A Simple Method to Find the Electron Conductance of a One-Atom Metallic Wire

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Abstract

We present a simple method to calculate the linear electron conductance of a one-atom metallic wire. As a matter of fact, the aforementioned conductance is determined by using the particle-in-a-box model and assuming the conduction electrons as non-interacting particles.

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1. Introduction

Quantum electrical conductors play a very important role in the context of nanoscience and nanotechnology. In particular, both metallic and semiconductor nanowires present a number of attractive features with significant potential applications [3,4]. But, unfortunately, there are still relevant open questions about the mechanisms underlying

the linear electrical conductance through nanowires. Indeed, appreciable research efforts on this subject are desirable from both the theoretical and experimental points of view. Key aspects relative to conductance quantization in nanowires should be fully investigated. Within this context, conductance quantization due to a single electron in a quasi-one-dimensional potential well presents notorious interest [1,2]. This fact will be exploited in the following to calculate the linear conductance of a one-atom metallic wire.

2. Theory

To a certain extent, we may assume a metallic one-atom wire as an ideal quasi-one-dimensional potential well (see refs.[1,2]). Consider a single electron inside this well. Under these conditions and in a first approximation, we can write:

$$\frac{\pi^2 \hbar^2 n^2}{2ml^2} = \frac{1}{2}mv_n^2 \quad (1)$$

where the left-hand side of (1) is the quantized electron energy and the right-hand side is the kinetic energy of the electron; m is the free-electron mass, l is the length of the potential well, and v_n is the magnitude of the quantized electron velocity. Eq.(1) is acceptable only for relatively high values of the quantum number n so that from eq.(1) it follows for $n \gg 1$:

$$v_n = \frac{\pi \hbar n}{ml} \quad (2)$$

As expected, eq.(2) is consistent with the fact that the magnitude of the corresponding quantized Fermi velocity reads (see, for example, ref.[2]):

$$v_{Fn} = \frac{\pi \hbar (2n+1)}{2ml} \quad (3)$$

for $n = 1, 2, \dots$. In effect, considering $n \gg 1$ in formula (3), then we have that $2n+1 \approx 2n$ so $v_{Fn} \approx v_n$ if $n \gg 1$.

Now one has that the (average) quantized time of motion of the electron is $\tau_n = l/v_n$. On the other hand, the averaged quantized electron conductivity is:

$$\sigma_n = \frac{e^2 N \tau_n}{m} \quad (4)$$

where e is the absolute value of the electron charge and $N = 1/(lA)$ is the average electron spatial density, A being the cross-sectional area of the wire. We have that $\sqrt{A} \ll l$ (quasi-one-dimensionality of the wire).

Since the quantized conductance is given by $G_n = \sigma_n A/l$, inserting relation (4) into this last formula with the expressions for N and τ_n as well as relation (2), then one gets that $G_n = G_0/n$ ($n \gg 1$) where $G_0 = 2e^2/h$ ($h = 2\pi\hbar$) is the fundamental conductance quantum. On the other hand, as a reasonable approach, we may assume the conduction electrons in the nanowire as non-interacting particles. Under this assumption, we have that the total conductance equals G_n multiplied by the number of electrons contained in a single atom, that is, $2n^2$. Therefore, we conclude that the total conductance (at zero bias) of the wire reads $\tilde{G}_n = 2G_0 n$ ($n \gg 1$). This relationship agrees with ref.[2] and is consistent with that conductance quantization in a metallic nanowire takes place if the diameter of the wire is on the same order of magnitude of the de Broglie wavelength of the conduction electrons, whose associated waves propagate in the transverse direction of the wire so that they constitute a well-defined quantum mode consisting of standing waves. Given that the contributions to the total conductance of all the modes are the same, then the total conductance is directly proportional to the number of modes so it is quantized. This was confirmed experimentally in ref.[3] for positive electrochemical potentials.

3. Conclusion

The preceding formulation shows that, in certain cases, relatively simple theoretical-analytical techniques are suitable to solve crucial problems. In particular, the particle-in-a-box model will be always fruitful for addressing a number of questions on nanophysics. By contrast, non-transparent computer simulations should be rejected.

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