Part 4. Two Terminal Quantum Wire Devices

Part 4. Two Terminal Quantum Wire Devices

Let's consider a quantum wire between two contacts. As we saw in Part 2, a quantum wire is a one-dimensional conductor. Here, we will assume that the wire has the same geometry as studied in Part 2: a rectangular cross section with area $L_x.L_y$. Electrons are confined by an infinite potential outside the wire, and can only flow along its length; arbitrarily chosen as the z-axis in Fig. 4.1.
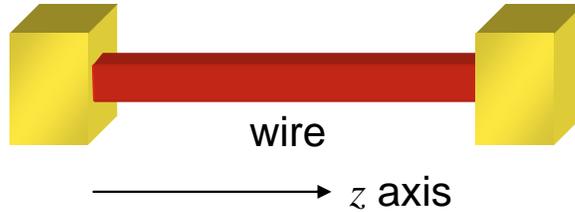
Fig. 4.1. A quantum wire between two contacts.

Under these assumptions, if we model the electrons by plane waves in the z direction we get

$$E = \frac{\pi^2 \hbar^2}{2m} \left(\frac{n_x^2}{L_x^2} + \frac{n_y^2}{L_y^2} \right) + \frac{\hbar^2 k_z^2}{2m}, \quad n_x, n_y = 1, 2, ... \tag{4.1}$$
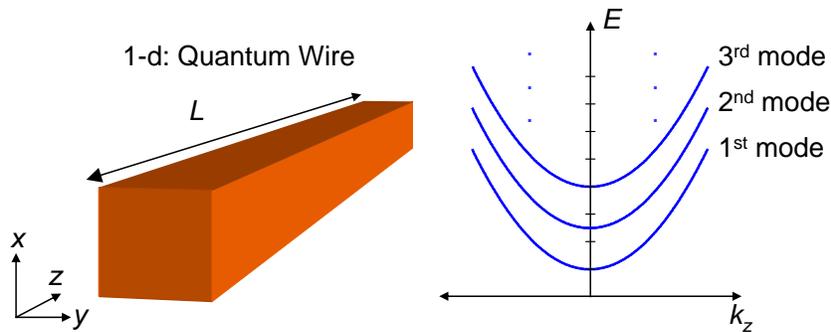
Fig. 4.2. Plane waves in a quantum wire have parabolic energy bands.

Recall that for current to flow there must be difference in the number of electrons in $+k_z$ and $-k_z$ states. As in Part 2, we define two *quasi* Fermi levels: F^+ for states with $k_z > 0$, F^- for states with $k_z < 0$. Thus, current flows when electrons traveling in the $+z$ direction are in equilibrium with each other, but not with electrons traveling in the $-z$ direction. For example, in Fig. 4.3, current is carried by the uncompensated electrons in the $+k_z$ states.
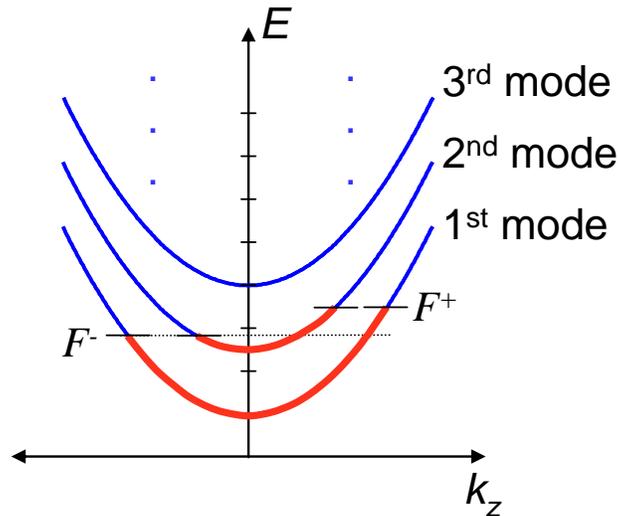
Fig. 4.3. Current flows when the quasi Fermi levels differ for $+k_z$ and $-k_z$. states.

Scattering and Ballistic Transport

Next, let's assume that electrons travel in the wire without scattering, *i.e.* the electrons do not collide with anything in the wire that changes their energy or momentum. This is known as 'ballistic' transport - the electron behaves like a projectile traveling through the conductor.

Electron scattering is usually caused by interactions between electrons and the nuclei. The probability of an electron collision is enhanced by defects and temperature (since the vibration of nuclei increases with temperature). Thus, the scattering rate can be decreased by lowering the temperature, and working with very pure materials. But all materials have some scattering probability. So, the smaller the conductor, the greater the probability that charge transport will be ballistic. Thus, ballistic transport is a nanoscale phenomenon and can be engineered in nanodevices.

For ballistic transport the electron has no interaction with the conductor. Thus, *the electron is not necessarily in equilibrium with the conductor*, i.e. the electron is not restricted to the lowest unoccupied energy states within the conductor.

But scattering can bump electrons from high energy states down to lower energies. There are two categories of scattering: elastic, where the scattering event may change the momentum of the electron but its energy remains constant; and inelastic, where the energy of the electron is not conserved. Equilibrium may be established by inelastic scattering.

Electron scattering is the mechanism underlying classical resistance. We will spend a lot more time on this topic later in this part.

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(a) Ballistic transport

electron

(b) Scattering
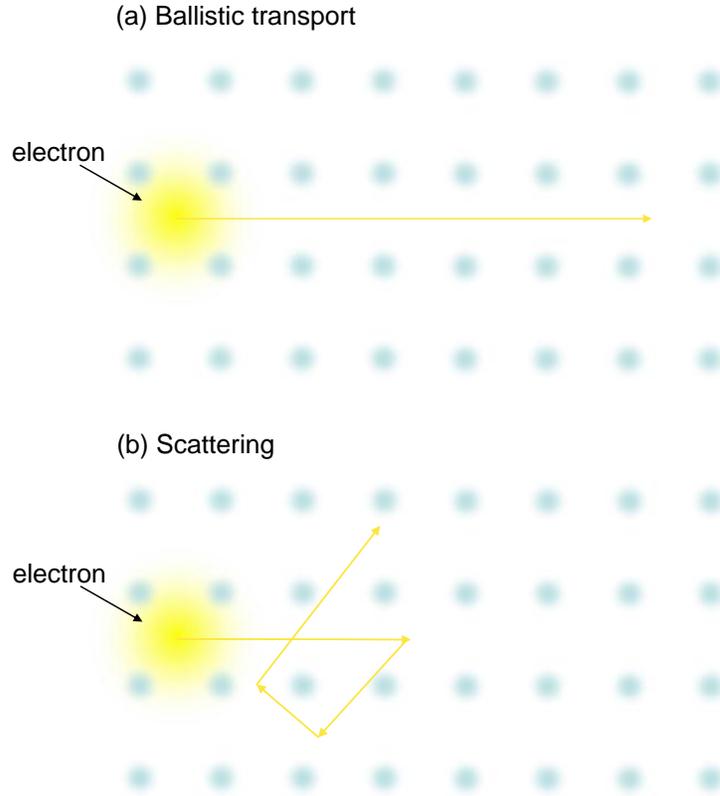
electron

Fig. 4.4. Here, we represent an electron traveling through a regular lattice of nuclei. If the electron travels ballistically it has no interaction with the lattice. It travels with a constant energy and momentum and will not necessarily be in equilibrium with the material. If, however, the electron is scattered by the lattice, then both its energy and momentum will change. Scattering assists the establishment of equilibrium within the material.

Equilibrium between contacts and the conductor

When the contact is connected with the wire, equilibrium must be established. For example, if F is higher than the chemical potential of the contact, μ, then electrons will diffuse from the wire into empty states in the contact. This is known as depletion. If the electrons are not replenished from another source, the loss of electrons lowers the Fermi level within the wire. In addition, since the wire has lost negative charge, it becomes positively charged, establishing an electric field that counteracts the diffusion of electrons out of the wire. Ultimately equilibrium is established when the Fermi level in the wire equals the chemical potential of the contact. If all the electrons diffuse out of the wire then the wire is said to be fully depleted.

If the chemical potential of the contact is higher than the Fermi level in the wire. Electrons diffuse into the wire from the contact, raising the Fermi level. This is known as accumulation. The addition of negative charge also establishes an electric field that counteracts the diffusion of electrons from the contact to the wire.

