Solution 5

Problem 1.

(a)

Consider electron a distance z away from another semi-infinite dielectric medium with ϵ. The surface of separation is the plane $z = 0$. The electron attracts positive charges to the dielectric medium surface. The net induced surface charge is much less than one electron's charge (hence $\lambda << 1$). Also, the induced surface charge is not uniform (larger right beneath the electron).

From here, knowing the electric lines of the electron and the boundary conditions

$$\begin{aligned} \partial_z \Phi|_{z\to+0} &= \epsilon \partial_z \Phi|_{z\to-0} \\ \partial_x \Phi|_{z\to+0} &= \partial_x \Phi|_{z\to-0} \\ \partial_y \Phi|_{z\to+0} &= \partial_y \Phi|_{z\to-0} \end{aligned} \tag{1}$$

it is not difficult to sketch the electric field lines for our system, see Figure 1.

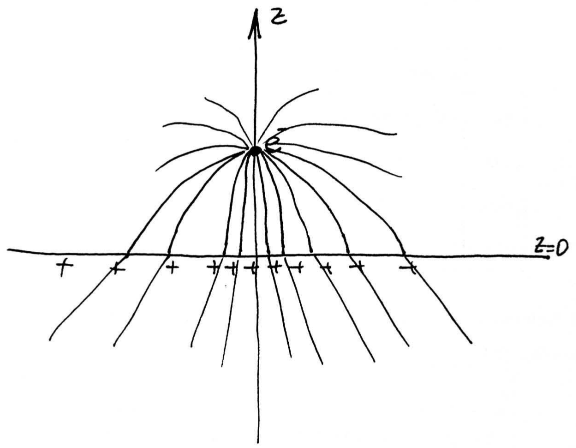

Figure 1:

In attempt to use the image method, it is natural to locate an image charge q' at a symmetrical position (at $-z$) from the electron (positioned at z).

Following Jackson,

$$q' = \frac{\epsilon - 1}{\epsilon + 1}\, e, \tag{2}$$

$$\tag{3}$$

From here, consider q' (at a distance $2z$ from q) as a source of an effective attraction of the electron to the surface of the dielectric and arrive at the expression

$$V(z) = -\frac{\epsilon - 1}{4(\epsilon + 1)} \frac{e^2}{z} = -\lambda \frac{e^2}{z}.$$

(b)

Start with Schrödinger equation

$$-\frac{\hbar^2}{2m}\Psi'' - \frac{\lambda e^2}{z}\Psi = E\Psi, \qquad z > 0 \tag{4}$$

where $\lambda = (\epsilon - 1)/4(\epsilon + 1)$ and the boundary condition is $\Psi(0) = 0$.

Choosing new variables $\tilde{z} = \lambda z/a_B$ and $\tilde{E} = E/\lambda^2 R_Y$, where a_B is the Bohr's radius and R_Y is the Rydberg's constant, we come to the equation:

$$\Psi'' + \frac{2}{\tilde{z}}\Psi + \tilde{E}\Psi = 0. \tag{5}$$

As we can see from Eq.(5) for $\tilde{z} \to \infty$, the solution should behave like $\Psi \sim e^{-k\tilde{z}}, \quad k > 0$. As to the behavior near zero, we know that $\Psi(0) = 0$ and we can look for the ground state function in the form

$$\Psi = C\tilde{z}^{\alpha} e^{-k\tilde{z}}, \quad k > 0$$

where C is the normalization constant.

Substituting this into the Eq.(5) we arrive at

$$(k^2 + \tilde{E})\ \tilde{z}^{\alpha} + 2(1 - \alpha k)\ \tilde{z}^{\alpha-1} + \alpha(\alpha - 1)\ z^{\alpha-2} = 0$$

and conclude that $\alpha = 1, k = 1$ and $\tilde{E} = -k^2 = -1$.

