ELSEVIER

Ultramicroscopy 73 (1998) 199–203

ultramicroscopy

Differential conductance in atomic-scale metallic contacts

A. García-Martín, T. López-Ciudad, J.A. Torres, A.J. Caamaño, J.I. Pascual, J.J. Sáenz*

Departamento de Física de la Materia Condensada, Universidad Autónoma de Madrid, E-28049 Madrid, Spain

Received 7 July 1997; received in revised form 10 November 1997

Abstract

We present exact free-electron calculations of the differential conductance of narrow necks connecting two three-dimensional electron gases. As the voltage increases, the initial quantized values of the conductance evolve into higher or lower noninteger multiples of $2e^2/h$. The contribution of electron tunneling through a region around the constriction is analyzed in terms of a simple model. We show that tunneling can change significatively the shape of the conductance–voltage characteristics. © 1998 Elsevier Science B.V. All rights reserved.

PACS: 61.16.Ch; 62.20.Fe; 73.40.Cg

1. Introduction

In the last few years, the physics of atomic-scale metallic contacts have been extensively investigated both from the experimental [1–6] and theoretical point of view [6–10]. However, the interpretation of the experimental results is still controversial [6]. Most of this work has been focused on the conductance at zero voltage. Very recently, it has been shown that differential conductance at high voltage should show a very interesting nonlinear behavior [11] similar to that observed for point contacts in two-dimensional electron gases (2DEG). In the 2DEG case the smearing of the quantized conductance plateaus from integer multiple of $2e^2/h$ to half-integer values was predicted by Glazman and Khaetskii [12] and observed experimentally by Patel et al. [13]. In atomic-scale contacts the theory [11] predicts a more complicated pattern due to the degeneracy of the transversal modes in the contact.

Some efforts have been done to measure the differential conductance G in atomic-scale contacts [3–5], with results that coincide in a systematic increase of the differential conductance with the voltage. In these experiments the applied voltages do not exceed a few hundreds mV, which, for metals, is a small percent of the Fermi energy E_F. In this work, we will discuss the nonlinear G characteristics in this range of relatively low voltages. We will also analyze the contribution of the electron transmission through the tunneling region around the constriction. This contribution to the conductance was not taken into account in previous approaches [11]. As we will see, tunneling effects

* Corresponding author. E-mail: juanjo.saenz@uam.es.

0304-3991/98/$19.00
PII S0304-3991(97)00156-3

can change significantly the G–V characteristics, mainly in nonelongated contacts.

2. Hard-wall exact calculation

Following Pascual et al. [11] we will assume the simple wide–narrow–wide (W–N–W) geometry sketched in Fig. 1. The narrow constriction is characterized by its length L and its circular section A_N. The wide leads have a section A_W. We assume that the voltage drops $V/2$ between the reservoirs and the constriction, while the potential remains constant inside the constriction itself (see Fig. 1) [11,12,14–16].

Assuming that the conduction is still ballistic for finite V, the zero-temperature conductance can be obtained from [11,12,14,15,17]

$$G(E_F,V) = \frac{\partial I(E_F, V)}{\partial V} = \frac{2e^2}{h}\frac{\partial}{\partial(eV)}\int_{E_{min}}^{E_F} t(\varepsilon, V)\,d\varepsilon,$$

$$t(\varepsilon, V) = \sum_w T_w(\varepsilon, V), \tag{1}$$

where E_F is the electron Fermi energy and $T_w(\varepsilon, V)$ is the transmission probability of an incoming electron with total energy ε and transverse energy ε_w. The sum runs over all the incident propagating modes w and the lower limit E_{min} is given by $\max\{(E_F - eV), 0\}$.