(a) Diffusion from wire to contact

(b) Diffusion from contact to wire
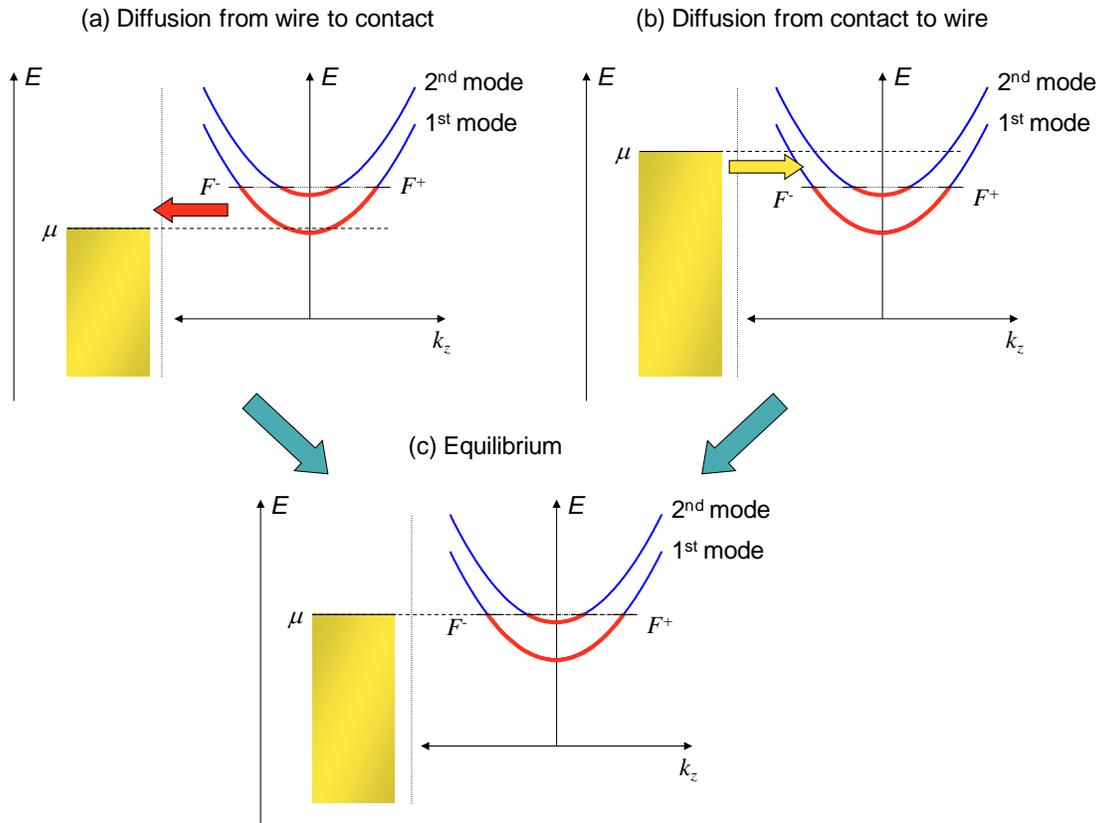
(c) Equilibrium

Fig. 4.5. Equilibrium is obtained at the interface between a contact and a conductor when the diffusion currents in and out of the conductor match.

Bias

Now, what happens when a voltage is applied between the contacts? Recall that applying voltage shifts the relative potential energies of each contact, i.e. $\mu_D - \mu_S = -qV_{DS}$, where the chemical potential of the source is μ_S and the chemical potential of the drain is μ_D.

As in the equilibrium case, charges flow from each contact, ballistically through the conductor and into the other contact. Thus, all states with $k_z > 0$ are injected by the source and have no relation with the drain. Similarly, electrons with $k_z < 0$ are injected by drain.

But now the injected currents do not balance. Conductor states in the energy range between μ_S and μ_D are uncompensated and only be filled by the source, yielding an electron current flowing from source to drain in Fig. 4.6.

The quasi Fermi level for electrons with $k_z > 0$, F^+ must equal the electrochemical potential of the left contact, *i.e.*

$$F^+ = \mu_S.$$

Similarly,

$$F^- = \mu_D.$$

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Thus, current can only flow when there is a difference between the chemical potentials of the contacts. This shouldn't be surprising, since the difference between chemical potentials is simply related to the voltage by $\mu_D - \mu_S = -qV_{DS}$.
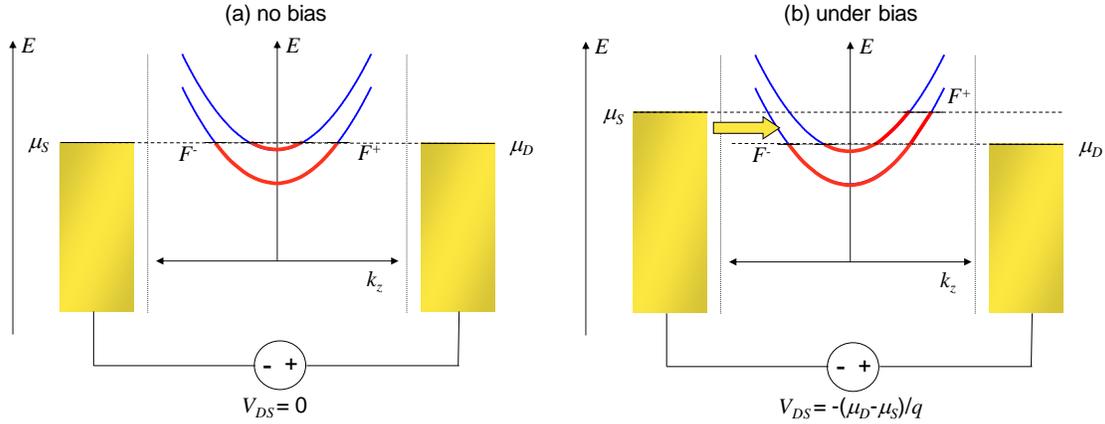
Fig. 4.6. Under bias the Fermi Levels of each contact shift. Diffusion from states in the contact with the higher potential causes a current.

The Spatial Profile of the Potential

As shown in Fig. 4.7, below, the wire may be described by its dispersion relation or by its density of states (DOS). The dispersion relation describes a band of conducting states. The bottom of the band is known as the conduction band edge. It corresponds to the lowest energy for a plane wave state in the wire. The conduction band edge is particularly important because its position controls the current flow in the wire. If it is below the source work function then electrons are readily injected into the wire. In contrast, if the conduction band edge is above the source workfunction, then current flow requires electrons with additional thermal energy.
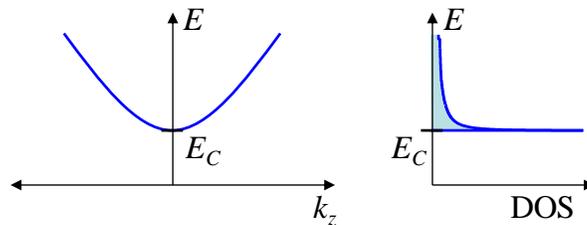
Fig. 4.7. Two representations of a 1-d quantum wire. The dispersion relation at left shows a band of energies available for conduction. The density of states at right drops to zero below the conduction band edge (E_C).

(a) No injection from source at T = 0K   **(b)** Electrons readily injected into wire
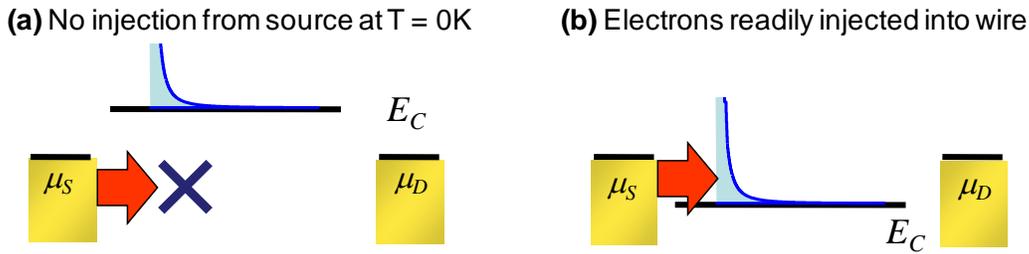
Fig. 4.8. The position of the conduction band edge, E_C, determines whether charge can be injected from the source into the wire.

The application of a bias may later the position of the conduction band edge by changing the local electrostatic potential, U. Two examples are shown in Fig. 4.9, below.
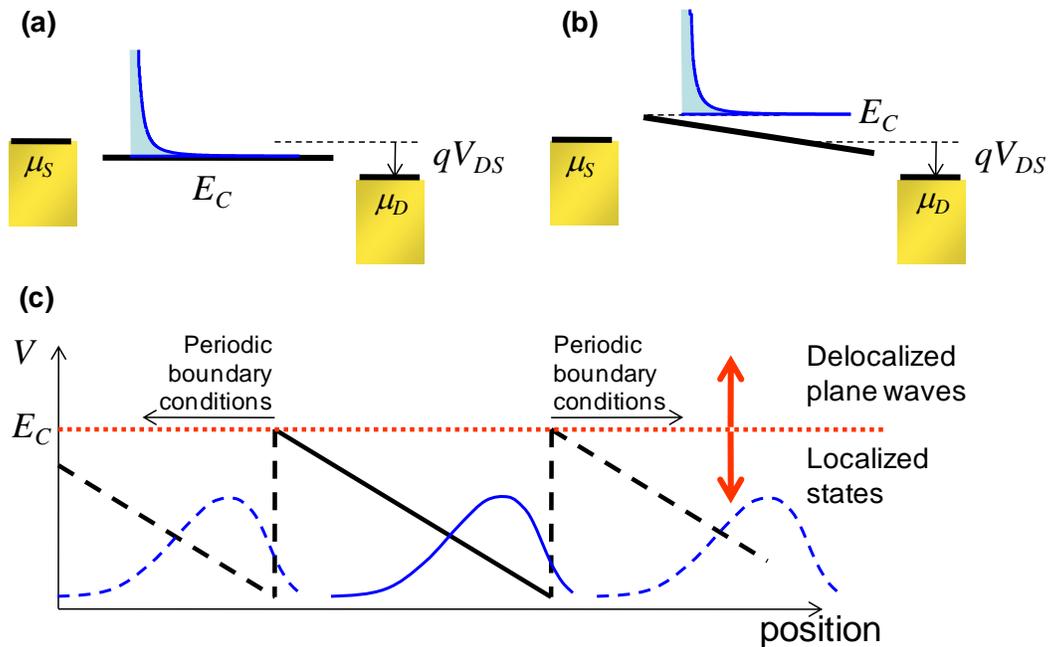
Fig. 4.9. (a) A metallic wire under bias. **(b)** An insulating or nanoscale wire under bias. Note that the conduction band edge corresponds to the maximum potential in the wire. This is explained in **(c)**, where we consider the electronic wavefunctions in the wire under bias. We have applied periodic boundary conditions to help demonstrate that electronic states with energies below the maximum potential are localized. These states may only be accessed by tunneling from the source. Electronic states above the maximum potential are delocalized plane waves. Consequently, the conduction band edge is positioned at the point of the maximum repulsive potential in the wire.

