GENERALIZED CONDUCTANCE SUM RULE IN ATOMIC BREAK JUNCTIONS

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Abstract When an atomic-size break junction is mechanically stretched, the total conductance of the contact remains approximately constant over a wide range of elongations, although at the same time the transmissions of the individual channels (valence orbitals of the junction atom) undergo strong variations. We propose a microscopic explanation of this phenomenon, based on Coulomb correlation effects between electrons in valence orbitals of the junction atom. The resulting approximate conductance quantization is closely related to the Friedel sum rule.

The progressing miniaturization of electronic circuits raises the question what controls the transport when a contact is shrunk to its minimal possible size, a single atom. Electrical single-atom contacts have recently been fabricated using the break junction technique [1]. By analyzing the subgap structure of superconducting contacts it was demonstrated that the valence orbitals of the junction atom act as the transmission channels for the electronic current and that the transmissions T_m of the individual orbitals $m = 1, \ldots, N$, add up to the total transmission of the contact, which was measured independently [1]. Naturally, the transmissions T_m can take any value $0 \leq T_m \leq 1$, since they depend on the microscopic details like the coupling matrix elements of the atomic orbitals to the leads. Therefore, it came as a surprise that in Al junctions the total conductance remained nearly constant with a value close to the conductance quantum $2e^2/h$, when the contact was mechanically stretched, although at the same time the individual channel transmissions T_m varied over a wide range [2]. As a consequence, certain conductance values are preferred in Al contacts as shown in Fig. 1. In the present work we prove a sum rule for the total conductance in atomic junctions where

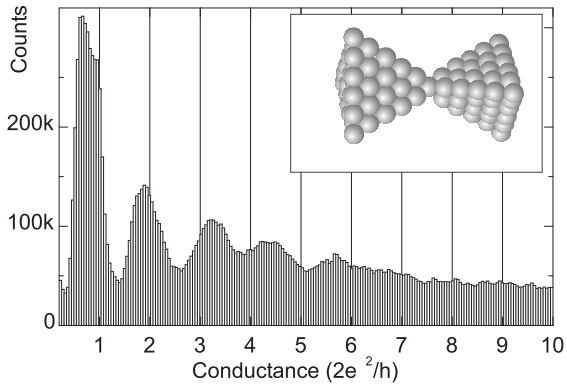

Figure 1 Histogram of the frequency of occurance of various conductance values of an Al atomic break junction during > 6200 opening sweeps of the contact; $T = 4.2$ K. The occurance of preferred conductance values close to multiples of the conductance quantum $2e^2/h$ is seen (courtesy: A. I. Yanson and J. M. v. Ruitenbeek [2]). The inset schematically shows the junction geometry.

the Coulomb repulsion between electrons in the valence orbitals of the junction atom is large. We propose that this correlation effect is the microscopic origin of the observed approximate conductance quantization.

In good metals the Coulomb interaction is screened on a length scale of a few Å. For electrons in the extended conduction band states of the leads it can, thus, be absorbed into a small renormalization of the Fermi liquid parameters. However, electrons traversing the contact are forced to pass through the orbitals of the junction atom, where their dynamics are strongly affected by the Coulomb electron-electron interaction because of the strong spatial confinement. As a model of the junction we, therefore, consider the Anderson-like Hamiltonian

$$\begin{aligned} H &= \sum_{k\sigma,\ \alpha=L,R} \varepsilon_k\ c^\dagger_{\alpha\ k\sigma} c_{\alpha\ k\sigma} + \sum_{m\sigma} \varepsilon_{d,m}\ d^\dagger_{m\sigma} d_{m\sigma} \qquad (1.1) \\ &+ \sum_{km\sigma,\ \alpha=L,R} \left[t^\alpha_{mk}\ d^\dagger_{m\sigma} c_{\alpha\ k\sigma} + \text{h.c.} \right] + \frac{U}{2} \sum_{(m,\sigma)\neq(m',\sigma')} \hat{n}_{m\sigma} \hat{n}_{m'\sigma'}\ , \end{aligned}$$

where $c^\dagger_{\alpha\ k\sigma}$ is the creation operator of an electron in the left or right lead ($\alpha = L, R$) with energy ε_k and spin σ. $d^\dagger_{m\sigma}$ creates an electron in one of the valence levels ε_m, $m = 1, \ldots, N$ of the junction atom, and $\hat{n}_{m\sigma} = d^\dagger_{m\sigma} d_{m\sigma}$. The transition matrix elements from a lead state (α, k) to a local level m is t^α_{mk}, and the Coulomb repulsion between two electrons in any of the junction atom's valence orbitals is denoted by U. To be explicit, we restrict ourselves to the case of $N = 2$ transmission channels here (A similar conductance sum rule can be proven for arbitrary N [3]).

The advanced local-orbital Green's function then takes the matrix form

$$\mathcal{G}_\sigma(\omega) = \begin{pmatrix} \omega - \varepsilon_{d,1} - i\Gamma_{11} - \Sigma_1(\omega) & -i\Gamma_{12} \\ -i\Gamma_{21} & \omega - \varepsilon_{d,2} - i\Gamma_{22} - \Sigma_2(\omega) \end{pmatrix}^{-1} \quad (1.2)$$

with the effective lead-to-orbital coupling matrix $\Gamma = (\Gamma_{mn})$, $\Gamma_{mn} = \pi \sum_{k,\,\alpha} t^{\alpha}_{mk} A_k(\omega) t^{\alpha\,*}_{kn}$, ($A_k(\omega)$: spectral density of lead state k). $\Sigma_m(\omega) = \Sigma'_m(\omega) + i\Sigma''_m(\omega)$ denotes the advanced self-energy due to Coulomb interaction U in the local orbitals. When a bias voltage V is applied, the current is given by [4]