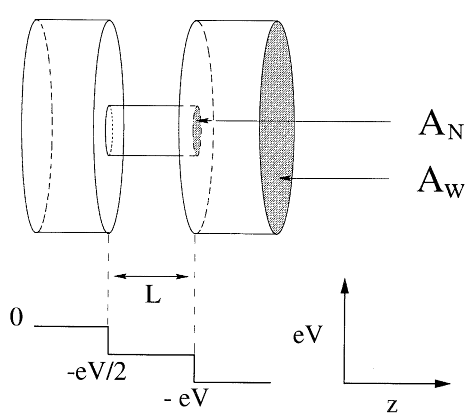

Fig. 1. Schematic representation of a W–N–W constriction in a three-dimensional electron gas. The potential energy profile along the contact is also sketched.

In the low voltage regime ($eV \ll E_F$) we can assume [15,18] that $t(\varepsilon, V)$ defined in Eq. (1) depends only on the energy difference between the incoming electrons and the bottom of the electrostatic confining potential, i.e. $t(\varepsilon, V) \approx t(\varepsilon + \frac{1}{2}eV)$. In this case, it is easy to show that

$$G(E_F, V) \approx \frac{1}{2}G\left(E_F + \frac{eV}{2}, 0\right) + \frac{1}{2}G\left(E_F - \frac{eV}{2}, 0\right) \tag{2}$$

$$\overset{V\to 0}{\approx} G(E_F) + \frac{1}{2}\frac{\partial^2 G(E)}{\partial(E)^2}\bigg|_{E=E_F}\left(\frac{eV}{2}\right)^2, \tag{3}$$

where $G(E) \equiv G(E, V=0)$. Notice that the absence of a linear term in the conductance is associated to our assumption of a symmetric potential drop.

The transmission probabilities $T_w(\varepsilon, 0)$ are calculated by solving the Schrödinger equation with hard-wall boundary conditions (i.e. the electron wave function is taken to be zero at the wall boundaries). This is done by a mode-matching technique together with a generalized scattering matrix approach [19]. In Fig. 2a we have plotted a typical staircase conductance–voltage (G–V) characteristics (Eq. (2)) for different sections A_N (Fig. 2b shows the same results projected on the G–V plane). The constriction length is $L \simeq 0.6\lambda_F$, which is a typical interatomic distance (for example, the atomic radius for Au is ≈ 1.7 Å while $E_F \approx 5.5$ eV and $\lambda_F \approx 5.2$ Å). Finite size effects induced by the wide leads manifest themselves as small kinks in the G–V curves. They appear as eV becomes of the order of the energy level spacing between transversal modes in the wide leads.

The analysis of the curvature $((\partial^2 G/\partial(E)^2)|_{E=E_F})$ of the G–V characteristics (see Eq. (3)) reveals a complicated oscillatory pattern (Fig. 2c) precursor of the smearing of the conductance plateaus observed at higher voltage [11]. The hard-wall condition inhibits the possibility of electron tunneling through the region around the constriction. Tunneling effects, however, could modify the predicted behavior.

3. Tunneling conductance

The exact quantum mechanical calculation for more realistic potentials is a difficult problem. Since