The first example in Fig. 4.9 demonstrates a metallic wire under bias. In this limit there is no potential variation along the wire. In (b) of Fig. 4.9 we present a wire with varying potential along its length. The conduction band edge, E_C, occurs at the point of maximum repulsive potential. This is explained in (c) of Fig. 4.9. Electronic wavefunctions in the

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wire with energies below E_C are localized and may only be accessed from the source by tunneling through a repulsive potential. Due to the relatively low rate of injection into these states we will ignore current through these modes in this class. Above E_C, however, the electron wavefunctions are delocalized plane waves which readily transport electrons between the contacts.

Determining the potential profile of the wire can be Consider a point, z, on the wire. The electrostatic potential at point z is given by

$$U(z) = -qV_{DS}\frac{C_D(z)}{C_{ES}(z)}$$

(4.2)

where C_D is the capacitance linking the point at z to the drain, and C_S is the capacitance linking the point at z to the source, and $C_{ES}(z)$ is the total electrostatic capacitance at z; $C_{ES}(z) = C_S(z) + C_D(z)$.

If we assume that source and drain capacitances can be modeled by parallel plate capacitors, we found in Eq. (3.15) that the potential varies linearly between the contacts. However, charging of the conductor can change the potential profile by opposing changes induced by the drain source voltage. Adding the effect of charging to Eq. (4.2) gives:

$$U = -qV_{DS}\frac{C_D}{C_{ES}} + \frac{q^2(N-N_0)}{C_{ES}}$$

(4.3)

Remember that all these electrostatic capacitances vary with position along the wire. Next, let's assume that applied bias is small and consequently the change in charge is small i.e. $\delta N = N - N_0$. We can relate δN to the density of states at the Fermi level in the wire, $g(E_F)$, and the change in potential, δU.

$$\delta N = -g(E_F)\delta U$$

(4.4)

Combining Eq. (4.4) with a small signal Eq. (4.3) gives

$$\delta U = -q\delta V_{DS}\frac{C_D}{C_{ES}} - \frac{q^2 g(E_F)}{C_{ES}}\delta U$$

(4.5)

Substituting the quantum capacitance $C_Q = q^2 g(E_F)$ and collecting terms gives

$$\delta U = -q\delta V_{DS}\frac{C_D}{C_{ES} + C_Q}$$

(4.6)

The equivalent circuit is shown in Fig. 4.10. Note that the quantum capacitance depends on the position of the Fermi level within the DOS. Because the potential shifts the DOS relative to the Fermi level, the quantum capacitance also depends on the potential.

In this class we'll consider two extreme cases: $C_Q \gg C_{ES}$ and $C_Q \ll C_{ES}$. The former case corresponds to a perfectly metallic wire. The later case can correspond to either a perfect insulator or a nanoscale conductor, which due to its size, has very few electronic states.
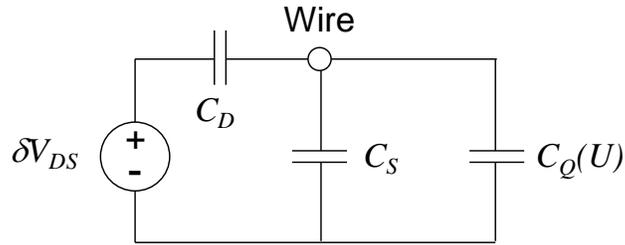
Fig. 4.10. The equivalent circuit to determine the potential in a nanowire under bias. When the quantum capacitance, C_Q, is large the potential in the wire varies little with applied bias. This corresponds to the behavior of a metallic wire. In insulators or smaller wires with fewer electronic states, the potential varies with position in the wire.

(i) Perfectly metallic wires

In the limit that $C_Q >> C_{ES}$, Eq. (4.6) reduces to $\delta U = 0$, meaning that the potential is fixed along the length of the wire by the large density of states at the Fermi Level. The potential of the wire relative to the contacts is then determined by the contact properties, in particular the coupling coefficients τ_S and τ_D. The potential is determined from the analysis of Fig. 3.25.
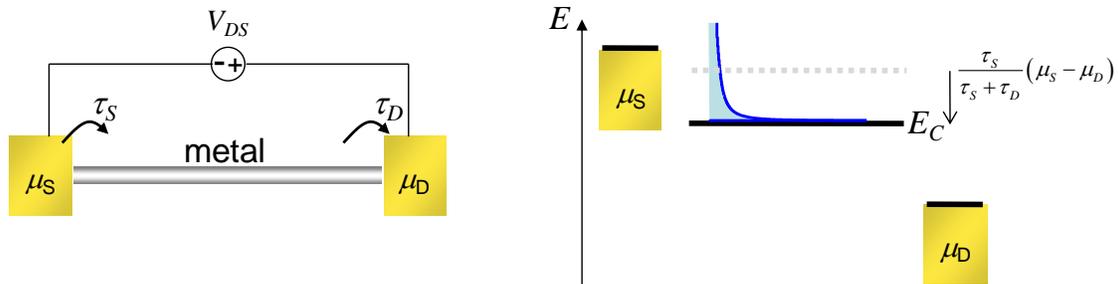
Fig. 4.11. The potential of a metallic wire is constant along its length. The position of the conduction band edge can be modeled by a voltage divider where the source and drain coupling coefficients τ_S and τ_D, respectively, represent the source and drain contact resistors.

(ii) The Insulator/Nanoscale Limit

The spacing between k states in a 1-d conductor is simply $\Delta k = 2\pi/L$, where L is the length of the wire. When L is small there are few states available for electrons. Consequently, insulators and many very small conductors have relatively few states for electrons at the Fermi level. We can ignore charging effects in these conductors. The potential is then simply described by Eq. (4.2).

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The quantum limit of conductance

We've seen that in a quantum wire, current flow requires a difference in the quasi Fermi levels for electrons moving with and against the current. Furthermore, only electrons between the quasi Fermi levels, i.e. $F^- < E < F^+$ carry current.
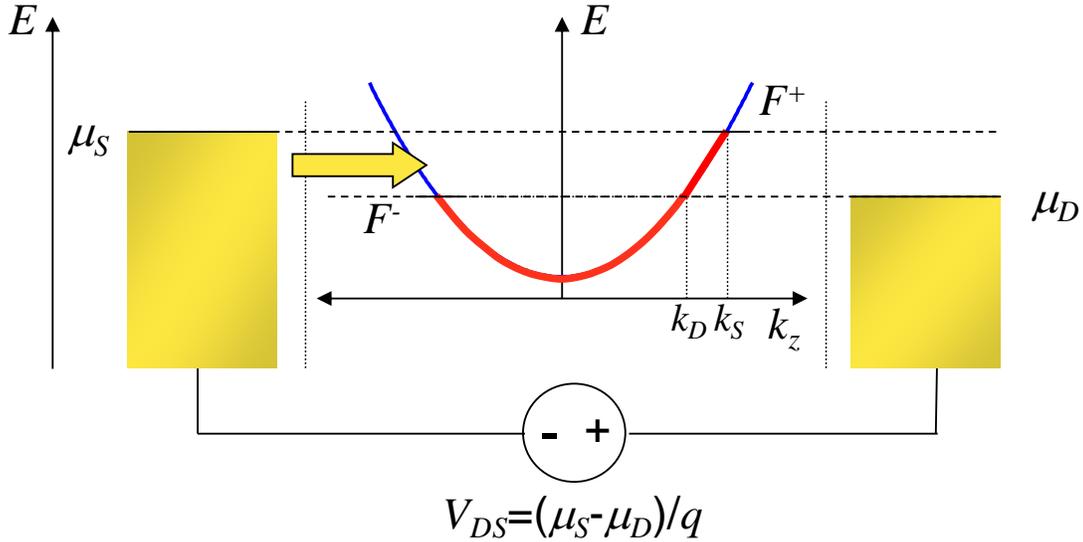
Fig. 4.12. In a single mode wire under bias, k states between k_D and k_S contain uncompensated electrons.

In general, the total current in a quantum wire is
$$I = qN/\tau \tag{4.7}$$
where N is the number of uncompensated electrons, and τ is their transit time (the time they take to cross from one end of the wire to the other). Let's use Eq. (4.7) to calculate the current in a single mode quantum wire at T=0K.

The velocity of electrons in the wire is given by the group velocity (see Problem 3)
$$v = \frac{1}{\hbar}\frac{dE}{dk} \tag{4.8}$$
As an aside, we note that if F^+-F^- is small, the current carrying electrons all move at approximately the equilibrium Fermi velocity.
$$v_F = \frac{1}{\hbar}\frac{dE}{dk}\bigg|_{E_F} \tag{4.9}$$

The transit time in Eq. (4.7) is related to the length of the wire, L, and the velocity of the uncompensated electrons:
$$\tau = \frac{L}{v} = L \bigg/ \left(\frac{1}{\hbar}\frac{dE}{dk}\right) \tag{4.10}$$

The number of uncompensated electrons is equal to the number of electrons in the states $k_D < k < k_S$, equivalent to $\mu_D < E < \mu_S$ in Fig. 4.12. Each k state occupies $\Delta k = 2\pi/L$. Recall also that there are two electrons per k state (one of each spin). Thus,

$$N = 2 \int_{k_D}^{k_S} \frac{dk}{2\pi/L} \tag{4.11}$$

Equation (4.7) is then,

$$I = 2q \int_{k_D}^{k_S} \frac{dk}{2\pi/L} \frac{1}{\hbar L} \frac{dE}{dk} \tag{4.12}$$

Simplifying gives

$$I = \frac{2q}{h} \int_{k_D}^{k_S} dk \frac{dE}{dk} \tag{4.13}$$

Changing the variable of integration to energy gives

$$I = \frac{2q}{h} \int_{\mu_D}^{\mu_S} dE$$

$$= \frac{2q}{h} (\mu_S - \mu_D) \tag{4.14}$$

Note $V_{DS} = -(\mu_D - \mu_S)/q$, thus

$$I = \frac{2q^2}{h} V \tag{4.15}$$

This expression demonstrates that the resistance of an ideal single mode wire is

$$R = \frac{h}{2q^2} \approx 12.9\,\text{k}\Omega \tag{4.16}$$

A multiple mode wire with M modes can be thought of as M single mode wires in parallel. Since parallel conductances add, the quantum limit is usually written as a conductance. For a multimode ballistic wire the conductance is

$$G_C = \frac{2q^2}{h} M \tag{4.17}$$

This is the famous quantum limited conductance. It yields the surprising conclusion that even ballistic conductors have a resistance, although this resistance is independent of the length of the conductor.

