

# Quantum transport through atomic wires

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We have investigated quantum transport through long wires in which a section consists of one or several Al atoms in a chain. The self-consistent ground state electronic potential is obtained using the first principles *ab initio* method and the conductance is calculated by solving a three-dimensional quantum scattering problem. We have observed quantized conductance when there are two or more Al atoms in the chain. Resistance is calculated for these wires at the Fermi level. © 1997 American Institute of Physics. [S0003-6951(97)01529-5]

It has been demonstrated by several laboratories<sup>1,2</sup> that atomic scale point contact with sizes of a few to  $\sim 50$  Å can have quantized conductance at room temperature. Atomic scale objects may thus have important implications to future quantum electronic applications. So far most investigations on atomic scale transport, both experimental and theoretical, are focused on transport properties of atomic contacts in the geometry of tip-substrate arrangement, such as those of scanning tunneling microscope (STM) or atomic force microscope.<sup>1,3-6</sup> In this regard, a complete first principles quantum scattering theory of the conductance of atomic scale objects is advanced by Lang<sup>7</sup> and his theoretical predictions for the case of a few Xe atoms sandwiched in between two substrates are in almost quantitative agreement with STM measurements.<sup>7</sup> While these theoretical investigations have provided many useful means of understanding concerning quantum transport properties of atomic scale wires in the geometry of a tip-substrate arrangement, there is clearly a need for further theoretical studies of this important problem. In particular, since the fabrication of free-standing atomic scale nanowires are becoming a reality as demonstrated by several groups,<sup>8,9</sup> a theoretical investigation of quantum transport through long atomic wires is important and useful, in addition to the geometry of tip-substrate arrangements. It is the purpose of this letter to report our investigations of the formation of atomic wires made of Al atoms.

In particular, we consider the model shown in Fig. 1 where a group of Al atoms in a chain is connected to the outside by two three-dimensional (3D) leads. Thus the whole system can be viewed as a long 3D wire with an atomic section in the middle. In our calculations, we shall use the jellium model for the 3D leads. Straight or other shaped quantum wires in the mesoscopic or ballistic transport regimes have been extensively investigated by many groups including the authors<sup>10</sup> using continuum models where atomic information is included into the effective mass of the electrons. In this work, however, we shall explicitly investigate quantum transport through the atoms.

Our calculation proceeds in two steps.<sup>11,12</sup> First, ground state properties of the atomic chain (the Al atoms) and the left and right leads each of length  $L$  are computed using a

preconditioned conjugate gradient (CG) minimization<sup>13</sup> of the Kohn–Sham total energy functional, where the valence electrons are treated explicitly and the core is introduced through a pseudopotential. We have fixed the ionic positions in our ground state calculation. The outcome of this step is the self-consistent Kohn–Sham electronic wavefunctions  $\psi_i(\mathbf{r})$  with a self-consistent effective potential  $V_{\text{eff}}(\mathbf{r}) \equiv \delta U / \delta \rho(\mathbf{r})$  which is seen by all the electrons. Here  $U[\rho]$  is the total self-consistent potential energy while  $\rho$  the electron density obtained from  $\{\psi_i\}$ .<sup>13,14</sup> We have used the parameterization of Ref. 15 for the exchange–correlation term, and a local pseudopotential<sup>16</sup> for the core. In the second step, we imagine that an incoming particle is launched in the left lead far away from the atomic chain of the wire. This particle traverses the wire defined by  $V_{\text{eff}}$  and we shall compute the transmission coefficients. Although for our 3D system, the quantum scattering calculation is quite involved, it is essentially a transfer matrix evaluation of the scattering probabilities. We have extended a recently reported method<sup>17</sup> for this purpose. With the transmission coefficients  $T_\alpha(E)$ , where subscript  $\alpha$  labels the transmission subbands, we can evaluate the conductance of the wire via the Landauer formula,<sup>18</sup>  $G(E) = 2e^2/h \sum_\alpha T_\alpha(E)$  where  $E$  is the incoming electron energy.

