Parity oscillation and relaxation in monatomic copper wires

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We present *ab initio* studies of the conductance in the ballistic limit for relaxed monatomic Cu wires. Our approach is based on density functional theory in the frame of the Korringa-Kohn-Rostoker Green's function method. Atomic relaxations are calculated by means of *ab initio* based many body potentials. We confirm the parity oscillation of the conductance and demonstrate that the effect is robust with respect to structural relaxation of the wire.

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I. INTRODUCTION

Newly developed experimental techniques such as scanning tunneling microscopy and mechanically controllable break junctions made it possible to fabricate metallic point contacts at the atomic scale. In this ultimate limit quantum effects dominate and can be directly visualized in the experiments. Upon elongation of the nanocontacts the conductance decreases stepwise with typical jumps of the order of the conductance quantum $g_0=2e^2/h$. This behavior is attributed to atomic rearrangements in the neck region of the constriction as a response to the applied stress. To analyze the results of experiments the conductance histograms have been introduced which in case of noble (Au, Ag, Cu) and alkali metals (Li, Na, K) show a dominant peak very close to g_0. This peak just before breaking corresponds to the monatomic wire suspended between the macroscopic electrodes.

Numerical simulations for monatomic sodium wires[1–3] as well as for noble metal wires[4] predicted an oscillation of the conductance as a function of the number of atoms (parity oscillation). In recent experiments by Smit *et al.*[5] parity oscillations indeed have been observed for Au, Pt, and Ir monatomic chains. Furthermore, calculations by Havu and co-workers[3] showed that the exact geometry of the atomic constriction and the attachment to the leads, especially the cone angle, influences the conductance oscillations. However, according to the theoretical study by Thygesen and Jacobsen[6] aluminum does not exhibit an even-odd effect in the conductance. As concerns the phase of oscillation, some authors found a perfect transmission for odd number of atoms and a reduced one for even number,[2,7] while others reported about the opposite behavior.[1,3] Major *et al.*[8] have shown by a mixed analytical *ab initio* treatment that the phase of the parity effect in monovalent wires is highly nonuniversal and depends on the fine details of the charge relaxation in the contact region.

Several studies of the parity effect use a parametrized description, such as jellium electrodes,[1,3] or a supercell geometry[2,4,6,9] to calculate the conductance. In this paper, we present *ab initio* calculations of the conductance in monatomic Cu chains suspended between metallic leads, where the electronic structure of both the electrodes and the wire is described without free parameters. Since one expects the conductance to be sensitive to the positions of the atoms in the chain, both unrelaxed and relaxed geometries of the wires were investigated. Based on this analysis we demonstrate the interplay between geometrical structure and electronic transport properties.

II. METHOD

We present electronic structure calculations based on density functional theory (DFT) in local density approximation (LDA) within a screened Korringa-Kohn-Rostoker (KKR) Green's function method. The KKR method is based on a scattering wave expansion in contrast to equivalent schemes using a local basis. A detailed description of the KKR method is given in Ref. 10. In comparison to our *ab initio* calculations, parametrized tight binding (TB) calculations are presented to elucidate the results.

The structures under consideration consist of two semi-infinite Cu leads, left and right, connected by a straight monatomic Cu wire of N atoms as it is shown in Fig. 1. The first atom of the wire is placed on the hollow site of the (001) surface of the lead. We studied wires in idealized and relaxed geometry. In the idealized geometry the distance between the atoms was chosen to be the nearest neighbor distance of fcc Cu similar to Ref. 4. In the relaxed geometry the equilibrium

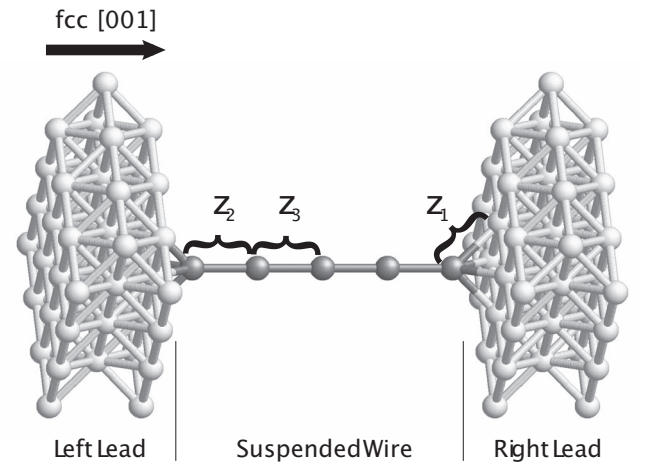

FIG. 1. Suspended metallic wire between two semi-infinite leads.

