# Microscopic Origin of Conducting Channels in Metallic Atomic-Size Contacts

J. C. Cuevas, A. Levy Yeyati, and A. Martín-Rodero

*Departamento de Física Teórica de la Materia Condensada C-V, Universidad Autónoma de Madrid, E-28049 Madrid, Spain*
(Received 20 August 1997)

We present a theoretical approach which allows one to determine the number and orbital character of conducting channels in metallic atomic contacts. We show how conducting channels arise from atomic orbitals with a significant contribution to bands around the Fermi level. Our theory predicts that the number of conducting channels with non-negligible transmission is three for Al and five for Nb one-atom contacts, in agreement with recent experiments. These results are shown to be robust with respect to disorder. The experimental values of the channel transmissions lie within the calculated distributions.
[S0031-9007(97)05206-X]

Metallic contacts of atomic dimensions, which can be produced by means of scanning tunneling microscope and break-junction techniques, have been the object of great attention in the last few years [1]. According to the scattering approach, the electronic transport in these mesoscopic structures can be described in terms of independent "conducting channels" characterized by certain transmission coefficients which vary between zero and one [2]. The complete understanding of their transport properties requires the knowledge of the transmission coefficients along *each* conducting channel. This information, which is not accessible by usual conductance measurements, has for the first time been obtained in recent experiments on superconducting Al contacts [3]. The possibility of extracting the individual transmissions from measuring the superconducting $I$-$V$ characteristic is based on the extreme sensitivity of the subgap structure to small changes in these parameters [4,5].

A remarkable conclusion of this experimental study is that, although the total conductance of an Al contact on the first plateau (presumably a one-atom contact [6]) can be close to one quanta of conductance, this situation does not correspond to a nearly open single channel, but rather to a situation with three partially open channels. The question naturally arises on the microscopic origin of this phenomenon for the specific case of Al. More generally, one would like to know what is the number of conducting channels for a given metal in a given contact geometry. The aim of this Letter is to provide theoretical insight into these questions.

Having a system of atomic dimensions it seems natural to choose an atomic orbital basis for the description of its electronic structure. This choice has proven useful in the context of scanning tunneling microscopy theory [7]. Furthermore, the use of a local basis in combination with Green function techniques provides an efficient way for obtaining the transport properties [4,7,8] in terms of microscopic parameters. In an atomic orbital basis the electronic Hamiltonian adopts the usual tight-binding form

$$\hat{H} = \sum_{i\alpha,\sigma} \epsilon_{i\alpha} c^{\dagger}_{i\alpha\sigma} c_{i\alpha\sigma} + \sum_{i\alpha \neq j\beta,\sigma} t_{i\alpha,j\beta} c^{\dagger}_{i\alpha,\sigma} c_{j\beta,\sigma} , \quad (1)$$

where $i$, $j$ run over the atomic sites and $\alpha$, $\beta$ denote the different atomic orbitals (the number of orbitals at each site will be denoted by $N_{\text{orb}}$). The hopping elements $t_{i\alpha,j\beta}$ are assumed to connect first-neighbor sites only. There exist in the literature several parametrization procedures for determining the tight-binding Hamitonian [9,10] which are known to accurately reproduce the band structure of bulk materials. As a starting point we follow the parametrization proposed in Ref. [10] considering as a minimal basis for each metal those atomic orbitals having a significant contribution to the electronic density of states (DOS) around the Fermi energy, $E_F$. Thus, for the case of superconducting metals of groups III and IV, like Al, Pb, etc., only $s$ and $p$ orbitals need to be considered; while for transition metals like Nb $d$ orbitals have to be included.

In an atomic contact the local environment in the neck region is very different to that of the bulk material and therefore the use of bulk parameters in the Hamiltonian requires some justification. In the first place, the inhomogeneity of the contact geometry can produce large deviations from the approximate local charge neutrality that typical metallic elements must exhibit. Within the tight-binding approximation this effect can be corrected imposing local charge neutrality through a self-consistent variation of the diagonal parameters $\epsilon_{i\alpha}$ [11]. As discussed below, this self-consistency in the neck region turns out to be crucial for the correct determination of the conducting channels. Regarding the hopping elements, $t_{i\alpha,j\beta}$, although we shall initially consider them as being equal to the bulk values in order to represent a neck geometry with bulk interatomic distances, we shall show that the results are robust with respect to fluctuations in the hopping elements induced by disorder in the atomic positions.

