Quantum Transport:
Atom to Transistor

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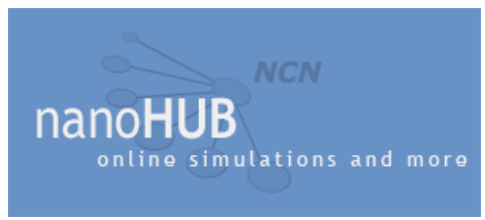
Lecture 22: Subbands: Minimum Resistance of a Wire and Velocity of (sub)band electrons

Ref. Chapter 6.3 & 6.4

Network for Computational Nanotechnology



Introduction

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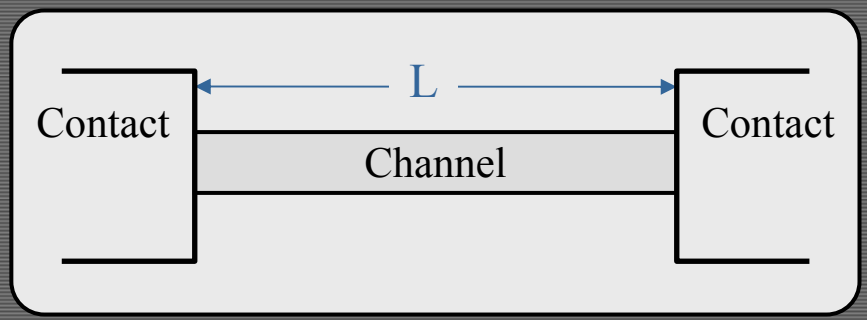
• Resistance of a conductor, of course, decreases as the length of the channel decreases. But at some point it reaches a minimum and decreases no further.



• The minimum resistance comes from the contact resistance. The smaller the device the more important this contact resistance. One might assume that this resistance may be eliminated by improving the contacts; this simply is not true. There is **a minimum contact resistance.**

• Minimum contact resistance is given by

$$R_{\min} = \frac{h}{2q^2}\frac{1}{[M(E)]_{E=E_f}}$$

where $[M(E)]_{E=E_f}$ is the number of subbands (modes) at the Fermi level.

• Similarly, conductance per spin per subband is $G_{\max} = q^2/h$ and the total conductance is:

$$G_{\max} = \frac{2q^2}{h}[M(E)]_{E=E_f}$$

Prelude to Modes

04:54

• Previously, at the beginning of the course, one level conductance was discussed for which the expression $G_{\max} = 2q^2/h$ was derived.

• Now that we've discussed subbands we can discuss the concept of modes

• Shouldn't the resistance decrease as the cross sectional area is increased? If yes, can we predict such thing from this relation?

$$R_{\min} = \frac{h}{2q^2}\frac{1}{[M(E)]_{E=E_f}}$$

Yes. As we increase the channel cross-section, the number of modes increases, so the resistance goes down.

• Even when talking about real world devices there is a *minimum* resistance, for example, with current FET's it is approximately 100Ω

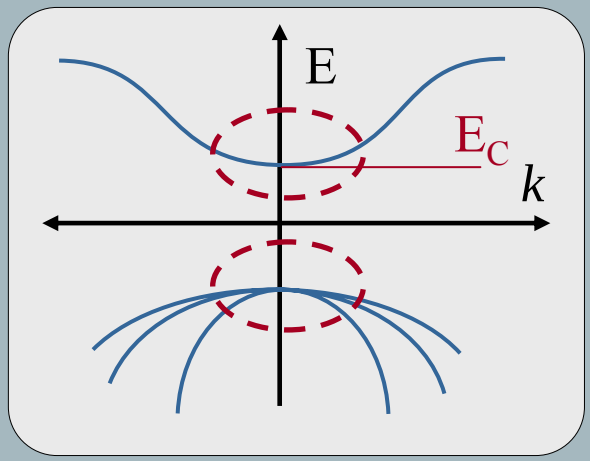
• The number of modes at a given energy equals the number of subbands available at that energy

• Let us review the major concepts of subbands and then move onto a general picture of conduction modes.

