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DSE3T (Nano Materials and Applications)

Topic – Electron Transport (Part – 1)

Introduction:

The research on transport properties of nanoelectronic devices has become a worldwide effort due to the possibility to fabricate structures at the nanometer scale. Metal-Oxide-Semiconductor transistors with channel lengths as small as 10 nm are now being actively studied both theoretically and experimentally. Remarkable experiments have been performed to measure the current I through single-quantum systems, such as molecules or semiconductor quantum dots. In these experiments, the molecules or the quantum dots are connected to metallic electrodes under bias φ using scanning tunnelling microscopy tips nanometer-size electrodes or break junctions.

Here we shall address a nano-device (e.g. the channel of a nano-transistor, molecules or quantum dots) connected to two electrodes with electrochemical potentials (i.e. non equilibrium Fermi levels) μ_L (left) and μ_R (right). When μ_L and μ_R are not equal due to an external bias ($\mu_L - \mu_R = e\varphi$), the nano-device is in a *non-equilibrium state* and there is a net electron flow through the system (Fig. 1). The two electrodes are macroscopic conducting leads (electron reservoirs) which can be simulated as semi-infinite metals or semiconductors. The reservoirs are large enough that the bulk μ_L and μ_R are not perturbed by the current I. We assume that the leads can be described by a one-particle Hamiltonian, and thus the electrons are viewed as non-interacting except for an overall mean-field potential. In contrast, electron- electron interactions usually play an important role in the nano-device because electrons are confined in a small region. Therefore their treatment represents a major challenge.

Description of the System:

Standard ab initio and semi-empirical methods used in the electronic structure calculations are not directly applicable to transport problems because (1) they usually apply to closed systems either periodic or finite and (2) the electronic system must be in equilibrium, whereas electronic conduction through

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nanostructures involves open systems (infinite and non-periodic) in non-equilibrium.

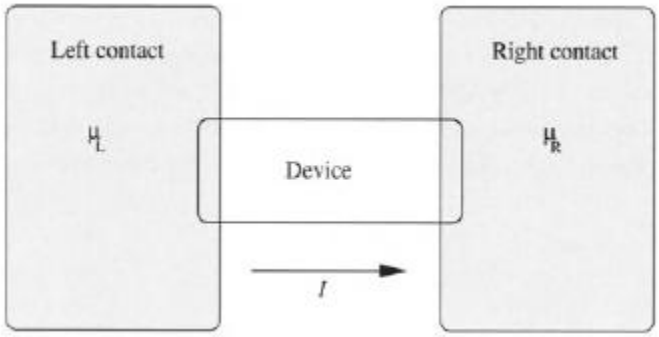

Fig. 1

The usual way to deal with open systems is to partition them into three regions, the device and the two contacts (Fig. 1), and to perform the calculations in three steps. The first one is to calculate the electronic structure of the contacts. It must be done only one time, for example at zero bias, because the contacts are defined in such a manner that a change in the applied bias just corresponds to a rigid energy shift of their electronic levels. This step requires computational methods which were mostly developed to study surfaces of metals or semiconductors. The second step is the resolution of the Schrödinger equation in the device region using a Hamiltonian which is renormalized to take into account the effect of the contacts on the device. This renormalization can be achieved by adding self-energy terms in the Hamiltonian. The resolution may be done iteratively when the calculation of the potential and of the eigenstates in the nano-device is performed self-consistently. The third step is the calculation of the current which leads to define a non-equilibrium density operator (or matrix) with the constraint that deep in the electrodes the electronic levels are filled according to their Fermi levels μ_L and μ_R.

This approach also works when the nano-device is connected to microscopic leads provided that these leads are coupled to macroscopic conductors acting as particle reservoirs. In that case it is often necessary to include a part of the leads into the device region (Fig. 1). In the general case, the device region includes the parts of the leads where the electron density differs importantly from the

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bulk or the free surface situation. In the case of metallic leads, these regions are small due to the strong screening of the electric fields.

Carrier transport in nanostrucutures, Weak Coupling Limit:

Here we consider the case where the nano-device is only weakly coupled to the two electrodes which allows to use perturbation theory. In many situations this approximation is well justified and is the basis of important theoretical developments to describe the conduction through small metallic or semiconducting islands.

