ECE609 Spring07

HOMEWORK 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:

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

The corresponding photon frequency is:

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

The corresponding wavelength equals:

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

The photon momentum, p, is:

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

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

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

since $E = p^2/(2m) = (1/2)mv^2$, we get for the velocity $v = 3.098 * 10^5 m.s^{-1}$.
For $\lambda = 645.5nm$, it comes $v = 0m.s^{-1}$ 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:
$$\begin{cases} \Psi_I = \exp(ikx) + r\exp(-ikx) \\ \Psi_{II} = E\exp(iKx) + F\exp(-iKx) \\ \Psi_{III} = t\exp(ikx) \end{cases}$$

2. 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 $R = 1 - T$.

3.
$$f(E) = \frac{U_0^2}{4E(E+U_0)}$$
and
$$g(E) = (2m(E+U_0))^{1/2}a/\hbar$$

4. Numerical application.

5. $T = 1$ 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 $E_1 = 0.7eV$, $E_2 = 50.8eV$, $E_3 = 134.3eV$.

6. If $E \to \infty$, $f(E) \to 0$, so $T \to 1$. 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:

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

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. $a >> 1/\alpha$ leads to $\exp(-\alpha a) << \exp(\alpha a)$, 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:

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

We set the error ϵ:

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

such as

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

$\epsilon(x) > 0$ 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 $\epsilon(1/2) = Log(4) \simeq 1.4$. When $\alpha a = 50$, we get

$$Log(T) = -100 + 1.4,$$

the formula is then exact at 1.4%.
At the classical limit $Log(T) \to -\infty$ then $T \to 0$.