Conduction Band Parabolic Model

10:07

• Recall, for the familiar E-k diagram (e.g. Si or Ge)…



• We are largely interested in the areas circled above because they determine the conduction and optical properties of a material. To simplify matters we create a parabolic model of the curvature in these areas

• Particularly, for the conduction band we use $E = E_C + h^2/2m_C \left(k_x^2 + k_y^2 + k_z^2\right)$

where E_C is the bottom of the conduction band and m_C is the effective mass (it is obtained by fitting the parabola to the E-k curve)

• Recall the concept of subbands. One or more dimensions is made considerably small such that k-space becomes discernibly discrete in that direction

• For example, if the z-dimension is made very small we get $k_z = p\,\pi/L_z$ and a quantum well results

$$E_p\left(k_x, k_y\right) = E_C + \frac{p^2\hbar^2\pi^2}{2m_C L_z^2} + \frac{\hbar^2}{2m_C}\left(k_x^2 + k_y^2\right)$$

Subband Confinement

15:45

• **CAVEAT:** Quantitative details of subband energies is often more complex than suggested by this simple model.

• To continue, further confinement in the y-direction results in a quantum wire

$$k_y = n\pi / L_y$$

$$E_{njp}(k_x) = E_C + \frac{p^2\hbar^2\pi^2}{2m_C L_z^2} + \frac{n^2\hbar^2\pi^2}{2m_C L_y^2} + \frac{\hbar^2}{2m_C}k_x^2$$

• One could argue that any solid should have subbands as well. But the primary point is that we only worry about discretization when

$$\frac{v^2\hbar^2\pi^2}{2m_C L},$$

(where v is an integer and L the length of a dimension), is equal to or greater than $k_B T$. Usually this is too fine to be experimentally observable in large structures.

Real World Subbands

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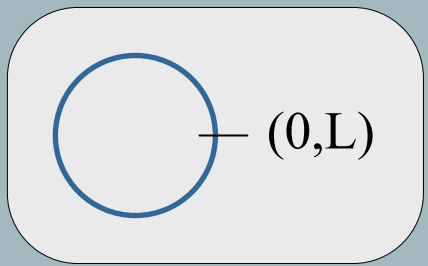
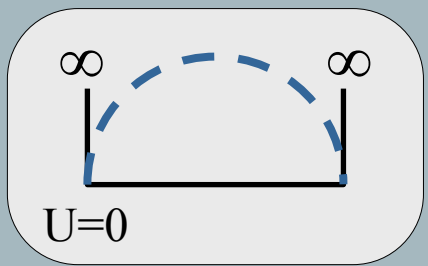
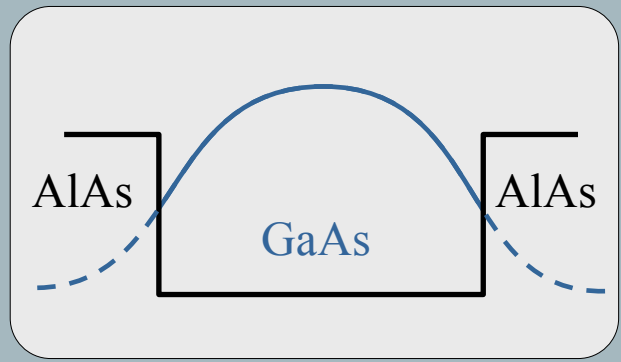
• Generally, there are two types of confinement which cause quantization in the real world. The first is described by periodic boundary conditions



The carbon nanotube is likely the only example of this. The second is described by two potential barriers often idealized as “infinite”



• GaAs sandwiched between two blocks of AlAs provides a real world example of this…

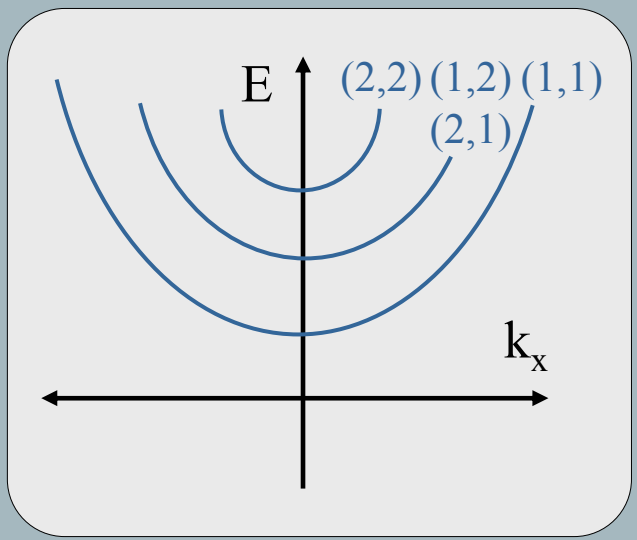


Of course, the “infinite” barrier is not really infinite and there is some leakage of the wavefunction (this is shown above)

