Distribution of conduction channels in nanoscale contacts: evolution towards the diffusive limit

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Highly stable atomic scale contacts are formed using a mechanically controlled break-junction (MCBJ) [9]. A notched lead wire 99.99% pure is glued on top of a flexible substrate. The rupture of the wire is carried out at 1.6 K in He exchange gas, thus preventing the freshly exposed surfaces from oxidizing. The contact can be reestablished and broken with picometer displacement resolution and stability.

It was shown that in one-atom contacts the \( \{ \tau_n \} \) can be obtained from the experimental current-voltage characteristic curve \( IV \) by fitting to the sum of \( N \) one-channel \( IV \) curves, \( I(V) = \sum_{n=1}^{N} (\tau_n, V) \) [3, 10], which have been calculated elsewhere for arbitrary transmission \( \tau \) [11].

Scheer et al. [3, 10] determined the transmission of a small number of channels for one-atom contacts using a steepest descent based method [12]. For larger contacts we have found that a simulated annealing algorithm is much more efficient. It is faster, a fact that becomes increasingly important as the number of channels to fit grows, and has the advantage of avoiding getting trapped at local minima. We use as acceptance criterion the root mean square deviation from the measured \( IV \) curve, \( \chi^2 \). The fit starts from a random initial position in the \( N \)-dimensional space spanned by \( \{ \tau_n \} \). Then a random walk is performed. At each step the new fit is accepted if \( \chi^2 \) is smaller than the previous one. If \( \chi^2 \) is larger the step can still be accepted, according to a Boltzmann-type factor, with a pseudo-temperature which is lowered in a smooth way. \( N \) is chosen large enough for the fit to result in several closed channels (\( \tau < 0.01 \)).

We show in fig. 1 a) \( IV \) curves for different contact realizations. These \( IV \) curves exhibit subharmonic gap structure for voltages below \( 2\Delta/e \) due to multiple Andreev reflections [11]. At low voltages the \( IV \) curves show a contribution from the supercurrent peak and is not taken into account.

In fig. 1 b) we show the channel transmissions obtained from the fit to the \( IV \) curves in fig. 1 a). Channel indexes are ordered in decreasing transmission. An estimate of...
15 is not very sensitive to the size of the contact and 16 the fits (lines). The value of the superconducting gap $\Delta = 1.35$ meV used in the fit is obtained from an IV curve in the tunnelling regime. The inset in a) shows the theoretical IV curves for a single channel used in the fitting procedure (taken from [11]). Bottom panel: corresponding sets $\{\tau_i\}$ obtained from the fits. The inset in b) shows a schematic representation of the MCBJ technique.

Previous experience for the case of one-atom contacts has demonstrated that band structure effects play a major role in the determination of the set $\{\tau_i\}$ for a given element [3, 14, 15, 16, 17]. It is thus interesting to analyze whether this is still the case for contacts in the intermediate range (larger than one atom but smaller than the mean free path). For this purpose we have performed model calculations of the set $\{\tau_i\}$ for idealized geometries of the nanocontacts.

As in previous studies we use a self-consistent parametrized tight-binding (TB) model in which the main features of the bulk band-structure are included [14]. We shall consider model geometries like the ones depicted in the insets of fig. 3 in which the neck of the contact is represented by several atomic layers of different cross section grown along the (111) direction on a fcc lattice. This central region is connected to the left and right electrodes represented by perfect semi-infinite crystals. The corresponding TB Hamiltonian can be written as $\hat{H} = \sum h_{i,j,\alpha,\beta}\hat{c}_i^\dagger\hat{c}_j$, where $\hat{H}_{L,R}$ and $\hat{H}_{\alpha}$ describe the uncoupled left and right electrodes and the central part of the contact respectively; $\hat{V}_{L,R}$ being a coupling term between the central region and the electrodes. The matrix elements $h_{i,j,\alpha,\beta}$, where $i, j$ and $\alpha, \beta$ design sites and orbitals respectively, are taken from fits to the bulk ab-initio band structure. As a self-consistency condition we impose local charge neutrality on each site. Disorder in the atomic positions at the central region can be included by rescaling the hopping elements according to the distortion of the different bond length with respect to the bulk values [18].
we show typical results for the transmission sets that are obtained for Pb contacts of intermediate cross section. The effect of an specific contact geometry is illustrated in the upper panels (fig. 3 a) and b)). As can be observed, a characteristic feature of Pb is the appearance of steps corresponding to partially open channels with similar transmission. For comparison we also show in this figure the corresponding results for Au contacts in order to remark the differences with the ballistic behavior observed in the case of Au.

In a second step we have analyzed the influence of atomic disorder in the calculated distributions $Q(T)$ for Pb and Au. The curves correspond to different values of the disorder parameter $\sigma$ described in text: 0 (black line), 0.05 (red), 0.1 (green) and 0.2 (blue). The symbols correspond to an average of the experimental results from 10 to 15$G_0$. The dashed line corresponds to the universal diffusive distribution.