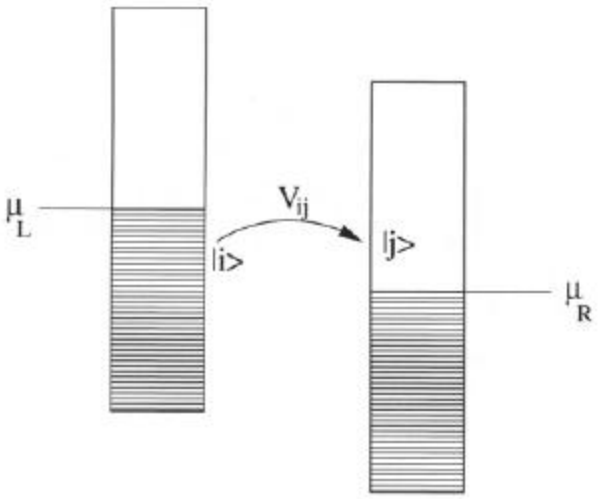

Fig. 2

Perturbation Theory. We treat here the transfer of electrons between two electrodes in perturbation theory (Fig. 2). We write the total Hamiltonian of the system as $H = H_0 + V$. where H_0 is the Hamiltonian of the free electrodes with their corresponding bias and V is their coupling which takes into account the presence of the nano-device. We assume that the left and right electrodes are characterized by quasi-continuum of states $|i\rangle$ and $|j\rangle$, respectively. The Fermi golden rule provides the transfer rate (probability per unit time) of an electron between these states

$$W_{ij} = \frac{2\pi}{\hbar}\left|V_{ij}\right|^2 \delta(E_i - E_j)$$

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Here $V_{ij} = \langle i|V|j\rangle$ and E_i, E_j are the energies of the states $|i\rangle$ and $|j\rangle$.

The current I is given by the net difference between the electron flow from the left to the right and the flow from the right to the left. Summing over all states and taking into account the occupation of the levels, we finally obtain

$$I = \frac{2\pi e}{\hbar}\sum_{i,j}\left|V_{ij}\right|^2\{f\left(E_j - \mu_R\right) - f(E_i - \mu_L)\}\delta(E_i - E_j)$$

where $f = (1 + e^{E/kT})^{-1}$ is the Fermi distribution function.

In the usual case of spin degeneracy, a factor 2 can be factorized. Introducing the density of states in the right and left electrodes as $n_R(E) = \sum_j \delta(E - E_j)$ and $n_L(E) = \sum_i \delta(E - E_i)$, we derive a well-known formula for the current as

$$I = \frac{2\pi e}{\hbar}\int |V(E)|^2\{f(E - \mu_R) - f(E - \mu_L)\}n_L(E)n_R(E)dE$$

where $V(E)$ is the coupling of the states at energy E (assuming that they are not degenerate).

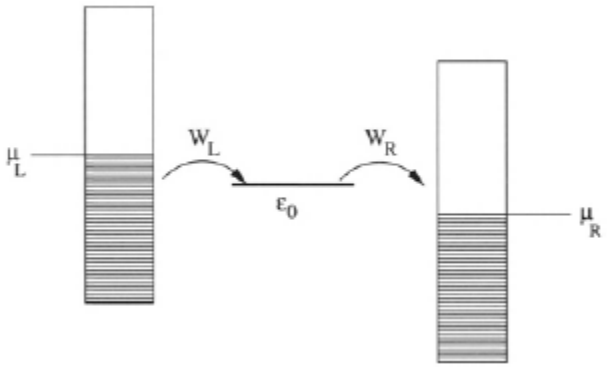

Fig. 3

Case of an Island with a Single Level. This is an example where we assume that the nano-device (called an island) is having only a single energy level E_0 which is located in between μ_L and μ_R. We define the transfer rates W_L and W_R through the left and right junctions, respectively (Fig. 3). Following the Fermi golden rule, we obtain

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$$W_L = \frac{2\pi}{\hbar}\sum_i |V_{i0}|^2 \delta(E_i - E_0) = \frac{\Gamma^L(E_0)}{\hbar}$$

$$W_R = \frac{2\pi}{\hbar}\sum_j |V_{0j}|^2 \delta(E_j - E_0) = \frac{\Gamma^R(E_0)}{\hbar}$$

Here Γ^L and Γ^R have the dimension of an energy and describe the coupling of the level E_0 with the electrodes. The net current through the left and right junctions is given by

$$I_L = (-e)[f(E_0 - \mu_L) - f_0]W_L$$

$$I_R = (-e)[f_0 - f(E_0 - \mu_R)]W_R$$

where f_0 is the mean occupation of the island state E_0. In a permanent regime, we have $I = I_L = I_R$ and we finally obtain

$$I = \frac{e}{\hbar}\{f(E_0 - \mu_R) - f(E_0 - \mu_L)\}\frac{\Gamma^L(E_0)\Gamma^R(E_0)}{\Gamma^L(E_0)+\Gamma^L(E_0)}$$

This simple expression shows that the difference between the chemical potentials in the two reservoirs creates a continuous flow of electrons through the island level for which the occupation f_0 is intermediate between $f(E_0 - \mu_L)$ and $f(E_0 - \mu_R)$.

