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# Resistance of a one-atom contact in the scanning tunneling microscope

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The resistance as a function of tip-sample separation in the scanning tunneling microscope is calculated for distances in the transition region between tunneling and point contact. A resistance plateau appears near point contact with value $A\pi\hbar/e^2$, where $A$ is of order unity, its exact value depending on the identity of the tip atom. Good agreement is found with the recent experimental data of Gimzewski and Möller.

We consider here the region of transition from the tunneling to the point-contact regimes in the scanning tunneling microscope,[1] where the initial contact takes place between a single tip atom and the sample surface.[2] We study the current that flows between two planar parallel metallic electrodes, one of which has an adsorbed atom (this electrode represents the tip), as a function of the distance between the electrodes, for the case of a small applied bias voltage. In this initial calculation, the atom will not be allowed to move relative to its electrode as the tip-sample separation is decreased, but will be kept at its large-separation equilibrium distance.

As we have done in our earlier studies of the scanning tunneling microscope,[3] we will use the jellium model to represent the metallic electrodes themselves. In contrast with these earlier studies, however, we can no longer use a tunneling-Hamiltonian formalism[4] to compute the current in terms of the wave functions determined separately for each electrode in the absence of the other, because this is only appropriate when the overlap of the wave functions of the two electrodes is small, that is, when the separation between the electrodes is large.

We proceed instead as follows. First, within the framework of the density functional formalism, we find the single-particle wave functions (we need only the standing-wave solutions at this point) and self-consistent density distribution for the pair of bare metallic electrodes, assuming them for simplicity to be identical ($r_s=2$ jellium model). This is the previously solved problem of the bimetallic junction.[5] Since our two bare electrodes are identical and since we are interested only in the zero-bias limit, however, we need not use the more general procedure of the authors of Ref. 5; the symmetry allows us instead to use the method of Lang and Kohn[6] that was employed earlier for the single bare surface.

We next use the procedure of Lang and Williams[7] to find the self-consistent density distribution and single-particle wave functions (again just standing-wave solutions) for the total system consisting of the two bare electrodes plus the atom. It will be recalled that this method was originally used to study an atom adsorbed on a single bare metallic surface, and proceeded by solving a Lippmann-Schwinger equation that involved a Green's function for the bare metal. The only significant difference in the present case is that the Green's function is the one appropriate to the bimetallic junction, instead of the single surface. This procedure provides us with the potential in which the electrons in our system will move in the zero-bias limit.

We now consider current-carrying states of the bimetallic junction without the atom. Deep in the left electrode (to make a particular choice) each such state consists of a plane wave moving to the right plus a reflected wave; deep in the right electrode it consists of a transmitted plane wave moving to the right. We consider all such waves whose energy is equal to the Fermi energy, but whose other quantum labels are different (the azimuthal quantum number $m$ and parallel-momentum label $\kappa$ defined in Ref. 7). We weight all of these states (continuum normalized as in Ref. 7) equally, and choose an overall normalization factor such that all of the plane waves moving to the right deep in the left electrode, taken together, yield a unit current density (atomic units).

We now solve the Lippmann-Schwinger equation again, using the procedure of Lang and Williams,[7] but this time to obtain the current-carrying states at the Fermi level in the presence of the atom, starting with the current-carrying states of the bimetallic junction without the atom. The potential that goes into this equation is the difference between the self-consistently determined potentials in the bimetallic junction with and without the atom.[8]

For small bias $V$ and zero temperature, the current density is given by[3] (using atomic units, with $|e|=\hbar=m=1$)

$$\mathbf{j}(\mathbf{r})=2V\int d\mu\,\delta(E_\mu-E_F)\mathrm{Im}\Psi_\mu^*(\mathbf{r})\nabla\Psi_\mu(\mathbf{r})\ ,$$

where $\Psi_\mu$ is a current-carrying state with quantum label $\mu$, which in our case represents energy $E$, azimuthal quantum number $m$, and parallel momentum label $\kappa$, and $\int d\mu$ is an integration over energy and a sum or integration over the other state labels as well. The factor 2 is for spins, which we do not include in our label $\mu$. We will be interested in the additional current density due to the presence of the atom, $\delta\mathbf{j}(\mathbf{r})=\mathbf{j}(\mathbf{r})-\mathbf{j}_0$, where $j_0$ is the current density for the bimetallic junction in the absence of the atom, and in the total additional current $\delta I$, which can be obtained by integration of $\delta\mathbf{j}$ over an appropriate surface. We can define the additional conductance[9] due to the presence of the atom as $\delta G=\delta I/V$, and it will be convenient to define an associated resistance $R\equiv 1/\delta G$.

