Lecture 18: Quantum Devices II – Tunneling Devices

Announcements

Homework 4/4:
• Due Now.
  • Email it to me if you have not already done so.

Literature Report 2/2
• Will be online after this lecture.
• You will have 2 weeks to complete the report.
  • It is due Thursday March 18th at 8:30 am.
  • Email it to me at john.labram@oregonstate.edu.

No Lectures in Week 10
• Today’s lecture is the final lecture of the course.
Last Time

- We studied the basics of quantum mechanics.

\[ E_n = \frac{\hbar^2 n^2}{8ma^2} \]

Lecture 18

- Finite Potential Wells.
- Tunneling.
- Resonant Tunneling Diodes.
- Quantum Cascade Lasers.
- Course Summary.
Finite Potential Wells

Last time we considered an electron confined to a region of space between two infinitely high potentials.

\[ E_n = \frac{\hbar^2 \pi^2 n^2}{8ma^2} \]

We found that the electrons can only possess energies with discreet values.

Infinite Potential Well

Last time we considered an electron confined to a region of space between two infinitely high potentials.

\[ E_n = \frac{\hbar^2 \pi^2 n^2}{8ma^2} \]
Finite Potential Well

- What about the more realistic situation where the electrons are in a potential well, but with the well height is finite?
- These systems can be created in reality.
- The best known system is GaAs/AlGaAs.

- Let’s consider a finite square well.
  - I.e. we are not going to worry about any band-bending or gradients in materials.
  - I.e., we can say describe the potential as:
    \[ V(x) = \begin{cases} 
    0 & \text{if } -a \leq x \leq a \\
    V_0 & \text{if } |x| > a 
    \end{cases} \]
  - We want to determine the wavefunction of an electron in the well.
Finite Potential Well

- As before, we are going to use the Time Independent Schrödinger Equation (TISE):
  \[ -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} + V \Psi = E \Psi \]  
  \hspace{1cm} (1)

- We should consider the equation in each section.

- In the well the potential is zero:
  \[ -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} + E \Psi = 0 \]  
  \hspace{1cm} (2)

- This leads to the same solution as last time:
  \[ \Psi(x) = A \cos(kx) + B \sin(kx) \]  
  \hspace{1cm} (3)
  \[ k = \frac{2mE}{\hbar^2} \]  
  \hspace{1cm} (4)

- Outside the well, the potential is \( V_0 \), hence:
  \[ -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} - (V_0 - E) \Psi = 0 \]  
  \hspace{1cm} (5)

- This has a different solution:
  \[ \Psi(x) = C \exp(\kappa x) + D \exp(-\kappa x) \]  
  \hspace{1cm} (6)
  \[ \kappa = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}} \]  
  \hspace{1cm} (7)

- Note we are using the Greek letter kappa (\( \kappa \)) which is not \( k \).

- We now need to determine these 4 constants: \( A, B, C, \) and \( D \).
Finite Potential Well

- Start with the solution outside the well, i.e. when $|x| > a$.
  
  $$\Psi(x) = C \exp(\kappa x) + D \exp(-\kappa x)$$

- We know the wavefunction should not $\to \infty$ as we move away from the well.

- We can then say:
  
  $$C = 0, \text{ if } x > a$$
  $$D = 0, \text{ if } x < a$$

- Leading to:
  
  $$\Psi(x) = \begin{cases} 
  D \exp(-\kappa x) & x > a \\
  C \exp(\kappa x) & x < a 
  \end{cases}$$

Because the wavefunction is defined outside of the well, we need to enforce the following properties:

- $\Psi(x)$ must be continuous at $x = \pm a$.
- $d\Psi(x)/dx$ must be continuous at $x = \pm a$.

E.g. let’s consider $x = a$:

Inside the well: 

$$\Psi(x) = A \cos(kx) + B \sin(kx)$$

Outside the well:

$$\Psi(x) = \begin{cases} 
  D \exp(-kx) & x > a \\
  C \exp(kx) & x < a 
  \end{cases}$$

I.e.:

$$\Psi(a) = A \cos(ka) + B \sin(ka) = D \exp(-kx)$$
Finite Potential Well

- By equating the wavefunctions and their derivatives at \( x = \pm a \), we get 4 equations:

\[
A \cos(ka) + B \sin(ka) = D \exp(-\kappa x) \tag{8}
\]
\[
-kA \sin(ka) + kB \cos(ka) = -\kappa D \exp(-\kappa x) \tag{9}
\]
\[
A \cos(ka) - B \sin(ka) = C \exp(-\kappa x) \tag{10}
\]
\[
kA \sin(ka) + kB \cos(ka) = -\kappa C \exp(-\kappa x) \tag{11}
\]