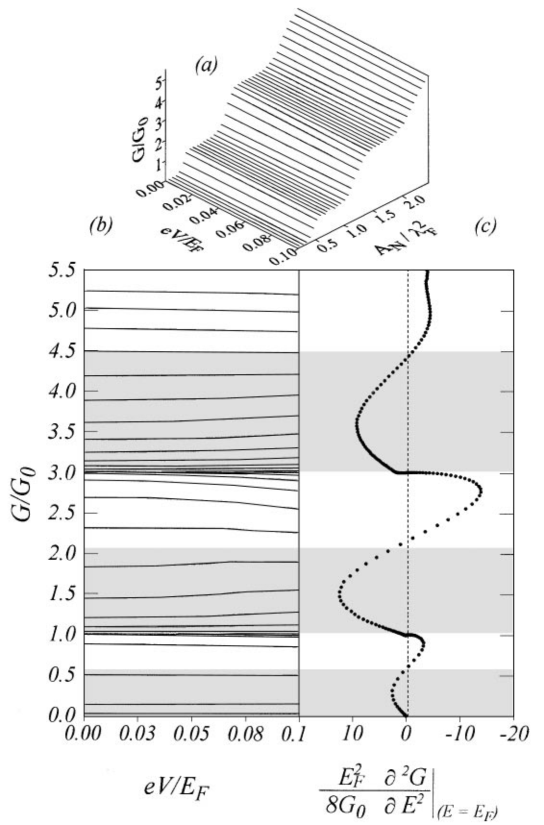

Fig. 2. (a) Differential conductance G/G_0 versus voltage for different contact cross sections A_N. (b) Same curves as in (a) projected over the G–V plane, showing their non-linear behavior. (c) Curvature of the G–V characteristics for different areas of the constriction A_N. The shadowed zones are those with positive curvature.

we are interested in a qualitative order-of-magnitude estimation of the tunneling effect, we will assume as a first approximation, that the current associated with the electron tunneling adds in parallel to that flowing through the constriction. The total conductance G_T will then be given by $G_T \approx G + G_{tun}$. The tunneling conductance G_{tun} can be estimated from a simple mean barrier approximation (MBA) [20,21]. At low voltages, we can approximate the exact transmission probabilities $T_w(\varepsilon, V)$ by those of a square barrier with an effective work function $\bar{\phi} - eV/2$, where $\bar{\phi}$ includes the image potential effects [20,21]: $T_w(\varepsilon, V) = T(\varepsilon - \varepsilon_w, V) \approx T(\varepsilon_z + eV/2)$, with

$$T(x) \approx \frac{16x(E_F + \bar{\phi} - x)}{(E_F + \bar{\phi})^2} \times \exp\left(-4\pi \frac{L}{\lambda_F}\sqrt{1 + \frac{\bar{\phi}}{E_F} - \frac{x}{E_F}}\right). \quad (4)$$

If the number of states in the wide leads is large enough, $t(\varepsilon, V) = \sum_w T_w(\varepsilon, V)$ can be written as an integral

$$t(\varepsilon, V) = \frac{\pi A_T}{(\lambda_F)^2}\int_{eV/2}^{\varepsilon + eV/2} \mathrm{d}x\, T(x) \approx \frac{\pi A_T}{(\lambda_F)^2}\int_{0}^{\varepsilon + eV/2} \mathrm{d}x\, T(x), \quad (5)$$

where $A_T = A_W - A_N$ is the total tunneling area.

Since, within this approach, $t(\varepsilon, V) \approx t(\varepsilon + eV/2)$, the tunneling contribution is also given by

$$G_{tun}(E_F, V) \overset{V \to 0}{\approx} G_{tun}(E_F) + \frac{1}{2}\frac{\partial^2 G_{tun}(E_F)}{\partial E_F^2}\left(\frac{eV}{2}\right)^2, \quad (6)$$

where, now, the two terms can be integrated exactly in terms of elementary functions. Assuming $(4\pi(L/\lambda_F)\sqrt{(\bar{\phi}/E_F)})^2 \gg 1$, we find

$$G_{tun}(E_F)/G_0 = \frac{\lambda_F}{2\pi L}\sqrt{\left(\frac{\bar{\phi}}{E_F}\right)}\left(\frac{\pi A_T}{\lambda_F^2}\right) \times 16\frac{\bar{\phi}}{E_F}\left(1 + \frac{\bar{\phi}}{E_F}\right)^{-2} \times \exp\left(-4\pi\frac{L}{\lambda_F}\sqrt{\frac{\bar{\phi}}{E_F}}\right), \quad (7)$$

which, except for the constant factor $(16\bar{\phi}E_F/(\bar{\phi} + E_F))$, is the same result obtained by Simmons within the current mean barrier approximation (CMBA) [20,21]. The quadratic term is simply given by

$$\frac{\partial^2 G_{tun}(E_F)}{\partial E_F^2} = G_{tun}(E_F) \times \left[\frac{E_F}{\bar{\phi}}\left(\frac{2\pi L}{\lambda_F}\right)^2\right]. \quad (8)$$

