HW9 solution

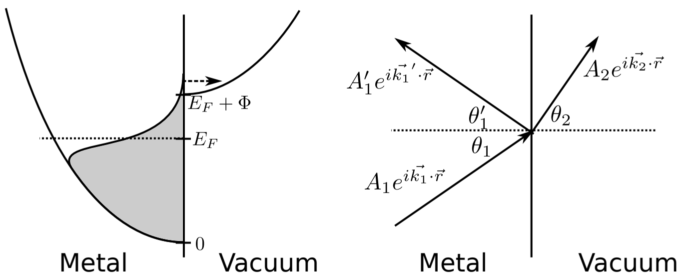
MTLE-6120: Spring 2018

Due: Apr 16, 2018

1. **Electrons crossing an interface**

An electron inside a free-electron metal is approaching its surface at incident angle θ_1 with respect to the normal, and is then either reflected or transmitted to vacuum with some probability. The work function of the metal is Φ, its Fermi level relative to the bottom of the band is E_F, and we choose to label the bottom of the metal's band as the reference energy $E = 0$. Assume that the electron mass is the free electron value m on both sides.

(Use this problem to develop an intuitive conection between wave optics and quantum electron mechanics discussed earlier in the course. Waves be waves!)



(a) What is the minimum electron energy E that can cross the interface at normal incidence ($\theta_1 = 0$)?

At normal incidence, the electron just needs enough energy to cross the barrier. So its energy must be $E \geq E_F + \Phi$.

(b) What are the dispersion relations $E(\vec{k})$ for electrons in the metal and in vacuum?

On both sides, the electron is free and has dispersion relation of the form $\hbar^2 k^2/(2m)$ relative to the bottom of the band. The bottom of the band is 0 in the metal and $E_F + \Phi$ in vacuum. Therefore:

$$E(\vec{k}) = \frac{\hbar^2 k^2}{2m} \qquad \text{metal}$$

$$E(\vec{k}) = \frac{\hbar^2 k^2}{2m} + E_F + \Phi \qquad \text{vacuum}$$

(c) For an electron of energy E sufficient to cross the interface, what are the magnitudes $|\vec{k}_1|$, $|\vec{k}_1'|$ and $|\vec{k}_2|$ of the incident, reflected and transmitted electron wavevectors respectively?

We just need to invert the equations of the previous part, noting that the incident and reflected waves are in the metal and the transmitted wave is in vacuum. Therefore:

$$|\vec{k}_1| = |\vec{k}_1'| = \frac{\sqrt{2mE}}{\hbar}$$

$$|\vec{k}_2| = \frac{\sqrt{2m(E - E_F - \Phi)}}{\hbar}$$

(d) Using the phase-matching condition that the components of $\vec{k}$ in the plane of the interface must be equal for all three electron waves, derive Snell's law for the electron of energy E (i.e. what is the relation between θ_1, θ_1' and θ_2). Express your answer only in terms of E, E_F, Φ and any fundamental constants.

Matching the wavevector components in the plane yields:

$$|\vec{k}_1|\sin\theta_1 = |\vec{k}_1'|\sin\theta_1' = |\vec{k}_2|\sin\theta_2$$

This immediately yields the condition for reflection:

$$\theta_1' = \theta_1$$

since $|\vec{k}_1| = |\vec{k}_1'|$. For transmission, the condition is:

$$\frac{\sin\theta_2}{\sin\theta_1} = \frac{|\vec{k}_1|}{|\vec{k}_2|} = \sqrt{\frac{E}{E - E_F - \Phi}}$$

(e) Write the matching conditions for the electron wavefunction across the interface and solve for the reflection and transmission amplitudes, $r \equiv A_1'/A_1$ and $t \equiv A_2/A_1$. Express the answer only in terms of $E, E_F, \Phi, \cos\theta_1$ and any fundamental constants. Hint: you only need to do this at one point, which you can set as $\vec{r} = 0$ for convenience.

The matching conditions are that the value and derivatives must be continuous. The matching conditions for the in-plane derivatives are redundant with the value condition because Snell's law above matched the in-plane wavevectors. So we only need the value and normal derivative matching condition.