- If you add (8) to (10)

\[
A \cos(ka) + B \sin(ka) + A \cos(ka) - B \sin(ka) = D \exp(-\kappa x) + C \exp(-\kappa x)
\]

\[
2A \cos(ka) = (C + D) \exp(-\kappa x) \tag{12}
\]

- Similar operations can be carried out to yield:

\[
2A \cos(ka) = (C + D) \exp(-\kappa x) \tag{12}
\]
\[
2kA \sin(ka) = \kappa(C + D) \exp(-\kappa x) \tag{13}
\]
\[
2B \sin(ka) = (D - C) \exp(-\kappa x) \tag{14}
\]
\[
2kB \cos(ka) = -\kappa(D - C) \exp(-\kappa x) \tag{15}
\]

- Divide (13) by (12):

\[
\frac{2kA \sin(ka)}{2A \cos(ka)} = \frac{\kappa(C + D) \exp(-\kappa x)}{(C + D) \exp(-\kappa x)}
\]

\[
k \tan(ka) = \kappa \quad \text{Unless } C = -D \text{ and } A = 0
\]
Finite Potential Well

- We get a similar result by dividing (15) by (14). Hence in total we have:

\[ k \tan(ka) = \kappa \quad \text{Unless } C = -D \text{ and } A = 0 \quad (16) \]

\[ k \cot(ka) = -\kappa \quad \text{Unless } C = D \text{ and } B = 0 \quad (17) \]

- Because we are seeking a solution which is generally true, we have two sets of solutions subject to the following conditions:

\[ k \tan(ka) = \kappa \quad \text{When } C = D \text{ and } B = 0 \quad (18) \]

\[ k \cot(ka) = -\kappa \quad \text{When } C = -D \text{ and } A = 0 \quad (19) \]

- We again see that there are only discreet solutions to these conditions, satisfied when:

\[ ka = n_1 \pi + \cos^{-1} \left( \frac{ka}{k_0 a} \right) \quad (20) \]

\[ ka = n_2 \pi + \sin^{-1} \left( \frac{ka}{k_0 a} \right) \quad (21) \]

- Where \( n_1 \) and \( n_2 \) are positive integers, and:

\[ k = \sqrt{\frac{2mE}{\hbar^2}} \quad (4) \quad k_0 = \sqrt{\frac{2mV_0}{\hbar^2}} \quad (22) \]

- Equations (20) and (21) have to be solved recursively.
Finite Potential Well

- What does this tell us?
  - Even in this experimentally-realizable situation, we should expect discreet energy levels rather than a continuum.
- How could we prove that this was occurring experimentally?

Optical Absorption

- Traditionally we picture semiconductor bands as follows:
- Aside from forbidden band gap energies, electrons can exist in a continuum of energies.
Optical Absorption

- But what if we reduced the size of the semiconductor until the states were quantized?
  - The lowest energy transition from valence band to conduction band has now increased.

Optical Absorption

- I.e. as we reduced the size of the semiconductor we observe a blue shift in the absorption spectrum.
  - This has been observed experimentally.

Dingle et. al. PRL 33 (1976) 827
Optical Absorption

- If we approximate the potential well as infinite, it is reasonably straightforward to calculate the blue shift as a function of quantum well size.

- Last time we determined the energy \( E \) electrons were permitted to have in an infinite well:
  \[
  E = \frac{\hbar^2 \pi^2 n^2}{8ma^2}
  \]

- We can equivalently say for states in the condition band \( E_n \):
  \[
  E_n = E_{xy} + \frac{\hbar^2 \pi^2 n^2}{8m_e^* a^2}
  \]
  - \( E_{xy} \): Band edge energy.
  - \( m_e^* \): Effective mass.

This has been verified experimentally.

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Dingle et. al. PRL 33 (1976) 827
Finite Potential Well

• So far we have established that a finite quantum well has discreet energy states
• But what about the wavefunction itself?
• It is not hard to run through the evaluation of $\Psi$ given what we know, but we will just take some results:
Wavefunction

• In particular, we notice that for certain states the probability is non-zero inside of the barrier.
• This means if we have an electron inside our well, it has a finite probability that when measured it will be found outside of the well.
• There is no analog for this in classical mechanics. It is a direct result of quantum mechanics.
• What does this mean?
  • That electrons can leak (tunnel) out of their well.

