

Part 3. Two Terminal Quantum Dot Devices

Part 3. Two Terminal Quantum Dot Devices

In this part of the class we are going to study electronic devices. We will examine devices consisting of a quantum dot or a quantum wire conductor between two contacts. We will calculate the current in these 'two terminal' devices as a function of voltage. Then we will add a third terminal, the gate, which is used to independently control the potential of the conductor. Then we can create transistors, the building-block of modern electronics. We will consider both nanotransistors and conventional transistors.

We will begin with the simplest case, a quantum dot between two contacts.

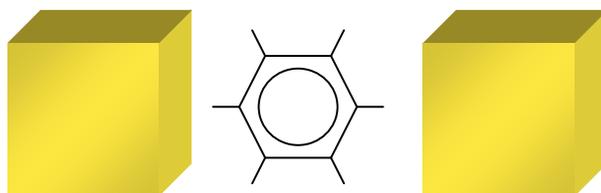


Fig. 3.1. A molecule between two contacts. We will model the molecule as a quantum dot.

Quantum Dot / Single Molecule Conductors

As we saw in Part 2, a quantum dot is a 0-d conductor; its electrons are confined in all dimensions. A good example of a quantum dot is a single molecule that is isolated in space. We can approximate our quantum dot or molecule by a square well that confines electrons in all dimensions. One consequence of this confinement is that the energy levels in the isolated quantum dot or molecule are discrete. Typically, however, the simple particle-in-a-box model does not generate sufficiently accurate estimates of the discrete energy levels in the dot. Rather, the material in the quantum dot or the structure of the molecule defines the actual energy levels.

Fig. 3.2 shows a typical square well with its energy levels. We will assume that these energy levels have already been accurately determined. Each energy level corresponds to a different molecular orbital. Energy levels of bound states within the well are measured with respect to the **Vacuum Energy**, typically defined as the potential energy of a free electron in a vacuum. Note that if an electric field is present the vacuum energy will vary with position.

Next we add electrons to the molecule. Each energy level takes two electrons, one of each spin. The **highest occupied molecular orbital (HOMO)** and the **lowest unoccupied molecular orbital (LUMO)** are particularly important. In most chemically stable materials, the HOMO is completely filled; partly filled HOMOs usually enhance the reactivity since they tend to readily accept or donate electrons.

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Earlier we stated that charge transport occurs only in partly filled states. This is best achieved by adding electrons to the LUMO, or subtracting electrons from the HOMO. Modifying the electron population in all other states requires much more energy. Hence we will ignore all molecular orbitals except for the HOMO and LUMO.

Fig. 3.2 also defines the **Ionization Potential** (I_P) of a molecule as the binding energy of an electron in the HOMO. The binding energy of electrons in the LUMO is defined as the **Electron Affinity** (E_A) of the molecule.

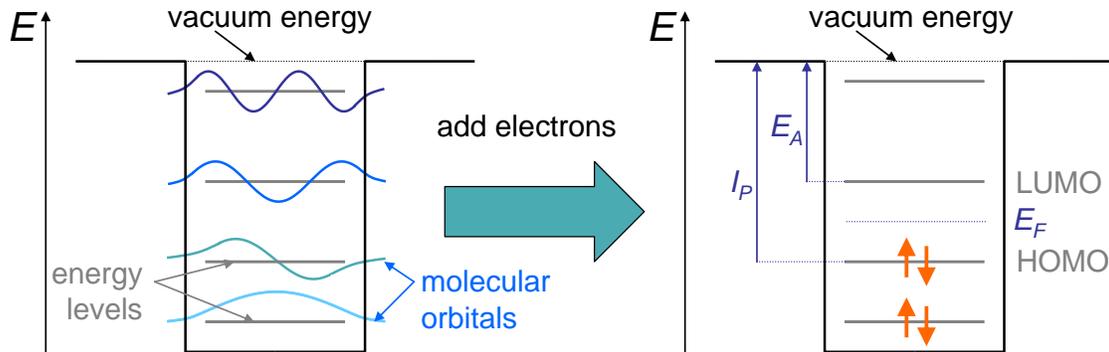


Fig. 3.2. A square well approximation of a molecule. Energy levels within the molecule are defined relative to the vacuum energy – the energy of a free electron at rest in a vacuum.

Contacts

There are three essential elements in a current-carrying device: a conductor, and at least two contacts to apply a potential across the conductor. By definition the contacts are large: each contact contains many more electrons and many more electron states than the conductor. For this reason a contact is often called a reservoir. We will assume that all electrons in a contact are in equilibrium. The energy required to promote an electron from the Fermi level in the contact to the vacuum energy is defined as the **work function** (Φ).

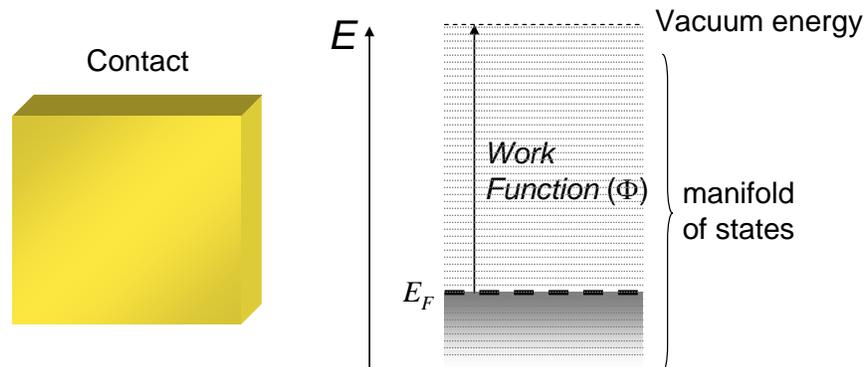


Fig. 3.3. An energy level model of a metallic contact. There are many states filled up with electrons to the Fermi energy. The minimum energy required to remove an electron from a metal is known as the work function.

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Metals are often employed as contacts, since metals generally possess very large numbers of both filled and unfilled states, enabling good conduction properties. Although the assumption of equilibrium within the contact cannot be exactly correct if a current flows through it, the large population of mobile electrons in the contact ensures that any deviations from equilibrium are small and the potential in the contact is approximately uniform. For example, consider a large metal contact. Its resistance is very small, and consequently any voltage drop in the contact must be relatively small.

Equilibrium between contacts and the conductor

In this section we will consider the combination of a molecule and a single contact.

In the absence of a voltage source, the isolated contact and molecule are at the same potential. Thus, their vacuum energies (the potential energy of a free electron) are identical in isolation.

When the contact is connected with the molecule, equilibrium must be established in the *combined* system. To prevent current flow, there must be a uniform Fermi energy in both the contact and the molecule.

But if the Fermi energies are different in the isolated contact and molecules, how is equilibrium obtained?

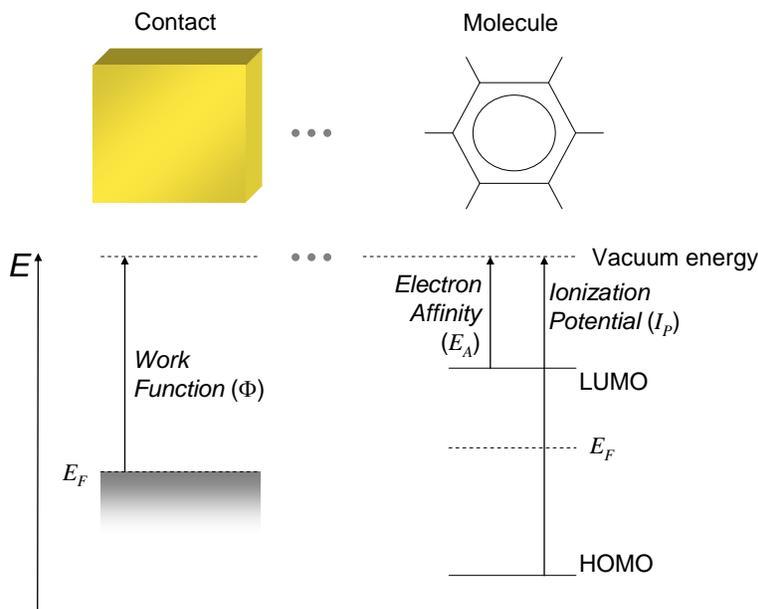


Fig. 3.4. The energy lineup of an isolated contact and an isolated molecule. If there is no voltage source in the system, the energy of a free electron is identical at the contact and molecule locations. Thus, the vacuum energies align. The Fermi energies may not, however. But at equilibrium, the Fermi energies are forced into alignment by charge transfer.

Since Fermi levels change with the addition or subtraction of charge, equilibrium is obtained by charge transfer between the contact and the molecule. Charge transfer changes the potential of the contact relative to the molecule, shifting the relative vacuum energies. This is known as ‘charging’. Charge transfer also affects the Fermi levels as electrons fill some states and empty out of others. Both charging and state filling effects can be modeled by capacitors. We’ll consider electron state filling first.

(i) The Quantum Capacitance

Under equilibrium conditions, the Fermi energy must be constant in the metal and the molecule. We can draw an analogy to flow between water tanks. The metal is like a very large tank. The molecule, with its much smaller density of states, behaves as a narrow column. When the metal and molecule are connected, water flows to align the filling levels.

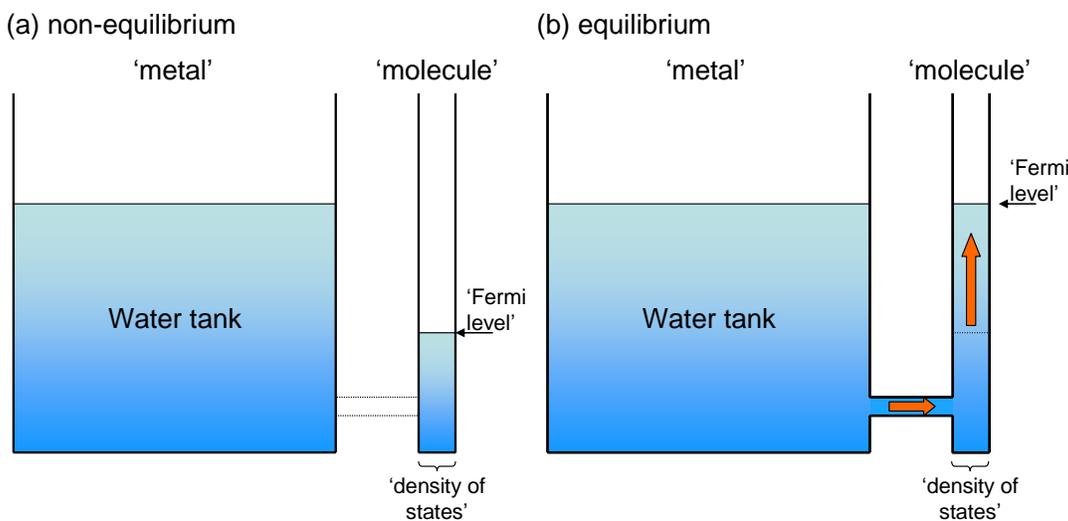


Fig. 3.5. An analogy for electron transfer at the interface between a metal and a molecule. The size of the water tank is equivalent to the density of states. The Fermi level is equivalent to the water level. If the ‘metal’ has a sufficiently large density of states, then the change in its water level is imperceptible.

But a molecule will not necessarily have a uniform density of states as shown in Fig. 3.5. It is also possible that only a fractional amount of charge will be transferred. For example, imagine that some fractional quantity δn electrons are transferred from the contact to the molecule. It is possible for the wavefunction of the transferred electron to include both the contact and the molecule. Since part of the shared wavefunction resides on the molecule, this is equivalent to a fractional charge transfer.

But if δn were equal to +1, the LUMO would be half full and hence the Fermi energy would lie on the LUMO, while if δn were -1, the HOMO would be half full and hence the Fermi energy would lie on the HOMO. In general, the number of charges on the molecule is given by

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$$n = \int_{-\infty}^{+\infty} g(E) f(E, E_F) dE \quad (3.1)$$

where $g(E)$ is the density of molecular states per unit energy. For small shifts in the Fermi energy, we can linearize Eq. (3.1) to determine the effect of charge transfer on E_F . We are interested in the quantity dE_F/dn . For degenerate systems we can simplify Eq. (3.1):

$$n = \int_{-\infty}^{E_F} g(E) dE \quad (3.2)$$

taking the derivative with respect to the Fermi energy gives:

$$\frac{dn}{dE_F} = g(E_F) \quad (3.3)$$

We can re-arrange this to get:

$$\delta E_F = \frac{\delta n}{g(E_F)} \quad (3.4)$$

Thus after charge transfer the Fermi energy within the molecule changes by $\delta n/g$, where g is the density of states per unit energy.

Sometimes it is convenient to model the effect of filling the density of states by the ‘quantum capacitance’ which we will define as:

$$C_Q = q^2 g(E_F) \quad (3.5)$$

i.e.

$$\delta E_F = \frac{q^2}{C_Q} \delta n \quad (3.6)$$

If the molecule has a large density of states at the Fermi level, its quantum capacitance is large, and more charge must be transferred to shift the Fermi level.

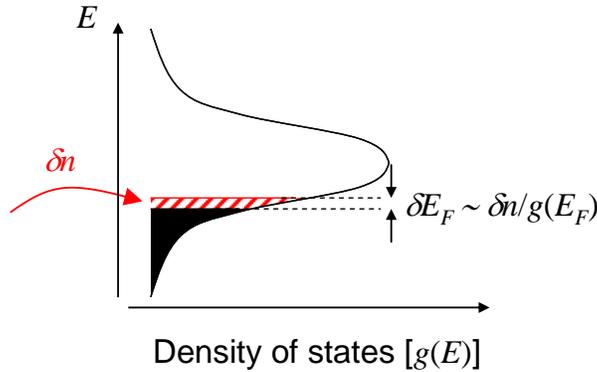


Fig. 3.6. Transferring charge changes the Fermi level in a conductor. The magnitude of the change is determined by the density of states at the Fermi level, and often expressed in terms of a ‘quantum capacitance’.

We can also calculate the quantum capacitance of the contact. Metallic contacts contain a large density of states at the Fermi level, meaning that a very large number of electrons must be transferred to shift its Fermi level. Thus, we say that the Fermi energy of the

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contact is ‘pinned’ by the density of states. Another way to express this is that the quantum capacitance of the contact is approximately infinite.

The quantum capacitance can be employed in an equivalent circuit for the metal-molecule junction. But we have generalized the circuit such that each node potential is the Fermi level, not just the electrostatic potential as in a conventional electrical circuit.