The value matching condition is:

$$A_1 + A_1' = A_2$$

while the normal derivative matching condition is:

$$i|\vec{k}_1|\cos\theta_1 A_1 - i|\vec{k}_1|\cos\theta_1' A_1' = i|\vec{k}_2|\cos\theta_2 A_2$$

which simplifies to:

$$A_1 - A_1' = A_2 \underbrace{\frac{|\vec{k}_2|\cos\theta_2}{|\vec{k}_1|\cos\theta_1}}_{x}.$$

For convenience, we define

$$x \equiv \frac{|\vec{k}_2|\cos\theta_2}{|\vec{k}_1|\cos\theta_1} = \frac{\sin\theta_1\sqrt{1-\sin^2\theta_2}}{\sin\theta_2\cos\theta_1} = \frac{\sqrt{1 - \frac{E}{E-E_F-\Phi}\sin^2\theta_1}}{\sqrt{\frac{E}{E-E_F-\Phi}}\cos\theta_1} = \sqrt{1 - \frac{E_F+\Phi}{E\cos^2\theta_1}}$$

We can now solve the two equations above for A_1' and A_2 in terms of A_1, which yield the reflection and transmission amplitudes:

$$r \equiv \frac{A_1'}{A_1} = \frac{1-x}{1+x} = \frac{1 - \sqrt{1 - \frac{E_F+\Phi}{E\cos^2\theta_1}}}{1 + \sqrt{1 - \frac{E_F+\Phi}{E\cos^2\theta_1}}}$$

$$t \equiv \frac{A_2}{A_1} = \frac{2}{1+x} = \frac{2}{1 + \sqrt{1 - \frac{E_F+\Phi}{E\cos^2\theta_1}}}$$

(f) What are the conditions for total internal reflection, and for zero reflection?

The condition for total internal reflection is that the transmitted ray no longer exist, which happens when $\sin\theta_2 \geq 1$ in the Snell's law equation above i.e.

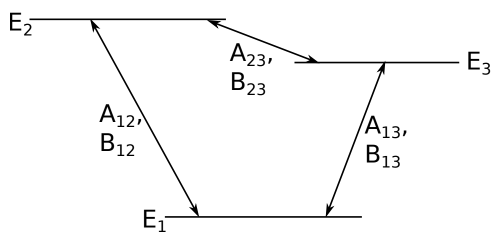
$$\sin\theta_2 = \sin\theta_1 \sqrt{\frac{E}{E - E_F - \Phi}} \geq 1 \quad \Rightarrow \quad \sin\theta_1 \geq \sqrt{\frac{E - E_F - \Phi}{E}}$$

The condition for zero reflection (Brewster angle), $r = 0$ yields $x = 1$ i.e.

$$\begin{aligned} 1 &= \sqrt{1 - \frac{E_F + \Phi}{E\cos^2\theta_1}} \\ \Rightarrow 2 &= \frac{E_F + \Phi}{E\cos^2\theta_1} \\ \Rightarrow \cos\theta_1 &= \sqrt{\frac{E_F + \Phi}{2E}} \\ \Rightarrow \sin\theta_1 &= \sqrt{1 - \frac{E_F + \Phi}{2E}} \end{aligned}$$

2. **Optical pumping and fluorescence**

Cosnider the minimal three-level system necessary for fluorescence (and lasing) as shown below. A pump light of intensity I_{pump} is tuned to a frequency matching $E_2 - E_1$, and assume the intensities at other frequencies are small enough that stimulated emission is negligible for the other transitions. Assume A and B coefficients for each pair of states as shown.



(a) Write the differential equations governing the kinetics of N_1, N_2 and N_3: the populations (electrons / volume) for the three states.

For each pair of states, there is a rate $AN_{\text{upper}} + BIN_{\text{upper}}$ going from the upper to lower state due to spontaneous and stimulated emission, and a rate BIN_{lower} going form the lower to the upper state due to absorption. This results in

$$\begin{aligned} \dot{N}_1 &= [A_{12}N_2 + B_{12}I_{\text{pump}}(N_2 - N_1)] + A_{13}N_3 \\ \dot{N}_2 &= -[A_{12}N_2 + B_{12}I_{\text{pump}}(N_2 - N_1)] - A_{23}N_2 \\ \dot{N}_3 &= A_{23}N_2 - A_{13}N_3 \end{aligned}$$

(b) In steady state, find the ratio N_3/N_1 in order to determine the condition for population inversion ($N_3 > N_1$). Find and interpret the $I_{\text{pump}} \to \infty$ limit of this criterion.