positions of the atoms for a fixed separation of the leads are determined by means of a quasi–*ab initio* molecular static method,[11–15] which is based on the second moment tight-binding approximation for many-body potentials.[16,17] In this approximation the many-body representation of the cohesive energy is used. The parameters of interatomic interactions are determined by fitting to the accurate first-principle calculations of the wire-surface properties, *ab initio* forces acting on adatoms and surface energy.[18] Thus, only *ab initio* data for low-dimensional systems are used to construct potentials. It was shown that *ab initio*-fitted many-body potentials and the KKR Green's function method can be combined to perform relaxations of metallic clusters on semi-infinite metal substrates.[19] Geometrical and electronic structure are calculated self-consistently.

Within the KKR method, the Green's function of the system was obtained in two steps. First, the Green's function $\mathring{G}^{jj'}_{LL'}(\mathbf{k}_{\|},E)$ of two semi-infinite leads separated by a vacuum spacer was calculated self-consistently. Here, index L stands for the angular momentum quantum numbers (l,m) and j denotes the layer index. In the second step a single nanowire was embedded between the two semi-infinite leads by solving the Dyson equation self-consistently:

$$G = \mathring{G} + \mathring{G}\Delta V G. \tag{1}$$

After the solution of the Dyson equation the Green's function G of the complete system (wire suspended between the leads) is obtained taking the full charge relaxation of a single wire in contact with the lead surfaces into account. ΔV is the change of the potential which is related to the wire in contact with the leads. ΔV is determined self-consistently. In terms of an angular momentum expansion the Green's function[10] is given by

$$G(\mathbf{r}+\mathbf{R}^n,\mathbf{r}'+\mathbf{R}^{n'};E) = \delta_{nn'}\sqrt{E}\sum_L R^n_L(\mathbf{r}_<;E)H^n_L(\mathbf{r}_>;E) + \sum_{LL'} R^n_L(\mathbf{r};E)G^{nn'}_{LL'}(E)R^{n'}_{L'}(\mathbf{r}';E), \tag{2}$$

where R^n_L, H^n_L are regular and irregular solutions of the Schrödinger equation for the potential site n and $G^{nn'}_{LL'}(E)$ is the structural Green's function, connecting the scattering paths between sites n and n'. The wave functions and Green's functions in the present calculations were expanded up to angular momenta $l_{\max}=3$, while the expansion of the charge density was taken into account up to $l_{\max}=6$. We assumed spherical potentials [atomic sphere approximation (ASA)]. Exchange and correlation effects were described using the LDA (Refs. 20 and 21) in the parametrization of Vosko, Wilk, and Nusair.[22]

The conductance of the nanowires suspended between the semi-infinite bulk electrodes was calculated using the Kubo linear response theory in the formulation of Baranger and Stone.[23] Following Ref. 23 the conductance g at zero temperature is given by

$$g = \frac{e^2\hbar^3}{8\pi M^2}\int_{A_{\text{right}}} d\mathbf{s}\int_{A_{\text{left}}} d\mathbf{s}'\, G^+(\mathbf{r},\mathbf{r}';E_F)\overleftrightarrow{\nabla}\overleftrightarrow{\nabla}' G^-(\mathbf{r}',\mathbf{r};E_F), \tag{3}$$

where $f(\mathbf{r})\overleftrightarrow{\nabla}g(\mathbf{r}) = f(\mathbf{r})\nabla g(\mathbf{r}) - g(\mathbf{r})\nabla f(\mathbf{r})$ and G^+, G^- are the advanced and retarded Green's functions, respectively. Formally, the conductance has to be calculated between two planes A_{left} and A_{right} positioned in the left and the right ideal semi-infinite lead. However, within the ASA we consider instead of integration over planes integrals over atomic layers. A description of the method and a detailed derivation can be found in Refs. 24 and 25. Combining Eqs. (2) and (3), we find

