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3.23 Electrical, Optical, and Magnetic Properties of Materials

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Homework # 3

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Homework is due on Wednesday October 3rd, 5pm

1 The Scanning Tunneling microscope

The purpose of this exercise is to show how from physical intuition we can create a physical model for a system, solve this model mathematically and then compare the prediction of the model with experiment. The physical system will be an electron moving from a piece of metal right through a vacuum region towards another piece of metal. What we want to calculate is the electrical current that tunnels through the vacuum layer.

1.1 Modeling the system

We have already seen the problem of an electron in an infinite well in one dimension. We solved for the eigenvalues and eigenfunctions. In reality an electron in a metal does not "hit" an infinite wall of potential but a finite wall. So we will model an electron in a piece of metal as being trapped inside a box with a finite height of potential. Inside the metal the electron will not feel any potential and outside it, i.e in the vacuum region, the potential energy of the electron will be V_0 . At this stage we will introduce the concept of **Fermi energy**. In a metal the Fermi energy is the highest occupied energy. This means that each eigenstate with an energy between 0 and E_F will be occupied by 2 electrons (because each energy state can be occupied by one "spin up" electron and one "spin down" electron). A sketch of the potential energy landscape seen by an electron in this problem is shown on figure 1.

1.2 Mathematical solution for our model

Important: Do not worry about the Fermi energy. We will come back to this notion later in the problem and you can just "forget" it right now.

In this part we would like to solve for the wavefunction of an electron in the potential landscape shown on figure 1. In our model we will take the **lowest occupied level** as our *reference energy*. The vacuum energy is called V_0 and corresponds to the potential energy of an electron in vacuum. We will consider the problem of an electron of energy E in the potential energy landscape shown on figure 1. Let us denote by **(I)**, **(II)** and **(III)** the three different regions of space as shown on figure 1.

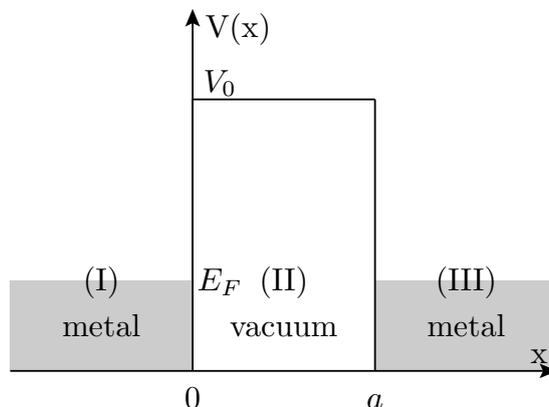


Figure 1: Sketch of a piece of metal (the STM tip on the left) hanging above another piece of metal (the surface to study on the right). Here the potential energy landscape felt by the electron in the different regions of space is shown.

1) Write down the stationary Schrodinger equation for the electron in the three different regions (I), (II) and (III).

solution:

In regions (I) and (III), the electron is free to move and so the potential is zero. Hence the stationary Schrodinger equation can be written as:

$$-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \psi(x) = E\psi(x) \text{ regions (I) and (III)}$$

In region (II), the electron feels a potential of intensity V_0 . The Schrodinger equation is then:

$$-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \psi(x) + V_0\psi(x) = E\psi(x) \text{ region (II)}$$

2) We will consider that $0 < E < V_0$, where E is the total energy of the electron (appearing on the right-hand side of the Schrodinger equation). Given this, express the general solution of the Schrodinger equation in respectively regions (I), (II) and (III) in terms of imaginary and/or real exponential functions.

solution:

In regions (I) and (III), the Schrodinger equation can be re-written as:

$$\frac{d^2}{dx^2} \psi(x) + k^2\psi(x) = 0 \text{ regions (I) and (III)}$$

where k is the wavevector of the electron ($k^2 = \frac{2mE}{\hbar^2}$).

In region (II), the Schrodinger equation looks the same as above but with a minus sign in front of the linear term in ψ :

$$\frac{d^2}{dx^2} \psi(x) - \kappa^2\psi(x) = E\psi(x) \text{ region (II)}$$

where κ is given by $\kappa^2 = \frac{2m(V_0-E)}{\hbar^2}$.

The first Schrodinger equation is well-known and we solved for it many times. The solution is a linear combination of complex exponentials like:

$$\psi(x) = Ae^{ikx} + Be^{-ikx} \text{ region (I)}$$

$$\psi(x) = Ee^{ikx} + Fe^{-ikx} \text{ region (III)}$$

The second Schrodinger equation is well-known in mathematics. The general solution for such an equation is a linear combination of real exponentials like:

$$\psi(x) = Ce^{\kappa x} + De^{-\kappa x} \text{ region (II)}$$

3) What we want to describe in our problem, is an electron coming from the left-hand side (in region (I)) and going through the vacuum layer towards the right-hand side (in region (II)). Considering that e^{ikx} describes a travelling wave going to the right and e^{-ikx} a travelling wave going to the left, we see that we will have to rule out some unphysical solutions in the general solution of question 2). Indeed, since the electron comes from the left, the initial wave e^{ikx} in region (I) will be reflected at the boundary between regions (I) and (II), and so there must be a wave like e^{-ikx} in region (I) to indicate the presence of a reflected wave. On top of having a reflected wave at the boundary between regions (I) and (II), some part of the wavefunction of the electron may tunnel through the vacuum layer and let a transmitted wave emerge in region (III). So in region (III), there must be a wave like e^{ikx} to indicate the presence of a transmitted wave. **But** there cannot exist any wave like e^{-ikx} in region (III) because it would describe an electron coming from the right! Having said that, can you simplify the general solution of the Schrodinger equation in region (III)?

