

ECE609 Spring06  
**HOMWORK 1 - SOLUTIONS**  
Review of Quantum Mechanics

## 1 The Photoelectric effect

1. The minimum photon energy,  $E_{ph}$ , equals the workfunction,  $W_0$ . This also equals:

$$E_{ph} = q * W_0 = 1.6 * 10^{-19} * 4.3 = 6.89 * 10^{-19} \text{ Joule}$$

The corresponding photon frequency is:

$$\nu = E_{ph}/h = 1040 \text{ THz}$$

The corresponding wavelength equals:

$$\lambda = hc/E_{ph} = 0.288 \mu.m$$

The photon momentum,  $p$ , is:

$$p = h/\lambda = 2.297 * 10^{-27} \text{ kg.m/s}$$

2. the wavelength threshold is  $\lambda_s = hc/W_0 = 621 \text{ nm}$ , so  $\lambda < \lambda_s$   
For  $\lambda = 546.1 \text{ nm}$ , we get for the Kinetic energy of the electron :

$$KE = hc/\lambda - W_0 = 0.273 \text{ eV},$$

since  $E = p^2/(2m) = (1/2)mv^2$ , we get for the velocity  $v = 3.098 * 10^5 \text{ m.s}^{-1}$ .

For  $\lambda = 645.5 \text{ nm}$ , it comes  $v = 0 \text{ m.s}^{-1}$  since  $\lambda > \lambda_s$  and then  $\nu < \nu_s$ .

## 2 Hydrogen atom

1. Normalization condition involves  $\int_0^\infty |\Psi|^2 4\pi r^2 dr = 1$ . It comes

$$4\pi C^2 \int_0^\infty r^2 \exp(-2r/a_0) dr = 1.$$

Using integrations by parts, we get

$$\int_0^\infty r^2 \exp(-2r/a_0) dr = a_0 \int_0^\infty r \exp(-2r/a_0) dr = a_0^2/2 \int_0^\infty \exp(-2r/a_0) dr = a_0^3/4,$$

then  $C = (1/(\pi a_0^3))^{1/2}$ .

2.  $dP = |\Psi|^2 4\pi r^2 dr$ , so  $dP/dr = (4/a_0^3) \exp(-2r/a_0) r^2$
3. if we call  $E(r) = dP/dr$ , a maximum of  $E(r)$  is obtained for  $dE(r_p)/dr = 0$ . It comes  $r_p = a_0$ .  
The Bohr radius (classical picture) corresponds, in fact, to an orbit where the probability to find an electron is maximal (quantum picture).

4.

$$P(0.9r_p < r < 1.1r_p) = (4/a_0^3) \int_{0.9a_0}^{1.1a_0} r^2 \exp(-2r/a_0) dr,$$

After calculations we get  $P = 0.108$  (10.8%).

5.

$$\langle r \rangle = (4/a_0^3) \int_0^\infty r^3 \exp(-2r/a_0) dr = 3a_0/2$$

6. We note that  $U(r) = -b^2/r$  where  $b = q^2/(4\pi\epsilon_0)$

$$\langle U \rangle = -b^2 \langle (1/r) \rangle = -b^2(4/a_0^3) \int_0^\infty r \exp(-2r/a_0) dr = -b^2/a_0 = -27.1eV.$$

We also note that (in spherical coordinates)

$$T = -\frac{\hbar^2}{2m} \frac{\partial}{r^2 \partial r} \left( \frac{r^2 \partial}{\partial r} \right),$$

we then get

$$\langle T \rangle = \frac{\hbar^2}{2m} \frac{1}{a_0^2} = 13.6eV.$$

Since  $E = T + V$ , it comes  $E = -13.6eV$ . This is equivalent to the fundamental energy obtained with the Bohr model.

### 3 Finite potential well

1. We get:

$$\begin{cases} \Psi_I = \exp(ikx) + r \exp(-ikx) \\ \Psi_{II} = E \exp(iKx) + F \exp(-iKx) \\ \Psi_{III} = t \exp(ikx) \end{cases}$$

Using the conditions of continuity:

$$\Psi_I(-a/2) = \Psi_{II}(-a/2); \quad d\Psi_I(-a/2)/dx = d\Psi_{II}(-a/2)/dx$$

and

$$\Psi_{II}(a/2) = \Psi_{III}(a/2); \quad d\Psi_{II}(a/2)/dx = d\Psi_{III}(a/2)/dx,$$

we obtain 4 equations with 4 unknowns  $r, E, F, t$ . We put the system into a matrix form and solve the linear system for the unknown  $t$ . The coefficient of transmission  $T$  is given by  $|t|^2$ :

$$T = \frac{1}{1 + \left( \frac{K^2 - k^2}{2Kk} \right)^2 \sin^2 Ka}$$

Since we know that  $R + T = 1$ , it comes  $R = 1 - T$ .