Beyond Perturbation Theory:

In the previous part, we assumed that the coupling between the contacts and the nano-device could be treated in perturbation. For metallic islands, this is valid when $\Gamma^L, \Gamma^R \ll U$ where U is the average Coulomb charging energy. For molecules or semiconductor nanostructures, there is a further requirement that $\Gamma^L, \Gamma^R \ll \Delta E$ where ΔE is the average splitting between quantum-confined states. But in many situations the coupling parameters Γ^L and Γ^R are of the same order of magnitude or larger than U and ΔE. Thus there is a need for a computational theory valid for any coupling strength.

In this section, we only consider the case of non-interacting electrons making use of the fact that most of the electronic structure calculations resolve single-

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particle equations. In this limit, the non-equilibrium Green's function formalism leads to simple expressions for the current.

Elastic Scattering Formalism. We consider once again the system of Fig. 1 divided into three regions. We neglect inelastic scattering processes within the islands and at the contacts, which turns out to be a good approximation for nano-devices in which the transport is often coherent. The elastic scattering formalism allows to calculate the current through the structure using the eigenstates of the total Hamiltonian $H = H_0 + V$ where H_0 is the Hamiltonian of the three uncoupled regions and V is their coupling. Among the eigenstates of H_0 we consider in the following two groups of states: (1) those $|i_+\rangle$ of energy E_i incident from the left lead, partially reflected back, and partially transmitted into the right lead and (2) the symmetric states $|j_-\rangle$ of energy E_j incident from the right lead (Fig. 4). Since the transport is coherent, the states $|i_+\rangle$ are in equilibrium with the left reservoir, i.e. they are occupied by electrons according to the Fermi function $f(E_i - \mu_L)$. Symmetrically, the states $|j_-\rangle$ are filled up according to the Fermi function $f(E_j - \mu_R)$.

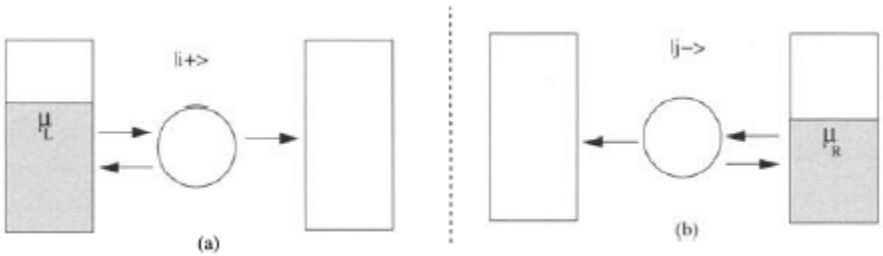

Fig. 4

The states $|i_+\rangle$ are solutions of the Schrödinger equation $(E_i - H)|i_+\rangle = V|i_+\rangle$. If $V = 0$, the solutions correspond to the eigenstates $|i\rangle$ of H_0 in the left lead given as $(E_i - H_0)|i\rangle = 0$. Thus the formal solution is written as

$$|i_+\rangle = |i\rangle + (E_i - H_0)^{-1} V|i_+\rangle$$

Now we define the (retarded) Green's functions which will be particularly useful in the following:

$$G(E) = \lim_{\eta \to 0+} (E - H + i\eta)^{-1}$$

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$$G_0(E) = \lim_{\eta \to 0+} (E - H_0 + i\eta)^{-1}$$

It can be shown that the Green's functions G and G_0 are connected by the so-called *Dyson's equation* as $G = G_0 + G_0 V G$.