An idealized geometry for a one-atom contact is depicted in Fig. 1. It consists of a close-packed fcc structure grown along the (111) direction (hereafter denoted as $z$ direction), starting from a central atom [12]. This
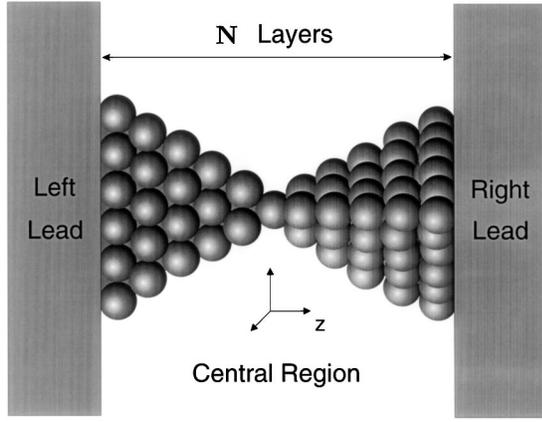
FIG. 1. Idealized geometry for a one-atom contact. The layers are numbered from 1 to $N$ starting from the left lead.

structure is connected to two semi-infinite crystals describing the metallic leads, $N$ being the number of atomic layers within the neck region. By taking different values of $N$ we can describe both the cases of long and short necks.

In order to obtain the dc current for a constant bias voltage applied between the leads, it is most convenient to use nonequilibrium Green function techniques [13]. Within this formalism the current can be written with an expression formally equivalent to that of scattering theory [14] by treating the coupling between the central region and the leads as a perturbation [15]. The current between the left lead and the central region is then given by

$$I = \frac{2e}{h} \int_{-\infty}^{\infty} T(E, V) [f_L(E) - f_R(E)] \, dE, \quad (2)$$

where $f_{L,R}$ are the Fermi-distribution functions for the (left, right) leads and $T(E, V)$ is an energy and voltage dependent transmission probability, which can be written in terms of the matrix elements of the (retarded, advanced) Green function matrix $\hat{G}^{r,a}(E) = [E \pm i0^+ - \hat{H}]^{-1}$ as

$$T(E, V) = 4 \mathrm{Tr} \left[ \mathrm{Im} \, \hat{\Sigma}_L \left( E - e \frac{V}{2} \right) \right.$$
$$\left. \times \hat{G}^r_{1N}(E) \, \mathrm{Im} \, \hat{\Sigma}_R \left( E + e \frac{V}{2} \right) \hat{G}^a_{N1}(E) \right].$$

In this expression $\hat{G}^r_{1N}$ and $\hat{G}^a_{N1}$ are matrices whose elements are the Green functions connecting layers 1 and $N$, $\hat{\Sigma}_{L,R}$ being self-energy matrices describing the coupling of the central region to the leads. These matrices have a dimension equal to the number of bonds connecting the central region to the leads ($M_{L,R}$) and have a simple expression in terms of the Green functions of the uncoupled leads, $g_{i\alpha,j\beta}$:

$$[\hat{\Sigma}_{L,R}(E)]_{i\alpha,j\beta} = \sum_{k,l \in L,R; \gamma, \delta} t_{i\alpha,k\gamma} g^a_{k\gamma,l\delta}(E) t_{l\delta,j\beta}.$$

The $g_{i\alpha,j\beta}$'s can be evaluated numerically by standard decimation techniques [16].

The voltage range which is probed in the experiments with superconducting contacts is of the order of the

gap parameter $\Delta$ (typically a few tenths of meV) [3]. For this bias range normal metallic systems will behave Ohmically. Even when the atomic-size contacts exhibit resonances around $E_F$ [11], their width will in general be much larger than $\Delta$ and linearization of Eq. (2) is appropriate. In this linear regime the contact normal conductance can be expressed as $G = (2e^2/h)T(E_F, 0)$. By using the cyclic property of the trace, $G$ can be written in the Landauer form $G = (2e^2/h) \mathrm{Tr}[\hat{t}(E_F)\hat{t}^\dagger(E_F)]$, where

$$\hat{t}(E) = 2[\mathrm{Im} \, \hat{\Sigma}_L(E)]^{1/2} \hat{G}^r_{1N}(E) [\mathrm{Im} \, \hat{\Sigma}_R(E)]^{1/2}. \quad (3)$$

The existence of $(\mathrm{Im} \, \hat{\Sigma})^{1/2}$ as a real matrix is warranted by $\mathrm{Im} \, \hat{\Sigma}$ being positive definite. Moreover, $\hat{t}\hat{t}^\dagger$ is a Hermitian matrix having $M_L$ real eigenvalues, $T_i$, which are bounded by zero and one [17]. Associated with these eigenvalues there will be $M_L$ eigenvectors, which in our model are linear combinations of the atomic orbitals in the layer which is in contact with the left lead. These eigenvectors define the way in which the atomic orbitals contribute to each conducting channel.