$$g = \frac{e^2\hbar^3}{8\pi M^2}\sum_{nn'}\sum_{L'L''}\sum_{L}(J^n_{LL''} - J^{*n}_{L''L})G^{nn'}_{LL'} \times \sum_{L'''}(J^{n'}_{L'L'''} - J^{*n'}_{L'''L'})G^{*nn'}_{L''L'''}, \tag{4}$$

where the sum n runs over all atoms in the atomic layer in the left lead, while the sum n' runs over the atoms in the atomic layer in the right lead. The star denotes complex conjugate, and we have dropped the energy dependence for simplicity. The current matrix elements

$$J^n_{LL''} = \frac{1}{\Delta}\int_{\text{WS}} d^3r R^n_L(\mathbf{r})\partial_z R^{*n}_L(\mathbf{r}), \tag{5}$$

are averaged over the distance Δ separating two nearest neighbor atomic layers in the z direction. The integration is performed over the Wigner-Seitz cell of atom n.

In the TB calculations we consider metallic leads with one s orbital. The Green's function of the wire with leads is given by[26]

$$G^{\pm}(E) = [(E \pm i0^+)I - H_{\text{wire}} - \Sigma(E)]^{-1}, \tag{6}$$

where I is the identity matrix and H_{wire} is the Hamiltonian for the isolated wire. The influence of the leads is taken into account by the self-energy $\Sigma = \Sigma_{\text{left}} + \Sigma_{\text{right}}$ with

$$\Sigma_{\text{left}} = (\tau_{\text{left}})^{\dagger} G^{\text{surf}}_{\text{left}} \tau_{\text{left}}, \tag{7}$$

where $G^{\text{surf}}_{\text{left}}$ is the surface Green's function of the isolated left lead, τ_{right} is the coupling matrix between left lead and wire and the symbol (†) denotes complex conjugate transpose. The self-energy Σ_{right} is defined analogously. The conductance at zero temperature and zero bias is calculated by the expression[26]

$$g = \frac{e^2}{h}\text{Tr}[\hat{T}(E_F)], \tag{8}$$

with E_F being the Fermi energy. Tr denotes the trace over all orbitals of the wire. The transmission matrix $\hat{T}$ is given by

$$\hat{T}(E) = \Gamma_{\text{left}} G^+ \Gamma_{\text{right}} G^-, \tag{9}$$

where $\Gamma_{\text{left}} = i[\Sigma_{\text{left}} - (\Sigma_{\text{left}})^{\dagger}]$.

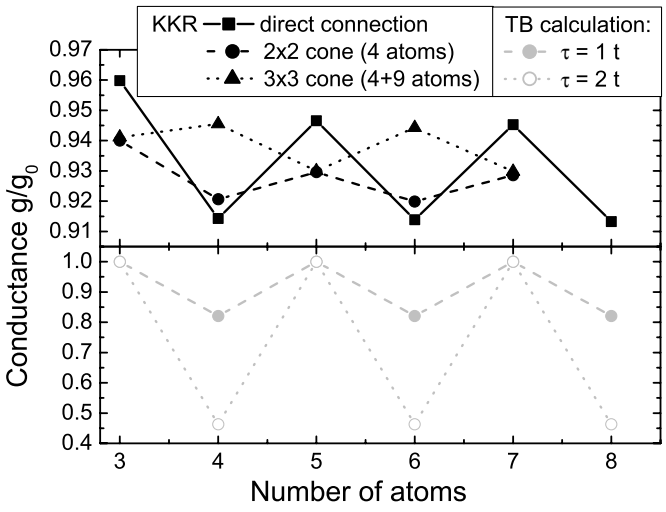

FIG. 2. Conductance versus the number of atoms in the atomic wire by means of a KKR Green's function method for three types of attachment—no cone (squares), 2×2 cone (circles), and 3×3 cone (triangles) (upper figure) and within a parametrized TB model (lower figure). The model parameters in the TB calculation are $\varepsilon_i=0$ and $t_i=t$ for all sites. The TB results are shown for two sets of coupling parameters $\tau_{\text{left}}=\tau_{\text{right}}=t$ (closed symbols) and $\tau_{\text{left}}=\tau_{\text{right}}=2t$ (open symbols).

