to

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

show that the acceleration of the electron is given by

$$\frac{dv}{dt} = \frac{F}{m^*}$$

and derive an expression for the effective mass m^*.

(d)

If $E(k) = U(1 - \cos(ka))$, where U is a positive constant, calculate the acceleration of electrons due to the force F as a function of k in the range $-\pi/a \leq k \leq \pi/a$. Hence show that the total momentum of the electrons in a full band does not change as a result of the imposition of the force F.

(a)

Explain what is meant by electronic bands and band gaps in solids. Under what circumstances can band gaps have a major effect on the properties of a solid? Discuss, using appropriate examples, how the electrical and optical properties of materials can depend on electronic band gaps.

(a)

Describe the differences in view point between the tight binding and nearly free electron models of electronic structure in materials. What features do they share? Explain physically how each model can account for the existence of band gaps in the electronic structure of materials.

(b)

Consider *N* atoms arranged in a ring with the atoms spaced a distance *a* apart. Electrons moving in this structure may be modelled by a one dimensional wavefunction $\psi(x)$, where *x* lies in the range $0 \leq x \leq Na$. The atoms lie at positions $x = \ell a$ where ℓ is an integer.

i.

Show that symmetry implies that

$$\psi(x + a) = \exp(i\phi)\psi(x)$$

where ϕ can take the values

$$\phi = \frac{2\pi p}{N}$$

only, where *p* is an integer.

ii.

Hence show that an expression of the form

$$\psi(x) = \exp(ikx)u(x)$$

with $k = 2\pi p/(Na)$ can be used to represent the electron, as long as the function *u*(*x*) satisfies a certain condition. What is this condition?

4.

(a)

i.

What feature of the density of states of electrons is characteristic of an intrinsic semiconductor?

ii.

How can intrinsic semiconductors be converted into *p*- and *n*-type extrinsic semiconductors? What changes in the density of states of electrons in the material are brought about by this conversion?

(b)

Theory shows that the density of electrons in the conduction band of a semiconductor (whether intrinsic or extrinsic) is given by

$$n_e = A(m_e T)^{3/2} \exp\left(\frac{\mu - E_C}{k_B T}\right)$$

where μ is the chemical potential of the electrons in the material, E_C is the energy of the bottom of the conduction band, k_B is Boltzmann's constant, T is temperature and m_e is the effective mass of the electrons. The constant A is given by $\frac{1}{4}(2k_B/(\pi\hbar^2))^{3/2}$.

The density of holes in the valence band is similarly given by

$$n_h = A(m_h T)^{3/2} \exp\left(\frac{E_V - \mu}{k_B T}\right)$$

where m_h is the effective mass of the holes, and E_V is the energy of the top of the valence band.

i.

For an intrinsic semiconductor, show that the chemical potential of the electrons is given by

$$\mu = \frac{1}{2}(E_C + E_V) + \frac{3}{4}k_B T \ln\left(\frac{m_h}{m_e}\right)$$

ii.

Calculate the chemical potential of electrons relative to the top of the valence band $(\mu - E_V)$ for intrinsic silicon at 300 K, if E_C-E_V=1.1 eV, and assuming that both m_e and m_h are equal to the mass of a free electron.

iii.

If the hole density in a sample of *p*-type silicon is 10^{22} m^{-3}, calculate the chemical potential, relative to the top of the valence band, of the electrons in this material at 300 K.

iv.

If a junction is formed between this *p*-type silicon and some intrinsic silicon, which way would electrons initially flow, and why?

5. (a) Describe what is meant by a hole, in the context of the theory of electrons in solids. Explain how a hole might be created or annihilated. Discuss the drift of a hole in an applied electric field and how this allows us to account for positive values of the Hall coefficient for some materials.

(b) Discuss the operation of a solar cell based on a simple *pn* junction.