The above two-step approach<sup>11</sup> is reasonable if several conditions are satisfied. Since  $V_{\text{eff}}$  is a self-consistent potential, the calculation makes sense if there are a large number of electrons which is the case here. Otherwise one may use a scattering theory based on Lippmann–Schwinger equation as

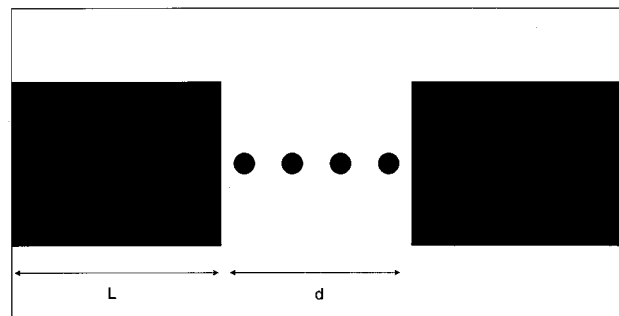


FIG. 1. Schematic plot of a long quantum wire where there is an atomic chain and two 3D jellium leads of length  $L$  each. The whole system is included in a supercell for plane wave based *ab initio* total energy calculations. The Al–Al bond length is 2.86 Å and the end atom jellium 1.375 Å. These values were used in Ref. 7.

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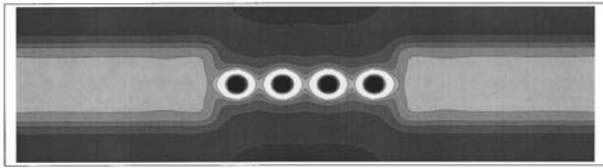


FIG. 2. The contour plot of the ground state effective potential  $V_{\text{eff}}$  obtained from the *ab initio* total energy calculation for a wire with four atoms. The bonding between the atoms and the leads are clearly seen. Relative potential strength is shown by the lighter (darker) region depicts lower (higher) values of  $V_{\text{eff}}$ . The scale ranges from  $-14$  (white) to  $+19$  eV (black), in intervals of  $3.67$  eV.

is usually done in nuclear scattering where a small number of particles are involved in the scattering process. Furthermore, since we consider cases in which each lead is asymptotically a perfect wire which is translationally invariant along the  $z$  direction, our ground state calculation produces truly precise  $V_{\text{eff}}$  when the length of the leads  $L$  is very large. Once satisfied, the eigenstates obtained from the ground state density functional calculation can thus be brought into the form of scattering states of the wire.<sup>12</sup>

Figure 2 shows the effective potential  $V_{\text{eff}}$  for a wire with four Al atoms. A jellium lead has a cross section area of  $4.65 \times 4.65 \text{ \AA}^2$ , length  $L = 12.47 \text{ \AA}$ , and its electron density is specified by the Al bulk value of  $r_s = 1.095 \text{ \AA}$  resulting in a total of 90 electrons in the jellium leads. The whole system (see Fig. 1) is put into a supercell of size  $8.82 \times 8.82 \times 36.27 \text{ \AA}^3$ , which we checked to be large enough, for the standard plane wave based *ab initio* calculations.<sup>13</sup> We have used an upper energy cutoff of 8 Rydbergs. Without the Al atoms, the two jellium leads are separated by a potential barrier provided by the vacuum in between. The potential  $V_{\text{eff}}$  in the 3D leads is affected by the atoms near the lead-atom junctions, but this effect is essentially damped out away from the junctions. This is clearly seen in Fig. 2, indicating that the length  $L$  of the leads is long enough to give a good approximation of the infinite length limit. In our self-consistent calculations of  $V_{\text{eff}}$ , the numerical convergence is guaranteed within a few  $\mu\text{eV}$ . In the leads,  $V_{\text{eff}}$  is essentially a well with a depth  $\sim -10.61$  eV below the Fermi level in the cross section plane ( $x, y$  plane) for the four atom wire. Similar values are obtained for other wires. In the atomic chain of the wire,  $V_{\text{eff}}$  has rather high peaks due to the ionic core of the atoms. Surrounding the peaks there is the usual attractive part of atomic potential. The bonding between the Al atoms, and between the Al atom and the jellium are clearly obtained. In the lateral direction, far away from the atomic chain, higher potential is seen which reflects the vacuum. For another number of Al atoms,  $V_{\text{eff}}$  is obtained analogously and exhibits similar features.