Tunneling Barriers

• What about if we constructed a thin barrier and directed electrons towards it?

• If it is thin enough, electrons should be able to move (tunnel) through the barrier.
Finite Barriers

• In this situation we would expect some electrons to be reflected and some to be transmitted.
• We can quantify transmission probability using a similar approach to before.

Moving electrons are described by plane waves. Hence to the left we say:

$$\Psi(x) = A e^{ikx} + B e^{-ikx}$$  \hspace{1cm} (23)

• Within the barrier ($0 < x < b$) we use the same solution as last time:

$$\Psi(x) = C \exp(\kappa x) + D \exp(-\kappa x)$$  \hspace{1cm} (24)

• To the right we also have a plane wave solution:

$$\Psi(x) = F e^{ikx}$$  \hspace{1cm} (25)
Tunneling

- In this case, we not necessarily aiming to solve the equation / energy levels.

- We want to know what % of electrons will make it from left to right.

- We identify this as the ratio of probabilities on each side. If we define this as the transmittance, $T$:

$$T = \frac{|F|^2}{|A|^2}$$

We can proceed as before, enforcing that both $\Psi$ and $d\Psi/dx$ are continuous at $x = 0, b$.

- This time we ill just take the results:

\begin{align*}
A + B &= C + D \quad (26) \\
A - B &= \frac{\kappa}{ik} (C - D) \quad (27) \\
C \exp(\kappa b) + D \exp(-\kappa b) &= F \exp(ikb) \quad (28) \\
C \exp(\kappa b) - D \exp(-\kappa b) &= \frac{\kappa}{ik} F \exp(ikb) \quad (29)
\end{align*}
Tunneling

• Adding (26) + (27), adding (28) + (29), and subtracting (29) from (28) give the following three equations:

\[ 2A = \left( 1 + \frac{\kappa}{ik} \right) C + \left( 1 - \frac{\kappa}{ik} \right) D \]  
\[ 2C \exp(\kappa b) = \left( 1 + \frac{\kappa}{ik} \right) F \exp(ikb) \]  
\[ 2D \exp(-\kappa b) = \left( 1 - \frac{\kappa}{ik} \right) F \exp(ikb) \]  

• Combining these equations we can get \( F/A \):

\[ \frac{F}{A} = \frac{4i\kappa k \exp(-ikb)}{(2i\kappa k + \kappa^2 - k^2) \exp(-\kappa b) + (2i\kappa k - \kappa^2 + k^2) \exp(\kappa b)} \]  

Tunneling Probability

• Equation (33) can be evaluated to give you an exact solution, but in most cases the tunneling probability is small, and the \( e^{-\kappa b} \) term in the denominator can be ignored.

• This makes it a lot easier to evaluate the tunneling probability:

\[ T = \frac{|F|^2}{|A|^2} = \frac{16E(V_0 - E)}{V_0^2} e^{-2\kappa b} \]  

• So while the potential height does feature in this equation, the probability is much more (exponentially) dependent on the barrier width \( b \).
Schottky Contacts

- We will not do it, but you could apply the same strategy to metal-semiconductor contacts

![Diagram of Schottky Contacts](image)

- We largely neglected this process in Lecture 10.

Flash Memory

- Let’s look at a specific example: a flash drive.
- Flash memory is non-volatile, meaning states are retained for long times.
- These devices operate using floating gate transistors.
Fowler–Nordheim Tunneling

- Consider the band diagram vertically.
- We will ignore band-bending, image force lowering and other non-idealities.
- We will assume the tunnel dielectric is \( \lesssim 5 \text{nm} \) thick.

Fowler–Nordheim Tunneling

- What happens if we ground the gate, and apply a voltage to the drain?
Fowler–Nordheim Tunneling

- Let’s just look at the semiconductor, tunnel dielectric and floating gate.

- Let’s look at the conduction band and consider where electrons are allowed:

- We now know that because if the barrier is thin enough the electrons will be able to tunnel through it.

- When tunneling through the entire barrier like this, the probability is primarily due to the thickness of the dielectric itself.

- Difficult to control tunneling with a voltage in this case.
Fowler–Nordheim Tunneling

• However if we apply a very large bias across this structure the effective tunneling distance can be reduced significantly.

Fowler–Nordheim Tunneling

• Tunneling across the top of the barrier like this is called **Fowler–Nordheim Tunneling**.
  
  • The important aspect of this phenomenon is that the angle of the tunnel barrier, and therefore the tunneling rate is highly dependent on the applied voltage.
  
