Name: Solution

SECOND EXAM

MSE102

Thursday October 18th 2004

BOTH SIDES of ONE 8.5x11" sheet and a calculator is allowed. Closed book.

1. SHORT ANSWER QUESTIONS
   a. For (a) a hydrogen molecule and (b) Cu metal, would you use the tight binding model or the nearly free electron model to describe the energy levels. Explain. [6]

The tight binding model describes the hydrogen molecule well as the molecular orbital can be accurately described as a superposition of atomic orbitals in which the probability of finding the electrons between the two atoms is high.

The nearly free electron model describes Cu well as the valence e^- feel a weak periodic potential due to the ionic lattice

   b. What is the general diffraction condition? Describe each parameter in the expression. [4]

$$2\underset{\sim}{k} \cdot \underset{\sim}{G} = |\underset{\sim}{G}|^2$$

or

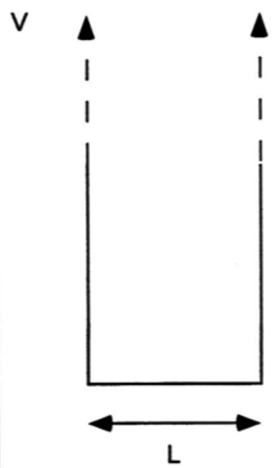
$$k' - k = \Delta k = \underset{\sim}{G}$$

$\underset{\sim}{k}$ ≡ wavevector of the incident beam

$\underset{\sim}{k}'$ ≡ wavevector of the diffracted beam

$\underset{\sim}{G}$ ≡ reciprocal lattice vector

c. Consider electrons in an infinite potential well of width L as described in lecture. So the uncertainty in the position is $\Delta x = L$. There must be a corresponding uncertainty in the momentum of the electron and hence it must have a certain kinetic energy. Calculate this energy from the uncertainty relationship and compare it with the value of the ground state energy. [10]



By uncertainty principle,

$$\Delta p \, \Delta x \sim \hbar$$

$$\Delta x \sim L$$

$$\therefore \Delta p \sim \frac{\hbar}{L}$$

$$\Delta E = \frac{\Delta p^2}{2m} = \frac{\hbar^2}{2mL^2}$$

$$E = \frac{\hbar^2}{2mL^2}$$

From particle in the box,

$$k = \frac{n\pi}{L} \quad ; \quad n = 1, 2, 3, \ldots\ldots$$

Due to the particle in the 1D box boundary conditions, pls refer to the lecture notes

$$E = \frac{\hbar^2}{2m}\left(\frac{n\pi}{L}\right)^2$$

$$E_1 = \frac{\hbar^2}{2m}\frac{\pi^2}{L^2} = \frac{h^2}{8mL^2}$$

i.e. $E = 4E_1$

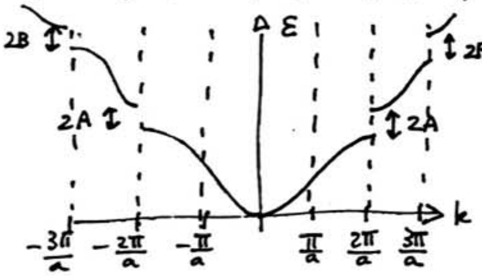
The energy calculated from the uncertainty principle is in the same order of magnitude as the ground state energy (1D box); as a result, we can determine and locate the ground state energy.

d. Consider electrons in a weak potential of the form $V(x) = A\cos\frac{4\pi x}{a} + B\cos\frac{6\pi x}{a}$. Sketch and label energy versus wavevector for electrons through the 3rd Brillouin zone. [5]. How many allowed energy states are there in the lowest energy band.[5]

So the weak periodic potential in general has the form: $V(x) = \sum_G V_G \cos Gx$ where $G = \frac{2\pi m}{a}$

In our case where $V(x) = A\cos\frac{4\pi x}{a} + B\cos\frac{6\pi x}{a}$,

$V_1 = 0$, $V_2 = A$, $V_3 = B$, $V_4 = 0$, ...



In the lowest energy band (which includes up to $|k| \le \frac{2\pi}{a}$), there are

$$\underbrace{2}_{\text{for spin}} \frac{\times(2\pi/a)}{\pi/L} = 4\frac{L}{a} = 4N \text{ allowed states.}$$

Problem #1.______/30
Problem#2._____/30
Total:_____/60

2. In the semiconductor industry, aluminum electrical interconnects are being replaced by copper ones for a variety of reasons. Aluminum and copper are both fcc metals.
   (a) Write down the primitive translation vectors for an fcc element in terms of its lattice parameter a. [3] Sketch the corresponding reciprocal lattice vectors. [3]

   Let us consider patterning the copper into a 10nm by 10nm by 10nm cube and apply the free electron model to these elements.

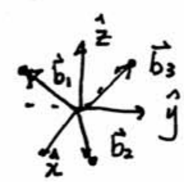
   (b) Write down the applicable Schrodinger equation. [4]
   (c) What are the wavefunctions and corresponding energies of the electrons in the cube. [6]
   (d) Sketch electron energy versus waevector k. [4]
   (e) Consider an electron in copper represented by a traveling wave with Fermi energy E_F, encountering the surface of a metal at which there is a potential step of height V_o ($V_o>E_F$). Set up the problem and give the form of the wavefunction outside the metal without solving the math. [10]

(a) For fcc real space lattice, the primitive translation vectors are:

$$\vec{a}_1 = \frac{a}{2}(\hat{x}+\hat{z}) \qquad \vec{a}_2 = \frac{a}{2}(\hat{x}+\hat{y}) \qquad \vec{a}_3 = \frac{a}{2}(\hat{y}+\hat{z})$$

whose corresponding reciprocal lattice vectors are:

$$\vec{b}_1 = \frac{2\pi}{a}(\hat{x}-\hat{y}+\hat{z}) \quad \vec{b}_2 = \frac{2\pi}{a}(\hat{x}+\hat{y}-\hat{z}) \quad \vec{b}_3 = \frac{2\pi}{a}(-\hat{x}+\hat{y}+\hat{z})$$