But a resistance implies that power is dissipated when a current flows. Given that electron transport in the wire is ballistic, where do the resistive power losses occur?

If we look at Fig. 4.12 we find that carriers entering the wire from the source propagate without change in potential until they reach the drain where they must come to equilibrium at chemical potential μ_D. Thus, the power is dissipated in the drain.

The quantum limit in conductance arises as a consequence of the interface between the contact with its (ideally) infinite modes and infinite number of electrons all at

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equilibrium, and a conductor with a small number of modes supporting non-equilibrium electrons. Thus, the quantum limit can be thought of as a contact resistance.

Of course, as the number of modes in the conductor increases, the contact resistance decreases. In the classical limit, it can be completely ignored.
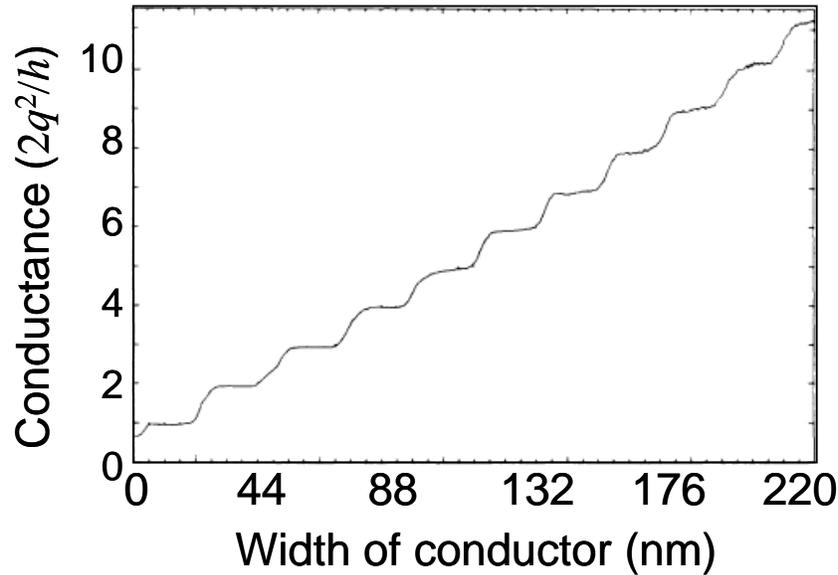
Fig. 4.13. Experimental data from van Wees, *et al* PRL **60,** 848 (1988) clearly showing conductance in a narrow conductor quantized in steps of $2q^2/h$.

The Landauer Formula[†]

We are now going to generalize the result of Eq. (4.15) by considering conduction at higher temperatures and in the presence of a scattering site.

Electrons flowing through the wire may be reflected by the scatterer. We define the transmission probability $\mathcal{T}$, of the scatterer, and assume that it acts equally on electrons flowing in either direction in the wire.
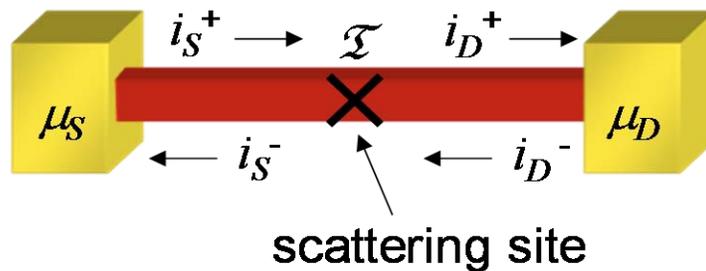
Fig. 4.14. A quantum wire containing a scatterer with transmission probability $\mathcal{T}$.

Let's define i_S^+ as the current carried by all electrons (compensated and uncompensated) in the $+k_z$ states in the wire adjacent to the source. Let i_S^- be the current carried by all electrons in the $-k_z$ states in the wire adjacent to the source. Similarly, we define i_D^+ and i_D^- as the currents entering and leaving the drain, respectively.

Generalizing Eq. (4.11) for wires with multiple modes and arbitrary temperatures, we calculate the number of electrons traveling in the $+k_z$ states adjacent to the source:

$$N_S^+ = 2\int_0^\infty \frac{dk}{2\pi/L} M\left(E(k)\right) f\left(E(k), \mu_S\right) \tag{4.18}$$

where the number of modes at energy E is $M(E)$, and as before $f(E,\mu)$ is the probability that a state of energy E is filled given the chemical potential μ. It follows that

$$i_S^+ = \frac{2q}{h}\int_0^\infty M\left(E\right) f\left(E, \mu_S\right) dE$$

$$i_D^- = \frac{2q}{h}\int_0^\infty M\left(E\right) f\left(E, \mu_D\right) dE \tag{4.19}$$

and

$$i_D^+ = \frac{2q}{h}\int_0^\infty \mathfrak{T} M\left(E\right) f\left(E, \mu_S\right) + \left(1-\mathfrak{T}\right) M\left(E\right) f\left(E, \mu_D\right) dE$$

$$i_S^- = \frac{2q}{h}\int_0^\infty \mathfrak{T} M\left(E\right) f\left(E, \mu_D\right) + \left(1-\mathfrak{T}\right) M\left(E\right) f\left(E, \mu_S\right) dE \tag{4.20}$$

The total current is $I = i_S^+ - i_S^- = i_D^+ - i_D$, this gives us the Landauer Formula

$$I = \frac{2q}{h}\int_0^\infty \mathfrak{T} M\left(E\right)\left(f\left(E, \mu_S\right) - f\left(E, \mu_D\right)\right) dE \tag{4.21}$$

Spatial variation of the electrochemical potential[†]

Next, we try to answer the question: *Where is the voltage dropped?*

Once again, let's consider a quantum wire at $T = 0$K. The wire has a single scatterer with transmission probability $\mathfrak{T}$. Uncompensated electrons emitted by the left contact are partly transmitted and partly reflected by the scatterer. Thus, to the right of the scatterer, only a fraction, $\mathfrak{T}$, of the $+k$ states in the energy range $\mu_D < E < \mu_S$ are filled. To the left of the scatterer, the fraction $(1-\mathfrak{T})$ of the $-k$ states in the energy range $\mu_D < E < \mu_S$ are filled; see Fig. 4.15(a).

After scattering the $+k$ states are no longer in equilibrium and the distribution of electrons in the $+k$ states can no longer be described by a quasi Fermi level. These electrons are said to be *hot*, and may travel some distance before they equilibrate. Similarly electrons in the $-k$ states are not in equilibrium to the left of the scatterer.

[†] This section is adapted from S. Datta, 'Electronic Transport in Mesoscopic Systems' Cambridge (1995).

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In Fig. 4.15(b) we plot the *average* quasi Fermi level of both $+k$ and $-k$ states. The change in the average quasi Fermi levels can be interpreted as a potential change in the vicinity of the scatterer of $(1-\mathfrak{T})(\mu_S-\mu_D)$.
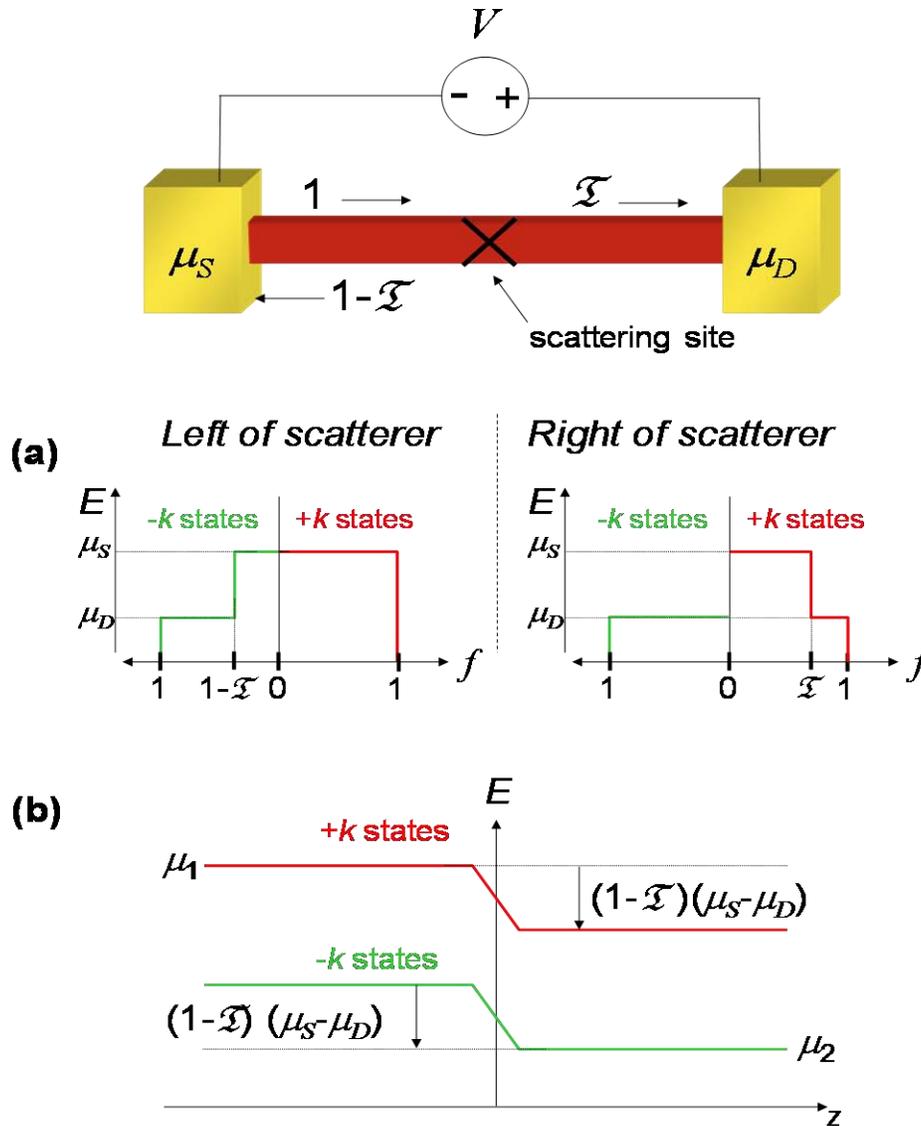
Fig. 4.15. (a) Distribution of electrons within a molecular wire that contains a scattering site. **(b)** The average quasi Fermi level of both $+k$ and $-k$ states changes at the scatterer. This can be interpreted as a change in potential at the scatterer. From S. Datta, 'Electronic Transport in Mesoscopic Systems' Cambridge (1995).