In the circuit below, the metal is modeled by a voltage source equal to the chemical potential μ_1 of the metal. Prior to contact, the Fermi level of the molecule is E_F^0 . The contact itself is modeled by a resistor that allows current to flow when the Fermi levels on either side of the contact are misaligned. Charge flowing from the metal to the molecule develops a potential across the quantum capacitance. But note that this is a change in the Fermi level, not an electrostatic potential. It is also important to note that the quantum capacitance usually depends on the Fermi level in the molecule. The only exception is if the density of states is constant as a function of energy. Thus, a constant value of C_Q can only be employed for small deviations between μ_1 and E_F^0 .

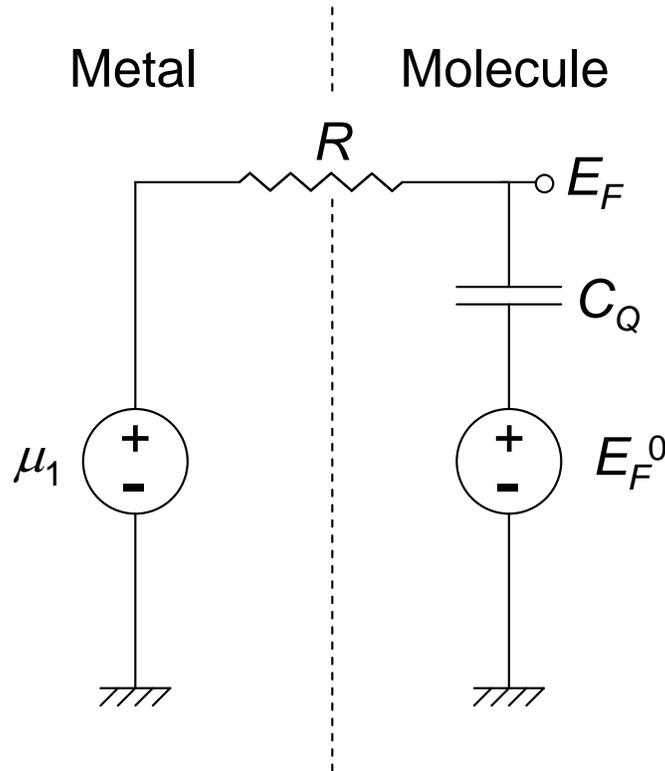


Fig. 3.7. A small signal model for the metal-molecule junction. The effects of charging are not included. The resistor will be characterized further in later sections.

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(ii) Electrostatic Capacitance

Unfortunately, the establishment of equilibrium between a contact and the molecule is not as simply as water flow between two tanks. Electrons, unlike water, are charged. Thus, the transfer of electrons from the contact to a molecule leaves a net positive charge on the contact and a net negative charge on the molecule.

Charging at the interface changes the potential of the molecule relative to the metal and is equivalent to shifting the entire water tanks up and down. Charging assists the establishment of equilibrium and it reduces the number of electrons that are transferred after contact is made.

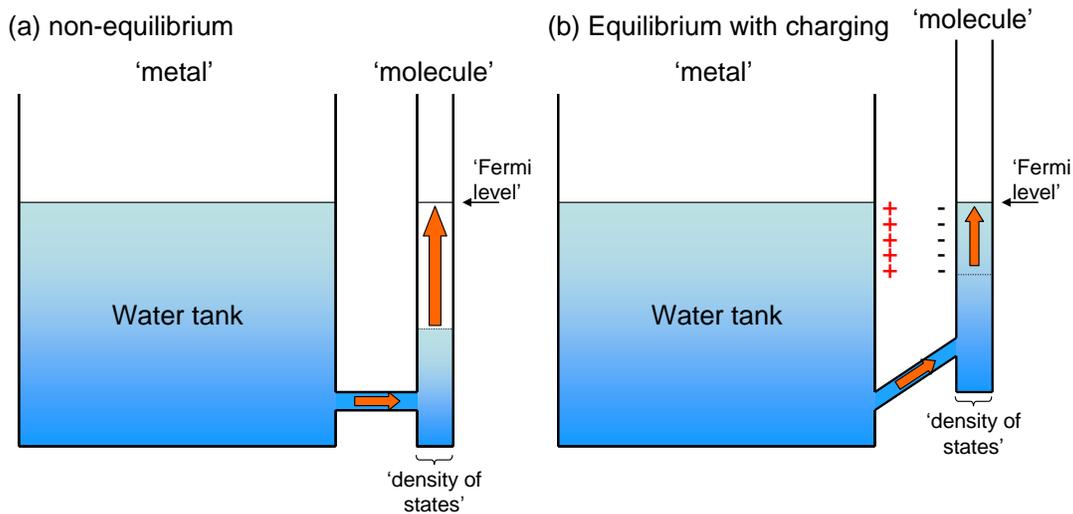


Fig. 3.8. Electrons carry charge and shift the potential when they are transferred between a metal and a molecule. The resulting change in potential is equivalent to lifting up the 'molecule' column of water. The water levels must ultimately match, but now less water is required to be transferred.

The contact and the molecule can be considered as the two plates of a capacitor. In Fig. 3.9 we label this capacitor, C_{ES} - the electrostatic capacitance, to distinguish it from the quantum capacitance discussed in the previous section.

When charge is transferred at the interface, the capacitor is charged, a voltage is established and the molecule changes potential. The change in the molecule's potential per electron transferred is known as the **charging energy** and is reflected in a shift in the vacuum energy. From the fundamental relation for a capacitor:

$$C_{ES} = \frac{Q}{V} \quad (3.7)$$

where V is the voltage across the capacitor. We can calculate the change in potential due to charging:

$$U_C = qV = \frac{q^2}{C_{ES}} \delta n. \quad (3.8)$$

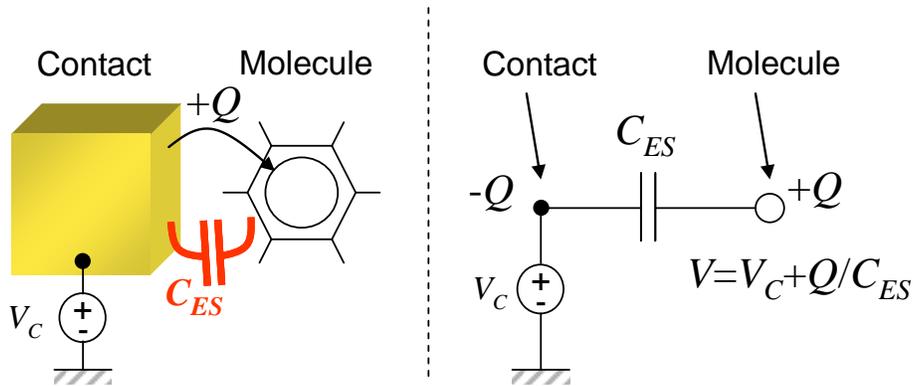


Fig. 3.9. A contact and a molecule can be modeled as two plates of a parallel capacitor. When charge is transferred, this electrostatic capacitance determines the change in electrostatic potential, and hence the shift in the vacuum energy.

We will find that δn is a dynamic quantity – it changes with current flow. It can be very important in nanodevices *because the electrostatic capacitance is so small*. For the small spacings between contact and conductor typical of nanoelectronics (e.g. 1 nm), the charging energy can be on the order of 1V per electron.

Summarizing these effects, we find that the Fermi energy of the neutral molecule, E_F^0 , is related to the Fermi energy of the metal-molecule combination, E_F , by

$$E_F = \delta n/g + \frac{q^2}{C_{ES}} \delta n + E_F^0 \tag{3.9}$$

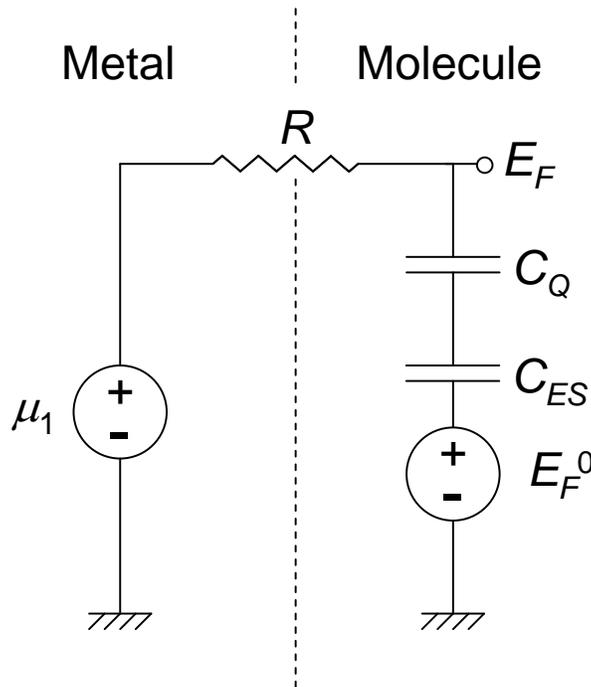


Fig. 3.10. A small signal model for the metal-molecule junction, including the effects of charging. The resistor will be characterized further in later sections.

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Or, in terms of the quantum capacitance:

$$E_F = \frac{q^2}{C_Q} \delta n + \frac{q^2}{C_{ES}} \delta n + E_F^0 \quad (3.10)$$

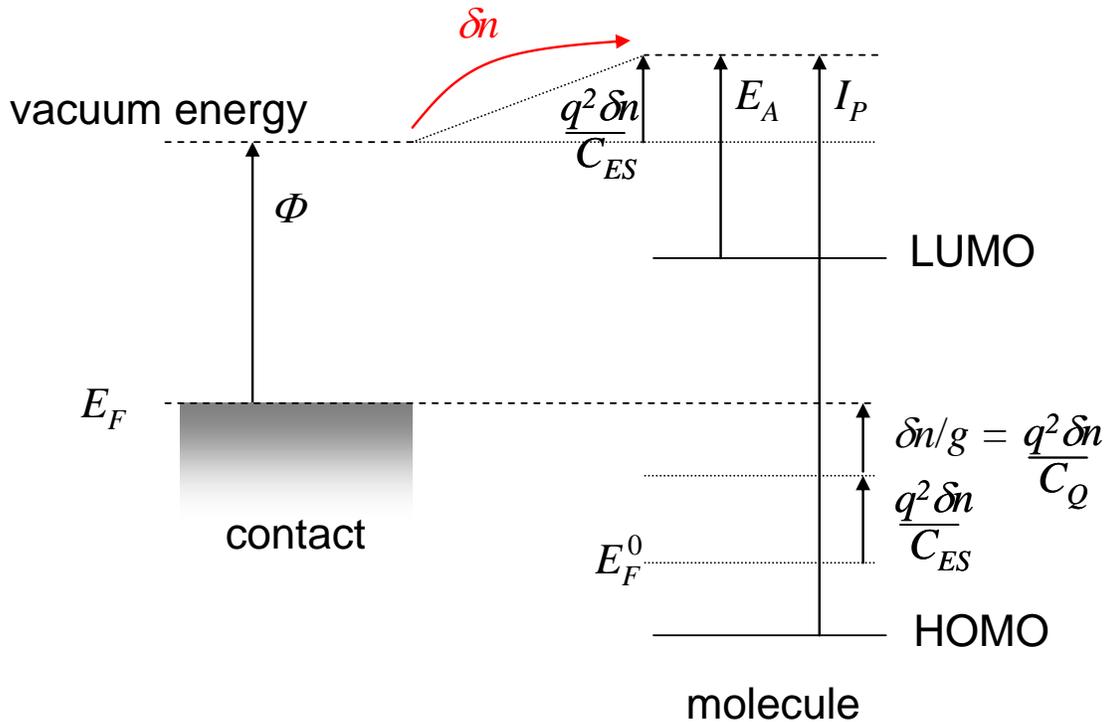


Fig. 3.11. Changes in energy level alignment when charge is transferred from the metal to a molecule. Charging of the molecule corresponds to applying a voltage across an interfacial capacitor, thereby changing the potential of the molecule. Consequently, the vacuum level shifts at the molecule's location, shifting all the molecular states along with it. In addition, the transferred charge fills some previous empty states in the molecule. Both effects change the Fermi energy in the molecule.

Calculation of the electrostatic capacitance

(i) Isolated point conductors

For small conductors like single molecules or quantum dots, it is sometimes convenient to calculate C_{ES} by assuming that the conductor is a sphere of radius R . From Gauss's law, the potential at a point with radius r from the center of the sphere is:

$$V = \frac{Q}{4\pi\epsilon r} \quad (3.11)$$

where $r > R$, ϵ is the dielectric constant and Q is the net charge on the sphere.

If we take the potential at infinity to be zero, then the potential of the sphere is $V = Q/4\pi\epsilon R$ and the capacitance is

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$$C_{ES} = \frac{Q}{V} = 4\pi\epsilon R \quad (3.12)$$

The notable aspect of Eq. (3.12) is that the electrostatic capacitance scales with the size of the conductor. Consequently, the charging energy of a small conductor can be very large. For example, Eq. (3.12) predicts that the capacitance of a sphere with a radius of $R = 1\text{nm}$ is approximately $C_{ES} = 10^{-19}\text{F}$. The charging energy is then $U_C = 1.6\text{eV}$ per charge.

(ii) Conductors positioned between source and drain electrodes

In general, the potential profile for an arbitrary distribution of charges must be calculated using Gauss's law. But we can often make some approximations. The source and drain contacts can sometimes be modeled as a parallel plate capacitor with

$$C = \frac{\epsilon A}{d} \quad (3.13)$$

where A is the area of each contact and d is their separation. This approximation is equivalent to assuming a uniform electric field between the source and drain electrodes. This is valid if $A \gg d$ and there is no net charge between the contacts. For source and drain electrodes separated by a distance l , the source and drain capacitances at a distance z from the source are:

$$C_S(z) = \frac{\epsilon A}{z}, \quad C_D(z) = \frac{\epsilon A}{l-z}. \quad (3.14)$$

The potential varies linearly as expected for a uniform electric field.

$$U(z) = -qV_{DS} \frac{1/C_S(z)}{1/C_D(z) + 1/C_S(z)} = -qV_{DS} \frac{z}{l}. \quad (3.15)$$

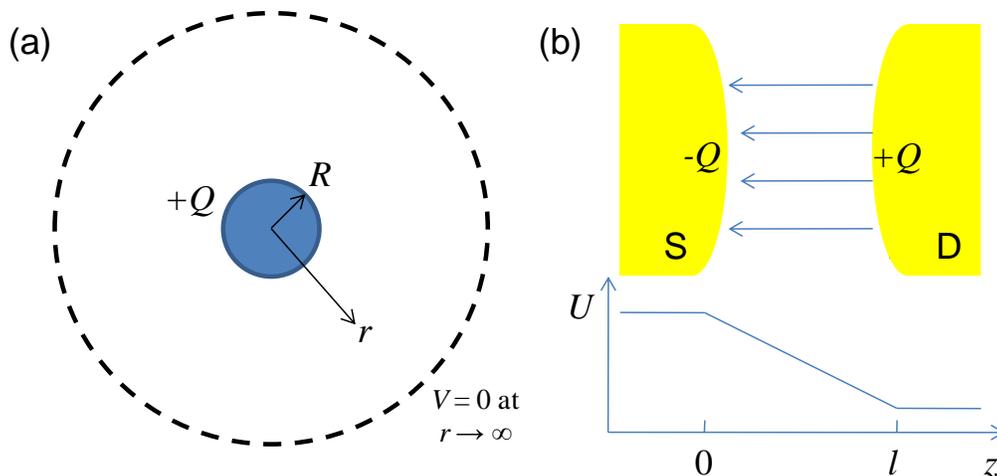


Fig. 3.12. (a) The capacitance of an isolated 0-d conductor is calculated by assuming the potential at infinity is zero. (b) A uniform electric field between the source and drain yields a linearly varying potential. The source and drain capacitors can be modeled by parallel plates.