  • This allows us to control the rate of tunneling by changing the voltage offset between the gate and semiconductor.
Resonant Tunneling Diodes

Double Barrier Structures

- With modern advances in deposition techniques, we are able to fabricate a wide range of interesting structures, with almost atomic resolution.
- E.g., we could make structure that have a conduction band that looks like this:

![Diagram of Double Barrier Structure]
Double Barrier Structures

- We could use similar strategies to before to evaluate the transmittance (but won’t).

![Diagram of double barrier structure]

- The method is explained well in a paper by Tsu and Esaki.\(^1\)


Double Barrier Structures

- Normally you will end up with this sort of behavior.

![Graph showing transmission vs energy]

- Energy is a proxy for voltage, meaning transmission is high for some voltages and not others.
Double Barrier Structures

- What does this mean for a device?
- It suggests that at certain voltages a lot of current should flow, while at others there should be very little.
- Note the logarithmic y-axis.
- So how do we make sense of this?
  - We need to think about the central quantum well.

![Graph showing the relationship between energy and transmittance](image)

Double Barrier Structures

- If the central layer is thin enough, we should expect the available electron states to be quantized, not a continuum:

![Diagram of double barrier structure](image)

- Remember this is just the conduction band. I.e. available, but unfilled states.
Double Barrier Structures

- The whole band structure would look something like:

  ![Diagram of a double barrier structure showing energy levels and electron distribution](image)

- Almost all electrons will be traveling at the band edge.

- At zero volts the bands are flat.
- There are no available states in the well at this energy, so the tunneling distance is long.
- Essentially this is a forbidden (or heavily attenuated) process.
Double Barrier Structures

• What about if we apply a voltage?

\[ E = eV_0 \]

\[ n = 1 \]
\[ n = 4 \]
\[ n = 3 \]
\[ n = 2 \]

• At a certain point the \( n = 1 \) state in the quantum well will line up with the electron in the left bulk semiconductor. We say it is resonant.

Double Barrier Structures

• What about as we increase the voltage further?

• Eventually the \( n = 1 \) state will drop below the electron and the path will again be blocked.
Resonant Tunneling Diodes

- These resonances give rise to a peak in current-voltage characteristics.

- These devices are called resonant tunneling diodes (RTDs) and they are characterized by a feature called negative differential resistance (NDR).

\[ R = \frac{dV}{dI} < 0 \]

Gunn Diodes

- RTDs have a few uses.
- Gunn diodes are probably the most common.
- They can be employed in a circuit with conventional components to create an unstable state.
- They can oscillate in the GHz.
- Hence they are good microwave sources.
Quantum Cascade Lasers

Triple Barrier Structures

- We will consider one final structure.
- Three barriers and two quantum wells:

$$n_1 = 1$$
$$n_2 = 2$$
$$n_3 = 3$$
$$n_4 = 4$$

- Let’s see what happens when we apply a voltage across this structure.
Triple Barrier Structures

- Let’s just look across the barriers for simplicity.

\[
\begin{align*}
V &= 0 \\
V &>> 0
\end{align*}
\]

- This process is called an **inter-sub-band transition**, and if we get everything aligned correctly, should potentially lead to photon emission.

Quantum Cascade Lasers

- One can manufacture more complicated stacks.

- Under the correct biasing conditions the electrons ”cascade” through the structure emitting light.
Quantum Cascade Lasers

- Light can be emitted at a range of frequencies, depending on design.

![Diagram showing frequency vs. wavelength and temperature for various types of quantum cascade lasers.](image)

Vitiello et al. Optics Express, 2015

- In reality the design and construction needs to be more sophisticated than the diagrams I have drawn here.

![Diagram showing a more detailed design of a quantum cascade laser.](image)

Faist et al. Science 1994

- See here for more details on QCLs:
  - [https://nanohub.org/resources/16812/watch?resid=17018&tmpl=component](https://nanohub.org/resources/16812/watch?resid=17018&tmpl=component)
PN Junctions

• How a pn-junction forms

• What happens to holes and electrons at the interface:
PN Junctions

• What happens when we apply an external voltage.

\[ J = J_0 \left[ \exp \left( \frac{eV}{k_B T} \right) - 1 \right] \]

- \( J = 0 \) for \( V = 0 \)
- \( J > 0 \) for \( V > 0 \)
- \( J < 0 \) for \( V < 0 \)

PN Junctions

• Studied a few non-idealities of pn-junctions and how they are manifest in electrical characteristics.

\[ J = J_0 \left[ \exp \left( \frac{e[V_d - IR_S]}{nk_B T} \right) - 1 \right] \]

- \( n = 2 \) (GR) - \( r_S \)-dominated
- \( n = 1 \) (DIFF)
- \( n = 2 \) (HLI)
PN Junctions

- How pn junctions breakdown when large reverse biases are applied.