But where is the heat dissipated?

It depends where the electrons relax into equilibrium. If the relaxation occurs within the contact, then once again all the heat is dissipated in the drain. Thus, although the average potential changes at the scatterer, heat is only dissipated where the electrons relax.

Ohm's law[†]

What happens when we increase the size of a conductor? Eventually, we should obtain Ohm's law as the quantum phenomena transform into the familiar model of classical conduction:

$$V = IR \tag{4.22}$$

But a linear relationship between V and I is not particularly profound. Almost any system can be linearized over a sufficiently narrow range of voltage or current. It is more significant to evaluate the resistance, R, in terms of macroscopic quantities such as cross-sectional area, A, and length, L.

You might recall that resistance is classically defined as:

$$R = \frac{\rho L}{A}. \tag{4.23}$$

where ρ, the resistivity, is some material dependent quantity, usually determined by a measurement. Let's see where this expression comes from – it will help illustrate differences between quantum and classical models of charge conduction.

At zero temperature, transmission formalism gives

$$G = \frac{2q^2}{h} M \mathcal{T}, \tag{4.24}$$

where M is the number of modes, and $\mathcal{T}$ is the net transmission coefficient. Rearranging this in terms of a resistance, we have

$$R = \frac{h}{2q^2} \frac{1}{M \mathcal{T}} \tag{4.25}$$

To determine the net transmission coefficient, let's break the conductor into a series of N elements labeled $i = 1 \dots N$, each containing a scattering site with transmission $\mathcal{T}_i$; see Fig. 4.16.
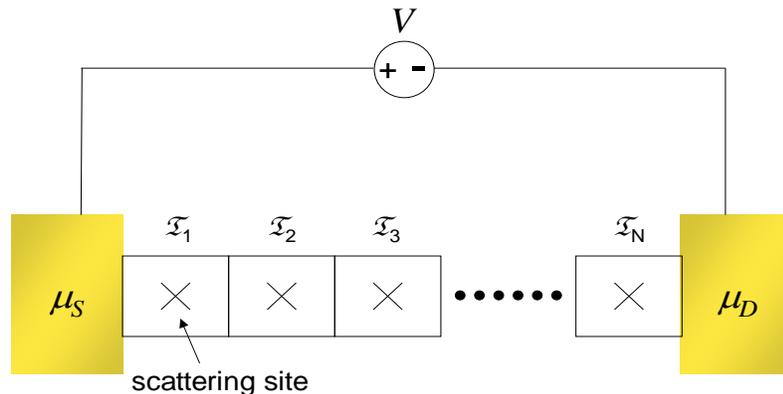
Fig. 4.16. The macroscopic conductor can be represented as a series of N scattering sites, each with transmission $\mathcal{T}_i$.

[†] This section is adapted from S. Datta, 'Electronic Transport in Mesoscopic Systems' Cambridge (1995).

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For many scatterers there will be many reflections to consider. If the scattering mechanism preserves the phase information of the electrons, then multiple reflections can yield interference effects. Such scattering is said to be coherent. Here, we will consider only incoherent scattering that randomizes the electron phase.

Let's begin with just two incoherent scatterers in series. The transmission for two incoherent scatterers in series is:

$$\mathcal{T}_{12} = \mathcal{T}_1\mathcal{T}_2 + \mathcal{T}_1\mathcal{T}_2\mathcal{R}_1\mathcal{R}_2 + \mathcal{T}_1\mathcal{T}_2\left(\mathcal{R}_1\mathcal{R}_2\right)^2 + \ldots \tag{4.26}$$

where $\mathcal{R}_i$ is the reflection from the ith scatterer, and $\mathcal{T}_i = (1-\mathcal{R}_i)$.
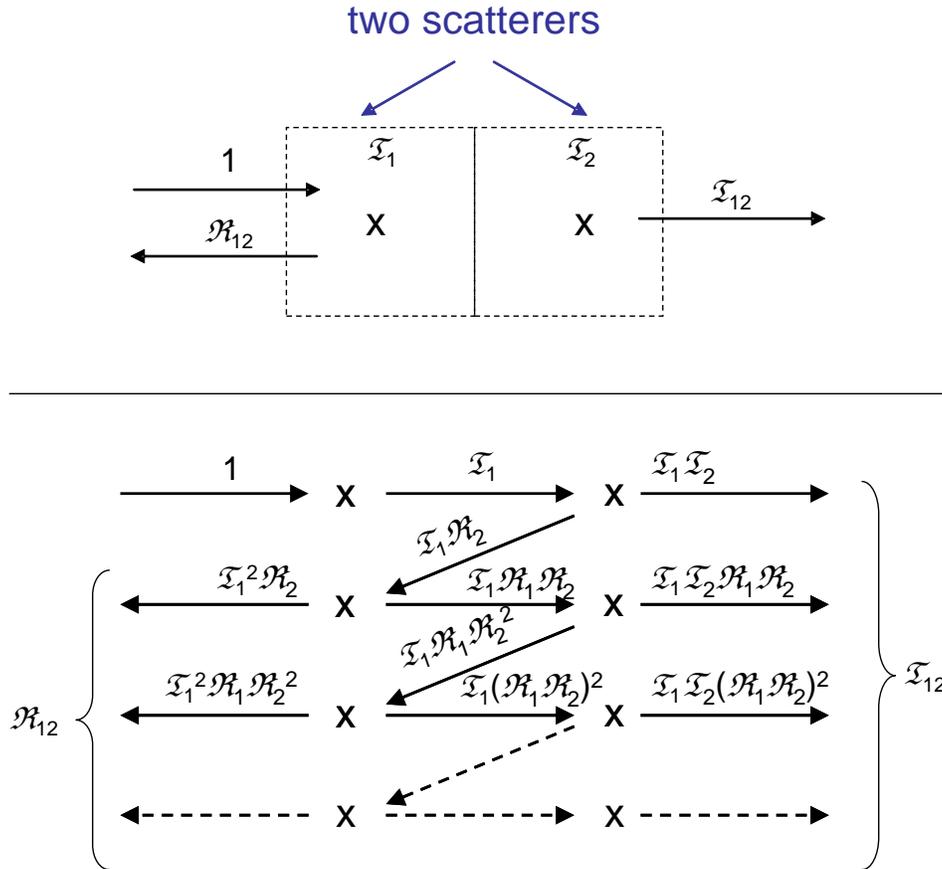
Fig. 4.17. Two scatterers generate an infinite number of reflections, but we can sum the geometric series. Adapted from S. Datta, 'Electronic Transport in Mesoscopic Systems' Cambridge (1995).

This geometric series simplifies to

$$\mathcal{T}_{12} = \frac{\mathcal{T}_1\mathcal{T}_2}{1 - \mathcal{R}_1\mathcal{R}_2}, \tag{4.27}$$

We can rearrange Eq. (4.27) to show

$$\frac{\mathcal{R}_{12}}{\mathcal{T}_{12}} = \frac{\mathcal{R}_1}{\mathcal{T}_1} + \frac{\mathcal{R}_2}{\mathcal{T}_2} \tag{4.28}$$

Thus, for N identical scatterers:

$$\frac{\mathfrak{R}}{\mathfrak{T}} = N\frac{\mathfrak{R}_i}{\mathfrak{T}_i} \tag{4.29}$$

Solving for the net transmission and using $\mathfrak{T} = (1-\mathfrak{R})$

$$\mathfrak{T} = \frac{\mathfrak{T}_i}{N(1-\mathfrak{T}_i)+\mathfrak{T}_i} \tag{4.30}$$

If we have λ scatterers per unit length, then

$$\mathfrak{T} = \frac{\mathfrak{T}_i}{\lambda L(1-\mathfrak{T}_i)+\mathfrak{T}_i} = \frac{L_0}{L+L_0} \tag{4.31}$$

Thus, Eq. (4.25) becomes

$$R = \frac{h}{2q^2}\frac{1}{M}\left(1+\frac{L}{L_0}\right) \tag{4.32}$$

where $L_0 = \mathfrak{T}/\lambda(1-\mathfrak{T})$ is a characteristic length. The length dependence of resistance is clear from Eq. (4.32). The dependence on cross sectional area is due to the number of current-carrying modes in the conductor

$$M \approx \frac{k_F^2}{4\pi}A, \tag{4.33}$$

where k_F is the Fermi wavevector.