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Current Flow in Two Terminal Quantum Dot/Single Molecule Devices

In this section we present a simplified model for conduction through a molecule. It is based on the ‘toy model’ of Datta, *et al.*[†] which despite its relative simplicity describes many of the essential features of single molecule current-voltage characteristics.

The contact/molecule/contact system at equilibrium is shown in Fig. 3.13. At equilibrium, $\mu_1 = E_F = \mu_2$. Since there are two contacts, this is an example of a two terminal device. In keeping with convention, we will label the electron injecting contact, the source, and the electron accepting contact, the drain. We will model the molecule by a quantum dot. This is accurate if the center of the molecule is much more conductive than its connections to the contacts.

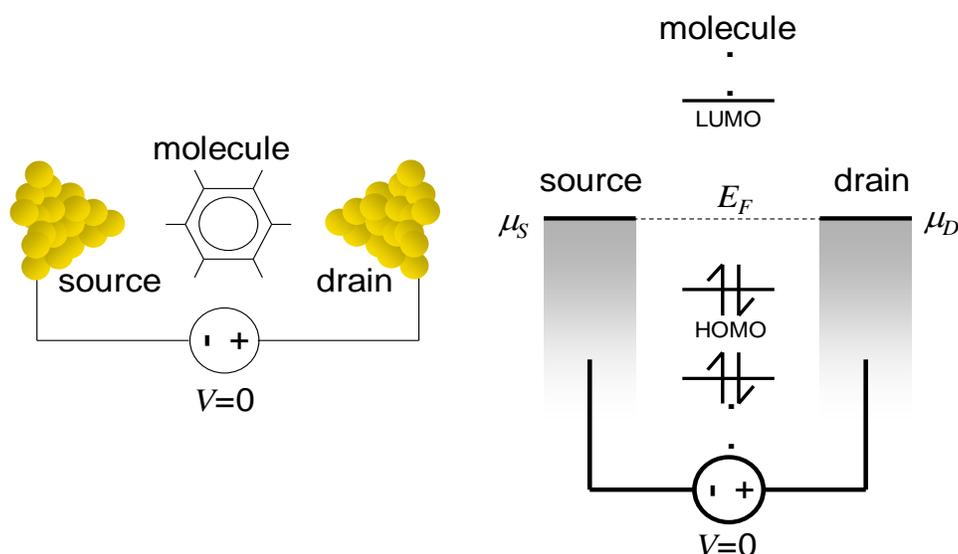


Fig. 3.13. A two terminal device with a molecular/quantum dot conductor. At equilibrium no current flows and the Fermi levels are aligned.

Now, when we apply a potential between the source and drain contacts we shift Fermi level of one contact with respect to the other, i.e.

$$\mu_D - \mu_S = -qV_{DS} \quad (3.16)$$

There are two effects on the molecule:

(i) *The electrostatic effect:* the potential at the molecule is changed by the electric field established between the contacts. The energy levels within the molecule move rigidly up or down relative to the contacts.

(ii) *The charging effect:* Out of equilibrium, a current will flow and the amount of charge on the molecule changes. It may increase if current flows through the LUMO, or decrease if current flows through the HOMO.

[†] S. Datta, ‘Quantum transport: atom to transistor’ Cambridge University Press (2005).

F. Zahid, M. Paulsson, and S. Datta, ‘Electrical conduction in molecules’. In *Advanced Semiconductors and Organic Nanotechniques*, ed. H. Korkoc. Academic Press (2003).

Unfortunately, these effects are linked: moving the molecular energy levels with respect to the contact energy levels changes the amount of charge supplied to the molecule by the contacts. But the charging energy associated with charge transfer in turn changes the potential of the molecule.

We will first consider static and charging effects independently.

(i) Electrostatics: The Capacitive Divider Model of Potential

Our two terminal device can be modeled by a quantum dot linked to the source and drain contacts by two capacitors, C_S and C_D , respectively. The values of these capacitors depend on the geometry of the device. If the molecule is equi-spaced between the contacts we might expect that $C_S \sim C_D$. On the other hand, if the molecule is closely attached to the source but far from the drain, we might expect $C_S \gg C_D$. (Recall that the capacitance of a simple parallel plate capacitor is inversely proportional to the spacing between the plates.)

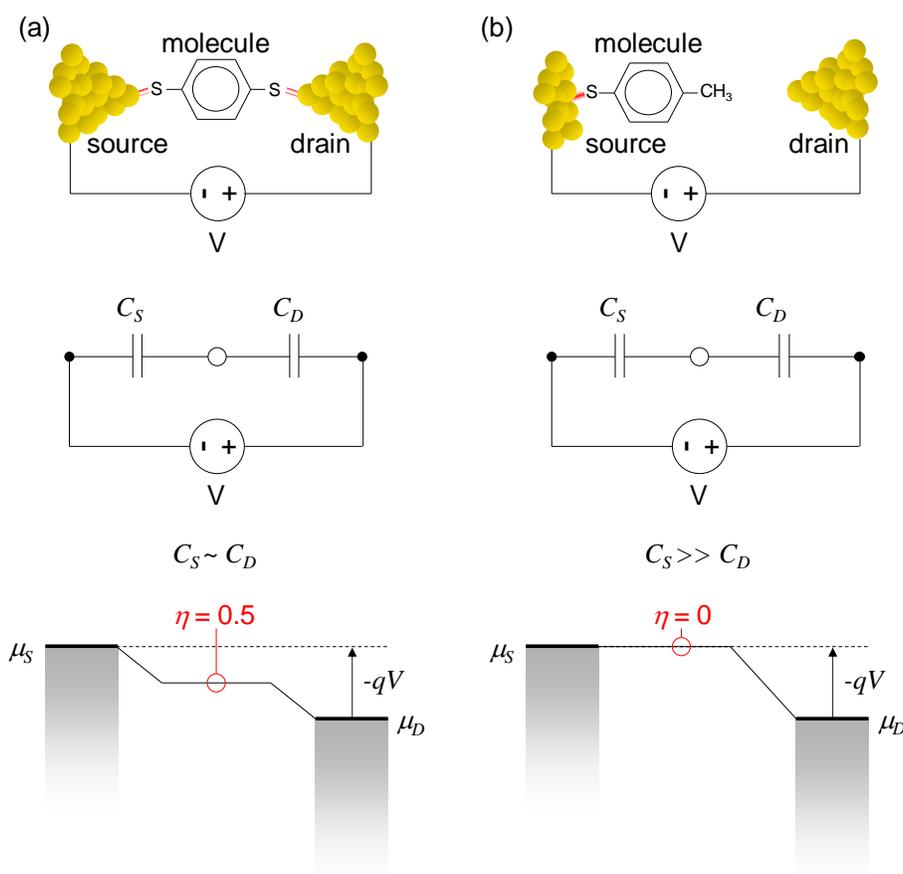


Fig. 3.14. Two single molecule two terminal devices accompanied by possible potential profiles in the molecular conductor. **(a)** symmetric contacts, **(b)** asymmetric contacts. We are concerned with the voltage in the center of the molecule. This is determined by the voltage division factor, η . It can be obtained by from a voltage divider constructed from capacitors. Adapted from F. Zahid, M. Paulsson, and S. Datta, 'Electrical conduction in molecules'. In *Advanced Semiconductors and Organic Nanotechniques*, ed. H. Korkoc. Academic Press (2003).

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These two potential profiles are shown in Fig. 3.14. The voltage is calculated from the capacitive divider. Thus, an applied voltage, V , shifts the chemical potentials of both the source and drain contacts:[†]

$$E_F = -\frac{1/C_S}{1/C_D + 1/C_S} qV_{DS} + \mu_s \quad (3.17)$$

It is convenient to use the Fermi energy of the molecule at equilibrium as a reference, i.e. if we set $E_F = 0$:

$$\begin{aligned} \mu_s &= +\frac{C_D}{C_S + C_D} qV_{DS} \\ \mu_D &= -\frac{C_S}{C_S + C_D} qV_{DS} \end{aligned} \quad (3.18)$$

We can define a voltage division factor, η .[†] It gives the fraction of the applied bias that is dropped between the molecule and the source contact, *i.e.*

$$\eta = \frac{C_D}{C_S + C_D} \quad (3.19)$$

As shown in Fig. 3.15, the voltage division factor determines in part whether conduction occurs through the HOMO or the LUMO. If $\eta = 0$, then the molecular energy levels are fixed with respect to the source contact. As the potential of the drain is increased, conduction eventually occurs through the HOMO. But if the potential of the drain is decreased, conduction can occur through the LUMO. The current-voltage characteristic of this device will exhibit a gap around zero bias that corresponds to the HOMO-LUMO gap.[†]

If $\eta = 0.5$, however, then irrespective of whether the bias is positive or negative, current always flows through the molecular energy level closest to the Fermi energy. In this situation, which is believed to correspond to most single molecule measurements,¹ the gap around zero bias is *not* the HOMO-LUMO gap, but, in this example, four times the Fermi energy – HOMO separation.[§]

The voltage division factor is a crude model of the potential profile, which more generally could be obtained from Poisson's equation. η is also likely to vary with bias. At high biases, there may be significant charge redistribution within the molecule, leading to a change in η .[†]

[†] F. Zahid, M. Paulsson, and S. Datta, 'Electrical conduction in molecules'. In *Advanced Semiconductors and Organic Nanotechniques*, ed. H. Korkoc. Academic Press (2003).

[§] It is possible to experimentally distinguish between $\eta = 0.5$ and $\eta = 0$ by choosing contact metals with different work functions. If the conductance gap is observed to change then it cannot be determined by the HOMO-LUMO gap, and hence $\eta \neq 0$

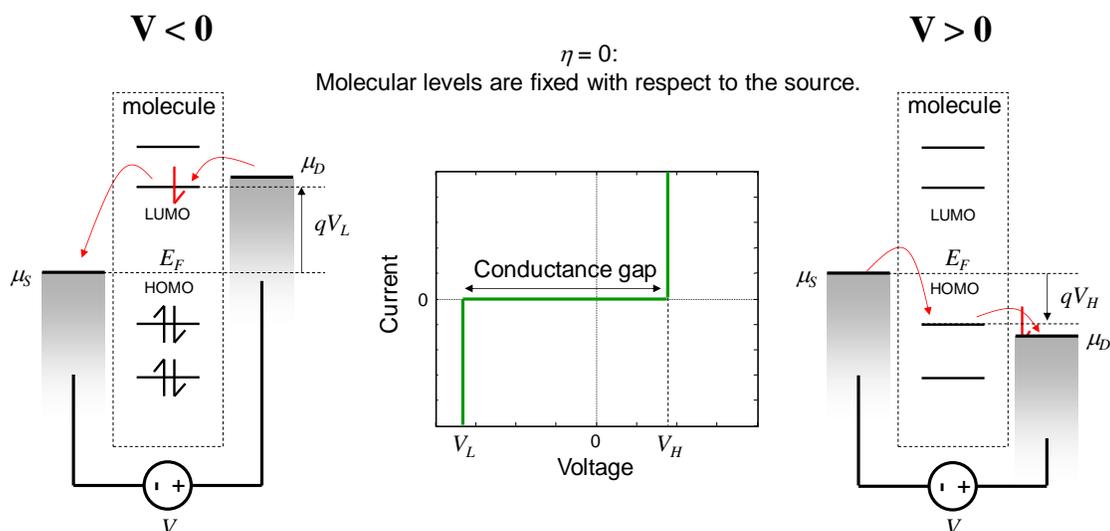


Fig. 3.15. The voltage division factor is crucial in determining the conduction level in a single molecule device. In this example, when $\eta = 0$, conduction always occurs through the HOMO when the applied bias is positive, and through the LUMO when the applied bias is negative. The conductance gap is determined by the HOMO-LUMO separation. Adapted from F. Zahid, M. Paulsson, and S. Datta, 'Electrical conduction in molecules'. In *Advanced Semiconductors and Organic Nanotechniques*, ed. H. Korkoc. Academic Press (2003).

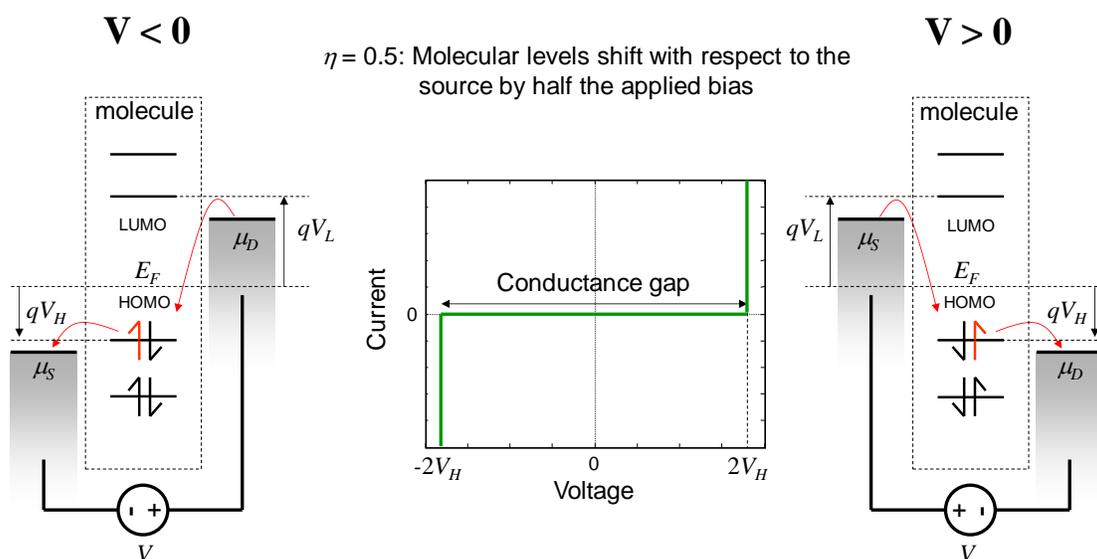


Fig. 3.16. When $\eta = 0.5$, conduction always occurs through the molecular orbital closet to the Fermi Energy. In this example that is the HOMO, irrespective of the polarity of the applied bias. Adapted from F. Zahid, M. Paulsson, and S. Datta, 'Electrical conduction in molecules'. In *Advanced Semiconductors and Organic Nanotechniques*, ed. H. Korkoc. Academic Press (2003).