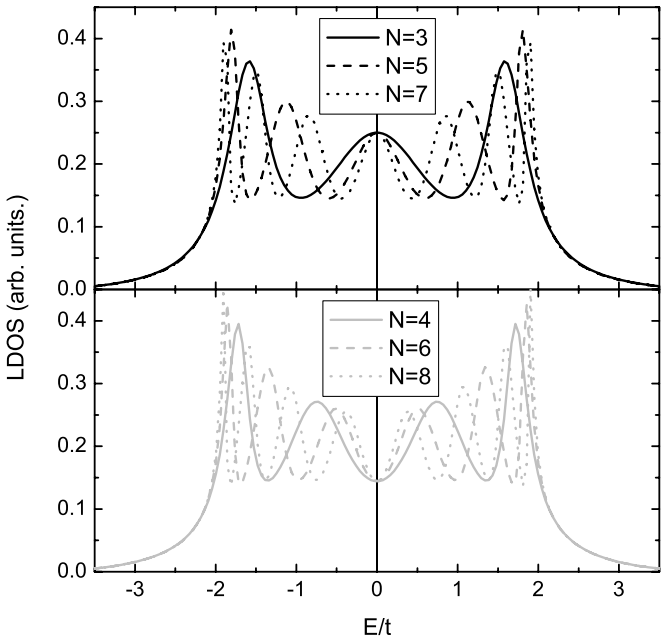

FIG. 3. Dependence of the LDOS for the atom next to the lead on the number of atoms in the atomic wires calculated within a TB model. The upper figure shows the LDOS for odd numbered atomic wires and the lower figure shows the LDOS for even numbered atomic wires. The model parameters are $\varepsilon_i=0$ and $t_i=t$ for all sites. The coupling parameters between leads and atomic wire are $\tau_{\text{left}}=\tau_{\text{right}}=t$.

III. RESULTS

A. Even-odd effect

As was mentioned in the Introduction, atomic wires should reveal quantum size effects in conductance as a function of length. In Fig. 2 results of the conductance through finite monatomic Cu chains bridging the macroscopic electrodes are presented. Both *ab initio* and TB model based calculations are shown. We observe that, independent of the computational approach, conductance oscillates with a period of two atoms. The origin of the effect is quantum interference of electron waves which propagate through the atomic constriction and are reflected at the interfaces between the wire and the electrodes. A simplified explanation of the effect was already given in a one-dimensional free-electron model (see Ref. 5). For monovalent metallic wires such as Na, Cu, Ag, Au, etc., the resulting oscillation has a period of two atoms, which is caused by a half-filled band at the Fermi energy. The phase of the oscillation, however, is a highly sensitive property and will be discussed later.

Let us consider the TB picture first (lower panel of Fig. 2). The model parameters in the calculations were chosen to be identical in the leads and in the wire, with the on site element $\varepsilon_i=0$ and the hopping integrals $t_i=t$. The results for different coupling parameters $\tau_{\text{left}}=\tau_{\text{right}}=t$ and $\tau_{\text{left}}=\tau_{\text{right}}=2t$ are shown in Fig. 2. The conductance is equal $g_0=2e^2/h$ for odd N and becomes smaller for even N. With increasing coupling parameters τ the conductance of the even numbered wires is further reduced.

The quantum effects due to the finite size of the atomic wires can also be seen in the local density of states (LDOS) shown in Fig. 3. As will be shown later, the correlation between the transmission and the LDOS is strongest for the atom of the chain close to the electrode (contact atom). Since we are describing monovalent metals with a half-filled s band, the Fermi energy is at $E/t=0$. The LDOS of the suspended wire shows peaks at points corresponding to the energy levels of the isolated wire. The singularities at energies equal to the eigenvalues of the isolated wire are shifted and broadened, which is caused by the coupling to the leads (see Ref. 26). Due to the symmetry of the system, the LDOS shows a maximum at the Fermi energy $E/t=0$ for wires with odd number of atoms and a minimum for even numbered wires. The peaks in the LDOS have a non-Lorentzian shape, since the self-energy is a function of E. The energy-dependent transmission $T(E)$ (not presented here) resembles the behavior of the LDOS shown in Fig. 3 with maxima at positions of the energy levels of the isolated wire. In particular, transmission reaches a maximum value of one at E_F for odd numbered chains and is smaller than one for even numbered chains (see Fig. 2).