Although the dimension of $\hat{t}\hat{t}^\dagger$ can be arbitrarily large depending on the size of the central region, the actual number of conducting channels (those with a nonvanishing transmission eigenvalue $T_i$) is limited by the number of orbitals in the narrowest section of the neck ($N_{\mathrm{orb}}$ when having a single atom contact). This fact can be shown by the following simple argument. As the division between "central region" and leads is somewhat arbitrary, one could always redefine the leads for the geometry of Fig. 1 in such a way that the new central region would consist only of the central atom. Then the new lead self-energy matrices $\hat{\Sigma}'_{L,R}$ would have a dimension of just $N_{\mathrm{orb}}$ and the new transmission matrix would admit only $N_{\mathrm{orb}}$ eigenmodes. Current conservation along each conducting channel ensures that the nonvanishing eigenvalues $T_i$ and $T'_i$ must be the same.

The above simple argument already allows an estimate of the maximum number of relevant conducting channels in a one-atom contact. Thus, for an $sp$-like metal like Al, this number should be typically four, while for a transition metal like Nb (having a negligible weight of $p$ orbitals at $E_F$) this number would be of order six. As discussed below, this rough estimate should be taken as an upper bound. The actual number of conducting channels can be smaller as some of the channels can carry no current due to symmetry considerations.

Let us first consider the case of an Al one-atom contact, which is the one analyzed experimentally in Ref. [3]. Al contacts have also been addressed theoretically in [18]. The atomic configuration for Al, $3s^2 3p^1$, gives rise to a conducting $sp$ band with three electrons per atom. The bulk DOS at $E_F$ has important contributions from both $3s$ and $3p$ orbitals, the $3s$ level being located $\sim 7$ eV below the $3p$ level [10]. While the above simple argument would predict a maximum number of four channels for a one-atom contact, the self-consistent calculation for the ideal geometry yields only three channels with
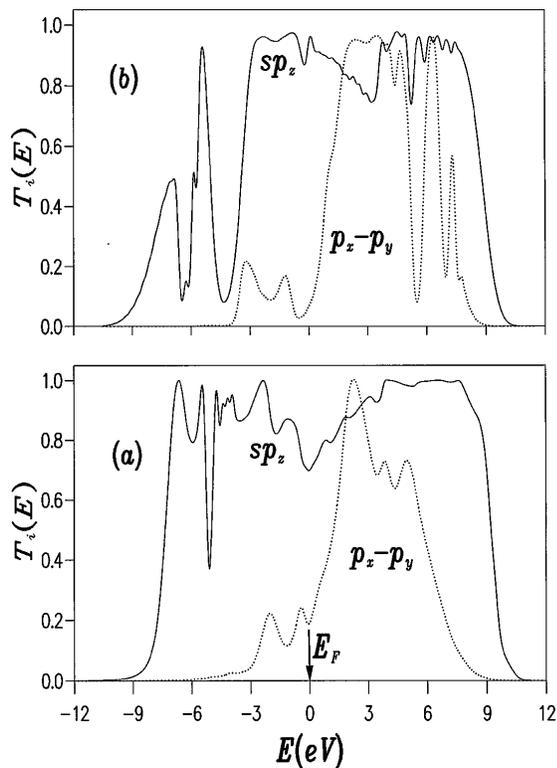
FIG. 2. Transmission eigenvalues as a function of energy for Al one-atom contacts in the two extreme cases of short (a) and long (b) necks. The solid curve corresponds to the nondegenerate $sp_z$ mode and the dotted curve corresponds to the twofold degenerate $p_x - p_y$ mode.

nonvanishing transmission. In Fig. 2 the transmission eigenvalues of the ideal (111) contact are shown as a function of energy for the two extreme cases of a short ($N = 1$) or a long ($N \rightarrow \infty$) neck geometry. There are certain features that are common to both cases: (i) there are three channels having a significant transmission around $E_F$, the fourth one being closed for every energy, (ii) the total transmission is close to one around $E_F$ increasing to almost three at higher energies, (iii) there is a nondegenerate mode which is widely open for almost every energy, and (iv) the second transmission eigenvalue is twofold degenerate and has a small value around $E_F$.