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(ii) Charging

Previously, we defined the charging energy as the change in the molecule's potential per additional electron. To calculate the net effect of charging we need the number of electrons transferred.

At equilibrium, the number of electrons on the molecule is determined by its Fermi energy.

$$N_0 = \int_{-\infty}^{\infty} g(E) f(E, E_F) dE \quad (3.20)$$

Under bias, the electron distribution on the molecule is no longer in equilibrium. We will define the number of electrons under bias as N .

Thus, the change in potential at the molecule due to charging is

$$U_C = \frac{q^2}{C_{ES}} (N - N_0) \quad (3.21)$$

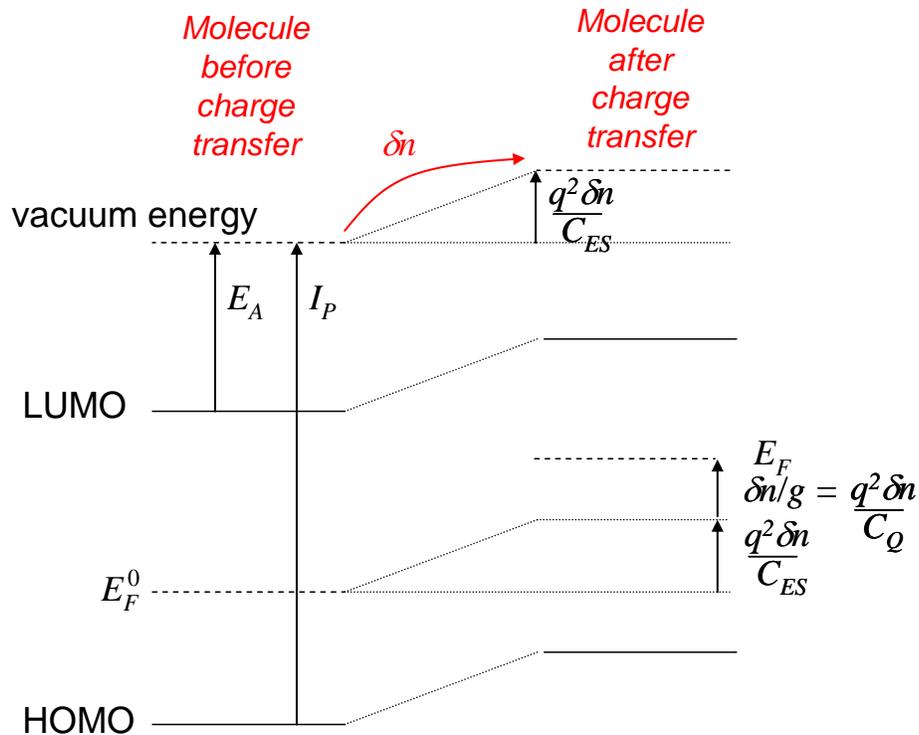


Fig. 3.17. The effect of charging on a molecule. The addition of electrons shifts the molecular potential (and hence all orbitals within the molecule) in order to repel the addition of more electrons. Note that although we have shown the expected change in the Fermi level, this is only meaningful if the molecule remains in equilibrium. Adapted from F. Zahid, M. Paulsson, and S. Datta, 'Electrical conduction in molecules'. In *Advanced Semiconductors and Organic Nanotechniques*, ed. H. Korkoc. Academic Press (2003).

Summary

The net change in potential at the molecule, U , is the sum of electrostatic and charging effects:

$$U = U_{ES} + U_C \quad (3.22)$$

By applying the source-drain voltage relative to a ground at the molecule we have forced $U_{ES} = 0$ in Fig. 3.16. But it will not always be possible to ignore electrostatic effects on U if the ground is positioned elsewhere. Analyses of transistors, for example, typically define the source to be ground.

We model the effect of the change in potential by rigidly shifting all the energy levels within the molecule, i.e.

$$g \rightarrow g(E - U) \quad (3.23)$$

Calculation of Current

Let's model the net current at each contact/molecule interface as the sum of two components: the contact current, which is the current that flows into the molecule, and the molecule current, which is the current that flows out of the molecule.

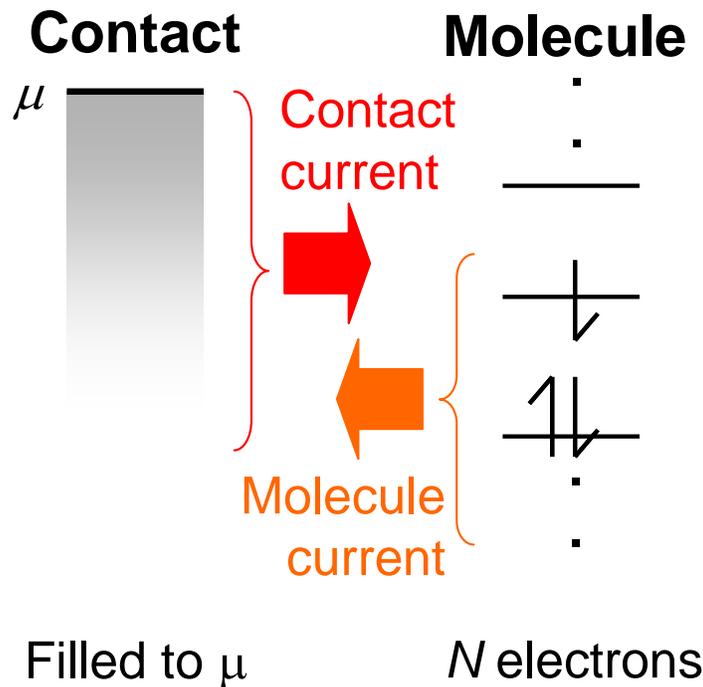


Fig. 3.18. The net current at a contact/molecule interface can be broken into a contact current – the current that flows out of the contact - and a molecule current – the current that flows out of the molecule. At equilibrium, these currents must balance.

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(i) The contact current

This current is the number of available states in the molecule filled per second. Electrons in the contact are filled to its chemical potential. They cannot jump into higher energy states in the molecule. The total number of electrons that can be transferred is simply equal to the number of states.

At the source contact, we get

$$N_S = \int_{-\infty}^{\infty} g(E-U)f(E, \mu_S)dE \quad (3.24)$$

where $g(E-U)$ is the molecular density of states shifted by the net potential change. Similarly, if at the drain contact then the number of electrons, N_D , that could be transferred level is

$$N_D = \int_{-\infty}^{\infty} g(E-U)f(E, \mu_D)dE \quad (3.25)$$

Let's define the transfer rate at the source and drain contacts as $1/\tau_S$ and $1/\tau_D$, respectively. Then the contact currents are

$$I_S^C = q \frac{N_S}{\tau_S}, \quad I_D^C = -q \frac{N_D}{\tau_D} \quad (3.26)$$

Note that we have defined electron flow out of the source and into the drain as positive.

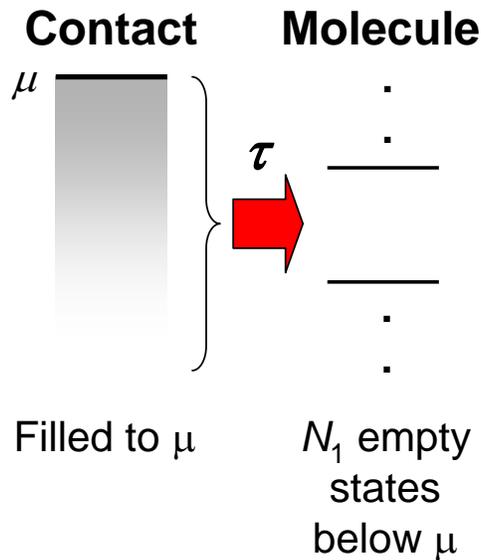


Fig. 3.19. The contact current is the rate of charge transfer from the contact to the molecule. Only states in the molecule with energies below the chemical potential of the contact may be filled. The transfer rate of a single electron from the contact is $1/\tau_S$.

(ii) The molecule current

Now, if we add electrons to the molecule, these electrons can flow back into the contact, creating a current opposing the contact current. The molecule current is the number of electrons transferred from the molecule to the contact per second.

Thus, the molecule currents into the source and drain contacts are

$$I_S^M = -q \frac{N}{\tau_S}, \quad I_D^M = q \frac{N}{\tau_D} \quad (3.27)$$

where we have again defined electron flow out of the source and into the drain as positive.

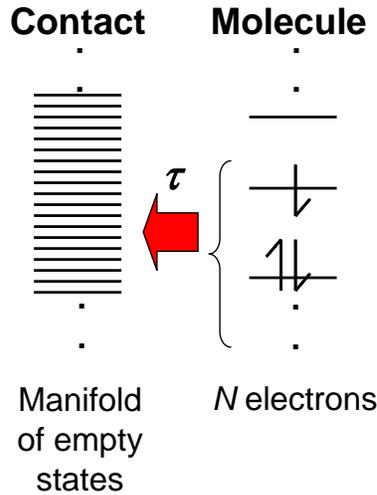


Fig. 3.20. The molecule current is the rate of charge transfer from the molecule to the contact. Note that the electrons on the molecule are not necessarily in equilibrium. The lifetime of a single electron on the molecule is τ .

From Eqns. (3.26) and (3.27) the net current at the source contact is

$$I_S = \frac{q}{\tau_S} (N_S - N) \quad (3.28)$$

and the net current at the drain contact is

$$I_D = \frac{q}{\tau_D} (N - N_D) \quad (3.29)$$

Note that we have assumed that the transfer rates in and out of each contact are identical. For example, let's define τ_S^M as the lifetime of an electron in the molecule and $1/\tau_S^C$ as the rate of electron transfer from the source contact. It is perhaps not obvious that $\tau_S^M = \tau_S^C$, but examination of the inflow and outflow currents at equilibrium confirms that it must be so. When the source-molecule junction is at equilibrium, no current flows. From Eqns. (3.20), (3.21) and (3.24), we have $N_S = N$. Thus, for $I_S = 0$ we must have $\tau_1^M = \tau_1^C$.

Part 3. Two Terminal Quantum Dot Devices

Equating the currents in Eqns. (3.28) and (3.29) gives[†]

$$I = q \int_{-\infty}^{\infty} g(E-U) \frac{1}{\tau_S + \tau_D} (f(E, \mu_S) - f(E, \mu_D)) dE \quad (3.30)$$

and

$$N = \int_{-\infty}^{\infty} g(E-U) \frac{\tau_D f(E, \mu_S) + \tau_S f(E, \mu_D)}{\tau_S + \tau_D} dE \quad (3.31)$$

The difficulty in evaluating the current is that it depends on U and hence N . But Eq. (3.31) is not a closed form solution for N , since the right hand side also contains a N dependence via U . Except in simple cases, this means we must iteratively solve for N , and then use the solution to get I . This will be discussed in greater detail in the problems accompanying this Part.

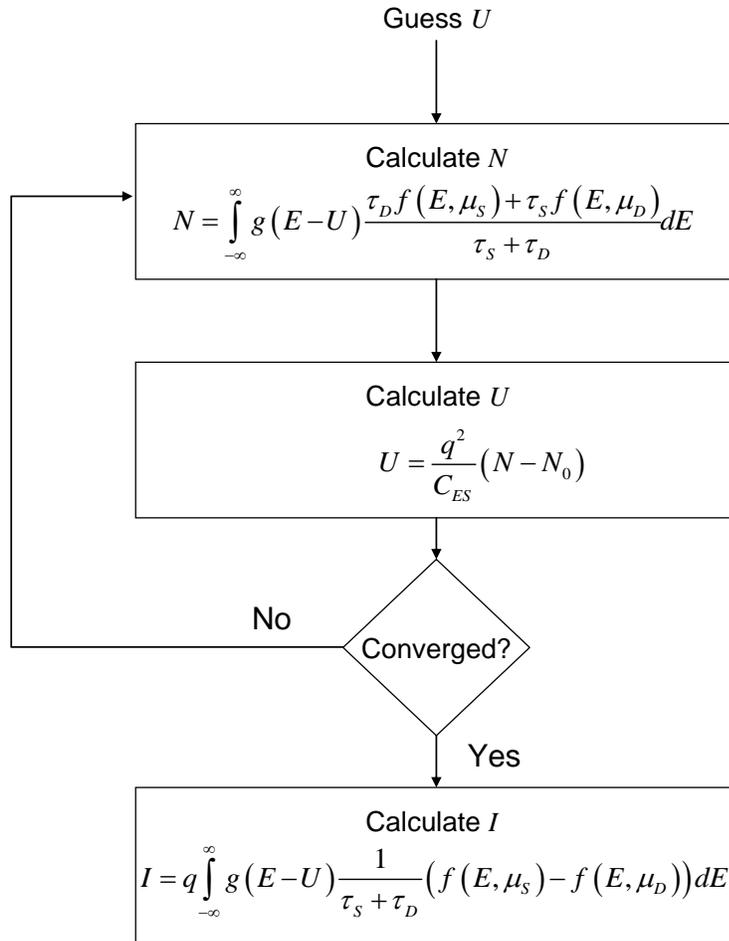


Fig. 3.21. A flow diagram describing an iterative solution to the IV characteristics of two terminal molecular devices. Adapted from F. Zahid, M. Paulsson, and S. Datta, 'Electrical conduction in molecules'. In *Advanced Semiconductors and Organic Nanotechniques*, ed. H. Korkoc. Academic Press (2003).

[†] F. Zahid, M. Paulsson, and S. Datta, 'Electrical conduction in molecules'. In *Advanced Semiconductors and Organic Nanotechniques*, ed. H. Korkoc. Academic Press (2003).

Analytic calculations of the effects of charging

The most accurate method to determine the IV characteristics of a quantum dot device is to solve for the potential and the charge density following the scheme of Fig. 3.21. This is often known as the self consistent approach since the calculation concludes when the initial guess for the potential U has been modified such that it is consistent with the value of U calculated from the charge density.

Unfortunately, numerical approaches can obscure the physics. In this section we will make some approximations to allow an analytic calculation of charging. We will assume operation at $T = 0\text{K}$, and discrete molecular energy levels, *i.e.* weak coupling between the molecule and the contacts such that $(\Gamma = \hbar/\tau) \rightarrow 0$.