In general, the atom of a chain next to the lead has a higher coordination number with respect to the atom in the chain and causes an increase of the effective coupling parameter τ. Therefore, we performed calculations for $\tau=2t$. The transmission $T(E)$ does not reveal significant changes as compared with the case of $\tau=t$ described above. The even-odd effect is still conserved as it is seen from Fig. 2. In addition the conductance of the even numbered wires is further reduced. The peaks, however, in the LDOS (Fig. 4) are broadened and shifted compared with Fig. 3. In contrast to the case of $\tau=t$ the LDOS has now a maximum at the Fermi energy for the even numbered atomic wires and a minimum

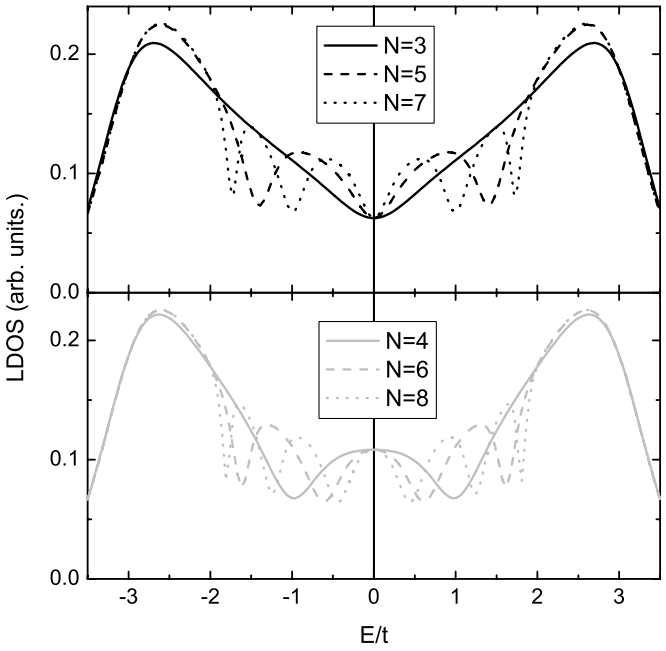

FIG. 4. LDOS for the atom next to the lead calculated within a TB model. All model parameters are the same as in Fig. 3 but with $\tau=2t$. Increasing coupling causes further shift and broadening of the peaks.

for odd numbered atomic wires. There is no more direct correspondence between the maxima and the energy levels of the isolated wire. Because of the non-Lorentzian broadening of the peaks the maxima are now situated between two energy levels of the isolated wires. The phase of the conductance, however, is still the same (Fig. 2, lower panel).

We proceed now with the results for the conductance of the *ab initio* calculations obtained by means of the KKR method. We consider straight wires with varying attachment to the leads: direct attachment of the wire to the leads without cone (Fig. 2, squares), attachment of the wire by a cone formed by 2×2 atoms (Fig. 2, circles), and attachment of the wire by a 3×3 cone consisting of all together 13 atoms (Fig. 2, triangles). The cones are constructed on the fcc lattice of the leads as described in Ref. 4. The conductance (upper panel of Fig. 2) shows for all configurations even-odd oscillations as in the TB model (lower panel) since in the case of an infinite Cu wire the half-filled band fixes the Fermi wave vector at $k_F=\pi/2a$. Perfect transmission, however, is never obtained in a realistic system because of charge redistribution in the constriction. The increased conductance value for the short three atom wire stems from additional tunneling contributions which are not taken into account in the TB calculation. The amplitude of the oscillation is about 3% of g_0 for the wire attached to the lead without cone and about 1% of g_0 for the connection with an atomistic cone.

