HW2 solution

MTLE-6120: Spring 2017

Due: Feb 13, 2017

1. **Photoelectric effect and quantum efficiency: Kasap 3.8**

   (a) Longest wavelength λ_0 corresponds to minimum photon energy E_0, which must equal the work function $\phi_0 = 1.9$ eV. So

   $$\lambda_0 = hc/E_0 = \frac{6.626 \times 10^{-34}\text{ Js} \cdot 3 \times 10^8\text{ m/s}}{1.9 \cdot 1.602 \times 10^{-19}\text{ J}} = 653\text{ nm}$$

   In fact, it is useful to note the value of $hc = 1241$ nm $\cdot$ eV to convert between wavelengths and photon energies. So $E_0 = 1.9$ eV corresponds to $1241/1.9 = 653$ nm.

   (b) Blue radiation of wavelength 450 nm has photon energy $1241/450 = 2.76$ eV. Since the work function is 1.9 eV, the ejected electrons have kinetic energy $2.76 - 1.9 = 0.86$ eV. It would therefore take a potential of 0.86 V to stop them.

   (c) Given intensity $\mathcal{I}$ on area A, the incident power is $\mathcal{I}A$. This corresponds to a photon incident rate of $\mathcal{I}A/E_{\text{photon}}$. The quantum efficiency QE determines the fraction of photons converted to electrons, so the electron generation rate is $\text{QE} \cdot \mathcal{I}A/E_{\text{photon}}$. Correspondingly the photocurrent is

   $$e\frac{\text{QE} \cdot \mathcal{I}A}{E_{\text{photon}}} = e\frac{(25\%)(30\text{ mW/cm}^2)(\pi(6\text{ mm})^2/4)}{2.76\text{ eV}} = \frac{(0.25)(300\text{ J/s/m}^2)(9\pi \times 10^{-6}\text{ m}^2)}{2.76\text{ V}} \approx 0.77\,\text{mA}$$

2. **Scattering by a δ-atom**

   (a) Consider an electron with energy $E = \frac{\hbar^2 k^2}{2m} > 0$ incident from the left $(-\infty)$ towards a δ-atom given by the potential $-V_0\delta(x)$, with strength parametrized using the parameter $q = 2mV_0/\hbar^2$. Find the wavefunction $\psi(x)$ (expressed in k and q, rather than E and V_0 for convenience). Can you normalize it?

   At $x \neq 0$, the wavefunctions are $e^{\pm ikx}$. So we can assume the general form

   $$\psi(x) = \begin{cases} Ae^{ikx} + Be^{-ikx}, & x < 0 \\ Ce^{ikx} + De^{-ikx}, & x > 0 \end{cases}$$

   The incident electron corresponds to Ae^{ikx}, which could reflect to Be^{-ikx} and transmit to Ce^{ikx}. But it cannot produce De^{-ikx}, which is an electron incident from the right $(+\infty)$, so set $D = 0$. At $x = 0$, the wavefunction should be continuous, which yields $A + B = C + D = C$, so that

   $$\psi(x) = \begin{cases} Ae^{ikx} + Be^{-ikx}, & x < 0 \\ (A+B)e^{ikx}, & x > 0 \end{cases}$$

   In class, we derived the derivative discontinuity condition

   $$\psi'(0^+) - \psi'(0^-) = \frac{-2mV_0}{\hbar^2}\psi(0) \equiv -q\psi(0)$$

Substituting $\psi(x)$ yields

$$ik(A+B) - (ikA - ikB) = -q(A+B)$$

which simplifies to $B = -qA/(2ik+q)$. Therefore

$$\psi(x) = A \begin{cases} e^{ikx} - \frac{q}{2ik+q} e^{-ikx}, & x < 0 \\ \frac{2ik}{2ik+q} e^{ikx}, & x > 0 \end{cases}$$

Usually A would now be deterined by normalizing the wavefunction. However, this wavefunction is present in all of space and cannot be normalized in the conventional way. (A naive attempt would lead to $A \to 0$.)

(b) What are the probabilities of the electron getting reflected and transmitted? Describe and explain their qualitative dependence on the energy of the electron. What would the corresponding probabilities be in the classical case?

The incident wave had amplitude A, and the reflected wave had amplitude B, so the reflection probability is

$$R \equiv \left|\frac{B}{A}\right|^2 = \frac{q^2}{4k^2+q^2}.$$

Similarly the transmission probability is

$$T \equiv \left|\frac{A+B}{A}\right|^2 = \frac{4k^2}{4k^2+q^2}.$$

As expected, $R + T = 1$.