Let's consider a LUMO state with energy E_{LUMO} that is above the equilibrium Fermi level. Under bias, the energy of the LUMO is altered by electrostatic and charging-induced changes in potential. When we apply the drain source potential, it is convenient to assume that the molecule is ground. Under this convention, the only change in the molecule's potential is due to charging. Graphically, the physics can be represented by plotting the energy level of the molecule in the presence and absence of charging. In Fig. 3.22, below, we shade the region between the charged and uncharged LUMOs. Now

$$U_C = \frac{q^2}{C_{ES}}(N - N_0), \quad (3.32)$$

and at $T = 0\text{K}$, $N_0 = 0$ for the LUMO in Fig. 3.22. Thus, the area of the shaded region is proportional to the charge on the molecule.

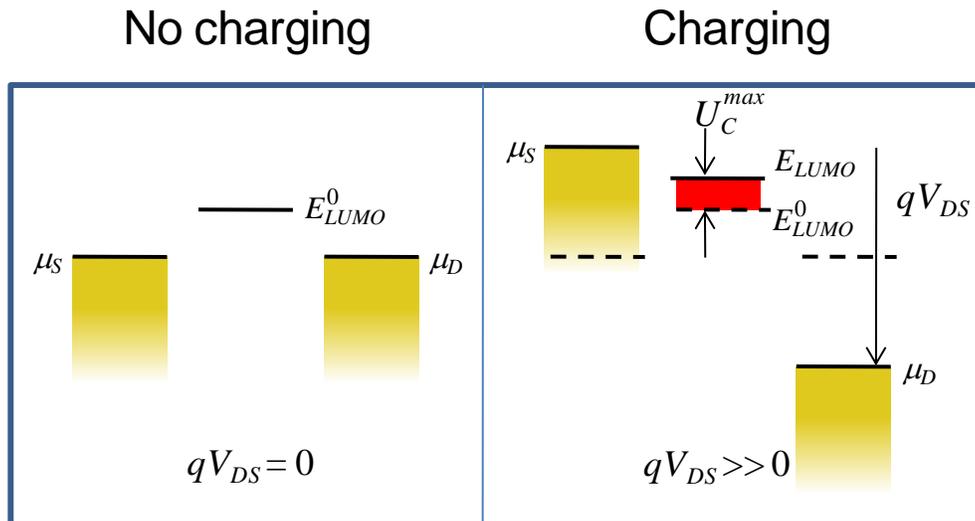


Fig. 3.22. Under bias, the energy levels of the molecule can be shifted by electrostatic and charging-induced changes in the potential. If we assume the molecule is ground, then the electrostatic changes in potential alter the source and the drain. Only charging then alters the molecular energy level. The difference between the charged and uncharged molecular energy levels is proportional to the charge on the molecule and is shaded red.

Part 3. Two Terminal Quantum Dot Devices

The graphical approach is a useful guide to the behavior of the device. There are three regions of operation, each shown below.

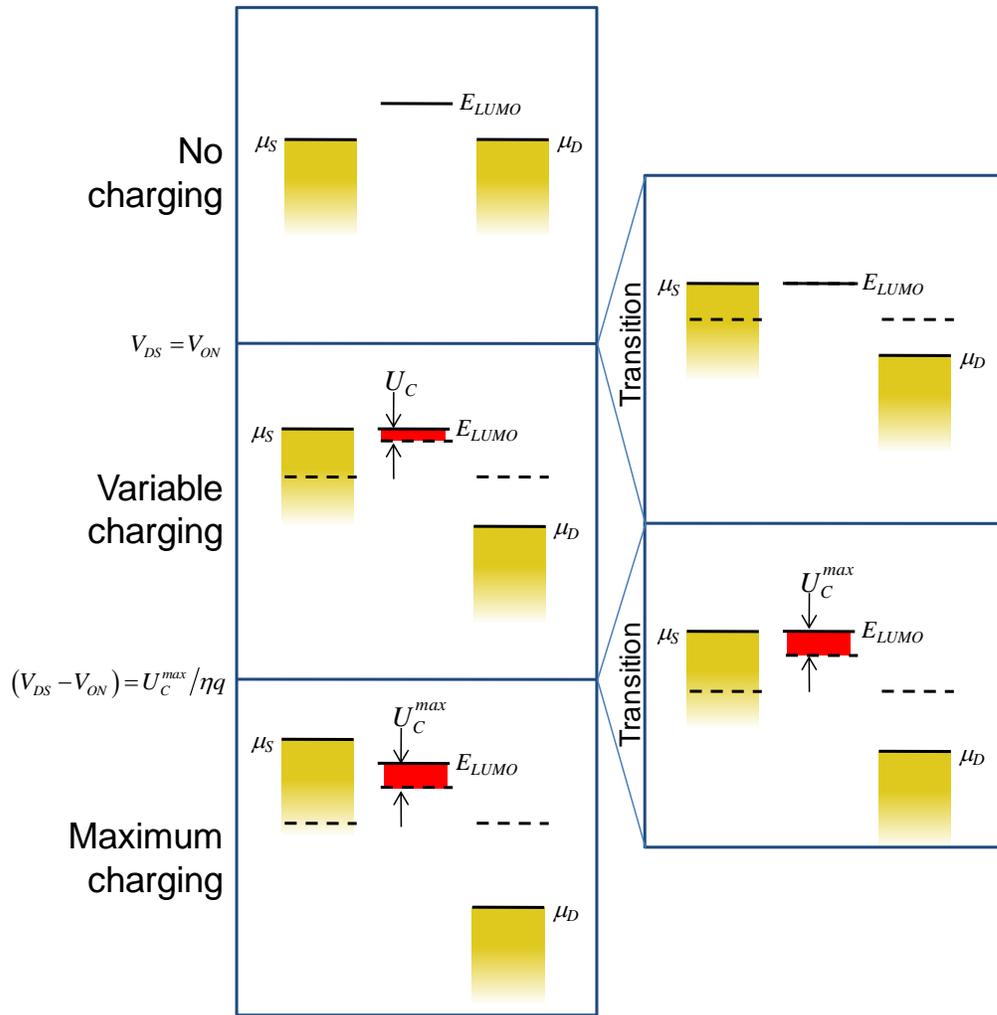


Fig. 3.23. The three regions of operation for a two terminal quantum dot device with discrete energy levels at $T = 0K$. Current flow requires the source to inject carriers into the molecular energy levels. The onset of current flow occurs when the chemical potential of the source is resonant with the LUMO. Additional drain-source bias charges the molecule, and the current increases linearly with the molecular charge. Finally, a maximum charge density is reached. Further increases in applied bias do not increase the charging energy or the current flow.

(i) No charging

At $T = 0K$ and $V_{DS} = 0$ there is no charge in the LUMO. Charging cannot occur unless electrons can be injected from the source into the LUMO. So as V_{DS} increases, charging remains negligible until the LUMO energy is aligned with the chemical potential of the source. Thus, for $\mu_S < E_{LUMO}$ the charging energy, $U_C = 0$.

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In this region, $I_{DS} = 0$. We define the bias at which current begins to flow as $V_{DS} = V_{ON}$. V_{ON} is given by

$$V_{ON} = \frac{E_{LUMO}^0 - \mu_S}{q\eta} \quad (3.33)$$

where E_{LUMO}^0 is the LUMO energy level at equilibrium.

(ii) Maximum charging

For $\mu_S > E_{LUMO}$, the charge on the LUMO is independent of further increases in V_{DS} . It is a maximum. From Eq. (3.31), the LUMO's maximum charge is

$$N^{max} = \frac{2\tau_D}{\tau_S + \tau_D} \quad (3.34)$$

Consequently, the charging energy is

$$U_C^{max} = \frac{2q^2}{C_{ES}} \frac{\tau_D}{\tau_S + \tau_D} \quad (3.35)$$

For all operation in forward bias, it is convenient to calculate the current from Eq. (3.29). At $T = 0K$, the charges injected by the drain $N_D = 0$. Consequently,

$$I_{DS} = \frac{qN^{max}}{\tau_D} = \frac{2q}{\tau_S + \tau_D} \quad (3.36)$$

Maximum charging occurs for voltages $\mu_S > E_{LUMO}$. We can rewrite this condition as

$$(V_{DS} - V_{ON}) > U_C^{max} / \eta q \quad (3.37)$$

(iii) Variable charging

Charging energies between $0 < U_C < U_C^{max}$ require that $\mu_S = E_{LUMO}$. Assuming that the molecule is taken as the electrostatic ground, then $\mu_S = E_{LUMO} = U_C$ for this region of operation. Calculating the current from Eq. (3.29) gives

$$I_{DS} = \frac{qN}{\tau_D} \quad (3.38)$$

Then, given that $U_C = q^2N / C_{ES}$, we can rearrange Eq. (3.38) to get

$$I_{DS} = \frac{C_{ES}U_C}{q\tau_D} \quad (3.39)$$

Then, from Eqs. (3.18) and (3.19) and noting that $\mu_S = E_{LUMO} = U_C$,

$$I_{DS} = \frac{C_{ES}}{\tau_D} \eta (V_{DS} - V_{ON}). \quad (3.40)$$

This region is valid for voltages

$$0 < (V_{DS} - V_{ON}) < U_C^{max} / \eta q. \quad (3.41)$$

The full IV characteristic is shown below. Under our assumptions the transitions between the three regions of operation are sharp. For $T > 0K$ and $(\Gamma = \hbar/\tau) > 0$ these transitions are blurred and are best calculated numerically; see the Problem Set.

Part 3. Two Terminal Quantum Dot Devices

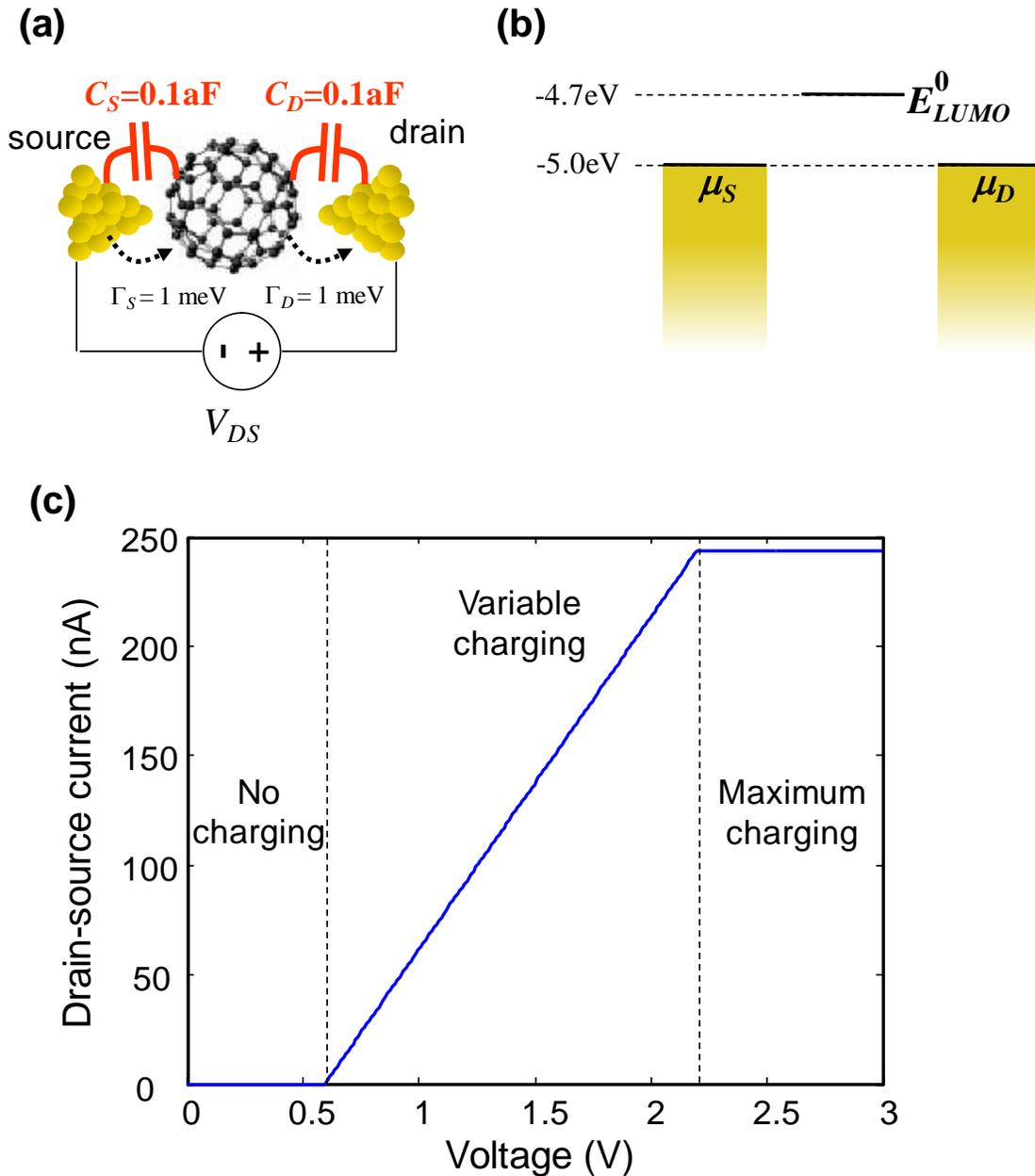


Fig. 3.24. (a) An example of a single molecule device subject to strong charging effects. The coupling between the molecule and the contacts is small relative to the applied voltage, *i.e.* $\Gamma_S/q = \Gamma_D/q = 1 \text{ mV}$. The source and drain capacitances yield a large charging potential per electron $q^2/C_{ES} = 0.8 \text{ eV}$. The voltage division factor is $\eta = 0.5$. (b) The offset between the LUMO and the contact work functions is 0.3 eV , consequently, $V_{ON} = 0.3/\eta = 0.6 \text{ V}$ (c) The current-voltage characteristic.

A small signal circuit model

In the discussion of the establishment of equilibrium between a contact and a molecule we introduced a generalized circuit model where each node potential is the Fermi level, not the electrostatic potential as in a conventional electrical circuit.

We can extend the model to two terminal, and even three terminal devices. It must be emphasized, however, that the model is only valid for small signals. In particular, the model is constrained to small V_{DS} . We assume that the density of states is constant and the modulation in V_{DS} must be smaller than kT/q so that we can ignore the tails of the Fermi distribution.

Let's consider current injected by the source

$$I_S = \frac{q}{\tau_S} (N_S - N) \quad (3.42)$$

This can be rewritten as

$$I_S = \frac{q}{\tau_S} \int_{-\infty}^{+\infty} g(E-U) (f(E, \mu_S) - f(E, E_F)) dE \quad (3.43)$$

For small differences between the source and drain potentials, and at $T = 0K$, we get

$$I_S = \frac{C_Q}{\tau_S} \frac{(\mu_S - E_F)}{q} \quad (3.44)$$

Thus, each contact/molecule interface is Ohmic in the small signal limit. Defining $R_S = \tau_S/C_Q$, and $R_D = \tau_D/C_Q$. We can model the contact/molecule/contact as shown in Fig. 3.25.