Quantum Wire Subbands

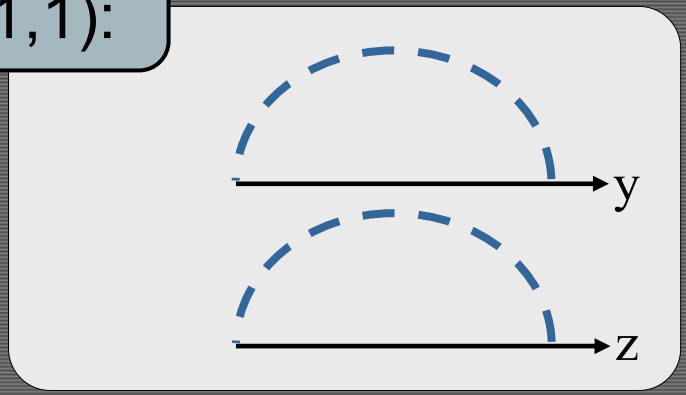
23:15

- For the quantum wire we get various subbands corresponding to different values of n and p or (n,p)

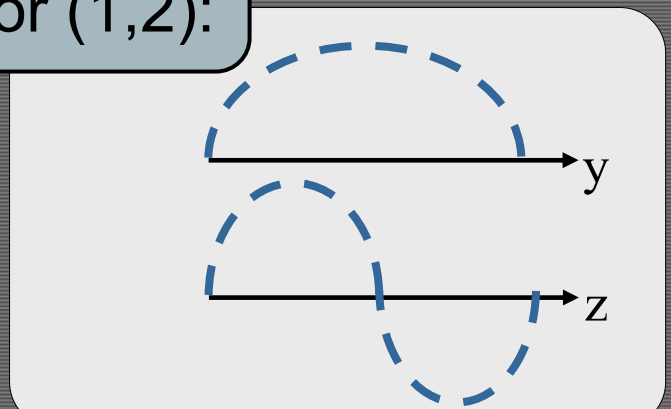


- The quantized wave functions in the y and z directions look like →

For (1,1):

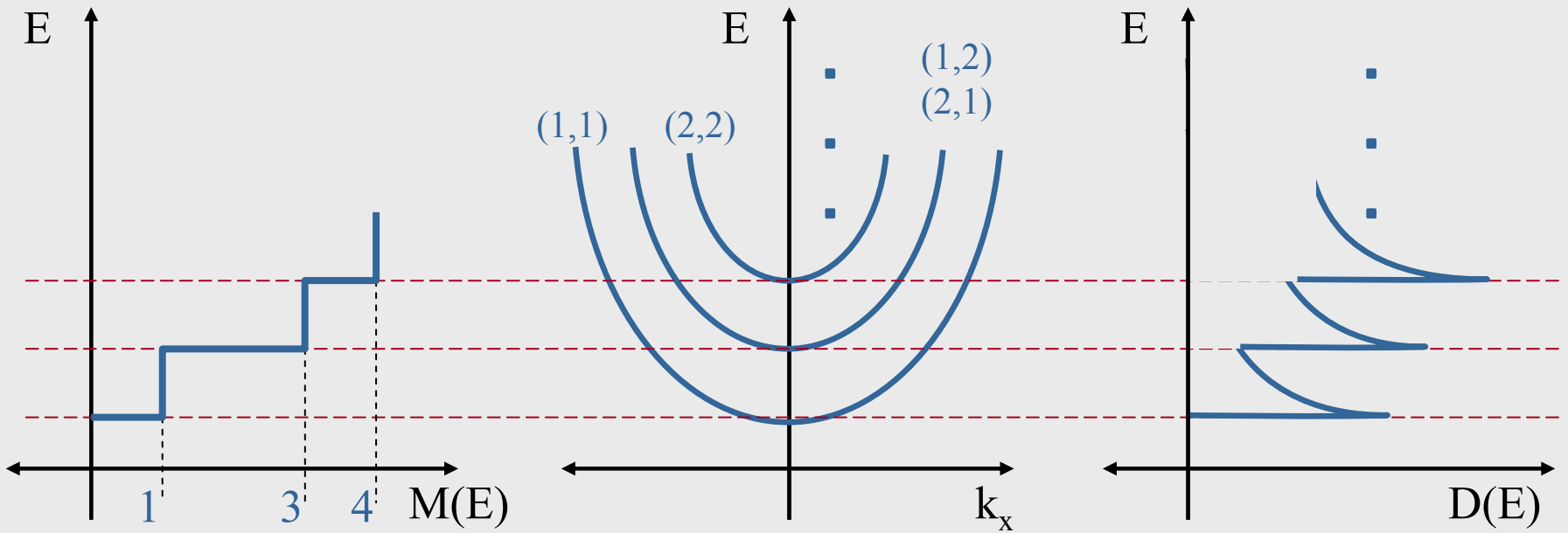


And For (1,2):