For energy $E \to 0$, $k = 0$, which corresponds to $R = 1$ and $T = 0$ i.e. perfect reflection. As energy increases, k increases, which causes R to decrease and T to increase. For energy $E \to \infty$, $k \to \infty$ which results in $R = 0$ and $T = 1$ i.e. perfect transmission. As the electron energy increases, it is less affected by the potential and has a greater tendency to continue in its original direction (transmission).

Classically the electron would always transmit $T = 1$ and $R = 0$. (It will roll into the bottom of the well gaining kinetic energy, and then roll back up converting that back to potential energy, and continue onwards with its original kinetic (and total) energy.)

(c) Consider the opposite potential $+V_0\delta(x)$. What is the electron wavefunction? What are the probabilities of the electron getting reflected and transmitted? What would the corresponding probabilities be in the classical case?

The only thing that changes is $V_0 \to -V_0$, which is equivalent to $q \to -q$. Therefore

$$\psi(x) = A \begin{cases} e^{ikx} + \frac{q}{2ik-q} e^{-ikx}, & x < 0 \\ \frac{2ik}{2ik-q} e^{ikx}, & x > 0 \end{cases}$$

The quantum reflection and transmission probabilities,

$$R = \frac{q^2}{4k^2+q^2} \qquad \text{and} \qquad T = \frac{4k^2}{4k^2+q^2},$$

remain unchanged!

Classically, the electron cannot cross an infinite potential and will always bounce back i.e. $T = 0$ and $R = 1$.

(d) Instead of a free electron with definite momentum k (and energy $E = \frac{\hbar^2 k^2}{2m}$) as considered above, consider a Gaussian wavepacket with coefficients

$$c_k = \frac{1}{\sqrt{\sigma_k\sqrt{2\pi}}} \exp \frac{-(k-k_0)^2}{2\sigma_k^2},$$

assuming that the spread in momentum $\sigma_k \ll k_0$ and q. Where is the electron as a function of time?

In class, we showed that for a wave $e^{i(kx-\omega t)}$, such a wavepacket takes the form

$$\frac{\exp\frac{-(x-\omega'(k_0)t)^2}{2\sigma_x^2}}{\sqrt{\sigma_x\sqrt{2\pi}}}e^{i(k_0x-\omega(k_0)t)}$$

with $\sigma_x = 1/\sigma_k$.

For a single k, we already solved for the wavefunction

$$\psi(x) = A\begin{cases} e^{ikx} - \frac{q}{2ik+q}e^{-ikx}, & x<0 \\ \frac{2ik}{2ik+q}e^{ikx}, & x>0 \end{cases}$$

which contains $e^{\pm ikx}$ pieces for $x<0$ and $x>0$. Within the wavepacket, all the k are close to k_0 within width $\sigma_k \ll k_0$ and q. This means that the coefficients of the reflected and transmitted piece are approximately the same for each k as for the center k_0 i.e.

$$\psi(x) \approx A\begin{cases} e^{ikx} - \frac{q}{2ik_0+q}e^{-ikx}, & x<0 \\ \frac{2ik_0}{2ik_0+q}e^{ikx}, & x>0 \end{cases}$$

for all k that are relevant.

Now, we can combine each of the pieces into a wavepacket using the derivation from class, taking care to flip the sign of k_0 for the negative propagating wave:

$$\psi_{\text{packet}}(x,t) \approx \frac{A}{\sqrt{\sigma_x\sqrt{2\pi}}}\begin{cases} \begin{array}{l}\exp\left(\frac{-(x-\omega'(k_0)t)^2}{2\sigma_x^2}\right)e^{i(k_0x-\omega(k_0)t)} \\ \quad -\frac{q}{2ik_0+q}\exp\left(\frac{-(x+\omega'(k_0)t)^2}{2\sigma_x^2}\right)e^{i(-k_0x-\omega(k_0)t)}\end{array}, & x<0 \\ \frac{2ik_0}{2ik_0+q}\exp\left(\frac{-(x-\omega'(k_0)t)^2}{2\sigma_x^2}\right)e^{i(k_0x-\omega(k_0)t)}, & x>0 \end{cases}$$

The first term for $x<0$ consists of a bunch centered at $x = v_g t$, where $v_g = \omega'(k_0) = \hbar k_0/m$, which has significant contribution for $x<0$ (the domain of this solution) only for $t<0$. So this is the incoming electron that lasts from $t=-\infty$ till $t=0$ when it 'collides' with the potential.

