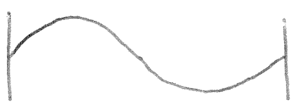
Problem set # 12 (2004)

#1 Dye laser

The molecule acts as a box of 4.18 nm where the electron is confined.

a) The wave functions are what we expect from a standing wave between two closed boundaries.

mode 1  $\lambda_1 = 2L$ $\quad k_1 = \frac{2\pi}{\lambda_1} = \frac{\pi}{L}$

mode 2  $\lambda_2 = L$ $\quad k_2 = \frac{2\pi}{L}$ $\quad$ with $L = 4.18$ nm

mode 3  $\lambda_3 = \frac{2}{3}L$ $\quad k_3 = 3\frac{\pi}{L}$

From the wave vectors, we can calculate the energies,

$$E_1 = \frac{\hbar^2 k_1^2}{2m} = \frac{(1.054\cdot 10^{-34}\,J\cdot s)^2 \cdot \left(\frac{\pi}{4.18\times 10^{-9}\,m}\right)^2}{2\cdot 9.11\times 10^{-31}\,kg} = 3.45\ J = 0.0215\ eV$$

replacing k_1 by k_2 and k_3, we get

$$\boxed{E_1 = 0.0215\ eV \quad E_2 = 0.0861\ eV \quad E_3 = 0.194\ eV}$$

#1 b) The energy of the emitted photon is egal to the difference in energy between the initial and final states of the electron.

$$E_{\lambda_{n=2 \rightarrow n=1}} = E_2 - E_1 = \underline{0.065 \text{ eV}}$$

This photon is about 50 times less energetic than a photon in the visible range. It corresponds to an Infrared photon.

c) We want to find the energy of the second transition:

$$E_{\lambda_{n=3 \rightarrow n=1}} = E_3 - E_1 = \underline{0,172 \text{ eV}}$$

where E_1 is the ground state energy, i.e. the lowest energy.

#2 Uncertainty principle for a particle in a box.

The box has length L, and the wave function in the ground state is $\psi_1(x) = A\sin(k_1 x) = \frac{A}{2i}\left(e^{ik_1x} - e^{-ik_1x}\right)$

(to get the other standing states, we just have to replace k_1 by k_n)

a) The different k_n must satisfy the fixed boundary condition in $x=L$.

$\rightarrow \quad \sin(k_n L) = 0 \quad \Rightarrow \quad k_n L = n\pi \quad \Rightarrow \quad \boxed{k_n = n\frac{\pi}{L}}$

b) In the ground state $(n=1)$, the wave function is

$$\psi_1(x) = \frac{A}{2i}\left(e^{ik_1x} - e^{-ik_1x}\right)$$

using the relation $|p_1| = \hbar|k_1|$, we can see that the wave function correspond to the sum of one travelling wave with momentum $p_{1+} = \hbar k_1$ and another with $p_{1-} = -\hbar k_1$

As for their probability, since probability is proportional to the square of the amplitude and since

\#2 b) continued

both travelling waves have the same coefficient in ψ, their probability will be equal!

So $\boxed{p_{1+} = \hbar k_1, \ p_{1-} = -\hbar k_1 \text{ in x-direction with equal probability.}}$

$$k_1 = \frac{\pi}{L}$$

c) Hence we don't know if we have p_{1+} or p_{1-}.

Then the uncertainty is $\Delta p = \frac{(p_{1+} - p_{1-})}{2} = \frac{2\pi\hbar}{2L} \ (= \hbar k_1)$

$$\boxed{\Delta p_x = \frac{\pi\hbar}{L}}$$

d) If $\Delta x = \frac{L}{2}$, then using $\frac{x_{max} - x_{min}}{2} = \frac{L}{2}$

$$\Delta x \, \Delta p = \frac{L}{2} \cdot \frac{\pi\hbar}{L} = \frac{\pi\hbar}{2}.$$

We hence get a relation satisfying to uncertainty principle. The extra factor of $\frac{\pi}{2}$ is small and we are close to the limit of the uncertainty principle.

#3 Size of the Hydrogen atom

a) To achieve this, we can use the Heisenberg Uncertainty Principle. We assume that the electron is confined in a box of length $2r$. This r will correspond to the radius where it is most probable to find the electron.

We have $\Delta x = r$. So $\Delta x \Delta p_x = \hbar \rightarrow \boxed{\Delta p_x = \frac{\hbar}{r}}$

b) Hence $\Delta p = \frac{\hbar}{r}$. Since the average ~~displacement~~ momentum of the electron is 0, this means that $\frac{1}{2}(p_{max} - p_{min}) = \Delta p$ and $p_{max} + p_{min} = 0$. So $p = \pm \frac{\hbar}{r}$ from what we have seen in #2.