Let us now write the total current as $I = I_+ + I_-$ separating the contribution from each group of states. The current I_+ comes from electrons in states $|i_+\rangle$, injected from the left side and scattered by the potential V. We get

$$I_+ = \frac{(-e)}{i\hbar} \sum_{i,j} \{\langle j|V|i_+\rangle\langle i_+|j\rangle - cc\} f(E_i - \mu_L)$$

where cc denotes the complex conjugate of the previous term. Introducing a new operator (called a *scattering operator*) defined as $t(E) = V + VG(E)V$, one finally obtains $I_+ = \frac{2\pi(-e)}{\hbar} \sum_{i,j} |\langle j|t(E_i)|i\rangle|^2 f(E_i - \mu_L)\delta(E_i - E_j)$

Using a similar expression for I_-, we finally get the total current as

$$I = \frac{2\pi e}{\hbar} \sum_{i,j} |\langle j|t(E_i)|i\rangle|^2 \{f\left(E_j - \mu_R\right) - f(E_i - \mu_L)\}\delta(E_i - E_j)$$

Let us now consider the common situation when the two leads are only coupled through the nanostructure ($\langle i|V|j\rangle = 0$). Here we have

$$t_{ij} = \langle i|t|j\rangle = \sum_{n,m} V_{in} G_{nm} V_{mj}$$

where n and m denote eigenstates of H_0 in the decoupled nano-device. Let us define the coupling matrices as

$$\Gamma_{nm}{}^{L}(E) = 2\pi \sum_i V_{ni} V_{im} \delta\,(E - E_i)$$

$$\Gamma_{nm}{}^{R}(E) = 2\pi \sum_j V_{nj} V_{jm} \delta\,(E - E_j)$$

The expressions lead to a compact expression for the current as

$$I = \frac{e}{h} \int \mathrm{Tr}[\Gamma^L G \Gamma^R G^\dagger]\{f(E - \mu_R) - f(E - \mu_L)\} dE$$

where the trace (Tr) of the matrix is taken over all the basis states within the decoupled nano-device subspace. This expression can finally be rewritten as

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$$I = \frac{e}{h}\int T(E)\{f(E-\mu_R) - f(E-\mu_L)\}dE$$

which is known as the generalization of the famous *Landauer formula* that relates the current to the transmission coefficient $T(E) = \mathrm{Tr}[\Gamma^L G \Gamma^R G^\dagger]$ across the nano-device region (a factor 2 is usually factorized in front of $\frac{e}{h}$ to account for the spin degeneracy).

Transport in Ballistic Conductor:

Electrical resistance characterizes the energy dissipation imposed upon the carriers when they pass through a device under the action of an electric field. It reflects the power lost in the device. Usually, when we want to study the transport properties of a macroscopic conductor, or a device which is not mesoscopic, we expect the resistive contribution of the device active layer to represent a non-negligible part of the overall measured resistance, and most often to be the prevailing part. Even if the contacts between the metal pads and the sample exhibit a substantial resistance value, we can get rid of it by using four-probe measurements, in which we pass the current through some terminals and we measure the voltage from the others. Then we obtain something which is not zero, which depends on the resistivity value of our sample and which scales with the device length according to Ohm's law. Now suppose that we want to measure the transport properties of a really small device, in which the electrons are truly ballistic. If nothing impedes the electron passing through the device we might expect the device resistance to go down to zero, and not to depend on the device length any longer. However, this is not the case. In fact, if we continuously reduce the resistance of something, we can expect that sooner or later the active layer resistance must become smaller than the contact resistance, which we need to link the small device to the macroscopic wires. Thus, we can expect that after a substantial enough reduction of device length, all the losses are due to the contact rather than to the "device" itself. We shall investigate this point in the case of quantum, ballistic devices.

The central assumption is that once an electron has entered into the *ballistic conductor*, it cannot be *reflected back*. As a matter of fact, this is not a completely new assumption, but a consequence which arises from the assumed

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ballistic character of the device: electrons do not experience any collision which can backscatter them; if we put one electron into the device going left, it cannot do anything but go to the left side since its momentum cannot change.

Quantized Conductance. It has been proposed that the conductance in a ballistic nano-device will be quantized in $\frac{2e^2}{h}$, given as $G = \frac{2e^2}{h}M$, where M is the number of *modes* or *channels* in the nanostructure.