solution:

The simplified solution, given that no wave traveling to the left can exist in region (III), is:

- $\psi(x) = Ae^{ikx} + Be^{-ikx}$ region (I)
- $\psi(x) = Ce^{\kappa x} + De^{-\kappa x}$ region (II)
- $\psi(x) = Ee^{ikx}$ region (III)

4) In this problem, the potential energy of the electron is a piecewise function, but the discontinuities between regions (I) and (II) and between regions (II) and (III) are **finite**. This means that the wavefunction and its first derivative will be continuous at the discontinuities, i.e $x = 0$ and $x = a$. Write down the four equations corresponding to the continuity conditions for the wavefunction and its first derivative at $x = 0$ and $x = a$.

solution:

At $x = 0$, we have the following continuity conditions:

- $A + B = C + D$ continuity of ψ
- $ik(A - B) = \kappa(C - D)$ continuity of $\frac{d\psi}{dx}$

At $x = a$, we have another set of continuity conditions:

- $Ce^{\kappa a} + De^{-\kappa a} = Ee^{ika}$ continuity of ψ
- $\kappa(Ce^{\kappa a} - De^{-\kappa a}) = ikEe^{ika}$ continuity of $\frac{d\psi}{dx}$

5) From question 4), we see that we end up with a system of 4 equations for 5 unknown. But what we are interested in, is the amount of transmitted wave (in region (III)) with respect to the incoming wave (in region (I)). So what we

can do is to divide the four equations of the system by the constant in front of the incoming wave e^{ikx} in region (I). That way we will define the *reflection coefficient* r as being the ratio between the coefficient in front of the reflected wave e^{-ikx} in region (I) and the coefficient in front of the incoming wave e^{ikx} in region (I). Similarly, we will define the *transmission coefficient* t , as being the ratio between the coefficient in front of the transmitted wave e^{ikx} in region (III) and the coefficient in front of the incoming wave e^{ikx} in region (I). Using those notation re-write the system of 4 equations for the 4 unknown ratios.

solution:

Introducing the notation $r = \frac{B}{A}$, $t = \frac{E}{A}$, $\alpha = \frac{C}{A}$ and $\beta = \frac{D}{A}$, we see that the four continuity conditions can be simplified to the following system of equations:

- $1 + r = \alpha + \beta$
- $ik(1 - r) = \kappa(\alpha - \beta)$
- $\alpha e^{\kappa a} + \beta e^{-\kappa a} = t e^{ika}$
- $\kappa(\alpha e^{\kappa a} - \beta e^{-\kappa a}) = ikt e^{ika}$

6) From the system of 4 equations in question 5), we can solve for t and find the following result:

$$|t|^2(E) = \frac{1}{1 + \frac{V_0^2}{4E(V_0 - E)} \sinh^2(a\sqrt{\frac{2m}{\hbar^2}(V_0 - E)})}$$

What we want to calculate now is the transmitted current density with **respect to the incoming density**. The classical expression for the current density of a single electron is: $j = -ev$, where $-e$ is the charge of the electron and v is its velocity. Can you express j in terms of the momentum p ? From that expression, express the quantum equivalent of the current density, i.e the quantum current density operator. Finally calculate the ratio $\frac{\langle j_t \rangle}{\langle j_i \rangle}$ between the expectation value of the quantum current density operator in region (III) and the expectation value of the quantum current density operator in region (I) (for the incoming wave only!).

Remark: if you feel uncomfortable with the normalization of the transmitted wave e^{ikx} (because you don't know what the boundaries of the integral are), it doesn't matter, because in this case you are interested in the ratio of two current densities that will each contain an integral of a complex exponential, and those two integrals will cancel out.

solution:

In classical mechanics, the current density for one electron is: $j = -ev = -\frac{e}{m}p$. To find the corresponding quantum operator, all we have to do is substitute p for $\frac{\hbar}{i} \frac{d}{dx}$. The quantum current density operator is then:

$$\hat{j} = -\frac{e\hbar}{mi} \frac{d}{dx} = \frac{ie\hbar}{m} \frac{d}{dx}$$

The ration between the expectation value of the quantum current density operator in region (III) and the expectation value of the quantum current density operator in region (I) is given by:

$$\frac{\langle j_t \rangle}{\langle j_i \rangle} = \frac{\int t^* e^{-ikx} \frac{ie\hbar}{m} \frac{d}{dx} (t e^{ikx}) dx}{\int e^{-ikx} \frac{ie\hbar}{m} \frac{d}{dx} (e^{ikx}) dx} = |t|^2$$