2.

$$f(E) = \frac{U_0^2}{4E(E + U_0)}$$

and

$$g(E) = (2m(E + U_0))^{1/2} a / \hbar$$

3. Numerical application.  
 4.  $T = 1$  for  $g(E) = n\pi$  ( $n$  positive integer); finally we get

$$E_n = n^2 \pi^2 \hbar^2 / (2ma^2) - U_0,$$

it comes  $E_1 = 0.7eV$ ,  $E_2 = 50.8eV$ ,  $E_3 = 134.3eV$ .

Calculate (analytically) the energy values for which  $T$  is equal to 1 (total transmission). What are the numerical expressions of these energy values (we consider only the values smaller than  $150eV$ ) ?

5. If  $E \rightarrow \infty$ ,  $f(E) \rightarrow 0$ , so  $T \rightarrow 1$ . At high energy, the electron "does not feel" the effect of the potential well. Same result than that obtained using classical mechanics.

#### 4 Finite potential wall (30pts)

1. We get:

$$\begin{cases} \Psi_I = \exp(ikx) + r \exp(-ikx) \\ \Psi_{II} = C \exp(i\alpha x) + D \exp(-\alpha x) \\ \Psi_{III} = t \exp(ikx) \end{cases}$$

with  $k = (2mE)^{1/2}/\hbar$  and  $\alpha = (2m(U_0 - E))^{1/2}/\hbar$ .

Using the conditions of continuity:

$$\Psi_I(0) = \Psi_{II}(0); \quad d\Psi_I(0)/dx = d\Psi_{II}(0)/dx$$

and

$$\Psi_{II}(a) = \Psi_{III}(a); \quad d\Psi_{II}(a)/dx = d\Psi_{III}(a)/dx,$$

we obtain 4 equations with 4 unknowns  $r, C, D, t$ . We put the system into a matrix form and solve the linear system for the unknown  $t$ . The coefficient of transmission  $T$  is given by  $|t|^2$ :

$$T = \frac{16}{|(1 + \frac{\alpha}{ik})(1 + \frac{ik}{\alpha}) \exp(-\alpha a) + (1 - \frac{\alpha}{ik})(1 - \frac{ik}{\alpha}) \exp(\alpha a)|^2}.$$

2.  $a \gg 1/\alpha$  leads to  $\exp(-\alpha a) \ll \exp(\alpha a)$ , so

$$T \simeq \frac{16 \exp(-2\alpha a)}{(4 + (\frac{\alpha}{k} - \frac{k}{\alpha})^2)}$$

or

$$T \simeq 16 \frac{E}{U_0} (1 - \frac{E}{U_0}) \exp(-2\alpha a).$$

3. From the previous result:

$$\text{Log}(T) = \text{Log} \left( 16 \frac{E}{U_0} (1 - \frac{E}{U_0}) \right) - 2\alpha a.$$

We set the error  $\epsilon$ :

$$\epsilon = \text{Log} \left( 16 \frac{E}{U_0} (1 - \frac{E}{U_0}) \right)$$

such as

$$\text{Log}(T) = -2\alpha a + \epsilon$$

$\epsilon(x) > 0$  is a necessary condition to obtain the maximum error; indeed  $T < \exp(-2\alpha a + \epsilon)$  only if  $\exp(\epsilon) > 1$ , then  $\epsilon > 0$ .

We set  $x = E/U_0$ ; Within the positive region,  $\epsilon(x)$  is maximal if  $d\epsilon(x)/dx = 0$ ; we get  $x = 1/2$ . So  $\epsilon(1/2) = \text{Log}(4) \simeq 1.4$ . When  $\alpha a = 50$ , we get

$$\text{Log}(T) = -100 + 1.4,$$

the formula is then exact at 1.4%.

At the classical limit  $\text{Log}(T) \rightarrow -\infty$  then  $T \rightarrow 0$ .