 

We consider here the simple case of a Na tip atom. The current density $\delta\mathbf{j}$ for this case is shown in Fig. 1, in the instance in which the tip-sample separation $s$, measured from the nucleus of the tip atom to the positive-background edge of the sample, is 5 bohrs (the distance $d$ between the center of the Na atom and the positive-background edge of the tip electrode is fixed at 3 bohrs, the equilibrium value for $s \rightarrow \infty$). The left edge of the box corresponds to the positive-background edge of the tip electrode, and the vertical line within the box corresponds to the background edge of the sample (the right-hand electrode). The presence of the Na atom is indicated schematically by two dashed circles with a cross at the position of the nucleus. For computational convenience, we only show results away from the immediate vicinity of the atom. At each point of a grid, the additional current density $\delta\mathbf{j}$ is represented by an arrow, with the length (and thickness as well) of the arrow made proportional to the magnitude of $\delta\mathbf{j}$. Note in particular the way in which the current spreads out in the sample, becoming less sharply peaked in planes parallel to the sample surface that are further from the tip.

In Fig. 2, the resistance $R$ defined above is shown as a function of tip-sample separation $s$. At large separations, $R$ changes exponentially with $s$. As $s$ is decreased toward $d$, the resistance levels out at a value of 32000 Ω. (For $s = d$, the atom is midway between the two metal surfaces, so this can in some sense be taken to define contact between the tip atom and the sample surface.) If the same calculation is done for a Ca atom, $R$ is found to level out at 18000 Ω. We can understand this leveling out, including the order of magnitude of the resistance, from discussions of Imry[10] and Landauer.[11] These authors point out

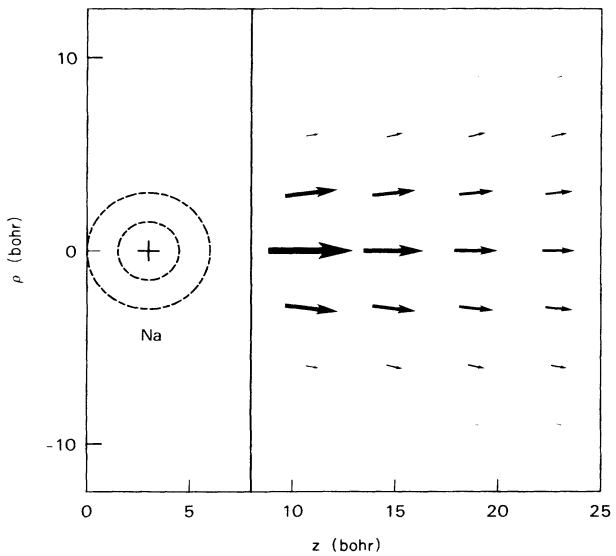


FIG. 1. Current density $\delta\mathbf{j}$ for the case of Na tip atom with tip-sample separation $s = 5$ bohrs. The length (and thickness) of each arrow is proportional to magnitude of $\delta\mathbf{j}$ evaluated at the spatial position corresponding to the center of the arrow. Coordinates $\rho$ and $z$ are parallel and perpendicular to surfaces, respectively.

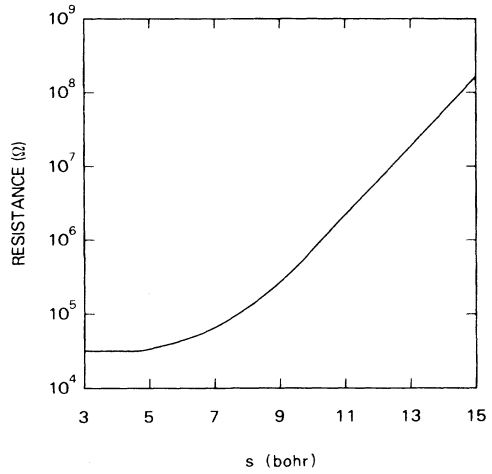


FIG. 2. Resistance $R \equiv 1/\delta G$ as a function of tip-sample separation $s$ for a Na tip atom.