Thus, for the ground state we have

$$\Psi_0 = 2\ \tilde{z}\ e^{-\tilde{z}}, \quad \tilde{E}_0 = -1. \tag{6}$$

As to the first excited state we can think of next polynomial behavior near $\tilde{z} \to 0$ which tends to 0, i.e. look for the solution in the form

$$\Psi = C\tilde{z}\ (\tilde{z} + b)\ e^{-k\tilde{z}}$$

where b is some constant. Doing same derivations as in the ground state, we arrive at the first excites state wave-function and energy:

$$\Psi_1 = \frac{1}{\sqrt{2}}\ \tilde{z}\ (1 - \tilde{z}/2)\ e^{-\tilde{z}/2}, \quad \tilde{E}_1 = -1/4. \tag{7}$$

As we can see in this new units for length, the effective Bohr radius $\tilde{a}_B = a_B/\lambda = 76 \mathring{A}$ and effective Rydberg energy $\tilde{R}_Y = \lambda^2 R_Y \cong 8K$ we have same two levels of energy spectrum as the hydrogen atom.

To find all energy levels, one has to consider confluent hypergeometric functions properties and get $\tilde{E} = -1/m^2, \quad m = 1, 2, \ldots.$

As to the wave function (w.f.) comparison, consider the equation for the radial function of the hydrogen atom (in units of a_B and R_Y for length and energy correspondingly):

$$R'' + \frac{2}{r}\, R' - \frac{l(l+1)}{r^2}\, R + (E + \frac{2}{r})\, R = 0.$$

Substituting $R(r) = \chi/r$ we come to the equation

$$\chi'' + \frac{2}{r}\, \chi' - \frac{l(l+1)}{r^2}\, \chi + E\chi = 0.$$

Thus, the equation for χ for cases $l = 0$ is identical to the equation (5) for Ψ above, giving same solutions up to factor r for $R_{n,0}$ and Ψ.

Problem 2.

(a)

From above, in effective Rydberg units $\tilde{R}_Y = \lambda^2 R_Y$ we have ground state with energy $E_0 = -1$ and the first excited level $E_1 = -1/4$, which gives the frequency of the transition between the states:

$$h\nu = 3\lambda^2 R_Y/4 \Longrightarrow \nu = 118.421 \text{ GHz}.$$

(b)

Consider states ($\tilde{z} = \lambda z/a_B$),

$$|0>= 2\tilde{z}e^{-\tilde{z}}, \qquad |1>= \frac{1}{\sqrt{2}}\, \tilde{z}(1 - \tilde{z}/2)e^{-\tilde{z}/2},$$

$$H_{pert} = eE_\perp z = \frac{eE_\perp a_B}{\lambda}\, \tilde{z}.$$

From here the first order perturbation theory gives for the ground state

$$E_0^{(1)} =< 0|H_{pert}|0 >= \frac{eE_\perp a_B}{\lambda} < 0|\tilde{z}|0 >= \frac{eE_\perp a_B}{\lambda}\; 4 \int_0^\infty \tilde{z}^3 e^{-2\tilde{z}} d\tilde{z} = \frac{3}{2}\, \frac{eE_\perp a_B}{\lambda}.$$

Similar computations for the first excited state give

$$E_1^{(1)} =< 1|H_{pert}|1 >= \frac{eE_\perp a_B}{\lambda} < 1|\tilde{z}|1 >= \frac{eE_\perp a_B}{\lambda}\, \frac{1}{2} \int_0^\infty \tilde{z}^3 (1 - \tilde{z}/2)^2 e^{-\tilde{z}} d\tilde{z} = 6\, \frac{eE_\perp a_B}{\lambda}.$$

Thus, for the shift in frequency we have:

$$\frac{\Delta\nu}{E_\perp} = \frac{E_1^{(1)} - E_0^{(1)}}{hE_\perp} = \frac{9}{2}\frac{a_B}{\lambda}\,\frac{e}{h}\,,$$

where

$$a_B = 0.5292 \cdot 10^{-8}\ \text{cm},$$
$$h = 4.1357 \cdot 10^{-15}\ \text{eV s},$$
$$\lambda = 0.00692756,$$

and thus

$$\frac{\Delta\nu}{E_\perp} = 0.8320\ \text{GHz cm/V}.$$

Problem 3.