$$I = \frac{e}{h} \sum_\sigma \int d\omega \Big[f(\omega) - f(\omega + \frac{eV}{\hbar}) \Big] \mathrm{Im\,tr}\,(\Gamma \cdot \mathcal{G}_\sigma(\omega)), \quad (1.3)$$

where $f(\omega)$ is the Fermi function. The hybridization t^{α}_{nk} induces an antiferromagnetic spin exchange coupling between an electron in any of the atomic orbitals and the conduction electrons. It is known from a renormalization group analysis of this problem, that the ground state of correlated quantum impurity models like Eq. (1.1) is a spin singlet [5]. Hence, for temperature T below a characteristic scale, $T < T_o$ the junction is a pure potential scatterer for electrons traversing the system, and the following Fermi liquid relations hold [6],

$$\Sigma''_m(\omega) = [(\hbar\omega)^2 + (\pi \mathbf{k}_B T)^2]/k_B T_o \qquad \omega, T \to 0 \quad (1.4)$$

$$\int_{-\infty}^{0} d\omega\ \mathrm{tr} \left\{ \frac{\partial \Sigma(\omega)}{\partial \omega} \cdot \mathcal{G}_\sigma(\omega) \right\} = 0 \qquad \text{(Luttinger theorem)} \quad (1.5)$$

The averaged total electron number on the junction atom for each spin species, $n_{d,\sigma}$, can now be evaluated using the general relation $\frac{d}{d\omega} \ln(\mathcal{G}^{-1}) = (1 - \frac{d\Sigma}{d\omega}) \cdot \mathcal{G}$ and the Luttinger theorem Eq. (1.5),

$$n_{d\sigma} = \mathrm{Im} \int_{-\infty}^{0} \frac{d\omega}{\pi} \mathrm{tr}\ \mathcal{G}_\sigma(\omega) = \frac{1}{\pi} \mathrm{Im} \Big[\mathrm{tr} \{ \ln\, \mathcal{G}_\sigma(\omega)^{-1} \} \Big]_{\omega=-\infty}^{\omega=0} . \quad (1.6)$$

Eq. (1.6) is a statement of the Friedel sum rule $n_{d\sigma} = \frac{1}{\pi} \sum_m \delta_{m\sigma}(0)$, since the scattering phase shift at the Fermi level in channel m is $\delta_{m\sigma}(0) = \arg[\Gamma \cdot \mathcal{G}_\sigma(0)]_{mm}$. It may be re-expressed, using $\mathrm{tr}\ \ln\, \mathcal{G}_\sigma{}^{-1} = \ln \det\, \mathcal{G}_\sigma{}^{-1}$, as

$$n_{d\sigma} = \frac{1}{\pi} \mathrm{arccot} \left[\frac{\mathrm{Re\ det}\ \mathcal{G}_\sigma(0)^{-1}}{\mathrm{Im\ det}\ \mathcal{G}_\sigma(0)^{-1}} \right] . \quad (1.7)$$

The scattering T-matrix of the junction atom, $\Gamma \cdot \mathcal{G}_\sigma$, which determines the conductance $G = dI/dV$ of the system via Eq. 1.3, is now evaluated

by expressing the inverse matrix Eq. (1.2) in terms of its determinant, and, using the Fermi liquid property Eq. (1.4), we obtain at the Fermi energy ($\omega = 0$, $T \ll T_o$),

$$\begin{aligned} \text{Im tr } (\Gamma \cdot \mathcal{G}_\sigma(0)) &= \sin^2(\pi n_{d\sigma}) \\ &+ \sin(2\pi n_{d\sigma}) \frac{\Gamma_{21}\Gamma_{12} - \Gamma_{11}\Gamma_{22}}{\Gamma_{11}(\varepsilon_{d,2} + \Sigma_2'(0)) + \Gamma_{22}(\varepsilon_{d,1} + \Sigma_1'(0))} \,. \end{aligned} \tag{1.8}$$

If the transition amplitudes t^α_{mk} are independent of the lead channels k, it follows directly from the definition of Γ_{mn} that the term $\propto \sin(2\pi n_{d\sigma})$ cancels. Eq. (1.8) is an exact result, valid for arbitrary microscopic parameters Γ_{mn}, $\varepsilon_{d,m}$, U, and $n_{d\sigma}$. It is the generalization of the well-known unitarity rule of the single-level Anderson impurity problem to the case of several impurity levels [3]. In metals in the single-atom junction geometry (inset of Fig. 1) [7], there is at least one of the local levels significantly below the Fermi level ($\varepsilon_{d,m_o} < 0$, $|\varepsilon_{d,m_o}|/\Gamma_{mn} < 1$). While in the non-interacting case the right-hand side of Eq. (1.8) can assume any value, a strong Coulomb repulsion U enforces $n_{d\sigma} \approx 1/2$, implying via Eqs. (1.8), (1.3) a conductance close to the conductance unit, i.e. $dI/dV \approx 2e^2/h$ (the factor 2 reflects spin summation). The physical origin of this quantization is that in the regime of large U charge fluctuations are suppressed and the low-energy spin fluctuations induce a Kondo-like resonance at the Fermi energy, (as seen from the resonant phase shift $\delta(0) = \pi/2$, which is implied by $n_{d\sigma} \approx 1/2$ through Eq. (1.6). Resonant transmission through the impurity complex is equivalent to unitary conductance per spin. This quantization holds for the total conductance and is exact in the limit $n_{d\sigma} = 1/2$, $T \ll T_o$. It will be approximate for the realistic parameters of a break junction.

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