The channels can be classified according to the orbital character of the eigenvectors on the central atom. In this way, the nondegenerate channel, widely open at $E_F$, is a combination with an amplitude $\sim 0.63$ on the $s$ and $\sim 0.77$ on the $p$ orbitals along the $z$ direction. The one with zero transmission corresponds to the orthogonal combination of these two orbitals. On the other hand, the two degenerate modes correspond to combinations of $p$ orbitals on a plane perpendicular to the $z$ direction. While the symmetry properties of the neck geometry are responsible for the decoupling between the $s - p_z$ and $p_x - p_y$ orbitals, the approximate fulfillment of the condition $\mathrm{Im}\,\Sigma'_{ss}\,\mathrm{Im}\,\Sigma'_{p_z p_z} = (\mathrm{Im}\,\Sigma'_{sp_z})^2$ accounts for the presence of a nonconducting channel (details will be given elsewhere).

The orbital character and energy dependence of the transmission eigenvalues is similar for the case of Pb, which is also an $sp$-like metal. However, in this case the Fermi level lies in the region where the three channels are almost open, giving rise to a total transmission larger than 2.

So far the possible effect of disorder in the atomic positions has been disregarded. We have studied this effect by introducing random fluctuations in the atomic positions of the idealized structure, assuming the distance dependence on the hopping parameters as suggested by Harrison [9]. Although there are certain features like the twofold degeneracy which, as expected, disappear with the inclusion of disorder, the gross features found for the ideal geometry are nevertheless robust. This fact is illustrated in the histograms shown in Fig. 3, which demonstrate that the decomposition of the total transmission consists of a widely open channel with $T_i$ between 0.6 and 0.9 and two low transmissive channels with $T_i$ between 0.1 and 0.3. These predictions are consistent with the experimental results for the first conductance plateau [3]. The fourth channel always has an extremely small transmission ($T_i < 10^{-4}$).

We have also analyzed the conducting channels of a Nb one-atom contact, as an example of transition metal contacts. As commented above, in this case the maximum number of conducting channels is expected to be six due to the fact that the DOS around $E_F$ mainly arises from the contributions of $5s$ and $4d$ orbitals [10]. The idealized one-atom contact geometry yields in this case a total transmission between 2 and 3 depending on the number of layers in the central region. The channel decomposition shows that this total transmission is mainly built up from the contribution of five conducting channels.
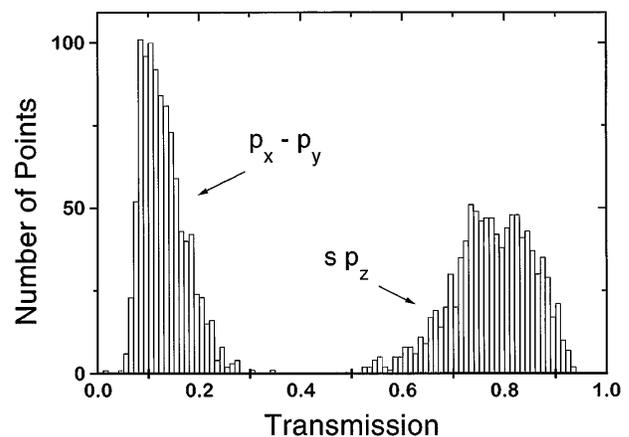


FIG. 3. Typical distributions of the transmission eigenvalues for an Al one-atom contact when disorder in the atomic positions is included (the maximum fluctuation in the hopping parameters is of the order of 100% with respect to the bulk values, which corresponds to variations of the order of 20% in the interatomic distances). The two modes corresponding to the twofold degenerate eigenvalue in the idealized case exhibit a similar distribution.
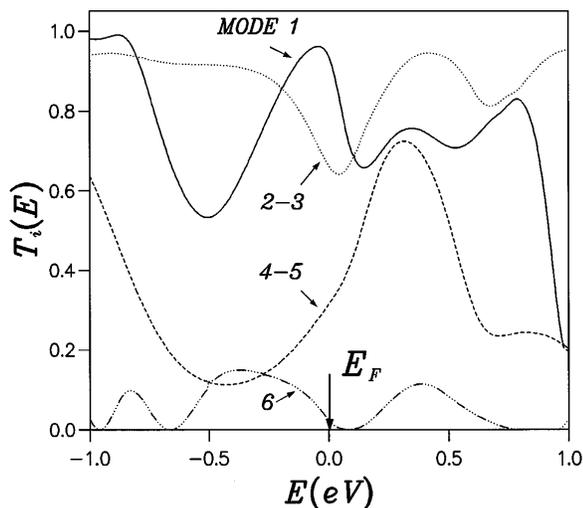
FIG. 4. Transmission eigenvalues as a function of energy for a Nb one-atom contact for the long neck case. Note the twofold degeneracy of modes 2-3 and of 4-5.