Quantum Wire Subbands, DOS and Modes

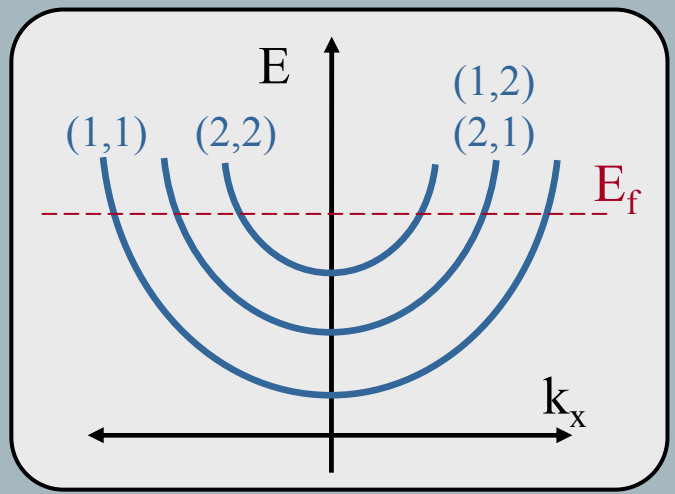
• Now, what does the density of states and modes distribution look like for a quantum wire? Clearly, as with the carbon nanotube, the density of states peaks where each subband is crossed. The mode distribution, on the other hand, has a staircase distribution increasing by integer amounts of 1 or more depending on the degeneracy of the subband



General Approach to Counting Modes

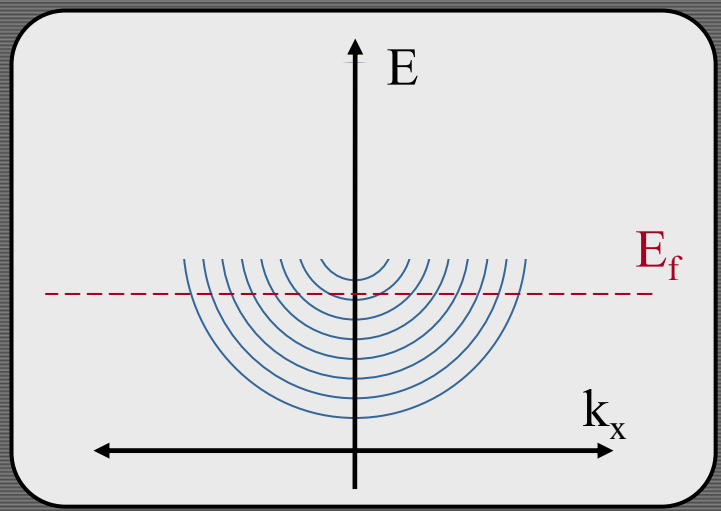
• From the previous diagram we can conclude that the number of modes available for conduction depends on the relative position of the Fermi energy. For example, if the Fermi energy is positioned as shown below we get $\left[M(E)\right]_{E=E_f} = 4$ and

$$G_{\max} = 4 \times {2q^2}/{h}$$



• As a conductor increases in size the subbands get closer together, with the Fermi energy remaining unchanged this means that the resistance goes down! (More modes lie below the Fermi energy)