Schottky Junctions

- Junction formation and band diagrams
Schottky Junctions

- Interface states and Fermi-Level pinning

- Electrostatics:

- Image force lowering:

ECE 615 – Semiconductor Devices I
Winter 2021 - John Labram
Schottky Junctions

• Emission and Injection mechanisms

\[ E \]

\[ E_C \]

\[ E_F \]

\[ e^+ \]

\[ e^- \]

\[ e^- \]

\[ e^- \]

\[ e^- \]

\[ e^- \]

Tunneling

Thermionic Tunneling

• Derivation of current-voltage characteristics:

\[ I(V) = I_s \exp \left( \frac{eV}{k_BT} \right) - 1 \]

\[ I_s = A^* T^2 \exp \left( - \frac{e\phi_{Bn}}{k_BT} \right) \]

MOS Capacitors

• Band diagrams of metal-oxide semiconductor capacitors.

\[ E_{VAC} \]

\[ e\phi_M \]

\[ e\phi_B \]

\[ e\chi_i \]

\[ e\chi_s \]

\[ e\phi_S \]

\[ E_C \]

\[ E_{FS} \]

\[ E_V \]

\[ d \]
MOS Capacitors

- Operating regimes of MOS capacitor:

Accumulation:

- Depletion:

Weak Inversion:

- Strong Inversion:

MOS Capacitors

- Quantitative description of charge density:

\[ F \left( \frac{e\phi_s}{k_BT} \frac{n_{po}}{p_{po}} \right) = \sqrt{2} \epsilon_r \epsilon_0 k_B T eL_D \left( \frac{e\phi_s}{k_BT} \frac{n_{po}}{p_{po}} \right) \]

\[ Q_{sc} = \frac{\sqrt{2} \epsilon_r \epsilon_0 k_B T eL_D}{eL_D} F \left( \frac{e\phi_s}{k_BT} \frac{n_{po}}{p_{po}} \right) \]

\[ C_D = \frac{\epsilon_r \epsilon_0}{\sqrt{2} L_D} \left( 1 - \exp \left( \frac{e\phi_s}{k_BT} \right) + \frac{n_{po}}{p_{po}} \left( \exp \left( \frac{e\phi_s}{k_BT} \right) - 1 \right) \right) F \left( \frac{e\phi_s}{k_BT} \frac{n_{po}}{p_{po}} \right) \]
MOS Capacitors

- We looked at “ideal” CV curves:

![Image of MOS Capacitors diagram]

- The how oxide charges can effect measurements:

Heterojunctions

- Classification of heterojunctions:

![Image of Heterojunctions diagram]
Heterojunctions

• How to draw the band diagram for a heterojunction 2-terminal device:

![Band Diagram of Heterojunction](image1)

Heterojunctions

• How we deal with interface states in heterojunctions:

![Interface States Diagram](image2)
Heterojunctions

- Electrostatics of anisotype heterojunction:
- How to deal with isotype junctions:

![Diagram of heterojunction](image)

Finally, we looked at the current voltage characteristics of heterojunctions.
Quantum Mechanics

- We studied the basics of quantum mechanics.

\[ E_n = \frac{\hbar^2 \pi^2 n^2}{8ma^2} \]

Quantum Devices

- Then we studied a few devices with exploit quantum tunnelling.
My Course Objectives

- The goal was to provide the following:
  - Overview of the theoretical operation of the most important (technologically) two-terminal electronic devices.
  - The basic models that are used to describe these devices quantitatively.
  - Start to look at some the issues that take us away from “ideal” behavior and strategies to quantify them.
  - In industry / research you are likely to use more specific, propriety models, typically solved numerically.
- The goal was not the following:
  - Get you to memorize a load of formulae, acronyms, etc. you will forget immediately after the exams.

Student Evaluation of Teaching

- Please complete the assessment when you get a chance.
- eSET is open now.
- These scores are taken very seriously by the College of Engineering.
- I’m not tenured → even more important for me.
- The College will not consider scores if less than 5 report.
  - In this case it is as if I have not taught the course.
  - So for a small class like this it is very important.
Thanks for Taking the Course!