The results demonstrate in agreement with Major *et al.*[8] that the phase of the even-odd effect depends on the fine details of charge relaxation in the region of attachment. While direct attachment and attachment via a 2×2 cone give rise to the same phase for the conductance oscillation the phase is changed for attachment of the wire by a 3×3 cone. This is probably also the reason for the opposite phase be-

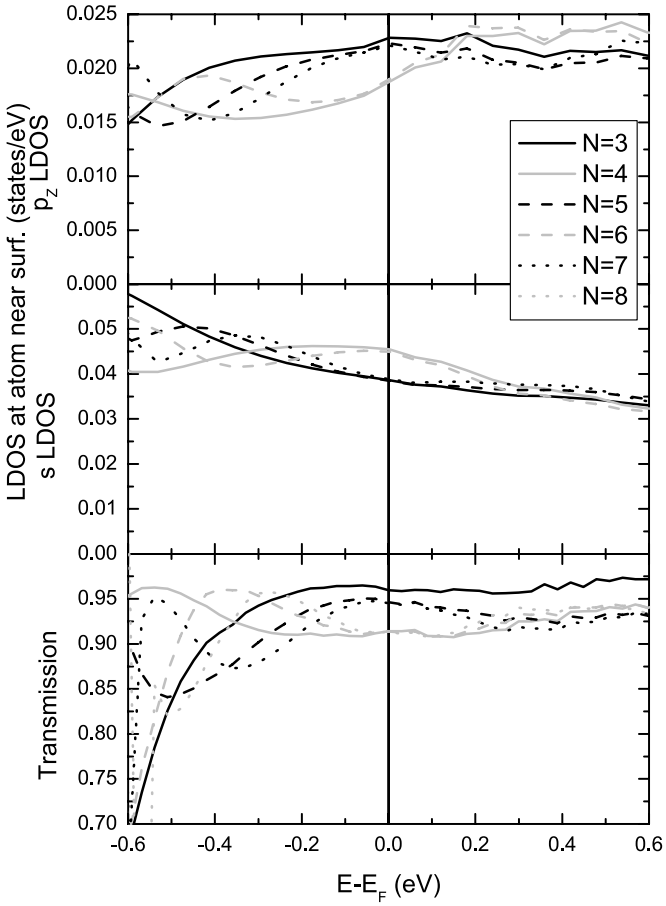

FIG. 5. Symmetry projected LDOS calculated by the KKR method for the atom next to the lead for odd numbered wires (black lines) and even numbered wires (gray lines) and transmission versus energy for different number N of atoms.

tween the *ab initio* results of Ref. 4 and the results of this paper for the 2×2 cone. The considered systems are in principle the same concerning the structure. The only difference consists in the scheme of calculation. The authors of Ref. 4 consider an in-plane supercell which means that the wire is periodically repeated. We consider a single wire. Consequently, the space for in-plane charge relaxation is slightly different which probably causes the opposite phase of the conductance.

The symmetry projected LDOS of the contact atom obtained within *ab initio* calculations and the energy-dependent transmission $T(E)$ are shown in Fig. 5. The open conductance channel of the wire has the symmetry of a unitary representation of the C_{4v} group. The projection of this channel to the contact atom consists of s and p_z contributions. Therefore the transmission $T(E)$ correlates with the s and p_z LDOS of the contact atom as it is clearly seen from Fig. 5. The maxima in the transmission correspond to the maxima in the p_z LDOS and to the minima of the s LDOS. We also observe from Fig. 5(a) that the p_z LDOS at the Fermi energy for different wires shows the same behavior as in case of the TB model with the coupling parameter $\tau=t$ (Fig. 3). The s LDOS [Fig. 5(b)], however, shows an inverted picture, where the even numbered wires have a larger LDOS at the

TABLE I. Distances between the atoms according to Fig. 1 in Å. z is the separation of the leads and d is the distance between the first atom in the wire and the surface of the leads.

	relaxed distances				unrelaxed distances	
z	z_1	z_2	z_3	d	$z_1=z_2=z_3$	d
10.94	2.10	2.21	2.19	1.07	2.15	1.17
11.45	2.21	2.23	2.21	1.28	2.22	1.29
11.96	2.32	2.28	2.25	1.45	2.29	1.40
12.45	2.41	2.34	2.29	1.60	2.36	1.51
12.95	2.50	2.41	2.34	1.72	2.43	1.62
13.46	2.56	2.52	2.39	1.82	2.50	1.73

Fermi energy than the odd numbered wires, similar to the results obtained within the TB model for $\tau=2t$ (Fig. 4), which indicates that s and p_z orbitals of the contact atom couple with different strength to the (001) surface of the lead.