Thus, we find that resistance can be broken into two components, a resistance due to the contacts, and a resistance that scales with the length of the conductor.

$$R = R_C + R_B = \frac{\rho L_0}{A} + \frac{\rho L}{A} \tag{4.34}$$

The contact resistance is the quantum effect that is familiar to us from Landauer theory. But in large conductors, the contact resistance is overwhelmed and we get the familiar classical expression for resistance.

The Drude or Semi-Classical Model of Charge Transport

Quantum models of charge conduction are rarely applied outside nanoelectronics. For traditional applications, the semi-classical model of the German physicist Paul Drude is usually sufficient. Drude proposed that conductors contain immobile positive ions embedded in a sea of electrons. Unlike the quantum view, where those electrons occupy various states with different energies, Drude viewed electrons as indistinguishable.

In the quantum model of charge transport, current is carried by only that fraction of electrons close to the Fermi energy. The current carrying electrons move at approximately the Fermi velocity, $v_F = \hbar k_F/m$. The remaining electrons are compensated, *i.e.* equal numbers flow in each direction yielding no net current.

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equilibrium   under bias
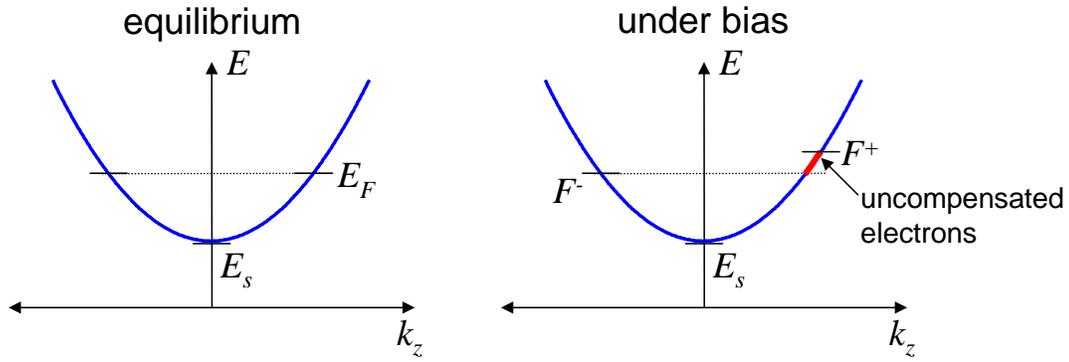
Fig. 4.18. Application of an electric field shifts the quasi Fermi levels for electrons moving with the field (F^+) and against the field (F^-).

But in the Drude model, current is carried by all electrons, moving at an average velocity known as the drift velocity, $\mathbf{v}_d$. Thus, the fundamental classical model for charge conduction is

$$\mathbf{J} = qn\mathbf{v}_d \qquad (4.35)$$

where n is the density of electrons.

In the Drude model, all the electrons travel in the direction of the electric field, gathering energy from the field. Eventually each electron collides with something, a positive ion or another electron, at which point, the electron is stopped. It is then accelerated once more by the electric field, traveling in this stop-start manner through the conductor.

Electric Field
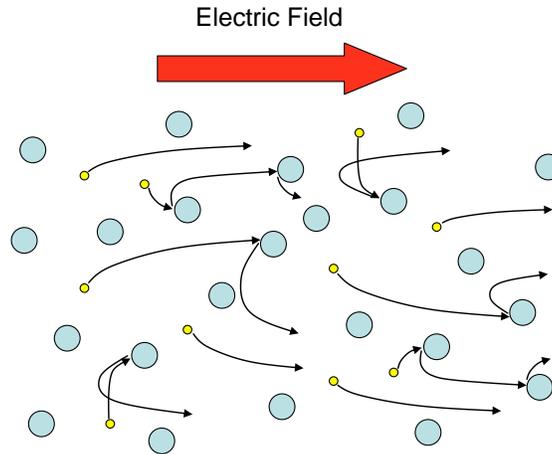
Fig. 4.19. Electron paths through scattering sites. The average time between collisions is the relaxation time, τ_m.

The conductivity of the material is characterized by τ_m, the relaxation time, the mean time between collisions.

The rate at which electrons gain momentum from the field, ε must be equal to the rate of losses due to scattering:[†]

[†] This derivation follows Ashcroft and Mermin, 'Solid State Physics', Saunders College Publishing (1976).

$$\frac{d\mathbf{p}}{dt}\bigg|_{scattering} = \frac{d\mathbf{p}}{dt}\bigg|_{field}. \tag{4.36}$$

$$\frac{mv_d}{\tau_m} = q\varepsilon, \tag{4.37}$$

Rearranging Eq. (4.37), we can express the drift velocity and current density in terms of the relaxation time.

$$\mathbf{J} = \frac{nq^2\tau_m}{m}\boldsymbol{\varepsilon} \tag{4.38}$$

Comparing to Ohm's law (expressed in terms of the conductivity, $\sigma = 1/\rho$)

$$\mathbf{J} = \sigma\boldsymbol{\varepsilon} \tag{4.39}$$

where

$$\sigma = \frac{nq^2\tau_m}{m} \tag{4.40}$$

Mobility

One of the most important simplifications of the Drude model is *mobility*, defined as the ratio of the electric field to the drift velocity.

$$v_d = \mu\varepsilon \tag{4.41}$$

Using Eq. (4.37) we obtain

$$\mu = \frac{q\tau_m}{m} \tag{4.42}$$

Mobility is a very common metric for the quality of transistor materials. It typically peaks at several thousand cm^2/Vs in high quality transistor materials such as GaAs or InP. But as we have seen, the actual charge carrier velocity, v_F, has little relation to the electric field. So, why are Drude parameters such as mobility and conductivity useful quantities?

Effective Mass

So far, both the classical and quantum models of conduction have assumed that the current carrying electrons occupy pure planewave states. The dispersion relation of real materials, however, varies from the ideal parabola. We can approximate any dispersion relation by a plane wave if we allow the mass of the electron to vary. We call the modified mass the *effective mass*. Under this approximation, the electron is thought of as a classical particle and various complex phenmomena are wrapped up in the effective mass. For example, given dispersion relation $E(k)$, a Taylor expansion about $k = 0$ yields:

$$E(k) = E(0) + k\frac{dE}{dk}\bigg|_{k=0} + \frac{1}{2}k^2\frac{d^2E}{dk^2}\bigg|_{k=0} + ... \tag{4.43}$$

Approximating the dispersion relation by a plane wave gives

$$E(k) = E_0 + \frac{\hbar^2 k^2}{2m*} \tag{4.44}$$

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Equating the quadratic terms in Eqns. (4.43) and (4.44) we get an expression for the effective mass

$$m^* = \hbar^2 \left(\frac{d^2 E}{dk^2} \right)^{-1} \tag{4.45}$$

The effective mass concept is commonly used in classical models of electron transport, especially models of mobility like Eq. (4.42).
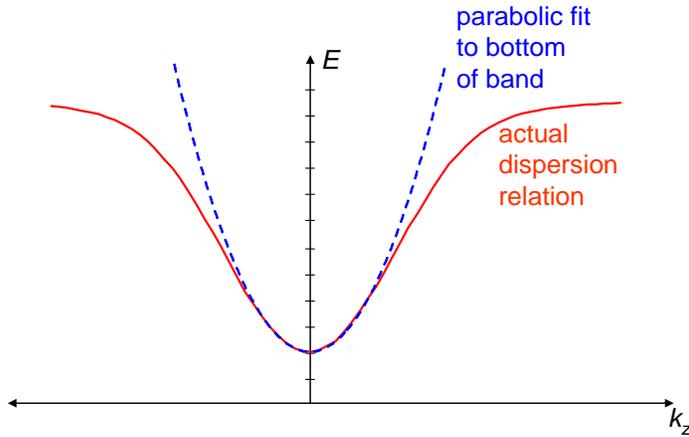
Fig. 4.20. We can model conduction in a material of arbitrary dispersion relation by assuming plane wave electron states with variable (effective) electron mass, m^*, obtained by fitting a parabola to the bottom of the band.

Comparing the quantum and Semi-Classical Drude models of conduction

(i) The mean free path

The Drude model gives a physically incorrect picture of charge conduction. Nevertheless it works quite well. The quantum model shows that rather than all the electrons moving at the drift velocity, as in the Drude model, only the uncompensated electrons carrying current, each moving at approximately the Fermi velocity:[3] Thus, the Drude model can be rearranged as

$$J = qn'v_F \tag{4.46}$$

where the uncompensated charge density is

$$n' = n \frac{v_d}{v_F} \tag{4.47}$$

We can also define the **mean free path**, L_m, as the average distance an electron travels between scattering events. The mean free path is related to the Fermi velocity by:

$$L_m = v_F \tau_m \tag{4.48}$$

Interestingly, the mean free path is approximately equal to the characteristic length L_0 in the derivation of Ohm's law.

(ii) Equilibrium and Non-equilibrium current flow

We can demonstrate the differences between the classical and ballistic limits using the analogy of water flow from one reservoir to another. The application of bias across a wire is equivalent to depressing the height of the drain reservoir relative to the source

reservoir. In the ballistic model water flowing from the source travels across the wire as a jet before relaxing to equilibrium in the drain. In the classical model the water minimizes its potential in channel.