As can be observed in Fig. 4, the $d$ bands cause a strong energy dependence of the transmission eigenvalues, with typical energy scales of the order of 0.5 eV. The $s$ and $d_{z^2}$ orbitals hybridize strongly and give rise to the conducting channel with the highest transmission around $E_F$ (mode 1 in Fig. 4). The almost closed channel (mode 6 in Fig. 4) corresponds to the orthogonal combination of these two orbitals. There also appears a twofold degenerate channel with transmission $\sim 0.7$ and another twofold degenerate channel with transmission $\sim 0.3$. Both the values of the total transmission and the number of relevant conducting channels are in good agreement with preliminary experimental results [19].

Our theory and the experimental results show that atomic contacts of metals which have an important contribution from $p$ and $d$ orbitals do not necessarily, even in the one-atom case, exhibit an integer number of perfectly transmitting modes. This situation is at variance with that of simple metals like Na, Au, Ag, etc., which can be described by a single $s$-like band around $E_F$ and exhibit well defined quantized conductance steps, at least at the lower plateaus [20]. Within our theory, in the one-atom contact geometry, simple metals would have a single conducting channel. The transmission of that channel is strongly pinned at one due to the charge neutrality condition [11].

In conclusion, we have presented a theoretical analysis of the conducting channels in metallic atomic-size contacts. We have shown that the number and character of these channels are determined by the orbital electronic structure and the local atomic environment around the neck region. For the case of $sp$-like metals like Al and Pb we predict the presence of three conducting channels in a one-atom contact, in good agreement with the

available experimental data [3]. For one-atom contacts of a transition metal like Nb we expect the presence of five conducting channels due to the contribution of $d$ orbitals. This result has been confirmed by recent experiments [19].

[1] For a review, see A. P. Sutton, Curr. Opin. Solid State Mater. Sci. **1**, 827 (1996).

[2] R. Landauer, Philos. Mag. **21**, 863 (1970).

[3] E. Scheer, P. Joyez, D. Esteve, C. Urbina, and M. H. Devoret, Phys. Rev. Lett. **78**, 3535 (1997).

[4] J. C. Cuevas, A. Martín-Rodero, and A. Levy Yeyati, Phys. Rev. B **54**, 7366 (1996).

[5] D. Averin and A. Bardas, Phys. Rev. Lett. **75**, 1831 (1995).

[6] J. M. Krans et al., Phys. Rev. B **48**, 14 721 (1993).

[7] J. Ferrer et al., Phys. Rev. B **38**, 10 113 (1988); P. Sautet and C. Joachim, Chem. Phys. Lett. **185**, 23 (1991); C. Sirvent et al., Phys. Rev. B **53**, 16 086 (1996).

[8] T. N. Todorov et al., J. Phys. Condens. Matter **5**, 2389 (1993).

[9] W. A. Harrison, *Electronic Structure and the Properties of Solids* (Freeman, San Francisco, 1980).

[10] D. A. Papaconstantopoulos, *Handbook of the Band Structure of Elemental Solids* (Plenum Press, New York, 1986).

[11] A. Levy Yeyati, A. Martín-Rodero, and F. Flores, Phys. Rev. B **56**, 10 369 (1997).

[12] Computer simulations show that this close-packed structure is a stable configuration; see, for instance, U. Landman et al., Science **248**, 454 (1990); T. N. Todorov and A. P. Sutton, Phys. Rev. Lett. **70**, 2138 (1993).

[13] C. Caroli et al., J. Phys. C **5**, 21 (1972).

[14] One of the advantages of the Green functions approach is that it does not require the existence of well defined asymptotic conducting channels; see, for instance, Y. V. Nazarov, in *Quantum Dynamics of Submicron Structures,* edited by H. A. Cerdeira (Kluwer, Dordrecht, The Netherlands, 1995).

[15] A. Levy Yeyati, Phys. Rev. B **45**, 14 189 (1992).

[16] F. Guinea et al., Phys. Rev. B **28**, 4397 (1983).

[17] These bounds can be derived using the general properties of the Green functions.

[18] N. D. Lang, Phys. Rev. B **52**, 5335 (1995); C. C. Wan et al., Appl. Phys. Lett. **71**, 419 (1997).

[19] B. Ludoph and J. M. van Ruitenbeek (private communication).

[20] J. M. Krans et al., Phys. Rev. B **48**, 14 721 (1993); L. Olesen et al., Phys. Rev. Lett. **72**, 2251 (1994); J. M. Krans et al., Physica (Amsterdam) **218B**, 228 (1996); G. Rubio, N. Agrait, and S. Vieira, Phys. Rev. Lett. **76**, 2302 (1996).