The tunneling probability between the two jellium leads without the atomic chain is very small, in the range of  $10^{-4}$  at the Fermi energy when the gap is  $5.33 \text{ \AA}$ . Introducing Al atoms between the leads “bridges” the vacuum gap and dramatically increases the conduction. For the system we have examined, there are six propagating modes in the leads below the Fermi energy. However due to the strong repulsive potential core in the atomic chain, only three propagating modes are available in this section. In this sense, the atomic

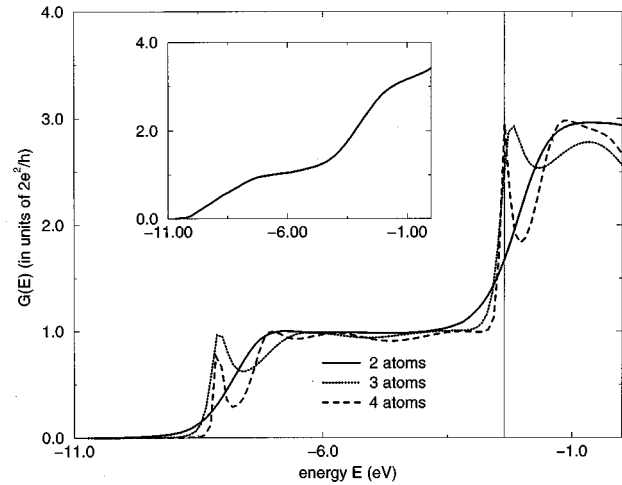


FIG. 3. Conductance  $G(E)$  as a function of incoming electron energy  $E$  for a wire with two Al atoms at the atomic chain (solid line); with three atoms (dotted line); with four atoms (dashed line). The vertical line indicates the position of the calculated Fermi level,  $E_f$ . Quantization of  $G(E)$  is obtained. Inset:  $G(E)$  for a wire with one Al atom in the atomic part.

chain provides a constriction to the jellium leads. The inset of Fig. 3 shows conductance  $G(E)$  as a function of the incoming electron energy  $E$  for the case of only one Al atom. The curve does not show good quantization and is essentially a monotonic increasing function of  $E$ . Thus with only one atom, the atomic part does not form a quantum “wire.” This could be because the length of the one atom region is too short such that a strong quasi-1D behavior has not formed. Quite different results are obtained where more than one Al atom is present. The curves in Fig. 3 shows  $G(E)$  for two, three, and four Al atoms in the atomic chain of the wire. In these cases, a clear conductance quantization is obtained. For all cases, the quantization is not perfect, since the junction between the jellium and the atomic chain provides some scattering to the incoming electron wave, as a result the reflection coefficient is nonzero. The scattering also leads to some resonance features near the onset of a plateau which is a familiar situation for mesoscopic quantum conductors where detailed discussions are available.<sup>19</sup> However, the main feature, namely the existence of conductance “plateau,” indicates that a quantum wire is formed.<sup>20</sup> We emphasize that the main features of the quantum transport are indeed due to the properties of the atomic chain, and the jellium leads only play a secondary role. Otherwise many more conductance plateaus would result since there are more transport channels in the ideal leads than there are in the atomic chain.

The values of resistance for these atomic wires can be obtained by inverting the conductance. At the Fermi level, we found  $R_1 \approx 4.7$ ;  $R_2 \approx 7.9$ ;  $R_3 \approx 5.1$ ; and  $R_4 \approx 5.3 \text{ K } \Omega$  where the subscript indicates the number of Al atoms in the atomic chain. For the wires studied here,  $E_f$  is found to locate at the transition region from the first plateau to the second. There, the two-atom wire has smaller  $G(E_f)$  leading to a larger resistance. While numerically of the same order, there are some differences between these values and those of Ref. 7 where chains with one to three Al atoms are studied. However we do not expect a direct agreement since we have studied long wires (jellium plus atoms) in 3D while Ref. 7

examined atomic chains in between planar jellium electrodes.

In summary, we have investigated the quantum transport properties of long atomic wires consisting of 3D incoming and outgoing jellium leads and an atomic chain with several Al atoms. Our theory is based on a self-consistent *ab initio* total energy calculation of the effective ground state potential of the wire, and a solution of a full quantum scattering problem. Our results show that the atomic chain of the wire breaks the vacuum barrier when there are no atoms between the leads, and this gives a dramatic increase of the conductance. Quantized conductance is observed when there are more than one atom in the atomic chain. Hence we may conclude that a “quantum wire” can actually be formed with two or more atoms connecting 3D leads.

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- <sup>20</sup>Notice that the plateau at  $2 \times 2e^2/h$  is missing, which is a result from 3D wires. For a perfect 3D wire with a square cross section, the transverse quantization gives conductance steps of 1,3,4,6,... in units of  $2e^2/h$ .