- From this $KE = \frac{p^2}{2m} = \frac{\hbar^2}{2mr^2}$ so $\boxed{KE = \frac{\hbar^2}{2mr^2}}$

c) - The potential energy is due to Coulomb interaction between the electron and the hydrogen nucleus which are of charge $-e$ and $+e$ respectively.

#3 continued

In general the potential energy is given by

$$PE = \frac{k q_1 q_2}{r} \quad \text{where } k = \frac{1}{4\pi\varepsilon_0} = 9\times10^9 \ \frac{N\cdot m^2}{C^2}$$

so $$PE = -\frac{ke^2}{r}$$

d). To find the r minimizing the total energy (this will be the most probable r, let call this a_0)

So $$\left.\frac{dE}{dr}\right|_{r=a_0} = 0 = \left(\frac{d\,KE}{dr} + \frac{d\,PE}{dr}\right)\Big|_{r=a_0} = \left(\frac{ke^2}{r^2} - \frac{\hbar^2}{mr^3}\right)_{r=a_0}$$

so $$\boxed{a_0 = \frac{\hbar^2}{mke^2} = 0.529\ \text{Å}}$$

This value is usually noted a_0 and called the Bohr radius.

A diameter of ~1 Å for the hydrogen atom is very reasonable, even if we use the uncertainty principle, we get an excellent result here.

e). So the energy at $r=a_0$ is $E_0 = -\frac{ke^2}{a_0} + \frac{\hbar^2}{2ma_0^2}$

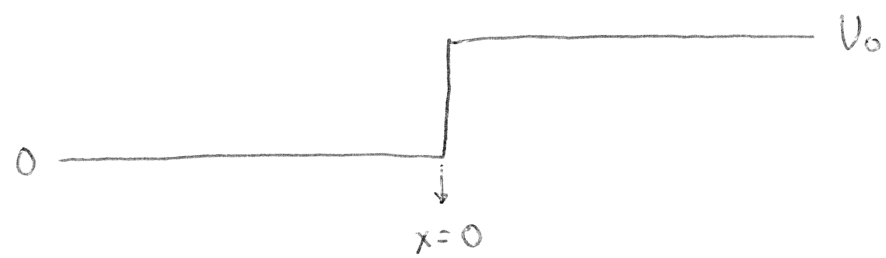
and $$E_0 = -\frac{9\times10^9 \frac{J\cdot m}{C^2}(1.6\times10^{-19}C)^2}{0.529\times10^{-10}\,m} + \frac{(1.054\cdot10^{-34}\,J\cdot s)^2}{2\cdot9.11\times10^{-31}kg\,(0.529\times10^{-10}\,m)^2}$$

$$= (-4.36 + 2.18)e^{-18}J = -27.22 + 13.62\ eV = -13.6\,eV$$

so $\boxed{E_0 \simeq E_{ionization} = -13.6\ eV}$ it represents the binding energy of the electron to the nucleus.

#4

Potential energy:



and $U_0 \in]-\infty, +\infty[$

a) We know that $KE = \frac{p^2}{2m} \rightarrow p = \sqrt{2mKE}$.

there are two cases, the incoming particle correspond to the first momentum of incoming particle

- $x \leq 0$, $KE = E \rightarrow \boxed{p_{x\leq 0} = p_1 = \sqrt{2mE}}$ → momentum of incoming particle
- $x \geq 0$, $KE = E - PE = E - U_0$ $\boxed{p_{x\geq 0} = p_2 = \sqrt{2m(E-U_0)}}$

the last value is a real number since $E > U_0$

b) $\underline{r}$ is the reflected amplitude of wave function.

It will give the probability of having a reflected particle at the boundary.

$\underline{t}$ is the amplitude of wave function for transmitted particle.

#4 c) Since $k = \frac{p}{\hbar}$

$$\boxed{k_1 = \frac{\sqrt{2mE}}{\hbar}} \qquad \boxed{k_2 = \frac{\sqrt{2m(E-U_0)}}{\hbar}}$$ → see part a)

d) $x \leq 0$ $\qquad \frac{d^2}{dx^2}\left(e^{ik_1x} + \underline{r}\, e^{-ik_1r}\right) = -k_1^2\left(e^{ik_1r} + \underline{r}\, e^{-ik_1r}\right)$

so $\quad -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi_1(x) + U(x)\psi_1(x) = \frac{\hbar^2 k_1^2}{2m}\psi_1(x) + 0(x)\psi(x)$

and $\quad \frac{\hbar^2 k_1^2}{2m} = E \qquad\qquad = E\,\psi_1(x)$ ✓

$x \geq 0$ $\quad -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi_2(x) + U(x)\psi_2(x) = \frac{\hbar^2 k_2^2}{2m}\psi_2(x) + U_0\,\psi_2(x)$

and $\quad \frac{\hbar^2 k_2^2}{2m} = E - U_0 \qquad\qquad = E\,\psi_2(x)$ ✓

e) In $x=0$, we must have $\psi_1(0) = \psi(0)$

so $\quad \boxed{1 + \underline{r} = \underline{t}}$ as usual!