The second term for $x<0$ is centered at $x=-v_g t$, which has significant contribution in $x<0$ only for $t>0$. This corresponds to the reflected electron bunch which is produced at $t=0$ upon collision with the potential.

The single term for $x>0$ is centered at $x=v_g t$, which contributes for $x>0$ when $t>0$. Of course, this corresponds to the electron bunch transmitted after collision with the potential at $t=0$.

Collecting by time, the electron comes in as a wavepacket of width $\sigma_x/\sqrt{2}$ (where $\sqrt{2}$ is because of wavefunction squared) centered at $x=v_g t$, moving with velocity $v_g\hat{x}$ towards $x=0$ till $t=0$. For $t>0$, the electron is **either** in the reflected bunch centered at $x=-v_g t$ moving with velocity $-v_g\hat{x}$ **or** in the transmitted bunch centered at $x=v_g t$ moving with velocity $v_g\hat{x}$. The probability of which bunch it is in is precisely given by the reflection and transmission probabilities, R and T.

3. **Photoemission from a δ-atom**

The δ-atom with potential $-V_0\delta(x)$ has a single bound state $e^{-\kappa|x|}\sqrt{\kappa}$ with $\kappa = mV_0/\hbar^2 \equiv q/2$ (as shown in class), and free states at any energy $E>0$ (previous problem). Now apply a time-varying electric field $\mathcal{E}e^{-i\omega t}$ in the x direction (from an EM wave, for example).

(a) For the atom in its ground state, what is the minimum ω that can free the electron?

The bound state energy is $E = \frac{-\hbar^2\kappa^2}{2m} = \frac{-\hbar^2 q^2}{8m}$, while the lowest energy free state is $E = 0$. So the ionization potential (analagous to work-function, but for an atom/molecule) is

$$\hbar\omega_{\min} = \phi_0 = \frac{\hbar^2 q^2}{8m}.$$

(b) For the free states solved in the previous problem, let us solve the normalization problem by assuming that the entire system is inside an infinite potential well of length L (centered at $x = 0$). What are the normalized wavefunctions and the condition(s) satisfied by the allowed k? (Hint: there are two classes of solutions: odd and even about $x = 0$. Also, you may not be able to solve for k explicitly in some cases; only write the condition satisfied by k in those cases.)

Our general solution was

$$\psi(x) = \begin{cases} Ae^{ikx} + Be^{-ikx}, & x < 0 \\ Ce^{ikx} + De^{-ikx}, & x > 0 \end{cases}.$$

This time we cannot zero any of the coefficients, because reflections at the outer walls can generate all the components. Value and derivative matching yield the conditions

$$A + B = C + D,$$
$$(ikC - ikD) - (ikA - ikB) = -q(A + B).$$

Additionally, $\psi(x)$ must now be zero at $x = \pm L/2$, which yields

$$Ae^{-ikL/2} + Be^{ikL/2} = 0 \qquad \Rightarrow \qquad A = -Be^{ikL},$$
$$Ce^{ikL/2} + De^{-ikL/2} = 0 \qquad \Rightarrow \qquad D = -Ce^{ikL}.$$

Therefore, we now have four homogeneous equations in A, B, C, D.
Substituting for A and D using the latter two equations into the first two:

$$B - Be^{ikL} = C - Ce^{ikL},$$
$$(ikC + ikCe^ikL) - (-ikB - ikBe^{ikL}) = -q(B - Be^{ikL}).$$

The first equation gives either $B = C$ or $e^{ikL} = 1$.
First, if we take $e^{ikL} = 1$, which corresponds to $k = 2n\pi/L$, the second equation becomes $C + B = 0$. The other relations also simplify to $A = -B$ and $C = -D$. The wavefunctions are then

$$\psi(x) = \begin{cases} -Be^{ikx} + Be^{-ikx}, & x < 0 \\ -Be^{ikx} + Be^{-ikx}, & x > 0 \end{cases},$$

which altogether is $\psi(x) = -B(e^{ikx} - e^{-ikx}) = -2iB\sin(kx) = c_0 \sin(kx)$ (say), since B is arbitrary anyway. The normalization condition is $|c_0|^2 = 1/\int_{-L/2}^{L/2} \mathrm{d}x \sin^2(kx) = 2/L$ (since $kL = 2n\pi$). Therefore the normalized wavefunctions are