(a)

Similar to previous problem, consider

$$H_{int} = \tilde{\lambda}\,\frac{e^2}{R^3}\,\frac{a_B^2}{\lambda^2}\,(\tilde{z}_1 - \tilde{z}_0)(\tilde{z}_2 - \tilde{z}_0),$$

where $\tilde{\lambda}$ is very close to one and $\lambda = 0.00692756$.

Considering the single electron states $|0>, |1>$ from above, for two electrons we have two degenerate states

$$|s_1> = |1>|0>, \qquad |s_2> = |0>|1>$$

with first electron in state $|1>$ and second electron in state $|0>$, and vice versa.

From here we see that the diagonal matrix elements

$$< s_1|H_{int}|s_1> \;=\; < s_2|H_{int}|s_2> = 0,$$

due to $< 0|(z_i - z_0)|0> = 0$.

For non-diagonal terms $< s_1|H_{int}|s_2> = < s_2|H_{int}|s_1>$, consider

$$< s_1|H_{int}|s_2> = \tilde{\lambda}\,\frac{e^2}{R^3}\,\frac{a_B^2}{\lambda^2}\,< 0|< 1|(\tilde{z}_1 - \tilde{z}_0)(\tilde{z}_2 - \tilde{z}_0)|0>|1> =$$

$$= \tilde{\lambda}\,\frac{e^2}{R^3}\,\frac{a_B^2}{\lambda^2}\,< 1|(\tilde{z}_1 - \tilde{z}_0)|0>< 0|(\tilde{z}_2 - \tilde{z}_0)|1>,$$

where

$$< 1|(\tilde{z}_1 - \tilde{z}_0)|0 >=< 0|(\tilde{z}_2 - \tilde{z}_0)|1 >= \sqrt{2} \int_0^\infty \tilde{z}^2(\tilde{z} - \tilde{z}_0)(1 - \tilde{z}/2)e^{-3\tilde{z}/2} d\tilde{z} = 32\sqrt{2}/81$$

or

$$< s_1|H_{int}|s_2 >= \left(\frac{32\sqrt{2}}{81}\right)^2 \tilde{\lambda} \, \frac{e^2}{R^3} \, \frac{a_B^2}{\lambda^2}$$

(b)

First order perturbation theory for the two degenerate cases gives the correction to the energy spectrum in the form

$$E^{(1)} = \frac{1}{2} \left[V_{11} + V_{22} \pm \sqrt{(V_{11} - V_{22})^2 + 4|V_{12}|^2}\right] ,$$

where the following notation is used $V_{11} =< s_1|H_{int}|s_1 >$, $V_{22} =< s_1|H_{int}|s_1 >$ and $V_{12} =< s_1|H_{int}|s_2 >$.

In our case this leaves just,

$$E^{(1)} = \pm|V_{12}| = \pm| < s_1|H_{int}|s_2 > | = \pm \left(\frac{32\sqrt{2}}{81}\right)^2 \tilde{\lambda} \, \frac{e^2}{R^3} \, \frac{a_B^2}{\lambda^2}$$

Thus, the oscillation frequency is

$$\nu = 2\tilde{\lambda} \, \frac{e^2}{R^3} \, \frac{a_B^2}{\lambda^2} \, \left(\frac{32\sqrt{2}}{81}\right)^2 \, \frac{1}{h} = \frac{4\tilde{\lambda}}{\lambda^2} \frac{a_B^3}{R^3} \frac{R_Y}{h} \left(\frac{32\sqrt{2}}{81}\right)^2 = 12.7\text{MHz}$$

where in addition to the numerical values from previous problem we used also $R_Y = 13.6057$eV. And time required for state $|1 > |0 >$ to evolve into $|0 > |1 >$ is

$$T = \frac{1}{2\nu} = 39.4 \text{ nano-s.}$$