#4 f) The derivatives must also be continuous:

$$\frac{d}{dx}\Psi_1(x)\Big|_{x=0} = \frac{d}{dx}\Psi_2(x)\Big|_{x=0}$$

$$ik_1\left(e^{ik_1x} - \underline{r}\,e^{ik_1x}\right)\Big|_{x=0} = ik_2\underline{t}\,e^{ik_2x}\Big|_{x=0}$$

$$\boxed{k_1(1-\underline{r}) = k_2\underline{t}}$$

g) So $1-\underline{r} = \frac{k_2}{k_1}\underline{t}$ and $1+\underline{r} = \underline{t}$ from f) and e)

adding these, we get $2 = \left(1+\frac{k_2}{k_1}\right)\underline{t} \Rightarrow \boxed{\underline{t} = \frac{2k_1}{k_1+k_2}}$

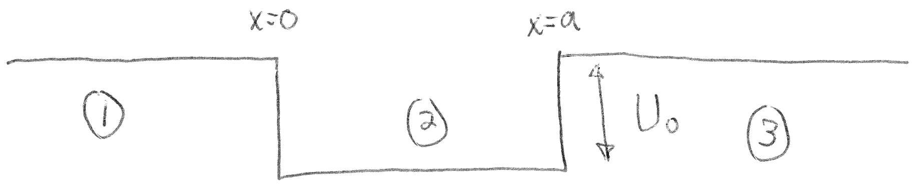
then, $\underline{r} = \underline{t} - 1 = \frac{2k_1 - k_1 - k_2}{k_1+k_2} \rightarrow \boxed{\underline{r} = \frac{k_1-k_2}{k_1+k_2}}$

h) The probability of being reflected is hence

$$P(\text{reflected}) = |\underline{r}|^2 = \left(\frac{k_1-k_2}{k_1+k_2}\right)^2$$

Classically the probability would always be $\underline{\underline{0}}$ since $E > U_0$, everything should be transmitted.

#5. $E > 0$, Potential given by



with $U_0 < 0$.

so $\psi_1(x) = e^{ikx} + \underline{R}\, e^{-ikx}$

$\psi_3(x) = \underline{T}\, e^{ikx}$

Want to find $\underline{R}$ and $\underline{T}$.

- 1st method, resolution of the Schroedinger equation

5.1 a) The wave function ψ_2 will have the fore

$$\psi_2(x) = \underline{C}\, e^{ik'x} + \underline{D}\, e^{-ik'x}$$

To find k and k', we use the relations involving kinetic energy:

$$KE = \frac{p^2}{2m} \quad \text{and} \quad k = \frac{p}{\hbar} \quad \rightarrow \quad k = \frac{1}{\hbar}\sqrt{2m\, KE}$$

Since in region 1 and 3 $PE = 0$, $KE = E$ and

$$\boxed{k = \frac{1}{\hbar}\sqrt{2mE}}$$

In region 2, $KE = E - U_0 > E$ and

$$\boxed{k' = \frac{1}{\hbar}\sqrt{2m(E - U_0)}}$$

5.1 b) Both the functions and their first derivative should be continuous at the boundaries. Hence

$$\psi_1(x=0) = \psi_2(x=0) \Rightarrow \boxed{1 + \underline{R} = \underline{C} + \underline{D}} \quad i)$$

$$\left.\frac{d\psi_1}{dx}\right|_{x=0} = \left.\frac{d\psi_2}{dx}\right|_{x=0} \Rightarrow \boxed{k(1-\underline{R}) = k'(\underline{C} - \underline{D})} \quad ii)$$

c) Same thing in $x=a$

$$\psi_3(x=a) = \psi_2(x=a) \Rightarrow \boxed{\underline{T}e^{ika} = \underline{C}e^{ik'a} + \underline{D}e^{-ik'a}} \quad iii)$$

and finally,

$$\left.\frac{d\psi_3}{dx}\right|_{x=a} = \left.\frac{d\psi_2}{dx}\right|_{x=a} \Rightarrow \boxed{k\underline{T}e^{ika} = k'\left(\underline{C}e^{ik'a} - \underline{D}e^{-ik'a}\right)} \quad iv)$$

d) We want to solve this for $\underline{R}$.