B. Relaxation

Up to now we have discussed idealized wires, with equal distances between the atoms. However, the realistic metallic nanowires are formed under continuous stretching which results in relaxation of the geometrical structure under stress and leads in general to different interatomic distances. In a recent publication[15] the relaxation effects in atomic wires and their influence on geometrical and electronic structure were discussed in detail. In this paper we present the study of transport properties.

A comparison of the unrelaxed and relaxed positions for the wire consisting of five atoms is presented in Table I. In the unrelaxed structure the nearest neighbor distances are chosen to be equal. In the relaxed structure the distance z_2 remains the same as in the unrelaxed structure. Starting from a total length $z=11.96A$ the distance z_1 is increased and z_3 reduced. The central atoms of the wire form a molecule with a weaker bond to the surface.

In Fig. 6 we show the variation of the conductance upon

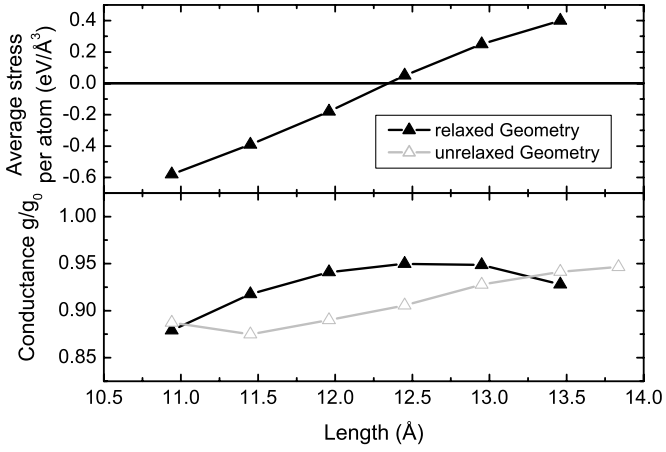

FIG. 6. Conductance and averaged stress per atom for a wire of five atoms.

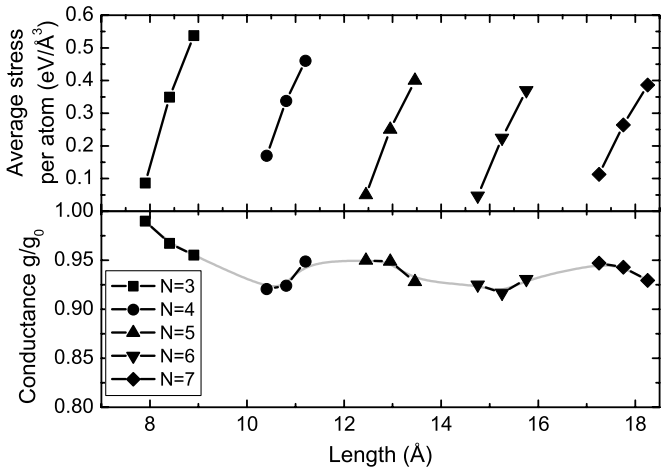

FIG. 7. Conductance and averaged stress per atom versus length of the wire for different number N of atoms.

stretching for the unrelaxed and relaxed wires consisting of five atoms in comparison with the averaged stress per atom. The general trend is an increasing conductance with increasing stress by order of magnitude 10%. The difference of the conductance due to relaxation is, however, only $0.05g_0$. For this reason the parity oscillation in noble metals is robust with respect to structural relaxation in the wire. This can be seen in Fig. 7, where we plot conductance and averaged stress per atom for the relaxed wire as a function of its length. The continuous stretching of the wire causes an increase of the stress until an additional atom is pulled out from the electrode and elongates the wire by one atom. At this moment the stress decreases rapidly. Compressed wires are not considered. Under the scenario of continuous stretching the parity oscillations of the conductance are still conserved with a smooth dependence on length. The amplitude of the oscillation is about 3% of g_0. The increased value for the three atom wire is caused by additional tunneling contributions. The conductance increases if the number of atoms in the wire changes from even to odd, followed by a decay if the number changes from odd to even.

IV. CONCLUSIONS

In summary, we performed *ab initio* calculations of the conductance of monatomic Cu nanowires upon stretching including a fully relaxed geometry. It was demonstrated that in agreement with experiments for monatomic Au wires[5] the even-odd effect in noble metals is robust against structural relaxation in the wire, since only one conducting channel of s,p_z character contributes to conductance.

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