BALLISTIC   CLASSICAL
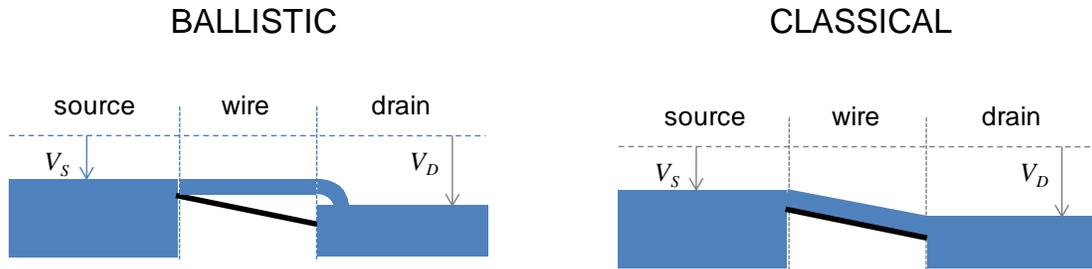
Fig. 4.21. A water flow analogy for ballistic and classical current flow. In the classical limit, the water is always in local equilibrium with the channel.

One way to think about classical transport is as the limit of a series of nanoscale ballistic wires interspersed by contacts. By definition, electrons in the contacts are in equilibrium. Thus contacts are different to the elastic scatterers we considered above, because electrons change energy in contacts. The limiting case of many closely spaced contacts is a continuously varying conduction band edge; see Fig. 4.22.

(a) Quantum model: series of ballistic wires

(b) Classical limit: continuously varying E_C
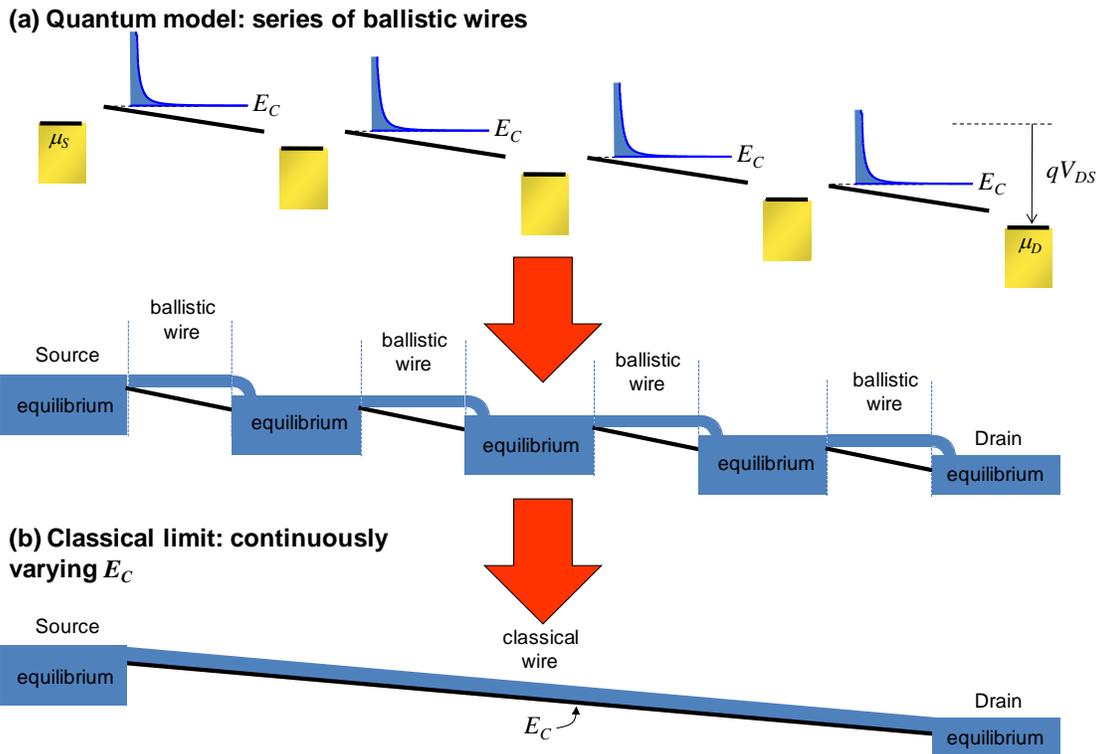
Fig. 4.22. In a classical wire, the conduction band edge varies continuously with position. The classical model can be imagined as the limiting case of many ballistic devices in series.

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(iii) The length scale of ballistic conduction

To determine whether we should use the ballistic or semi-classical models of charge transport we need to know the likelihood of electron scattering in the channel. This depends on the channel length, and the quality of the semiconductor.

The number of scattering events in the channel is given by τ/τ_m where τ is the transit time of the electron, and τ_m is its average scattering time. Relating the transit time to the carrier velocity, and τ_m to the definition of mobility in Eq. (4.42) gives:

$$\frac{\tau}{\tau_m} = \frac{l/v}{m_{eff}\,\mu/q} = \frac{l^2/\mu V_{SD}}{m_{eff}\,\mu/q} = \frac{ql^2}{m_{eff}V_{SD}\mu^2} \tag{4.49}$$

This expression is plotted in Fig. 4.23 assuming a Si conductor with $V_{DS} = 1\text{V}$, $\mu = 300 \text{ cm}^2/\text{Vs}$ and $m_{eff} = 0.5 \times m_0$, where m_0 is the mass of the electron. It shows that silicon is expected to cross into the ballistic regime for lengths of approximately $l < 50\text{nm}$.
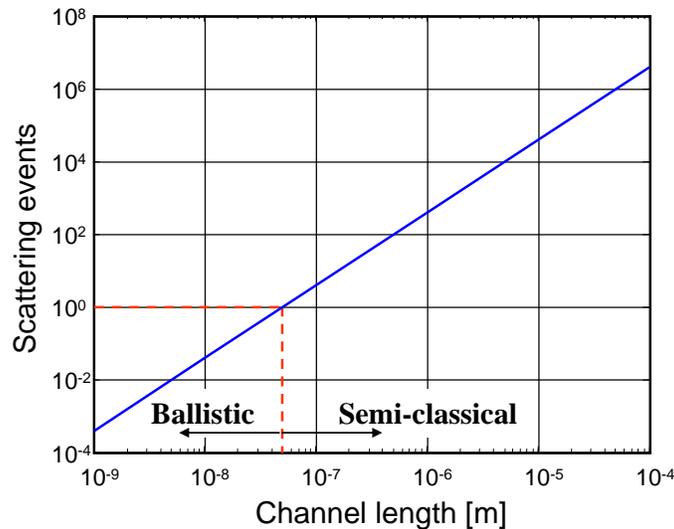
Fig. 4.23. The expected number of electron scattering events in Si as a function of the channel length. The threshold of ballistic operation occurs for channel lengths of approximately 50nm.

Problems

1. Consider the metal/nanowire/metal device shown below. Assume the nanowire is an ideal 1-dimensional conductor with no scattering.
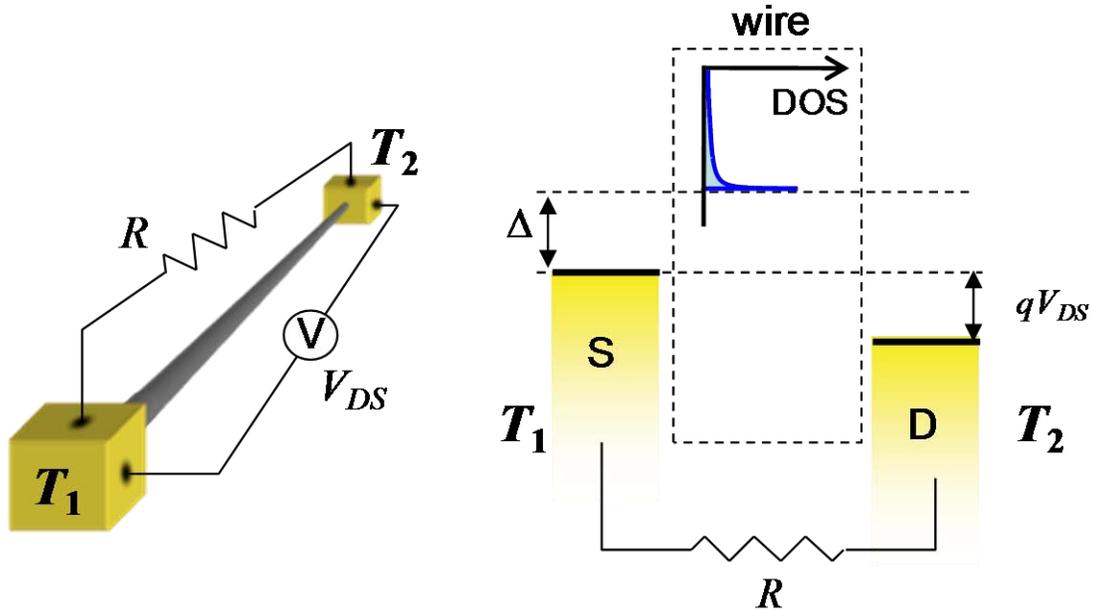
Fig. 4.24. A thermoelectric nanowire.

The source contact is heated to temperature T_1, while the drain contact remains at temperature T_2. Assume that the energy separation between the source and the bottom of the conduction band (Δ) is independent of bias. Assume also that $\Delta \gg kT_1$.

(a) The contacts are now shorted together, i.e. $R \rightarrow 0$. What is the current that flows? (This is the 'short circuit current').

(b) Next assume the contacts are returned to open circuit, i.e. $R \rightarrow \infty$. What is the voltage between the contacts? (This is the 'open circuit voltage')

2. The dispersion relation for a relativistic particle is given by $E = \sqrt{p^2 c^2 + (m_0 c^2)^2}$ where $E = \hbar \omega$ and $p = \hbar k$. Find the group velocity of this particle.

3. The group velocity is given by $v_g = \dfrac{d}{dt}\langle x \rangle$. Show that $\dfrac{d}{dt}\langle x \rangle = \left\langle \dfrac{1}{\hbar}\dfrac{dE}{dk} \right\rangle$.

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4. Find the effective mass for an electron in a conductor with the dispersion relation:

$$E(k) = 5 - 2V\cos(ka) \; , \; |k| < \frac{\pi}{a}$$

where V and a are positive constants.