4. Results and discussion

The electron tunneling has two main effects on the conductance–voltage characteristics. First, it increases the conductance at zero voltage leading, in general, to nonquantized conductance values. On the other hand, the nonlinear oscillating behavior of the conductance can be strongly modified by the, always positive, quadratic term of the tunneling contribution. For a typical Au work function $\phi = 5.37$ eV and taking into account image potential effects as disscused by Simmons [20] and Miskovsky et al. [21], we find an effective barrier $\bar{\phi}$ as small as 1.1 eV, i.e. $\bar{\phi} \approx 0.2E_F$. In Fig. 3 we have plotted $G_{N\text{-}L} = (G_T(E_F, V) - G_T(E_F, 0))$ for three different sections of the narrow constriction A_N corresponding to the first conductance plateau in the hard-wall calculation. For tunneling areas of the order or larger than $A_T \approx 19\lambda_F^2$ the nonlinear conductance $G_{N\text{-}L}$ becomes positive. At the same time, the conductance at zero voltage changes from $\approx G_0$ to $\approx 1.5G_0$.

This effect of the tunnel on the G–V characteristics can be also seen in plots of the *normalized* differential conductance d(log I)/d(log V) versus eV for different values of A_N. This quantity is commonly used in scanning tunneling microscopy STM spectroscopy experiments. In Fig. 4 we have plotted these curves for the same parameters in Fig. 3, without tunneling (Fig. 4a), and with different tunneling areas, $A_T = 19\lambda_F^2$ (Fig. 4b) and $A_T = 66\lambda_F^2$ (Fig. 4c). In absence of tunneling (Fig. 4a) d(log I)/d(log V) oscillates around 1 due to the oscillations of $(\partial^2 G(E)/\partial(E)^2)|_{E=E_F}$ discussed above. However, as the tunnel area increases from $A_T = 0$ to $A_T = 66\lambda_F$, the quadratic (positive) contribution of the tunneling current increases and, for certain A_T, tunneling becomes the dominant contribution to the nonlinear conductance. We see how tunneling modifies these curves decreasing the range of the oscillations and leading to values that are *always* greater than unity.

From the results above, we can conclude that tunneling areas of the order of $\approx 8 \times 8$ atoms ($\approx 19\lambda_F^2$) are enough to remove the predicted decrease of the conductance for a single-atom point contact [11]. If a single-atom contact were made by an STM tip, this would imply radius of the order

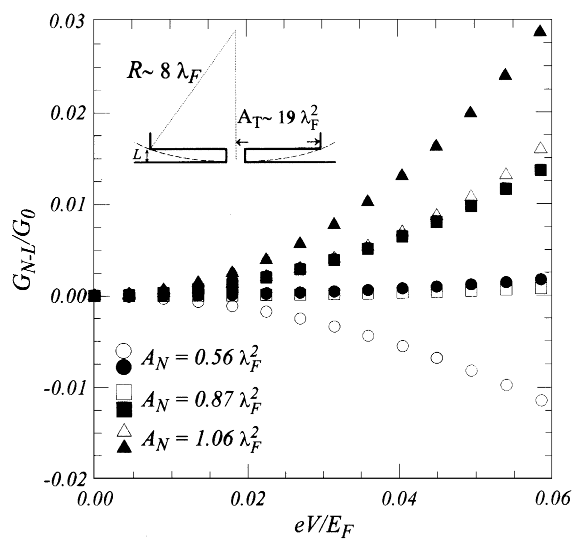

Fig. 3. Traces of the nonlinear term of the differential conductance with (filled symbols) and without (open symbols) tunneling. Inset: schematic view of the contact.