that there will be a "constriction" resistance $\pi\hbar/e^2 = 12900$ Ω associated with an ideal conduction channel, sufficiently narrow to be regarded as one dimensional, which connects two large reservoirs. Our atom, in the instance in which it is midway between the two electrodes, contacting both, forms a rough approximation to this.[12]

Now Kalmeyer and Laughlin[13] have studied the differential conductance for a 3D square well within a square barrier with 1D symmetry.[14] At the energy corresponding to the peak of a resonance of the well, they show numerically, for barriers that are fairly thick on the scale of interest here, and with the assumption that the extent of the well is small, that the differential conductance is almost exactly equal to $e^2/(\pi\hbar)$ for two spin directions when the well is at the center of the barrier (they actually consider spinless electrons, and we have just doubled their result). The well resonance thus acts like the spatially narrow conduction channel envisioned in Refs. 10 and 11. In the present study, however, we are considering atomic potentials that are of similar spatial extent to the barrier created by the bimetallic junction, and so the conditions assumed in their study do not hold here.[15] If we write our limiting resistance values as $R_{\rm lim} = A\pi\hbar/e^2$, then it is presumably for this reason that the $A$ values found in the present study (e.g., 2.5 for Na) are higher than unity.[16,17]

We now discuss the relation of this calculation to the experiment of Gimzewski and Möller[2] using a Ag sample surface and an Ir tip (though the identity of the tip atom itself was not determined). These authors fix the voltage on the tip (at 20 mV) and start with the tip at a distance from the surface at which the current has some particular value (1 nA). (Thus the starting resistance is 20 MΩ.) They then measure the current as a function of the distance $\Delta z$ that the tip is moved *toward* the surface, starting at this initial separation (which defines $\Delta z = 0$). A plot of their experimental data is given in Fig. 3. For small $\Delta z$ (large separations from the surface) the conductance varies exponentially with distance. At larger $\Delta z$ (smaller separations) the curve starts to bend over, and reaches a

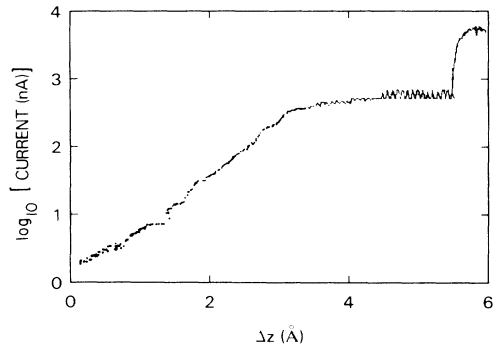


FIG. 3. Tunneling current ($\log_{10}I$) vs distance $\Delta z$ *toward* surface measured from the point at which the resistance is 20 MΩ, for a clean Ir tip and polycrystalline Ag surface at constant bias voltage of magnitude 20 mV. The results were obtained by Gimzewski and Möller as discussed in the experiment in Ref. 2, but these data are selected to show the resistance plateau more clearly. A high-gain electrometer was used to measure the lower currents corresponding to $\Delta z < 3.5$ Å, while a low-gain electrometer was used for the currents found at larger $\Delta z$. The high-gain data was digitized from a graph and replotted in producing this figure. There was an offset between the two electrometers so that the high-gain data should be shifted vertically to produce more closely a (0,0) curve intercept (i.e., $I \sim 1$ nA at $\Delta z = 0$).

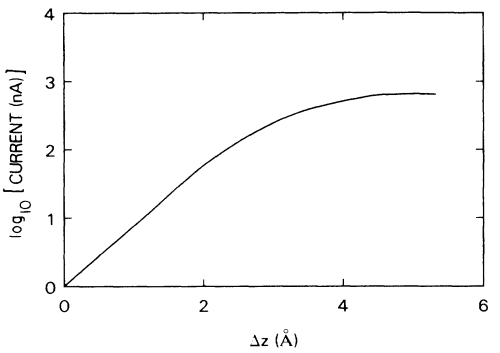


FIG. 4. Tunneling current ($\log_{10}\delta I$) vs distance $\Delta z$ *toward* surface measured from the point at which the resistance is 20 MΩ, calculated for a Na tip atom as described in the text (assuming a bias voltage of magnitude 20 mV).

plateau, with the resistance at the plateau ~35000 Ω (corresponding to $A \sim 2.7$).

At $\Delta z \sim 5.5$ Å there is a jump in the current. For $\Delta z$ smaller than this, the current versus distance characteristics were found to be reversible, while for $\Delta z$ larger a significant hysteresis was observed. These results suggest that the current jump is associated with significant atom motion and adhesion between the tip atom and the sample. Since we are not allowing atom motion in our calculation, we will be interested here only in the region before the current jump.