(b) If we pattern the copper into a cube whose side is $L \times L \times L$ where
& $L = 10\,nm$, the confinement into a cube limits the values of the
(c) wavevectors according to Schrödinger's eqn & the relevant boundary conditions.

$$-\frac{\hbar^2}{2m}\nabla^2\psi(\underline{r}) = E\psi(\underline{r}) \quad \text{for} \quad \begin{matrix} 0 \le x \le L \\ 0 \le y \le L \\ 0 \le z \le L \end{matrix} \quad \text{and } \psi(\underline{r}) = 0 \text{ otherwise.}$$

We know that we can perform separation of variables so that $\psi(\underline{r}) = \phi_1(x)\,\phi_2(y)\,\phi_3(z)$

For example. $\phi_1(x=0) = 0 = \phi_1(x=L)$ & the corresponding Schrödinger equation yields

$$\phi_1(x) = \underbrace{C}_{\text{constant}} \sin\frac{n_x\pi x}{L}$$

Similarly for the y and z functions: $\phi_2(y) = C'\sin\frac{n_y\pi y}{L}$ & $\phi_3(z) = C''\sin\frac{n_z\pi z}{L}$

Therefore, the solution looks like: $\psi(\underline{r}) = C\sin\frac{n_x\pi x}{L}\sin\frac{n_y\pi y}{L}\sin\frac{n_z\pi z}{L}$

Normalizing this wavefunction over all space: $\int\psi^*(\underline{r})\,\psi(\underline{r})\,d^3\underline{r} = 1$

$$\int_0^L\int_0^L\int_0^L |C|^2 \sin^2\frac{n_x\pi x}{L}\sin^2\frac{n_y\pi y}{L}\sin^2\frac{n_z\pi z}{L} = 1 \quad\Rightarrow\quad C = \sqrt{\left(\frac{2}{L}\right)^3} = \left(\frac{2}{L}\right)^{3/2}$$

and therefore

$$\psi(\underline{r}) = \left(\frac{2}{L}\right)^{3/2}\sin\frac{n_x\pi x}{L}\sin\frac{n_y\pi y}{L}\sin\frac{n_z\pi z}{L}$$

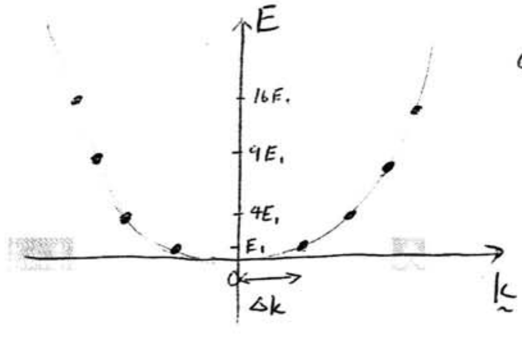
$$E = \frac{\hbar^2}{2m}\left(\frac{\pi}{L}\right)^2(n_x^2+n_y^2+n_z^2)$$

(d) Since this is the free electron model, the shape is parabollic

$$E = \frac{\hbar^2}{2m}(k_x^2 + k_y^2 + k_z^2) = \frac{\hbar^2}{2m}\left(\frac{\pi}{L}\right)^2 (n_x^2 + n_y^2 + n_z^2)$$

where n_x, n_y, n_z are positive integers.

It means there is no energy state at $\underset{\sim}{k} = 0$ point, and not all $\underset{\sim}{k}$'s are allowed. $\boxed{2\text{pts}}$ (discrete)

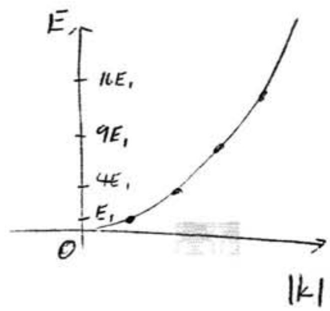


axes are given $\boxed{2\text{pts}}$

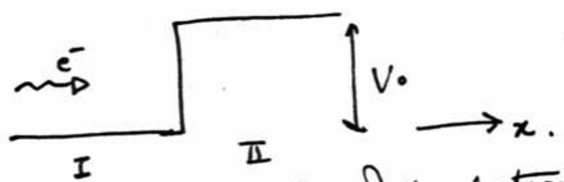
if $\underset{\sim}{k}$ is [100]

$\Delta k = \frac{\pi}{L}$

You can sketch like below, too, to make sure $|\underset{\sim}{k}| > 0$



(e)



If the Fermi energy ε_F of the electron is $< V_0$, then the resulting wavefunction in region II has to be an exponentially damped function.

If we were to solve Schrödinger's eqn, (for simplicity let's look at 1D)

(I) $-\frac{\hbar^2}{2m}\nabla^2\psi(x) = E\psi(x)$

(II) $-\frac{\hbar^2}{2m}\nabla^2\psi(x) + V_0\psi(x) = E\psi(x)$

$$-\frac{\hbar^2}{2m}\nabla^2\psi(x) = \underbrace{(\varepsilon_F - V_0)}_{\text{this is negative!}}\psi(x)$$

Therefore solutions look like $\psi(x) = Ae^{Kx} + Be^{-Kx}$ where $K = V_0 - \varepsilon_F > 0$

But physically the probability that an e^- exists outside the box decreases as we get away from the boundary so $A \to 0$ $\therefore$ $\psi(x) \sim e^{-Kx}$ for $K = V_0 - \varepsilon_F$!