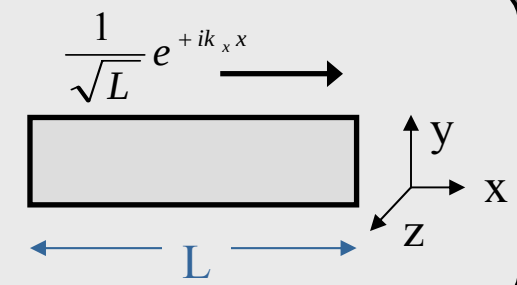
Bigger Conductor

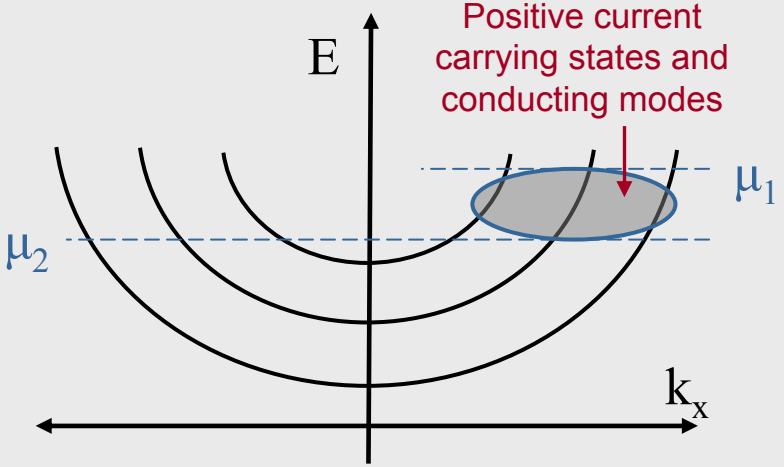


Current and Modes

• When voltage is applied, the current carried by a material is dependent upon the number of modes between μ_1 and μ_2

Quantum Wire of Length L





• Given a quantum wire of length L, how do we calculate the current carried?

• First, the number of electrons available for conduction is given by

$$n = \sum_{k_x} 1/L$$

This follows from a consideration of electron density

$$\rho = \sum_{\alpha} |\phi_\alpha|^2 f_0(\varepsilon_\alpha - \mu)$$

at near absolute zero with $\phi_\alpha = 1/\sqrt{L}\, e^{ik_x x}$

(to be explained further in subsequent lectures)

Current for a Single Mode I

• If we look at a single mode in a subband (n, p), for the quantum wire energy relation

$$E_{n,p}(k_x) = E_C + \frac{n^2\hbar^2\pi^2}{2m_C L_y^2} + \frac{p^2\hbar^2\pi^2}{2m_C L_z^2} + \frac{\hbar^2}{2m_L}k_x^2$$

The conduction current may be written as

$$I = -qnv = \frac{-q}{L}\sum_{k_x} v_x(k_x)$$

Where $v_x(k_x)$ is the group velocity of an electron at state k_x in the mode of interest

• For a long conductor, this summation is replaced by the integral

$$I = \frac{-q}{L}\int dk_x v_x(k_x) \times \frac{L}{2\pi}$$

(recall, the spacing between two points in k-space is $(2\pi)/L$)

• But, velocity is

$$v_x(k_x) = \frac{\hbar k_x}{m_C}$$

$$\therefore I = -q\int \frac{dk_x}{2\pi}\cdot\frac{\hbar k_x}{m_C}$$

Current for a Single Mode II

40:00

• Furthermore, given

$$E_{n,p}(k_x) = E_C + \frac{n^2\hbar^2\pi^2}{2m_C L_y^2} + \frac{p^2\hbar^2\pi^2}{2m_C L_z^2} + \frac{\hbar^2}{2m_C}k_x^2$$

$$\therefore dE = \frac{\hbar^2}{m_C}k_x dk_x$$

$$\text{and } I = -q\int\frac{dE}{2\pi\hbar} = \frac{-q}{h}\int dE$$

• More generally, we can write the maximum current for a single mode as

$$I = \frac{-q}{h}(\mu_1 - \mu_2) = \frac{q^2}{h}V$$

where V is the bias voltage

• Conclusion: What is the current carried by electrons in a certain energy range? It is q/h multiplied by that energy range. For the provided example $\int dE = \mu_1 - \mu_2$. Since only the positive velocity states are occupied between μ_1 and μ_2, this represents the excess positive going electrons. Below μ_2 both the positive and negative velocity states are equally occupied and their contributions cancel.

General Conclusion For Current

45:00

• Importantly, the current carried by a subband is independent of the subband shape, it need not be parabolic, the relation holds for all cases!

$$I = \frac{-q}{h}\int dE$$

• This is because the correct velocity is the group velocity:

$$v_x(k_x) = \frac{1}{\hbar}\frac{\partial E}{\partial k_x}$$

thus

$$I = -q\int \frac{dk_x v_x(k_x)}{2\pi}$$

$$= -q\int \frac{dk_x}{2\pi\hbar}\frac{\partial E}{\partial k_x} = \frac{-q}{h}\int dE$$

• Overall the amount of current is dictated by the number of modes between μ_1 and μ_2. Each mode contributes $\frac{-q}{h}\int dE$

for a total current of

$$I = \frac{-q}{h}(\mu_1 - \mu_2)\cdot[M(E)]_{E=E_f}$$