We now replot the calculated curve of Fig. 2 so that it is on the same type of scale as Fig. 3. That is, we find the separation $s_0$ at which $R = 20$ MΩ and write $\Delta z \equiv s_0 - s$; we then plot a current equal to $V/R(s)$, with $V = 20$ mV, versus $\Delta z$, in Fig. 4. The separation in our model at which the atom is midway between the two electrodes corresponds to $\Delta z = 5.3$ Å. This would clearly define a region of significant atom motion in the model, in that if the tip electrode were retracted, the adatom would be equally likely to stay on the sample surface as on the tip surface. (There should be significant bistability a little before this.) This value of $\Delta z$ corresponds fairly well to that at which the current jump occurs in the experiment. The value of the current at the plateau and the general shape of the curve agree rather well with the experimental data in Fig. 3. This suggests that the model we have presented gives an essentially correct picture of the transition from the tunneling to the point-contact regimes in the scanning tunneling microscope.

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[1]For reviews of scanning tunneling microscopy, see G. Binnig and H. Rohrer, IBM J. Res. Dev. **30**, 355 (1986); P. K. Hansma and J. Tersoff, J. Appl. Phys. **61**, R1 (1987).

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[4]J. Bardeen, Phys. Rev. Lett. **6**, 57 (1961).

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[8]All image effects are omitted.

[9]If we were to have a four-probe measurement, with the electrochemical potential drop measured only across a quantum-mechanically coherent scattering element between two reservoirs, then we would have to use the Landauer conductance formula—see M. Büttiker, Y. Imry, R. Landauer, and S. Pinhas, Phys. Rev. B **31**, 6207 (1985); M. Büttiker, Phys. Rev. Lett. **57**, 1761 (1986).

[10]Y. Imry, in *Directions in Condensed Matter Physics: Memorial Volume in Honor of Shang-keng Ma,* edited by G. Grinstein and G. Mazenko (World Scientific, Singapore, 1986), pp. 101–163.

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[12]Discussions of this constriction (or spreading) resistance from a different point of view are summarized in an article on point-contact spectroscopy in metals by A. G. M. Jansen, A. P. van Gelder, and P. Wyder [J. Phys. C **13**, 6073 (1980)]. If the size of the constriction is large compared with the mean free path of the electrons, then it is known as the Maxwell resistance; in the opposite limit, which is the one of interest to us here, it is known as the Sharvin resistance.

[13]V. Kalmeyer and R. B. Laughlin, Phys. Rev. B **35**, 9805 (1987).

[14]Cf. also B. Ricco and M. Ya. Azbel, Phys. Rev. B **29**, 1970

(1984) (1D case); J. Halbritter, Surf. Sci. **122**, 80 (1982); H. Knauer, J. Richter, and P. Seidel, Phys. Status Solidi (a) **44**, 303 (1977).

[15]In fact, for the Na case actually studied, for $s=d$ (atom midway between the electrodes), the self-consistent potential *along the z direction* does not even present a tunneling barrier to electrons at the Fermi level. Also, if we remove the atom in this instance ($s=d$), the conductance over an effective area of one atom for just the pair of flat electrodes is $\sim 20\%$ of the additional conductance $\delta G$ due to the presence of the atom, while the analysis of Ref. 13 is appropriate to the case in which this residual conductance is negligible.

[16]To make a comparison with the study of Ref. 13, the present calculation was redone with a 3D exponential potential well, instead of the self-consistent atom potential, embedded in the bimetallic junction barrier, with parameters chosen to put a resonance peak associated with the well at the Fermi level. It was found that the $A$ value as defined in the text was very close to unity when the barrier was made thick enough by moving the two electrodes apart (always keeping the atom midway between the electrodes and the resonance peak at the Fermi level), but that $A$ increased to values similar to those actually computed in the present study when this barrier thickness was decreased so that it was comparable to the well diameter.

[17]It might be thought that another reason that the $A$ value found for our atoms is higher than unity is that the peaks in the density of states resonances might not be at the Fermi level, in view of the fact that Kalmeyer and Laughlin (Ref. 13) have shown the differential *conductance* to be a Lorentzian centered at the energy of the state-density peak. The $m=0$ state-density peak for Na, however, is very close to the Fermi level when $s=d$.