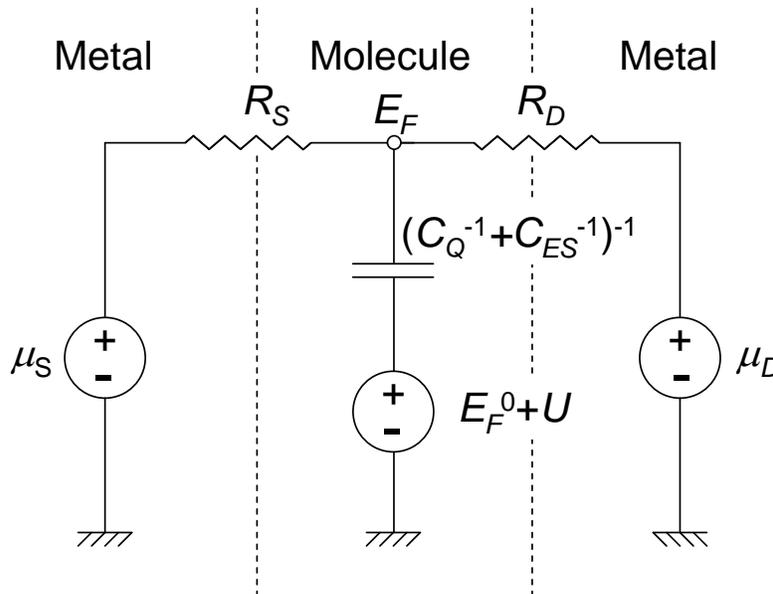


Fig. 3.25. A small signal model for two terminal metal/molecule/metal circuits. Note that the potential U must be determined separately (e.g. by using a capacitive divider circuit).

Part 3. Two Terminal Quantum Dot Devices

The Ideal Contact Limit[†]

Interfaces between molecules and contacts vary widely in quality. Much depends on how close we can bring the molecule to the contact surface. Here, we have modeled the source and drain interfaces with the parameters τ_S and τ_D . If electron injection is unencumbered by barriers or defects then these lifetimes will be very short. We might expect that the current should increase indefinitely as the injection rates decrease. But in fact we find a limit – known as the quantum limit of conductance. We will examine this limit rigorously in the next section but for the moment, we will demonstrate that it also holds in this system.

We model ideal contacts by considering the current under the limit that $\tau_S = \tau_D \rightarrow 0$. Note that the uncertainty principle requires that the uncertainty in energy must increase if the lifetime of an electron on the molecule decreases. Thus, the density of states must change as the lifetime of an electron on a molecule changes.

Let's assume that the energy level in the isolated molecule is discrete. In Part 2, we found a Lorentzian density of states for a single molecular orbital with net decay rate $\tau_S^{-1} + \tau_D^{-1}$:

$$g(E-U)dE = \frac{2}{\pi} \frac{(\hbar/2\tau_S + \hbar/2\tau_D)}{(E-U-E_0)^2 + (\hbar/2\tau_S + \hbar/2\tau_D)^2} dE \quad (3.45)$$

If we take the limit, we find that the molecular density of states is uniform in energy:

$$\lim_{\tau_S = \tau_D \rightarrow 0} g(E-U)dE = \frac{8}{h} \frac{1}{1/\tau_S + 1/\tau_D} dE \quad (3.46)$$

Substituting into Eq. (3.30) for $\tau_S = \tau_D$ gives

$$I = \frac{2q}{h} \int_{-\infty}^{+\infty} f(E, \mu_S) - f(E, \mu_D) dE \quad (3.47)$$

At $T = 0K$,

$$f(E, \mu) = u(\mu - E) \quad (3.48)$$

where u is the unit step function, and the integral in Eq. (3.47) gives

$$I = \frac{2q}{h} (\mu_S - \mu_D) \quad (3.49)$$

Note $-qV_{DS} = (\mu_D - \mu_S)$, thus the conductance through a single molecular orbital is

$$G = \frac{2q^2}{h} \quad (3.50)$$

The equivalent resistance is $G^{-1} = 12.9 \text{ k}\Omega$. Thus, even for ideal contacts, this structure is resistive. We will see this expression again in the next section. It is the famous quantum limited conductance.

[†] This derivation of the quantum limit of conductance is due to S. Datta, 'Quantum transport: atom to transistor' Cambridge University Press (2005).

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Problems

1. (a) A $1\text{nm} \times 1\text{nm}$ molecule is 30\AA away from a metal contact. Calculate the electrostatic capacitance using the parallel plate model of the capacitor. Find the change in potential per charge added to the molecule, $U_{ES}/\delta n$.

(b) A $50\text{nm} \times 50\text{nm}$ molecule is 30\AA away from a metal contact. Calculate the electrostatic capacitance using the parallel plate model of the capacitor. Find the change in potential per charge added to the molecule, $U_{ES}/\delta n$.

(c) A $100\text{nm} \times 100\text{nm}$ molecule is 30\AA away from a metal contact. Calculate the electrostatic capacitance using the parallel plate model of the capacitor. Find the change in potential per charge added to the molecule, $U_{ES}/\delta n$.

2.(a) Assume the molecule in problem 1(a) has a uniform density of states of $g(E) = 3 \times 10^{20}/\text{eV}$ and Fermi level at $E_F^0 = -5.7\text{eV}$ in isolated space. The metal has a work function of 5eV . Sketch all of the energy levels in equilibrium after the metal contact and molecule are brought into contact. Find the number of charges, δn , transferred from the molecule to the metal (or vice versa.).

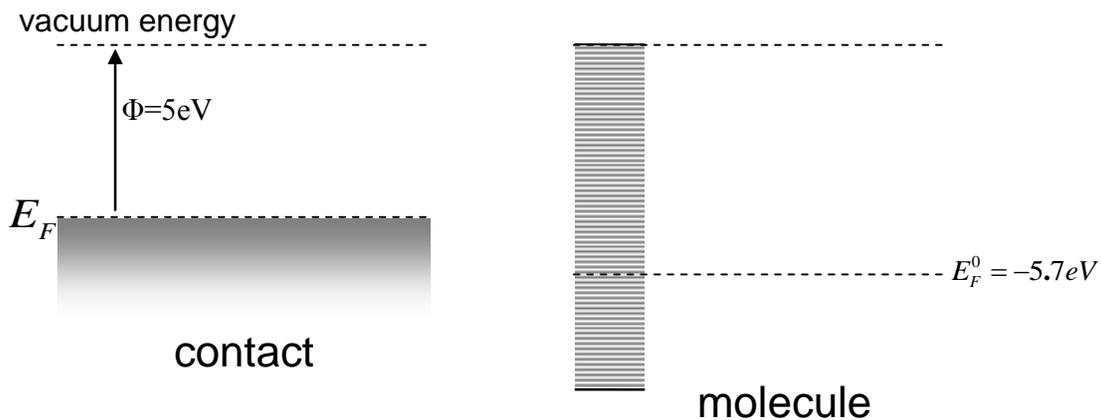


Fig. 3.26. A separated contact and molecule. The molecule has a uniform density of states.

(b) Repeat part (a) for the molecule in problem 1(b) using the same density of states and Fermi levels.

(c) Repeat part (a) for the molecule in problem 1(c) using the same density of states and Fermi levels.

Part 3. Two Terminal Quantum Dot Devices

3. Consider the molecule illustrated below with $E_A = 2\text{eV}$, $I_P = 5\text{eV}$, and $E_F^0 = 3.5\text{eV}$.

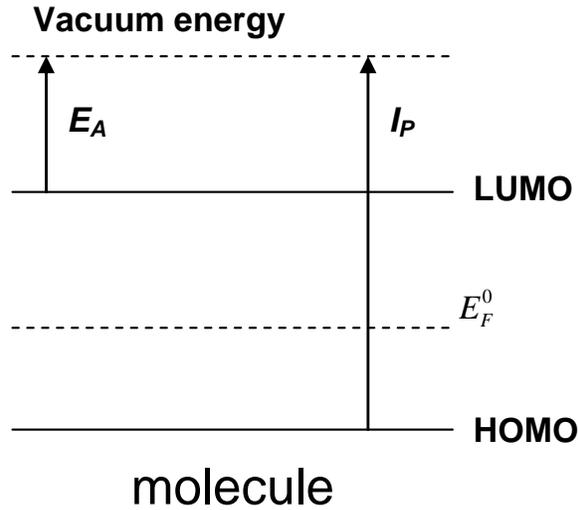


Fig. 3.27. Energy levels within a molecule.

- (a) What is C_Q when the electron lifetime is $\tau = \infty, 1\text{ps}, 1\text{fs}$?
- (b) For each of the lifetimes in part (a), what is the equilibrium Fermi level when $\delta n = 0.1$ charge is added to the molecule.
- (c) What is the equilibrium Fermi level when $\tau_{HOMO} = .1\text{ps}$ and $\tau_{LUMO} = 1\text{ps}$?

4. A quantum well is brought into contact with a metal electrode as shown in the figure below.

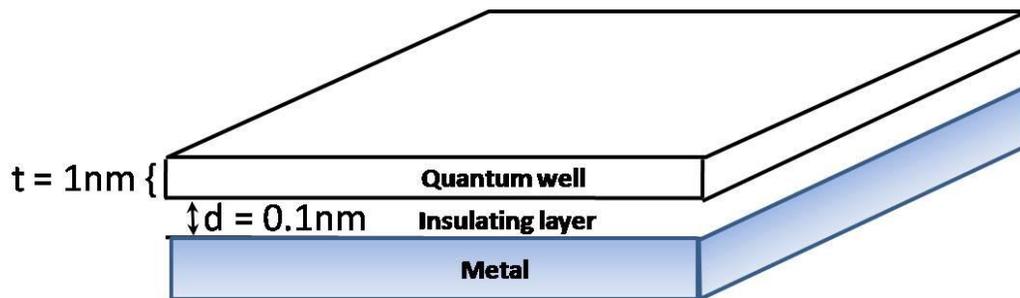


Fig. 3.28. The quantum well in contact with a metal surface.

- (a) Calculate the DOS in the well between 0 and 2eV assuming an infinite confining potential and that the potential inside the well is zero.

Continued....

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(b) On contact charge can flow between the metal and the quantum well. But assume that on contact the well is still separated from the metal by a 0.1nm thick layer with dielectric constant $5 \times 8.84 \times 10^{-12}$ F/m. Calculate the surface charge density at equilibrium, for an initial separation of (i) 0.6eV and (ii) -0.6eV, between the quantum well E_F and the chemical potential of the metal. Assume $T=0$.

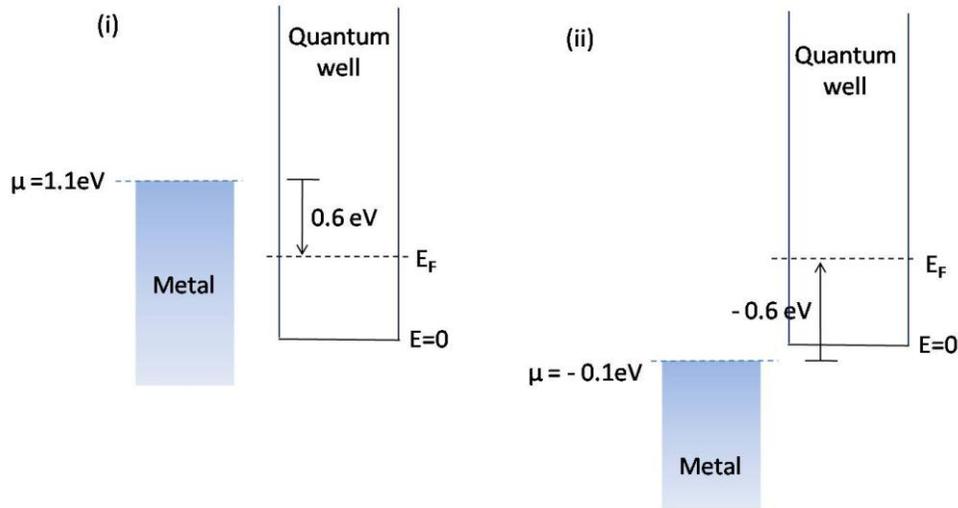


Fig. 3.29. Two different energetic alignments between the quantum well and the metal.

(c) Plot the vacuum energy shift at each interface at equilibrium, for part b (i) and (ii), above.

The next question is adapted from an example in ‘Introductory Applied Quantum and Statistical Mechanics’ by Hagelstein, Senturia and Orlando, Wiley Interscience 2004.

5. In this problem we consider charge injection from a *discrete energy level* rather than a metal. Consider charge transport through a quantum dot buried within an insulator. The materials are GaAs|GaAlAs|GaAs|GaAlAs|GaAs with thicknesses $1000\text{\AA}|40\text{\AA}|100\text{\AA}|40\text{\AA}|1000\text{\AA}$. The potential landscape of this device is modeled as below with $V_0=0.3 \text{ eV}$, $b=50\text{\AA}$, and $a=90\text{\AA}$. Let the effective mass of an electron in GaAs and GaAlAs be $0.07m_e$, where m_e is the mass of an electron.

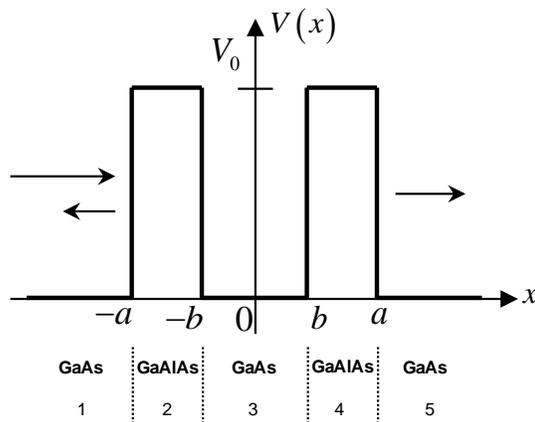


Fig. 3.30. The energy levels for a quantum dot buried within a tunnel barrier.

Part 3. Two Terminal Quantum Dot Devices

Considering only energies below V_0 , the wavefunction is piecewise continuous with

$$\begin{cases} \psi_1 = e^{ikx} + Be^{-ikx} \\ \psi_2 = Ce^{-\alpha x} + De^{\alpha x} \\ \psi_3 = Fe^{ikx} + Ge^{-ikx} \\ \psi_4 = He^{-\alpha x} + Ie^{\alpha x} \\ \psi_5 = Je^{ikx} \end{cases}, \text{ where } k = \frac{\sqrt{2mE}}{\hbar} \text{ and } \alpha = \frac{\sqrt{2m(V_0 - E)}}{\hbar}$$

(a) Match the boundary conditions and find \bar{M} such that $\bar{M}\bar{C} = \bar{A}$, where

$$\bar{C} = \begin{pmatrix} B \\ C \\ D \\ F \\ G \\ H \\ I \\ J \end{pmatrix} \text{ and } \bar{A} = \begin{pmatrix} e^{-ika} \\ ike^{-ika} \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

(b) The transmission coefficient is $T = |J|^2 = |\bar{C}(8)|^2$, where $\bar{C} = \bar{M}^{-1}\bar{A}$. Determine T numerically or otherwise. It is plotted below as a function of electron energy, E . Verify that the resonant energies where $T = 1$ are within a factor of two of the eigenenergies of an infinite square well with width $L=2b$. Note that this approximation for the resonant energies works better for deeper square wells (V_0 big).