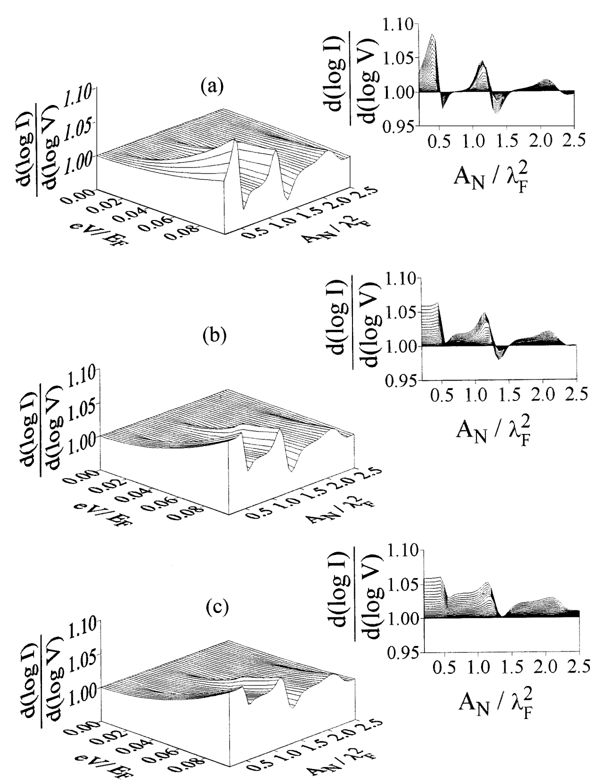

Fig. 4. Normalized differential conductance d(log I)/d(log V) versus the contact area A_N. The insets show the projection over the conductance–area plane (a) without tunneling, (b) $A_T = 19\lambda_F^2$, (c) $A_T = 66\lambda_F^2$.

of ≈ 40 Å (see inset in Fig. 3). The existence of larger tunneling areas could explain the systematic increase of the differential conductance observed in some experiments [4,5]. Only in the case of very sharp contacts a conductance decrease would be observable.

In conclusion, we have studied the behavior of the differential conductance and the normalized differential conductance of a ballistic constriction. We have shown that tunneling can change significantly the qualitative behavior of the G–V characteristics of atomic-scale metallic contacts. Tunneling effects must be taken into account in any systematic experimental and theoretical study of the conductance of atomic-scale contacts.

Acknowledgements

This work has been supported by the DGICyT through contract No. PB95-0061. A.G.-M. acknowledges partial financial support from the postgraduate grant program of the Universidad Autónoma de Madrid.