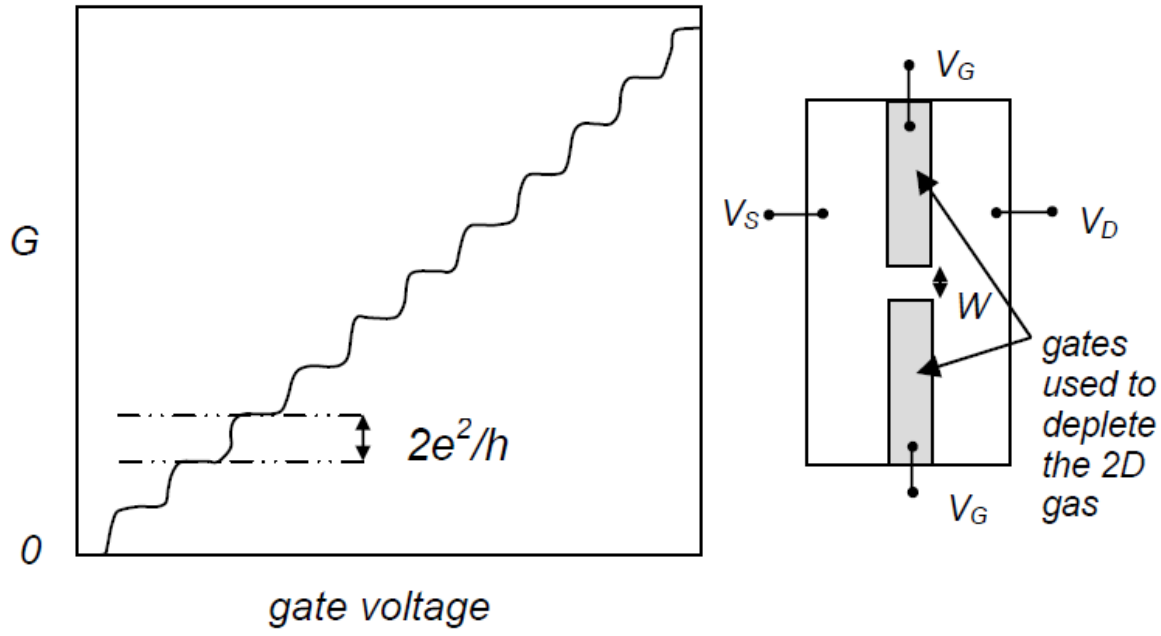

Fig. 5

This quantized conductance has already been experimentally observed. In 2D devices such as Si MOSFETs or heterostructures, if we fabricate a local constriction such as schematized in the right part of Fig. 5, we obtain something which is 1D. In addition, if we can operate the gates above or by the sides of the constriction, we can change its effective width by depleting its sides. As we deplete the edges the free space becomes more constrained and the 1D subband bottom energies E_n correspondingly increase, so that we can really control the number of open channels below the Fermi energy. Thus, whenever we change the gate voltage so as to make one energy E_n go below the Fermi level, we add

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one channel and expect a quantized conductance increase by a factor $\frac{2e^2}{h}$ as shown in the left part of Fig. 5.

Explanation from Landauer Formula. Incorporating the spin degeneracy Landauer formula gives us $I = \frac{2e}{h}\int T(E)\{f(E-\mu_R) - f(E-\mu_L)\}dE$. Assuming the transmission coefficient $T(E)$ independent of energy E, this expression can be simplified to $I = \frac{2e}{h}M(E)T(\mu_L - \mu_R)$ where $M(E)$ is the number of modes in the nano-device. Since we can relate the external bias as $\mu_L - \mu_R = e\varphi$, therefore we get $I = \frac{2e^2}{h}M(E)T\varphi$ or the conductance is given as $G = \frac{I}{V} = \frac{I}{\varphi} = \frac{2e^2}{h}MT$. For a true ballistic conductor, $T = 1$ and we finally obtain the formula for quantized conductance as $G = \frac{2e^2}{h}M$.

Coulomb Blockade Effect:

The application of a mean-field theory to the transport through nanostructures is better justified when the coupling is strong ($\Gamma^L, \Gamma^R \gg U$). However, as already mentioned, many experiments actually belong to an intermediate regime where the coupling coefficients and the charging energy have similar magnitudes. Therefore our aim in this part is to point out the main deficiencies of computational methods of the electronic structure to describe the *Coulomb blockade effect* which is the more obvious consequence of electron-electron interactions in nanostructures. We shall consider the limit $\Gamma^L, \Gamma^R \ll U$ in order to compare with the predictions of the orthodox theory. It will give us the opportunity to judge the mean-field approaches in the worst situation. Here the current I is the resultant of several tunnelling processes under applied bias φ. For example, an electron can tunnel from the left electrode to the island, which goes from a configuration of energy $E_n(q, \varphi)$ to a configuration of energy $E_m(q-1, \varphi)$. We define the transition levels as