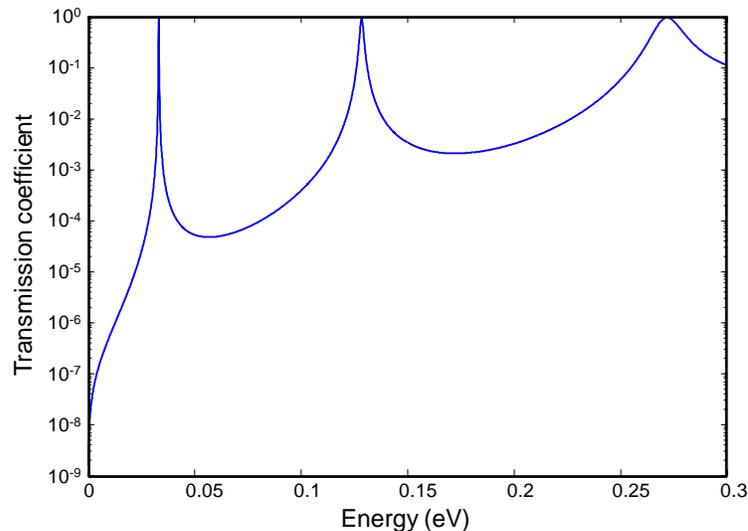


Fig. 3.31. Your solution to part (b) should look like this.

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(c) Why do the widths of the resonances in the transmission coefficient increase at higher electron energy?

(d) Now suppose we apply a voltage across this device. Electrons at the bottom of the conduction band E_C in the GaAs on the left side will give net current flow which is proportional to the transmission coefficient T .

Let's first consider only one discrete energy level E_0 in the dot as shown in part (a) of the figure below. Assume the potential drop is linear (electric field F is constant) across the whole device, as shown in part (b) of the figure below.

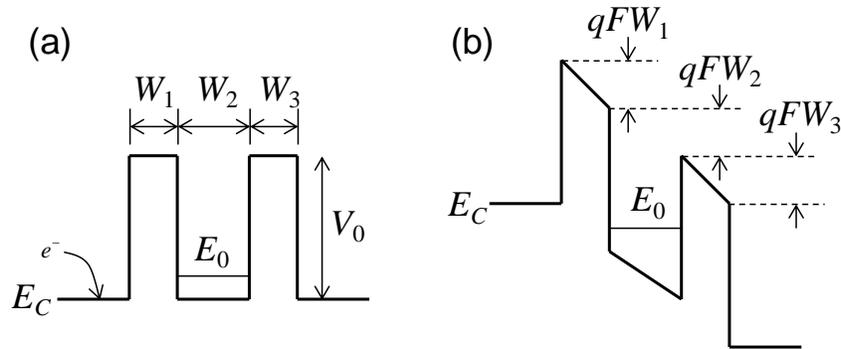


Fig. 3.32. (a) The Quantum Dot structure at zero bias, and (b) under an applied bias.

Sketch out qualitatively what you think the current-vs-voltage curve will look like. It should look quite different to the IV characteristic of a quantum dot with metal contacts. Explain the difference.

(e) Approximating E_0 as the ground state of an infinite square well, what is the expression for the resonant voltage in terms of W_2 , assuming $W_1=W_3$?

(f) Without solving for the wavefunction, sketch qualitatively what the probability density of the lowest eigenstate of an infinite well will look like when distorted by an electric field. Where in the well has the highest probability of finding an electron?

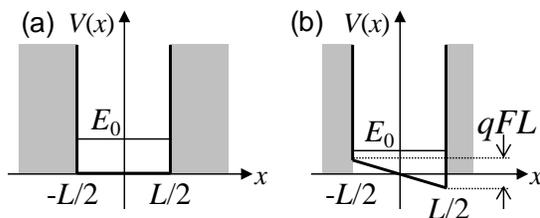


Fig. 3.33. The quantum dot under bias.

(g) Now, if we consider the multiple discrete energy levels in the dot, what will the current-voltage curve look like?

(h) Analytically determine the current through the dot at the 0.27eV resonance. Hint: consider the width of the resonance.

Part 3. Two Terminal Quantum Dot Devices

6. Consider the two terminal molecular device shown below. Note that this calculation differs from the previous calculation of charging by considering transport through the HOMO rather than the LUMO.

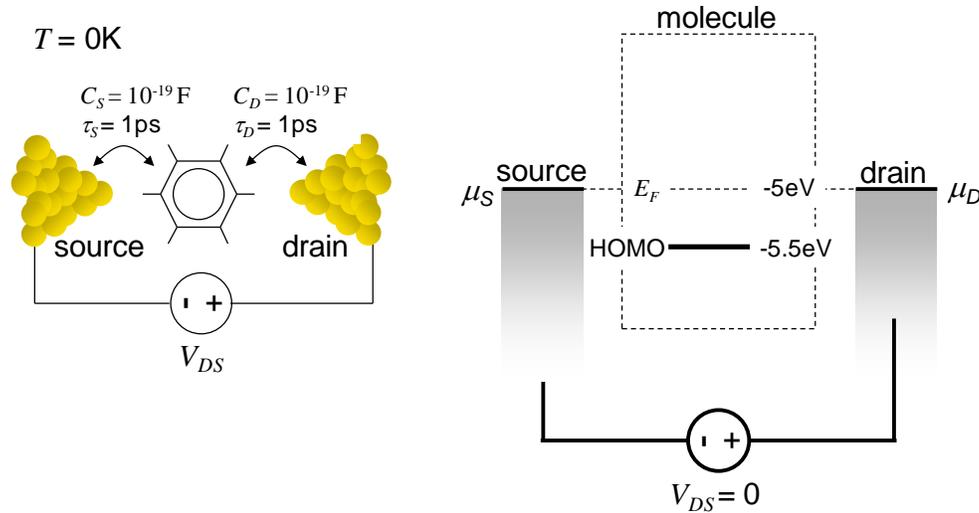


Fig. 3.34. The device structure for an analytical calculation of charging effects.

- (a) Estimate the width of the HOMO from τ_s and τ_D .
- (b) Assuming that the molecule can be modeled as a point source conductor of radius 2nm, calculate the charging energy per electron. Compare to the charging energy determined from the capacitance values shown in Fig. 3.34.
- (c) Assuming that the charging energy is negligible, calculate the I_{DS} - V_{DS} characteristic and plot it.
- (d) Now consider charging with $q^2/C_{ES} = 1\text{eV}$. How does charging alter the maximum current and turn on voltage (the lowest value of V_{DS} when current flows)?
- (e) Show that the number of electrons on the HOMO is at least
- $$N = 2 \frac{\tau_D}{\tau_s + \tau_D}$$
- (f) What is the maximum charging energy when $q^2/C_{ES} = 1\text{eV}$?
- (g) Assuming that the charging energy is negligible, plot the energy level of the HOMO together with the source and drain workfunctions for $V_{DS} = 2\text{V}$. On the same plot, indicate the energy level of the HOMO when $q^2/C_{ES} = 1\text{eV}$ and $V_{DS} = 2\text{V}$. What is the charging energy at this bias?
- (h) Calculate the I_{DS} - V_{DS} characteristic when $q^2/C_{ES} = 1\text{eV}$. Plot it on top of the I_{DS} - V_{DS} characteristic calculated for negligible charging.

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7. Consider the two terminal molecular device shown in the figure below. This question considers conduction through both the HOMO and LUMO as well as the effect of mismatched source and drain injection rates and capacitances.

Note that: $T = 0\text{K}$; $C_S = 2C_D$; $\tau_S = 1\text{ps}$; $\tau_D = 9\text{ps}$

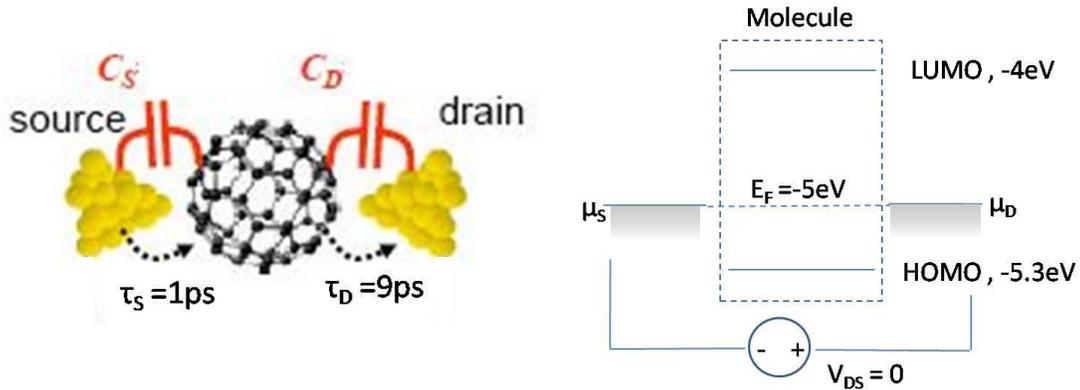


Fig. 3.35. A two terminal molecular device.

- Estimate the width of the HOMO and LUMO from τ_S and τ_D .
- If $C_D = 1\text{pF}$ calculate the charging energy per electron.
- Plot the current-voltage characteristic (IV) from $V_{DS} = -10\text{V}$ to $V_{DS} = 10\text{V}$ assuming that the charging energy equals zero.
- Assume the charging energy is now 1eV per electron. What is C_D ?
- Plot the IV from $V_{DS} = 0\text{V}$ to $V_{DS} = 10\text{V}$ assuming that the charging energy is 1eV per electron.
- Plot the IV from $V_{DS} = -10\text{V}$ to $V_{DS} = 0\text{V}$ assuming that the charging energy is 1eV per electron. **Hint:** you should find a region of this IV characteristic in which the HOMO and LUMO are charging together, increasing the current but leaving the net charge on the molecule unchanged. Consequently, your IV characteristic should exhibit a step change in current at a particular voltage.

Part 3. Two Terminal Quantum Dot Devices

8. A quantum wire with square cross-section with a 1-nm thickness side is bent and fused into a circular ring with radius $R=2\text{nm}$ as shown below.

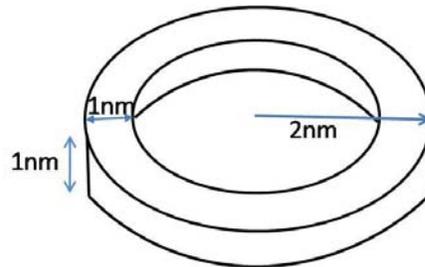


Fig. 3.36. A quantum wire bent into a ring.

(a) Plot the DOS in the wire from $E = 0$ to $E = 0.8\text{eV}$. Assume an infinite confining potential and that the potential in the ring is $V = 0$.

(b) Next the ring is placed between contacts as shown. What is the charging energy?

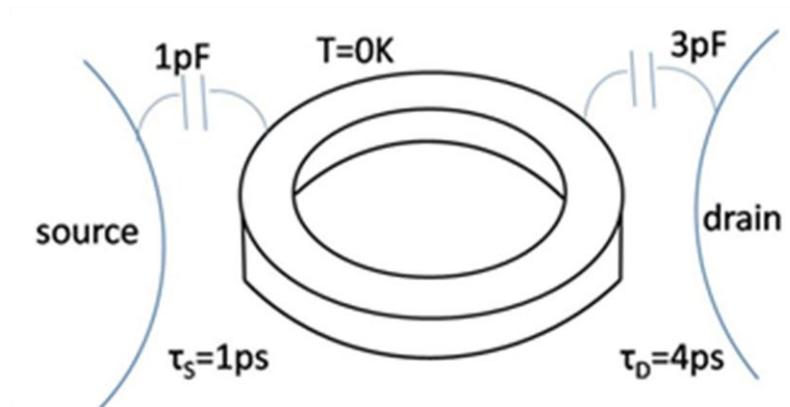


Fig. 3.37. The ring between contacts.

(c) Plot the current versus voltage for V from 0 to 1.1 V.

(d) A magnetic field is applied perpendicular to the ring. Sketch the changes in the IV .

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The next three questions have been adapted from F. Zahid, M. Paulsson, and S. Datta, 'Electrical conduction in molecules'. In *Advanced Semiconductors and Organic Nanotechniques*, ed. H. Korkoc. Academic Press (2003).

9. (a) Numerically calculate the current-voltage and conductance-voltage characteristics for the system shown in Fig. 3.38 with the following parameters:

$$\begin{aligned} \eta &= 0.5 \\ E_F &= -5.0 \text{ eV} \\ \text{HOMO} &= -5.5 \text{ eV} \\ \Gamma_S = \Gamma_D &= 0.1 \text{ eV} \\ T &= 298\text{K} \end{aligned}$$

Set the charging energy to zero, i.e. take $C_{ES} \rightarrow \infty$.

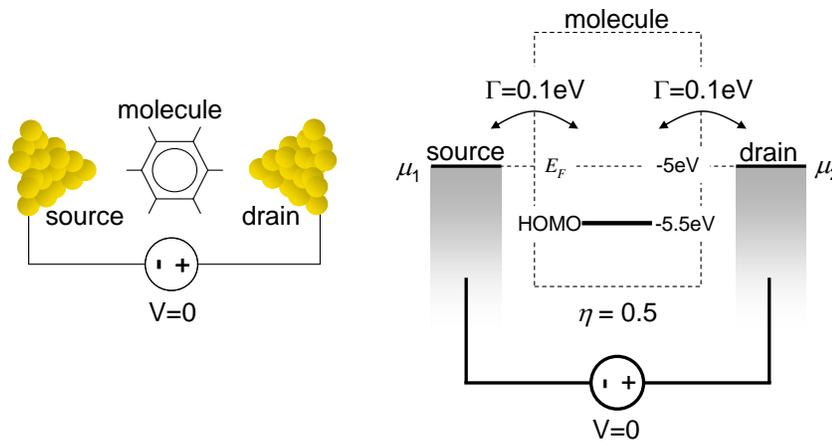


Fig. 3.38. The two terminal molecular device for this problem.