In steady state, $\dot{N}_1 = \dot{N}_2 = \dot{N}_3 = 0$, so that

$$\begin{aligned} 0 &= [A_{12}N_2 + B_{12}I_{\text{pump}}(N_2 - N_1)] + A_{13}N_3 \\ 0 &= -[A_{12}N_2 + B_{12}I_{\text{pump}}(N_2 - N_1)] - A_{23}N_2 \end{aligned}$$

$$0 = A_{23}N_2 - A_{13}N_3$$

Since we want to compare N_3 and N_1, use the last equation to replace N_2 in favor of N_3 in the second equation (same result if done in first equation). This gives the population inversion criterion:

$$\frac{N_3}{N_1} = \frac{B_{12}I_{\text{pump}}}{A_{13}\left(1 + \frac{A_{12}+B_{12}I_{\text{pump}}}{A_{23}}\right)} > 1$$

In the limit of $I_{\text{pump}} \to \infty$:

$$\frac{N_3}{N_1} = \frac{A_{23}}{A_{13}} > 1$$

which simply means that the spontaneous emission rate from $3 \to 1$ must be slower than that from $2 \to 3$ (which feeds state 3). Therefore, having a forbidden transition (selection rule) is useful to slow down $3 \to 1$.

(c) What is the net power density (rate of energy change per unit volume) absorbed from the pump light into the electrons? Assume that stimulated emission puts energy back into I_{pump} (best case scenario for efficiency), while the energy from spontaneous emission is lost. Just write the answer in terms of instantaneous N_1, N_2, N_3 (don't solve for the Ns).

The net rate per unit volume at which photons are being taken from the pump (absorption - stimulated emission) is $B_{12}I_{\text{pump}}(N_1 - N_2)$. These photons have energy $(E_2 - E_1)$, so the net absorbed power density is $B_{12}I_{\text{pump}}(N_1 - N_2)(E_2 - E_1)$.

(d) Similarly, what is the power density output from the $3 \to 1$ transition (fluorescence)? Again, just express in terms of N_1, N_2, N_3 as needed.

The rate of the fluorescence transition is $A_{13}N_3$ and the photon energy is $E_3 - E_1$, so that the power density emitted is $A_{13}N_3(E_3 - E_1)$.

(e) What is the energy efficiency of the fluorescence process in steady state, and how does it depend on I_{pump}? (This time, solve for the Ns in terms of the A, B parameters and interpret!)

The energy efficiency is the power density emitted / power density absorbed

$$\begin{aligned}
\text{Efficiency} &= \frac{A_{13}N_3(E_3 - E_1)}{B_{12}I_{\text{pump}}(N_1 - N_2)(E_2 - E_1)} \\
&= \frac{A_{13}N_3(E_3 - E_1)}{B_{12}I_{\text{pump}}\left(N_1 - N_3\frac{A_{13}}{A_{23}}\right)(E_2 - E_1)} && \text{last steady state equation} \\
&= \frac{A_{13}\frac{N_3}{N_1}(E_3 - E_1)}{B_{12}I_{\text{pump}}\left(1 - \frac{N_3}{N_1}\cdot\frac{A_{13}}{A_{23}}\right)(E_2 - E_1)} \\
&= \frac{A_{13}\frac{B_{12}I_{\text{pump}}}{A_{13}\left(1+\frac{A_{12}+B_{12}I_{\text{pump}}}{A_{23}}\right)}(E_3 - E_1)}{B_{12}I_{\text{pump}}\left(1 - \frac{B_{12}I_{\text{pump}}}{A_{13}\left(1+\frac{A_{12}+B_{12}I_{\text{pump}}}{A_{23}}\right)}\cdot\frac{A_{13}}{A_{23}}\right)(E_2 - E_1)} && \text{using part (b) solution} \\
&= \frac{A_{23}}{A_{23} + A_{12}} \cdot \frac{E_3 - E_1}{E_2 - E_1}
\end{aligned}$$

The result is independent of the pump power and depends only on the ratio of two A parameters, and the energies. The first factor expresses the fraction of electrons excited to state 2 that end up in state 3 instead of going back to state 1 via spontaneous emission. The second factor accounts for the fact that the energy of the emitted photon is smaller than the absorbed one.