$$\psi(x) = \sqrt{\frac{2}{L}} \sin kx.$$

These solutions are odd about $x = 0$.
Second, if we instead take the condition $B = C$, the derivative matching equation simplifies to

$$\frac{2k}{q} = \frac{e^{ikL} - 1}{i(1 + e^{ikL})} = \tan\frac{kL}{2},$$

We cannot explicitly solve for k in this case. But, we can use the remaining conditions to write the wavefunction with a single coefficient. We have $A = -Be^{ikL}$, $C = B$ and $D = -Ce^{ikL} = -B^{eiKL}$. Therefore

$$\psi(x) = \begin{cases} -Be^{ik(x+L)} + Be^{-ikx}, & x < 0 \\ Be^{ikx} - Be^{ik(L-x)}, & x > 0 \end{cases},$$

which altogether is $\psi(x) = B(e^{ik|x|} - e^{ik(L-|x|)}) = Be^{ikL/2}(e^{ik(|x|-L/2)} - e^{ik(L/2-|x|)}) = 2iBe^{ikL/2}\sin(k(|x| - L/2)) = c_0 \sin(k(|x| - L/2))$ (say), sinc B is arbitrary anyway. The normalization constraint is

$$\begin{aligned}
1/|c_0|^2 &= \int_{-L/2}^{L/2} \mathrm{d}x \sin^2(k(|x| - L/2)) \\
&= 2\int_0^{L/2} \mathrm{d}x \sin^2(k(x - L/2)) && \text{(even about } x = 0) \\
&= 2\int_0^{L/2} \mathrm{d}y \sin^2(ky) && (y = L/2 - x) \\
&= \int_0^{L/2} \mathrm{d}y(1 - \cos ky) \\
&= \frac{L}{2} - \frac{1}{k}\sin\frac{kL}{2} \\
&= \frac{1}{k}\left(\frac{kL}{2} - \sin\frac{kL}{2}\right).
\end{aligned}$$

Thus the normalized wavefunctions are

$$\psi(x) = \sqrt{\frac{k}{\frac{kL}{2} - \sin\frac{kL}{2}}}\sin\left[k\left(|x| - \frac{L}{2}\right)\right].$$

These solutions are even about $x = 0$.

Note that in both cases above, the k are now quantized even for $E > 0$, because these states are now bound by the box of size L.

(c) What are the matrix elements $\langle\psi_f|H'|\psi_i\rangle$ of the perturbation Hamiltonian $H' = -e\mathcal{E}x$ between the bound state (initial) and the free states (final) determined above? Use $L \gg 1/k, 1/\kappa$ to simplify the integrals. (We are going to take $L \to \infty$ below.) Are there any selection rules?

The matrix elements are defined by

$$\langle\psi_f|H'|\psi_i\rangle = (-e\mathcal{E})\int \mathrm{d}x \psi_f^*(x) x \psi_i(x)$$

where $\psi_i(x) = e^{-\kappa|x|}/\sqrt{\kappa}$ is bound state.

Now, $\psi_i(x)$ is an even function and x is odd, so $\psi_f(x)$ must be odd for the product of all three to be even. If $\psi_f(x)$ is even, the product is odd, and its integral from $-L/2$ to $L/2$ is zero. So the complicated even solutions determined above have zero matrix element! We no longer need to deal with them. This is the selection rule, which is the 1D equivalent of $\Delta l = \pm 1$ for 3D atoms.

For the simpler odd solution, the matrix element is

$$\begin{aligned}
\langle\psi_f|H'|\psi_i\rangle &= -e\mathcal{E}\int_{-L/2}^{L/2} \mathrm{d}x \sqrt{\frac{2}{L}}\sin(kx) x e^{-\kappa|x|}\sqrt{\kappa} \\
&= -e\mathcal{E}\sqrt{\frac{2\kappa}{L}}\int_{-L/2}^{L/2} \mathrm{d}x \sin(kx) x e^{-\kappa|x|} \\
&= -e\mathcal{E}\sqrt{\frac{2\kappa}{L}}\int_0^{L/2} \mathrm{d}x 2\sin(kx) x e^{-\kappa x} \\
&= ie\mathcal{E}\sqrt{\frac{2\kappa}{L}}\int_0^{L/2} \mathrm{d}x (e^{ikx} - e^{-ikx}) x e^{-\kappa x} \\
&= ie\mathcal{E}\sqrt{\frac{2\kappa}{L}}\int_0^{L/2} \mathrm{d}x (e^{-(\kappa - ik)x} - e^{-(\kappa + ik)x}) x \quad \approx ie\mathcal{E}\sqrt{\frac{2\kappa}{L}}\int_0^{\infty} \mathrm{d}x (e^{-(\kappa - ik)x} - e^{-(\kappa + ik)x}) x
\end{aligned}$$

since the integrand from $L/2$ to ∞ is negligible when $L \gg 1/k, 1/\kappa$.