Hints

(1) Despite the statement that $\Gamma_S = \Gamma_D = 0.1 \text{ eV}$, the HOMO in this problem is assumed to be infinitely sharp. Simplify Eqns. (3.30) and (3.31) for $g(E-U) = 2\delta(E-U-\varepsilon)$, where ε is the energy of the HOMO.

(2) You will need to implement the flow chart shown in Fig. 3.21. If your solution for U oscillates and does not converge, try setting

$$U = U_{old} + \alpha(U_{calc} - U_{old}),$$

where U_{calc} is the solution to Eq. (3.21), U_{old} is the previous iteration's estimate of U and α is a small number that may be reduced to obtain convergence.

(b) Repeat the numerical calculation of part (a) with $q^2/C_{ES} = 1 \text{ eV}$.

(c) Explain the origin of the conductance gap. What determines its magnitude?

(d) Write an analytic expression for the maximum current when $q^2/C_{ES} = 0$.

(e) Explain why the conductance is much lower when the charging energy is non-zero.

Part 3. Two Terminal Quantum Dot Devices

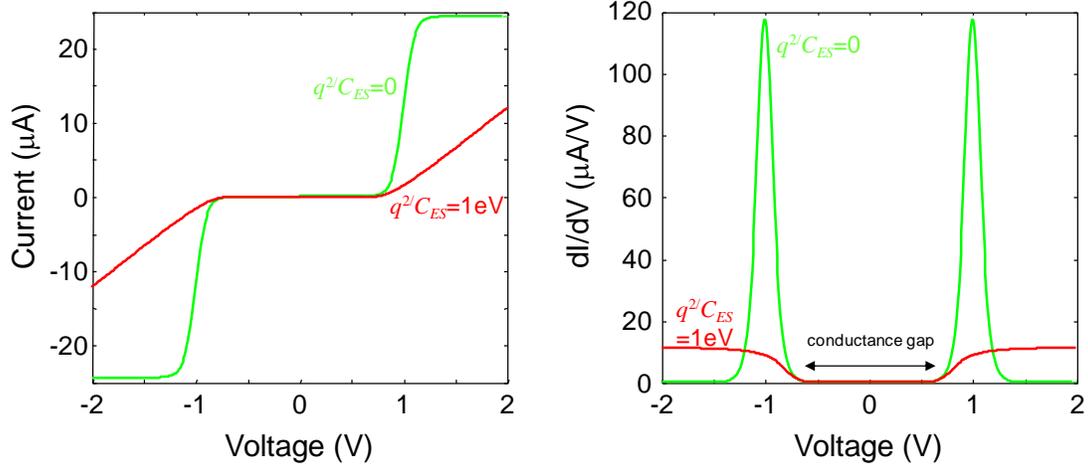


Fig. 3.39. Your solution should look like this.

10. Next, we add a LUMO level at -1.5 eV.

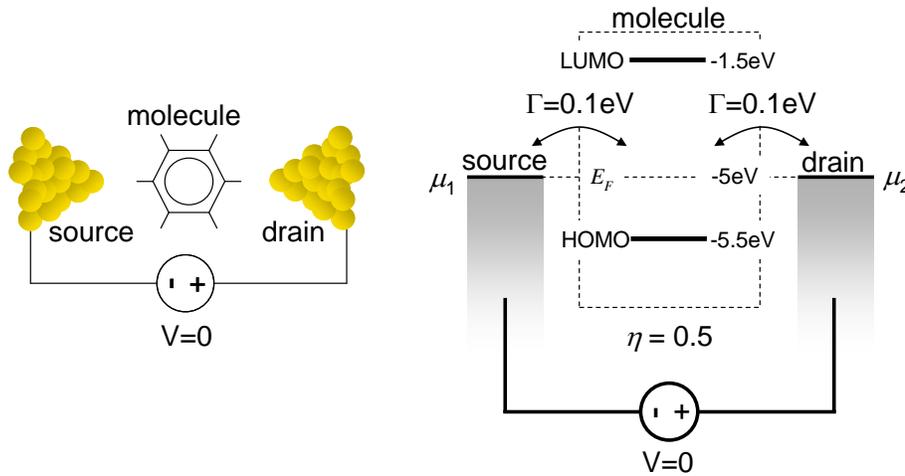


Fig. 3.40. The two terminal molecular device for this problem.

(a) Numerically calculate the current-voltage and conductance-voltage characteristics for $q^2/C_{ES} = 1$ eV and $E_F = -2.5$ eV.

(b) Repeat the numerical calculation for $q^2/C_{ES} = 1$ eV and $E_F = -3.5$ eV.

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(c) Repeat the numerical calculation for $q^2/C_{ES} = 1$ eV and $E_F = -5.0$ eV (same as Q8.b).

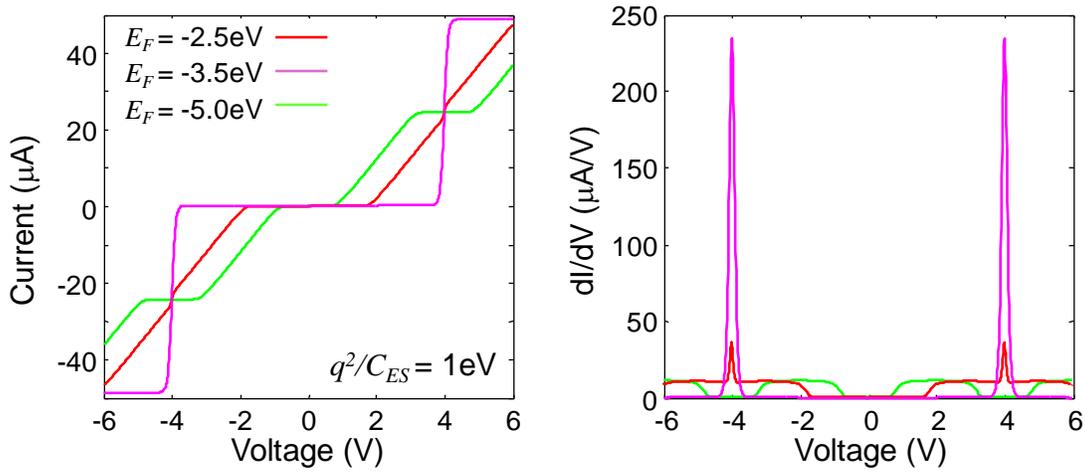


Fig. 3.41. Your solution should look like this.

(d) Why are the current-voltage characteristics uniform? Hint: what would happen if $\eta \neq 0.5$? Identify the origin of the transitions in the IV curve.

(e) Why is the effect of charging absent when $E_F = -3.5$ eV?

11. Next, we consider a Lorentzian density of states rather than simply a discrete level.

$$g(E)dE = \frac{1}{\pi} \frac{\Gamma}{(E - \varepsilon)^2 + (\Gamma/2)^2} dE \quad (51)$$

where $\Gamma = \Gamma_S + \Gamma_D$ and ε is the center of the HOMO. Ignore the LUMO, *i.e.* consider the system from problem 9.

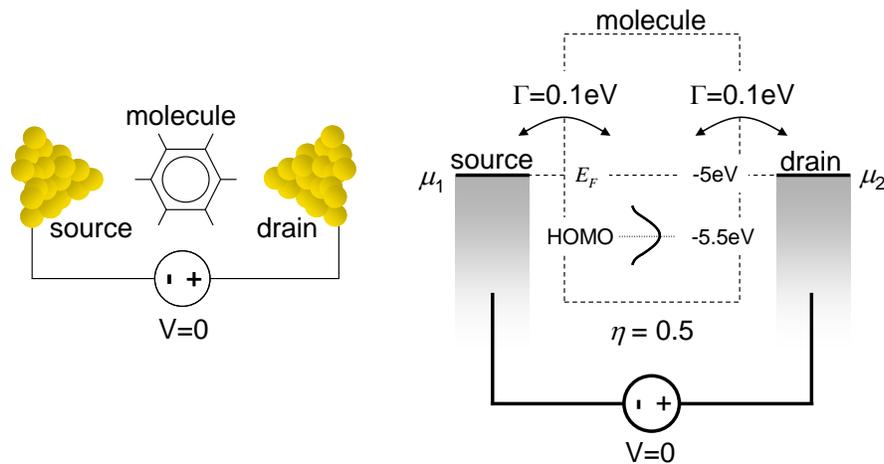


Fig. 3.42. The two terminal molecular device for this problem.

Part 3. Two Terminal Quantum Dot Devices

(a) Numerically compare the current-voltage and conductance-voltage characteristics for a discrete and broadened HOMO with $q^2/C_{ES} = 1$ eV.

(b) How would you expect the IV to change if $\Gamma_S > \Gamma_D$? Explain.

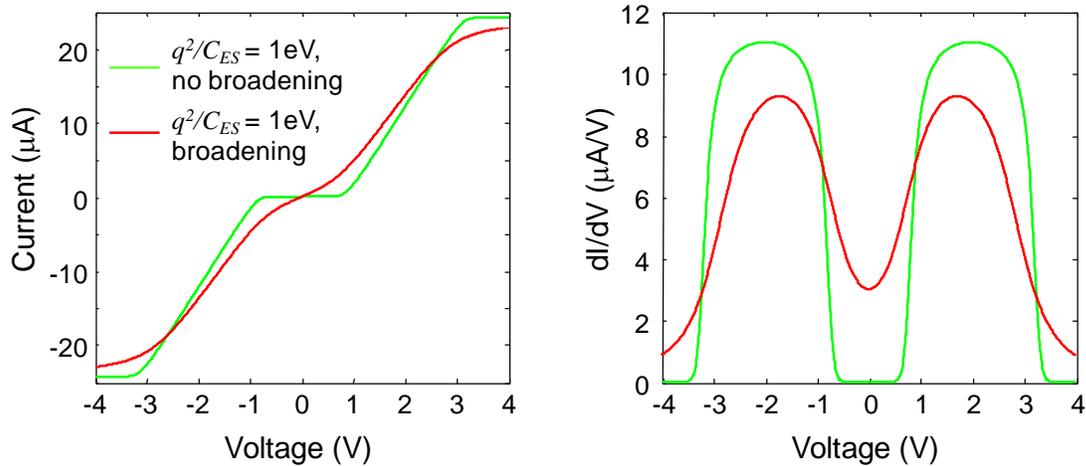


Fig. 3.43. Your solution should look like this.

12. The following problem considers a 2-terminal conductor under illumination. The light produces an electron transfer rate of αN_H from the HOMO to the LUMO. The light also causes an electron transfer rate of αN_L from the LUMO to the HOMO, where α is proportional to the intensity of the illumination, and the electron populations in the LUMO and HOMO are N_L and N_H , respectively.

Assume $C_S = C_D$, that the LUMO and HOMO are delta functions, and $T = 300$ K. Also, assume that under equilibrium in the dark, the Fermi Energy is midway between the HOMO and LUMO.

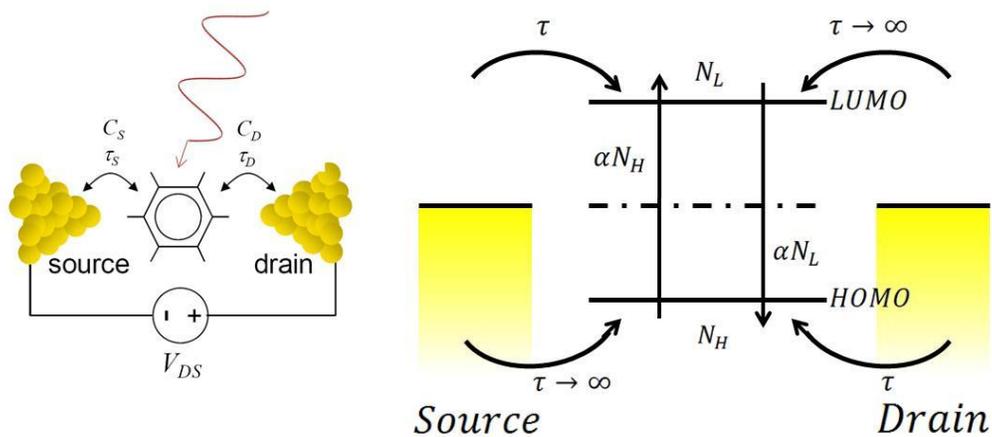


Fig. 3.44. A model of a single molecule solar cell.

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Next, imagine that the contacts are engineered to have the following characteristics:

Transfer rate between Drain and HOMO = $1/\tau$.

Transfer rate between Drain and LUMO = 0.

Transfer rate between Source and HOMO = 0.

Transfer rate between Source and LUMO = $1/\tau$.

(a) Determine the short circuit current for this system. (*i.e.* let $V_{DS} = 0$, what is the current that flows through the external short circuit?)

(b) Determine the open circuit voltage for this system. (*i.e.* Disconnect the voltage source, what is the voltage that appears across the terminals of the molecule?)

(c) Repeat (a) and (b) with the addition of an additional electron transfer rate βN_L from the LUMO to the HOMO, where β is independent of the intensity of the illumination.

13. This problem refers to the 2 terminal molecular conductor below.

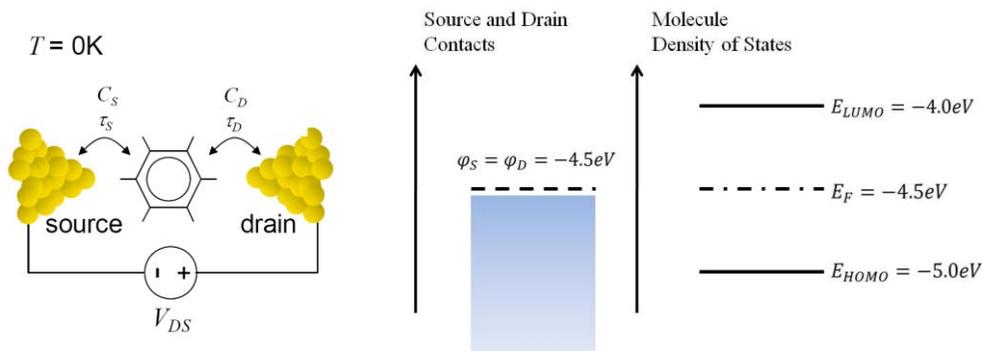


Fig. 3.45 Equilibrium between a molecule and a contact requires charge transfer.

(a) When $\tau_S = 10$ fs, $\tau_D = 5$ fs, calculate the actual molecular density of states versus energy. Determine the full width half maximum of HOMO and LUMO.

(b) Based on the actual density of states calculated in part c), find the number of electrons and the charging energy when the molecule is brought into contact with the metal electrode and reached equilibrium (no applied voltage). Also sketch the energy diagram at equilibrium. Assume that the charging energy per electron is 1eV and $\tau_S = 10$ fs, $\tau_D = 5$ fs.

Hint: You will need your calculator to solve this. You might use $\int \frac{1}{1+x^2} dx = \tan^{-1}(x)$.

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