1.3 Physical discussion

7) In question 6), we have been expressing the expectation value of the current density operator when the electron is described by a wavefunction ψ corresponding to eigenenergy E . As I explained in the first section of this problem, in a metal, all the eigenenergies E up to the Fermi energy E_F are occupied by two electrons. If the two metals (on both side of the vacuum region) have the **same value for E_F** , what do you think will be the "net" current tunneling through the vacuum region? Explain your answer.

solution:

From question 6), we conclude that the probability that an electron tunnel through the vacuum layer is given by $|t|^2(E)$ (for a given energy E between 0 and V_0). Up to now, we have been discussing an electron coming from the left hand side and tunneling towards the right hand side. But because of the symmetry of the problem, we see that an electron coming from the right hand side can also tunnel towards the left hand side, with the exact same probability. Since the Fermi energy indicates the highest energy state occupied in the metal, we see that if the two metals have the same Fermi energy, then the "net current" going through the vacuum layer is zero. Indeed, an electron coming from the left hand side with an energy E is "canceled out" by an electron coming from the right hand side with the same energy E .

8) From question 7), we see that in order to break the symmetry of the problem and create a net current from the tip towards the surface, we need to introduce a bias. This is achieved by connecting the two pieces of metal to a generator that will introduce a little potential difference V between the two metals. If one wants a net flow of electrons from the left to the right, can you show on a diagram what the shift in the Fermi energies of the two metals should be?

Remark: In a given potential configuration, an electron always goes where the potential is smaller in order to minimize its total energy.

solution:

From what has been explained in question 7), we see that in order to get a "net current" flowing from the left to the right, we need to raise the Fermi energy in the tip (the metal on the left hand side), and lower the Fermi energy at the surface (the metal on the right hand side). To achieved this, we connect the two metals to a generator and apply a bias V . Everything is indicated on figure 2.

9) Now let us imagine that the bias between the two metals is really small. If this is the case then most of the net current result from the motion of electrons from the left to the right with an energy corresponding to the Fermi energy $E = E_F$. Let us introduce $\phi = V_0 - E_F$. ϕ is called the "work function" of the metal. Can you simplify the expression obtained in question 6) (at $E = E_F$) when the argument of the sinh is big (Remember that $\sinh(x) \approx \frac{e^x}{2}$ when $x \gg 0$)? Give a result in terms of ϕ , E_F , V_0 , a and fundamental constants like \hbar , and m . In this simplified expression, what is the *characteristic decay length* of the current density? For a (100) surface of Aluminum, the work function is $\phi \approx 4.20\text{eV}$. Can you give an estimate for the characteristic decay length? From this value, conclude about the capability of an STM device to image a surface up to atomic dimensions.

solution:

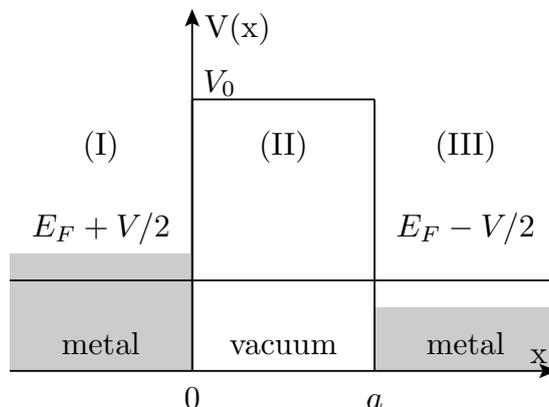


Figure 2: In order to have a net flow of electron from the left to the right, we apply a bias between the two metals. The Fermi energy is raised on the left hand side by $V/2$ and lowered on the right hand side by $V/2$, where V is the applied bias.

Replacing E by E_F in the expression for $|t|^2$ and expanding the $\sinh(x)$ in $\frac{e^x}{2}$, we find that:

$$|t|^2 \approx \frac{16\phi}{V_0^2} e^{-2a\sqrt{\frac{2m\phi}{\hbar^2}}}$$

From this expression, we see that the characteristic decay length is $l = \frac{1}{2\sqrt{\frac{2m\phi}{\hbar^2}}}$. For the (100) surface of Aluminum, we end up with: $l \approx 0.47\text{\AA}$. From this value we can safely conclude that an STM device is more than capable of imaging a surface up to atomic dimensions.

10) From question 9) we come to the conclusion that, when a small bias exists between the two metals, the current density is exponentially depending on the distance a between the two metals and so the device (the STM) is extremely sensitive to the distance between the tip and the metal surface. From there, can you think of a measurement setup that would allow us to image the surface?

solution:

A practical measurement setup would be to use an electronic system (a feedback loop) that would monitor in live the current and act on the tip (i.e raising or lowering the tip) in order to keep the current constant. That way someone would image the surface by following the z coordinate of the tip with respect to displacement in x and y directions.