References

[1] C.J. Muller, J.M. van Ruitenbeek, L.J. de Jongh, Phys. Rev. Lett. 69 (1992) 140; N. Agraït, J.G. Rodrigo, S. Vieira, Phys. Rev. B 47 (1993) 12 345; J.I. Pascual, J. Méndez, J. Gómez-Herrero, A.M. Baró, N. García, Vu Thien Bhin, Phys. Rev. Lett. 71 (1993) 1852; L. Olesen, E. Lægsgaard, I. Stensgaard, F. Besenbacher, J. Schiøtz, P. Stoltze, K.W. Jacobsen, J.K. Nørskov, Phys. Rev. Lett. 72 (1994) 2251; J.L. Costa-Krämer, N. García, P. García-Mochales, P.A. Serena, Surf. Sci. Lett. 342 (1995) L1144; A. Stalder, U. Dürig, Appl. Phys. Lett. 68 (1996) 637; G. Rubio, N. Agraït, S. Vieira, Phys. Rev. Lett. 76 (1996) 2302.
[2] J.M. Krans, J.M. van Ruitenbeek, V.V. Fisun, I.K. Janson, L.J. de Jongh, Nature 375 (1995) 6534.
[3] V.V. Dremov, S.Yu. Shapoval, JETP Lett. 61 (1995) 336.
[4] J.I. Pascual, J. Méndez, J. Gómez-Herrero, A.M. Baró, N. García, U. Landman, W.D. Luedke, E.N. Bogachek, H.P. Cheng, Science 267 (1995) 1793.
[5] J.L. Costa-Krämer, N. García, P. García-Mochales, P.A. Serena, M.I. Marqués, A. Correia, Phys. Rev. B 55 (1997) 5416.
[6] P.A. Serena (Ed.), Proceedings of the NATO Advanced Research Workshop on Nanowires, Madrid, 1996, Kluwer, Dordrecht, in press; J.M. van Ruitenbeek, in: Mesoscopic Electron Transport, NATO-ASI Series, Kluwer Academic Publishers, Dordrecht, 1997.
[7] U. Landman, W.D. Luedke, N.A. Burham, R.J. Colton, Science 248 (1990) 454; Phys. Rev. Lett. 77 (1996) 1362; T.N. Todorov, A.P. Sutton, Phys. Rev. Lett. 70 (1993) 2138; Phys. Rev. B 54 (1996) R14 234; A.M. Bratkovsky, A.P. Sutton, T.N. Todorov, Phys. Rev. B 52 (1995) 5036; C. Sirvent, J.G. Rodrigo, S. Vieira, L. Jurczyszyn, N. Mingo, F. Flores, Phys. Rev. B 53 (1996) 16 086.
[8] J.A. Torres, J.I. Pascual, J.J. Sáenz, Phys. Rev. B 49 (1994) 16581; E.N. Bogachek, A.M. Zagoskin, I.O. Kulik, Sov. J. Low Temp. Phys. 16 (1990) 796.
[9] J.A. Torres, J.J. Sáenz, Phys. Rev. Lett. 77 (1996) 2245; Physica B 218 (1996) 234; A. García-Martín, J.A. Torres, J.J. Sáenz, Phys. Rev B 54 (1996) 13448.
[10] M. Brandbyge, J. Schiøtz, M.R. Sørensen, P. Stoltze, K.W. Jacobsen, J.K. Nørskov, L. Olesen, E. Lægsgaard, I. Stensgaard, F. Besenbacher, Phys. Rev. B 52 (1995) 8499; A.M. Bratkovsky, S.N. Rashkeev, Phys. Rev. B 53 (1996) 13074.
[11] J.I. Pascual, J.A. Torres, J.J. Sáenz, Phys. Rev. B 55 (1997) R16029.
[12] L.I. Glazman, A.V. Khaetskii, Europhys. Lett. 9 (1989) 263.
[13] N.K. Patel, L. Martín-Moreno, M. Pepper, R. Newbury, J.E.F. Frost, D.A. Ritchie, G.A.C. Jones, J.T.M.B. Janses, J. Singleton, J.A.A.J. Perboom, J. Phys: Condens. Matter 2 (1990) 7247; Phys. Rev. B 44 (1991) 13549.
[14] L. Martín-Moreno, J.T. Nicholls, N.K. Patel, M. Pepper, J. Phys.: Condens. Matter 4 (1992) 1323.
[15] Hongqui Xu, Phys. Rev. B 47 (1993) 15630.
[16] Recent self-consistent calculations for a one-dimensional chain connecting two three-dimensional electron reservoirs show that the potential drop is concentrated *inside* the reservoirs, provide there are no defects along the chain [P.L. Pernas, A. Martín-Rodero, F. Flores, Phys. Rev. B 41 (1990) 8553; P.L. Pernas, Ph.D. Thesis, Universidad Autónoma de Madrid, 1992].
[17] E. Castaño, G. Kirczenow, Phys. Rev. B 41 (1990) 3874.
[18] At higher voltages ($eV \leqslant E_F$) the exact calculation of Eq. (1) shows an overall decrease of the conductance which cannot be explained in terms of the simple approximation (see Ref. [11]). However, for the range of voltages discussed in this work, there are no significant differences between exact and approximate results.
[19] A. Weisshaar, J. Lary, S. M. Goodnick, V.K. Tripathi. J. Appl. Phys. 60 (1991) 335; J.A. Torres, J.J. Sáenz, in preparation.
[20] J.G. Simmons, J. Appl. Phys. 6 (1963) 1793.
[21] N.M. Miskovsky, P.H. Cutler, T.E. Feuchtwang, A.A. Lucas, Appl. Phys. A 27 (1982) 139.