① $k \cdot i) + ii) \Rightarrow$

$$2k = k(\underline{C} + \underline{D}) + k'(\underline{C} - \underline{D})$$
$$= (k+k')\underline{C} + (k-k')\underline{D}$$

$$\boxed{\underline{C} = \frac{(k'-k)}{k+k'}\underline{D} + \frac{2k}{k+k'}} \quad v)$$

② $k \cdot i) - ii)$

using v)

$$2k\underline{R} = (k-k')\underline{C} + (k+k')\underline{D}$$
$$= \left(-\frac{(k-k')^2}{k+k'} + k+k'\right)\underline{D} + \frac{2k(k-k')}{k+k'}$$
$$= \frac{4kk'}{k+k'}\underline{D} + \frac{2k(k-k')}{k+k'}$$

5.1 d) continued

so $$\boxed{\underline{R} = \frac{2k'}{k+k'}\underline{D} + \frac{(k-k')}{k+k'}} \quad \text{vi)}$$

using v)

(3) $k \cdot$ iii) $-$ iv) $\quad 0 = \underline{C}\,e^{ik'a}(k-k') + \underline{D}\,e^{-ik'a}(k+k')$

$$= e^{ik'a}(k-k')\cdot\left(\frac{(k'-k)}{k+k'}\underline{D} + \frac{2k}{k+k'}\right) + \underline{D}\,e^{ik'a}(k+k')$$

So

$$-2k\,\frac{(k-k')}{k+k'}e^{ik'a} = \underline{D}\left(-e^{ik'a}\frac{(k'-k)^2}{k+k'} + e^{-ik'a}(k+k')\right)$$

so $$\boxed{\underline{D} = \frac{2k}{k+k'}\left(\frac{k-k'}{k+k'} + \frac{k+k'}{k'-k}e^{-2ik'a}\right)^{-1}} \quad \text{vii)}$$

(4) Replacing $\underline{D}$ in eq. vi), we get

$$\underline{R} = \frac{2k'}{k+k'}\cdot\frac{2k}{k+k'}\left(\frac{k-k'}{k+k'} + \frac{k+k'}{k'-k}e^{-2ik'a}\right)^{-1} + \frac{k-k'}{k+k'}$$

$$= \frac{4kk'}{(k+k')^2}\cdot\left(\frac{k+k'}{k'-k}e^{-2ik'a}\right)^{-1}\left(-\frac{(k'-k)^2}{(k+k')^2}e^{2ik'a} + 1\right)^{-1} + \frac{k-k'}{k+k'}$$

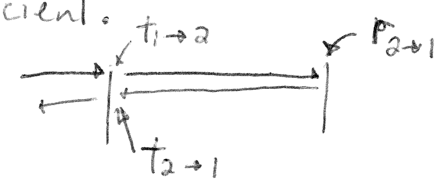
$$\boxed{\underline{R} = \frac{\left(\frac{2k}{k+k'}\right)\left(\frac{2k'}{k+k'}\right)\left(\frac{k'-k}{k+k'}\right)e^{2ik'a}}{\left(1 - \left(\frac{k'-k}{k+k'}\right)^2 e^{2ik'a}\right)} + \frac{k-k'}{k+k'}}$$

#5.2 2^{nd} method, using the sum over history.

a) We know that the reflexion coefficient will be $\underline{r}_{1\to2} = \underline{r}_{12}$, and the wave will have momentum $-\hbar k$.

so $$\boxed{\psi_{r_a}(x) = \underline{r}_{12}\, e^{-ikx}}$$

b) For the wave reflected at $x=a$, we'll still have momentum $-\hbar k$ in the end. The change will be in the coefficient.



→ also an extra phase of $2k'a$

$$\boxed{\psi_{r_b}(x) = t_{1\to2}\, t_{2\to1}\, r_{2\to1}\, e^{i2k'a}\, e^{-ikx}}$$

c) Summing all reflexions, the ratio will be $(r_{2\to1})^2 e^{i2k'a}$

and $$\sum_{i=0}^{\infty} x^i = \frac{1}{1-x}$$

We can use this for the wave in b) and then add the wave found in a).

Hence,

$$\boxed{\underline{R} = \underline{r}_{12} + \frac{t_{12}\, t_{21}\, r_{21}\, e^{i2k'a}}{1 - r_{21}^2\, e^{i2k'a}}}$$

This is the same as what we have seen for string waves!

5.2 c) continued

using #4. $r_{12} = \frac{k-k'}{k+k'}$ $r_{21} = \frac{k'-k}{k+k'}$ $t_{12} = \frac{2k}{k+k'}$ $t_{21} = \frac{2k'}{k+k'}$.

So

$$\boxed{\underline{R} = \frac{k-k'}{k+k'} + \frac{\left(\frac{2k}{k+k'}\right)\left(\frac{2k'}{k+k'}\right)\left(\frac{k'-k}{k+k'}\right)e^{i2k'a}}{1 - \left(\frac{k'-k}{k+k'}\right)^2 e^{i2k'a}}}$$

The same as in #5.1 !