As a result of these previous calculations one can conclude that, even in the absence of atomic disorder, Pb contacts deviate strongly from the ballistic behavior observed in the case of Au.

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Once the TB Hamiltonian has been built the conductance $G(E) = G_0 \text{Tr} \left[ \hat{T}(E)\hat{\Gamma}(E) \right]$ is calculated in terms of the matrix elements of the Green function operator $\hat{\Gamma}(E) = \lim_{\eta \to 0} [E + i\eta - \hat{H}]^{-1}$ using:

$$\hat{\Gamma}(E) = 2\hat{\Gamma}_L^{1/2}(E)\hat{G}_L^r(E)\hat{\Gamma}_R^{1/2}(E),$$

where $\hat{\Gamma}_L,\hat{\Gamma}_R$ are the matrix tunneling rates connecting the central region to the leads [14]. The transmission matrix $\hat{T}\hat{\Gamma}$ can then be diagonalized in order to obtain the transmission eigenchannels and eigenvalues $\tau_n$.

In fig. 3 we show typical results for the transmission sets that are obtained for Pb contacts of intermediate cross section. The effect of an specific contact geometry is illustrated in the upper panels (fig. 3 a) and b)). As can be observed, a characteristic feature of Pb is the appearance of steps corresponding to partially open channels with similar transmission. For comparison we also show in this figure the corresponding results for Au contacts in order to remark the differences with a monovalent metal. Although the detailed structure of these curves is strongly dependent on the specific geometry, the behavior for Pb is clearly in contrast to the one observed in Au where partially open channels are rarely observed. These differences can be directly related to the particular band structure of both metals. While in the case of Au the channels can be associated with a single band of s-character at the Fermi energy, in Pb the channels arise from the contribution of several bands with sp-character. In fact, for the same geometry the total number of channels with significant transmission is larger for Pb than for Au. When the cross section of the contact is increased (fig. 3 c)) the partially open channels in Pb tend to define a rather continuous distribution which fairly resembles that of a diffusive conductor. In panel d) we compare the corresponding distributions $Q(T)$ with the result expected for a diffusive wire.

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is in fairly good agreement with the calculated one for the case $\sigma = 0.1$, which roughly corresponds to a mean free path $l_0 \sim 10$ nm. This rather low degree of disorder is consistent with what is known both from molecular-dynamics simulations and images made by transmission electron microscopy of metallic nanocontacts [5].

It should be stressed that these distributions still exhibit some deviations with respect to the universal curve, specially for high transmission. We can associate these deviations with the fact that the size of the contact is still considerably smaller than the mean free path.

In contrast to the case of Pb, Au exhibits a clear deviation from the universal distribution even for the larger values of $\sigma$ considered. Notice that $\sigma = 0.2$ already corresponds to an unexpectedly high degree of disorder [19].

As a final issue we estimate the effect of disorder on the bulk electrodes by means of a phenomenological model. In this model the electrodes are diffusive conductors characterized by a classical probability $P_{cl}(t)$ for returning to the contact region after a given time $t$. Modelling the electrode as a cone with opening angle $\gamma$ this probability is given by

$$ P_{cl}(t) = \frac{v_F}{\langle v_\perp \rangle} \left\{ 2\sqrt{3\pi k_F^2 (Dr)^{3/2}} (1 - \cos \gamma) \right\}, $$

where $k_F$ and $v_F$ are the Fermi wavevector and velocity respectively and $D = v_F l_0/3$ is the diffusive constant [20]. Following the arguments of ref. [20] the correction to the transmission distribution can be written as

$$ \delta P(T) = \left\langle \sum_n \delta (T - \tau_n) (1 - \tau_n) \right\rangle p_{\text{return}}, $$

where $\tau_n = l_0/v_F$ is the elastic scattering time and $p_{\text{return}} = \int_{\tau_n}^{\infty} P_{cl}(t) dt$. Assuming that typically $\gamma \sim 45^\circ$ and that $l_0$ can range from $\sim 10$ nm to $\sim 4$ nm in Pb, one obtains $p_{\text{return}} \sim 0.005 - 0.02$ leading to a rather small correction which hardly modifies the theoretical results already shown in fig. 4.

In conclusion, we have presented a combined experimental and theoretical analysis of the conduction channel distribution of nanoscale contacts with several atoms in cross section. The experimental method demonstrates the applicability of the technique developed by Scheer et al. [3, 10] to much larger contacts. It is found that for Pb contacts the distribution tends rather fast to the universal diffusive limit. We show that this behavior can be associated with the specific band structure of Pb which favors the appearance of partially open channels in contrast to what is predicted for monovalent metals like Au.

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