$$\begin{aligned}
\langle\psi_f|H'|\psi_i\rangle &\approx ie\mathcal{E}\sqrt{\frac{2\kappa}{L}}\left(\frac{1}{(\kappa-ik)^2}-\frac{1}{(\kappa+ik)^2}\right) \\
&= ie\mathcal{E}\sqrt{\frac{2\kappa}{L}}\frac{(\kappa+ik)^2-(\kappa-ik)^2}{(\kappa^2+k^2)^2} \\
&= ie\mathcal{E}\sqrt{\frac{2\kappa}{L}}\frac{4ik\kappa}{(\kappa^2+k^2)^2} \\
&= -e\mathcal{E}\sqrt{\frac{2\kappa^3}{L}}\frac{4k}{(\kappa^2+k^2)^2}
\end{aligned}$$

(d) Using Fermi's Golden rule, calculate the rate of photo-excitation out of the bound state. This requires summing over the final states which have separation in k that is proportional to $1/L$. Take the limit $L \to \infty$ so that this becomes an integral. Describe the frequency dependence of the photoemission rate.

The photoemission rate is

$$\begin{aligned}
\Gamma_i &= \frac{2\pi}{\hbar}\sum_f |\langle\psi_f|H'|\psi_i\rangle|^2\delta(E_f-E_i-\hbar\omega) \\
&= \frac{2\pi}{\hbar}\sum_k \left|-e\mathcal{E}\sqrt{\frac{2\kappa^3}{L}}\frac{4k}{(\kappa^2+k^2)^2}\right|^2 \delta\left(\frac{\hbar^2k^2}{2m}+\frac{\hbar^2\kappa^2}{2m}-\hbar\omega\right) \\
&= \sum_k \frac{2\pi}{L}\frac{32\kappa^3(e\mathcal{E}k)^2}{\hbar(\kappa^2+k^2)^4}\delta\left(\frac{\hbar^2k^2}{2m}+\phi_0-\hbar\omega\right)
\end{aligned}$$

Now, $k = 2n\pi/L$ with a spacing of $2\pi/L$. When $L\to\infty$, $\sum_k 2\pi/L \to \int \mathrm{d}k$.

$$\Gamma_i = \int_0^\infty \mathrm{d}k\frac{32\kappa^3(e\mathcal{E}k)^2}{\hbar(\kappa^2+k^2)^4}\delta\left(\frac{\hbar^2k^2}{2m}-(\hbar\omega-\phi_0)\right)$$

Substitute k and κ in terms of corresponding energies i.e. $E = \hbar^2k^2/2m$ and $\phi_0 = \hbar^2\kappa^2/2m$.

$$\begin{aligned}
\Gamma_i &= \int_0^\infty \mathrm{d}E\frac{\sqrt{2m}}{\hbar\sqrt{E}}\frac{32\left(\frac{\sqrt{2m\phi_0}}{\hbar}\right)^3 e^2\mathcal{E}^2\frac{2mE}{\hbar^2}}{\hbar\left(\frac{2m(E+\phi_0)}{\hbar^2}\right)^4}\delta\left(E-(\hbar\omega-\phi_0)\right) \\
&= \frac{32\hbar\phi_0^{3/2}e^2\mathcal{E}^2}{2m}\int_0^\infty \frac{\mathrm{d}E\sqrt{E}}{(E+\phi_0)^4}\delta\left(E-(\hbar\omega-\phi_0)\right) \\
&= \frac{32\hbar\phi_0^{3/2}e^2\mathcal{E}^2}{2m}\frac{\sqrt{\hbar\omega-\phi_0}}{(\hbar\omega)^4} \qquad (\hbar\omega > \phi_0) \\
&= \frac{16e^2\mathcal{E}^2}{\hbar^3 m\omega^4}\sqrt{\phi_0^3(\hbar\omega-\phi_0)}
\end{aligned}$$

The rate is zero for $\hbar\omega < \phi_0$ (the work function), then it increases sharply with a square root dependence on the frequency relative to the threshold, reaching a maximum for $\hbar\omega = 8\phi_0/7$, and then it decreases as ω^{-4} for large frequencies.