$$\epsilon_{nm}(q|q-1) = E_m(q-1, \varphi) - E_n(q, \varphi)$$

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Here we consider the simplest model of a nano-device characterized by a single level two-fold degenerate due to the spin. We assume that this level is empty in the neutral state and that the total energy of the system can be written as

$$E(n) = nE_0 + \frac{1}{2}Un^2$$

where n is the number of electron in the island ($= 0,1,2$) and U is the *Coulomb charging energy* which takes into account the dielectric environment of the nanostructure. We suppose for simplicity that the triplet and singlet states for $n = 2$ have the same energy. We also neglect the dependence of the energy levels with the applied bias. Following the transition levels we define two ionization energies as $\varepsilon(0|-1) = E_0 + \frac{1}{2}U$ and $\varepsilon(-1|-2) = E_0 + \frac{3}{2}U$ and and the current is determined by the position of the chemical potentials with respect to these levels.

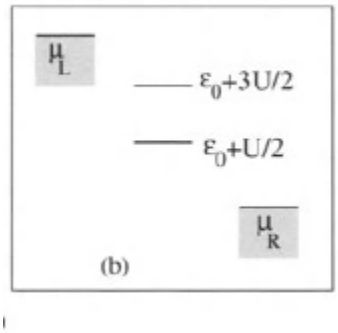

Fig. 6

Orthodox Model. We consider the situation of Fig. 6 where a bias voltage shifts the chemical potential μ_L of the left electrode. When $\mu_L > \varepsilon(0|-1) > \mu_R$, the current flows through the nanostructure which is in the charge state 0 or -1 with the respective probabilities σ_0 and σ_1 respectively. These probabilities can be calculated as $\sigma_0 = \frac{\Gamma^R}{\Gamma^R+2\Gamma^L}$ and $\sigma_1 = \frac{2\Gamma^L}{\Gamma^R+2\Gamma^L}$, where for simplicity we assume that the coupling coefficients Γ^R and Γ^L are independent of the energy. In these conditions, the current is given by $I = -\frac{e}{\hbar}\frac{2\Gamma^R\Gamma^L}{\Gamma^R+2\Gamma^L}$.

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When $\mu_L > \varepsilon(-1|-2) > \varepsilon(0|-1) > \mu_R$, the there will be three possible charge states 0, -1 and -2 with the respective probabilities $\sigma_0 = (\frac{\Gamma^R}{\Gamma^R+\Gamma^L})^2$, $\sigma_1 = \frac{2\Gamma^R\Gamma^L}{(\Gamma^R+\Gamma^L)^2}$ and $\sigma_2 = (\frac{\Gamma^L}{\Gamma^R+\Gamma^L})^2$ and the current becomes $I = -\frac{e}{\hbar}\frac{2\Gamma^R\Gamma^L}{\Gamma^R+\Gamma^L}$.

The current vs voltage characteristics in the limit $T \to 0$ K is shown in Fig. 7 for two sets of values for Γ^R and Γ^L. It is a staircase function due to the use of a perturbation theory. The true characteristic should be with a broadening of the steps of the order of Γ^R and Γ^L (neglecting Kondo effect).

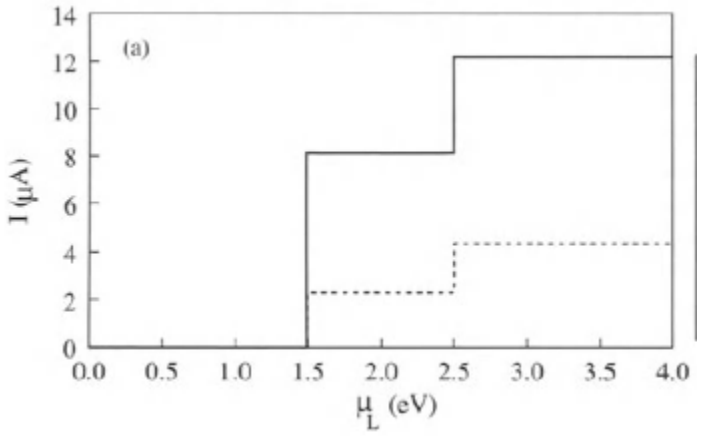

Fig. 7

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This concludes part 1 of this e-report.

The discussion will be continuing in the part 2 of this e-report.

Reference(s):

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(All the figures have been collected from the above mentioned references)