5. Graphene exhibits a photon-like dispersion relation. Assume the carrier velocity is independent of the carrier's energy and equal to the speed of light, c. Based on the high velocity of carriers in graphene it is often argued that graphene transistors will be faster than similar transistors constructed from other materials.

(a) Draw the dispersion relation of a graphene wire. Assume the wire has only one mode.

(b) Given a wire of length, l, constructed of ballistic graphene, assume we inject a carrier pulse as shown below. f is the distribution function, *i.e.* when $f = 1$ each state is completely full. What is the applied voltage?
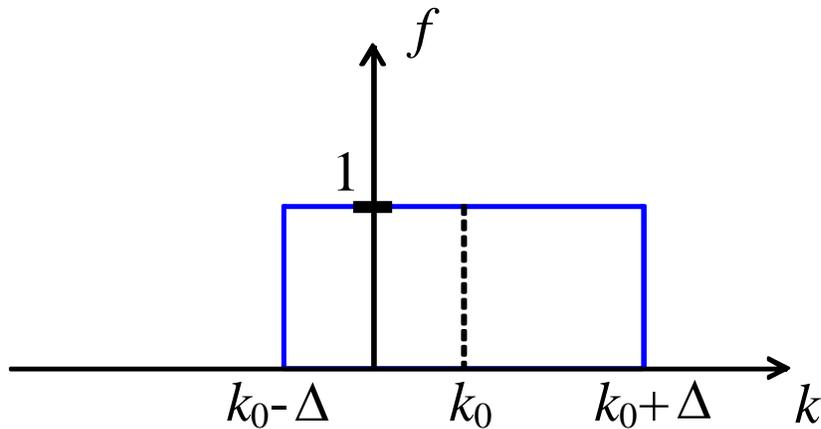
Fig. 4.25. The electron distribution in the graphene wire.

(c) How many carriers are contained in the pulse?

(d) Determine the current carried by the wire from the group velocity and number of carriers.

(e) What is the conductance of the wire?

(f) Now assume that the graphene is used to drive a load capacitance of value C. What is the time constant of the system? How does the graphene wire compare to other 1d wires?

6. This problem refers to the ballistic 1-D wire below. The X's in the wire are representative of elastic scattering sites, each with transmission, T. Assume $E_C < \mu_S, \mu_D$ where
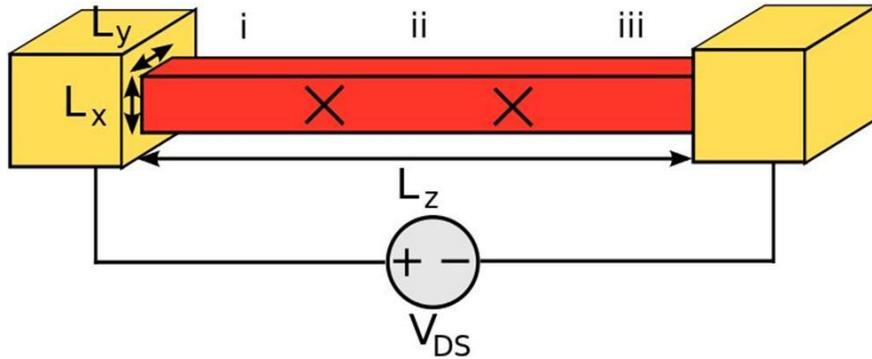
Fig. 4.26. A ballistic nanowire with two scattering sites.

(a) For T = 1.0, plot the filling function at positions (i), (ii), and (iii) along the z-axis.
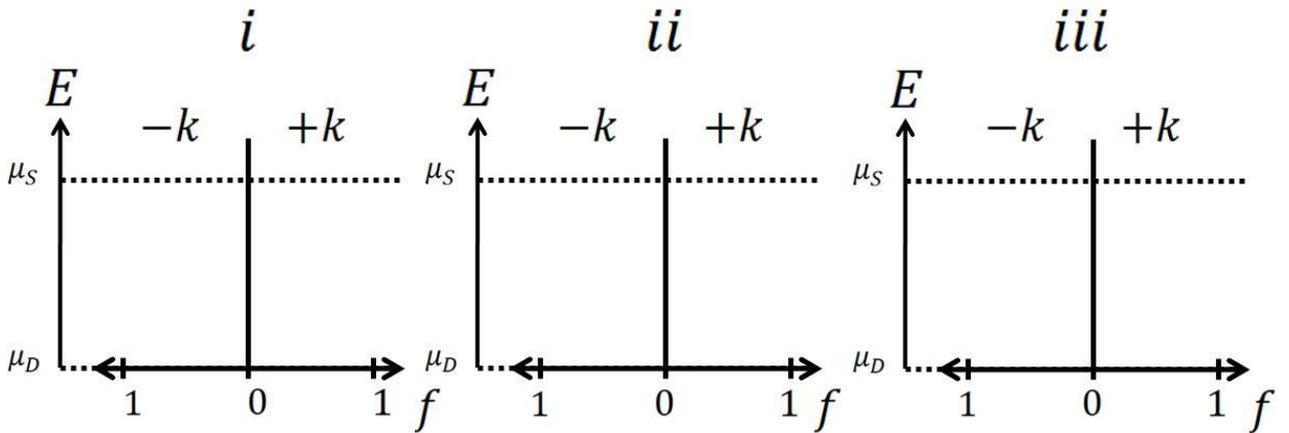
(b) For T = 0.5, plot the filling function at positions (i), (ii), and (iii) along the z-axis.
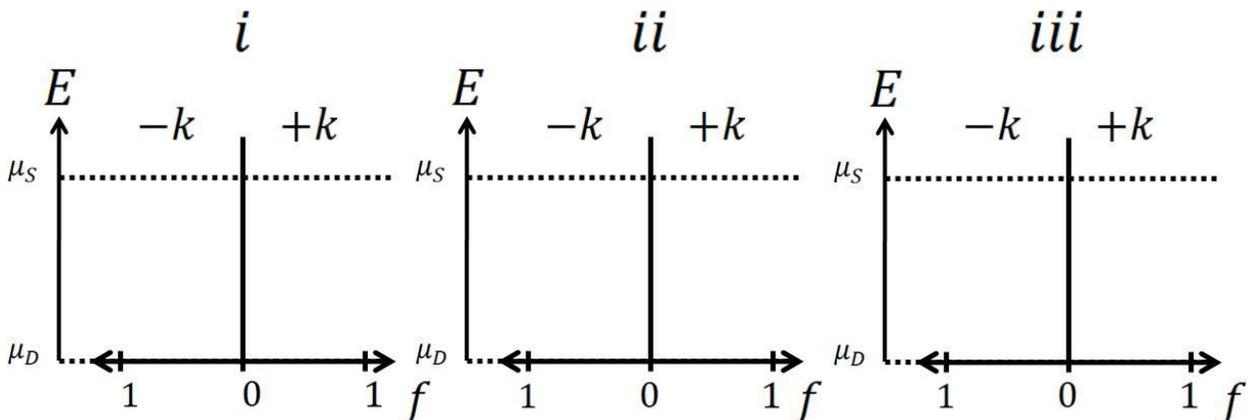
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(c) Consider a very large number of scattering sites along the wire, each with $T = 0.5$. Plot the filling function at the source (i), at the midpoint of the wire (ii), and at the drain (iii).

$$i \qquad\qquad ii \qquad\qquad iii$$

$E \qquad -k \quad +k \qquad\qquad E \qquad -k \quad +k \qquad\qquad E \qquad -k \quad +k$

$\mu_S \qquad\qquad\qquad\qquad \mu_S \qquad\qquad\qquad\qquad \mu_S$

$\mu_D \qquad\qquad\qquad \mu_D \qquad\qquad\qquad \mu_D$

$\quad 1 \qquad 0 \qquad 1\ f \qquad 1 \qquad 0 \qquad 1\ f \qquad 1 \qquad 0 \qquad 1\ f$
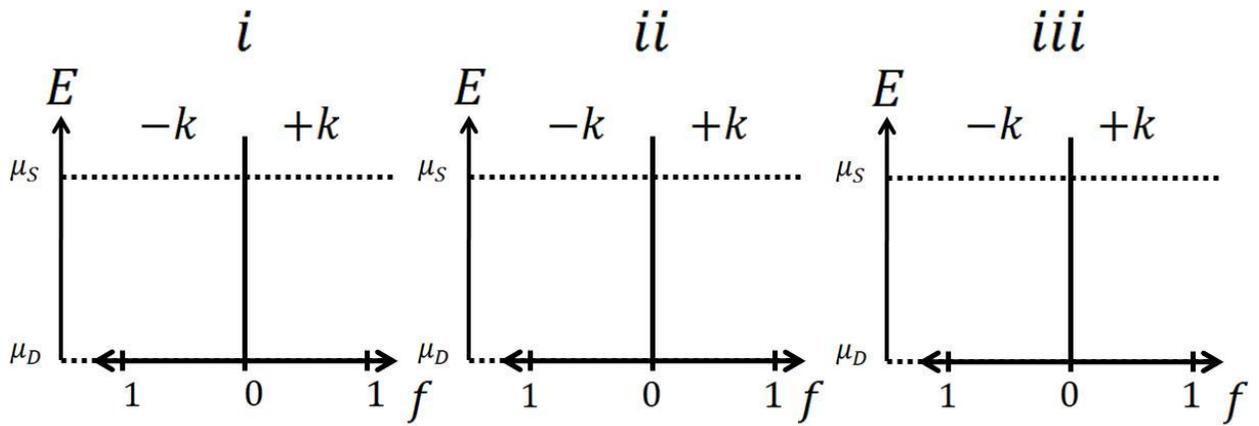
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