Comment on "First-principles treatments of electron transport properties for nanoscale junctions"

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(Received 16 May 2003; published 9 October 2003)

The use of a jellium model for the electrodes gives a good account of the conductance of a gold nanowire linking two metallic electrodes. The statement to the contrary in the recent paper of Fujimoto and Hirose [Phys. Rev. B **67**, 195315 (2003)] is based on an incorrect positioning of the edge of the jellium relative to the outermost lattice plane of the electrode it represents.

DOI: 10.1103/PhysRevB.68.157301 PACS number(s): 73.63.Nm, 68.37.Ef, 73.40.Jn

The recent paper by Fujimoto and Hirose[1] makes an unfortunate error in discussing the use of the jellium model for the electrodes, which has the effect of making it appear that this model is not adequate to treat the problem of the conductance of gold nanowires. In fact it is entirely adequate, and gives results quite similar to those found in the authors' more elaborate treatment.

The main point is that the quantity D discussed in Sec. III of Ref. 1, which represents the distance between the jellium surface (positive-background edge) and the plane of gold atoms (called the "square basis of the nanowires" in Ref. 1) contacting the nanowire is *not*, as Fujimoto and Hirose suggest, arbitrary or unknown, but by construction of the jellium model, has a *perfectly definite value*. In their case, this value is $(1/4)a_0 = 1.93$ a.u. (a_0 is the gold lattice constant). If the correct value of $D = 1.93$ a.u. is used in Fig. 6 of Ref. 1, which gives conductance vs D, then a conductance value of $\approx 0.98 G_0$ is found, which is to be compared with what the authors call the "true" value of $\approx 1 G_0$. This shows also that the effect on transport of the interface between the jellium and the gold layer that seems to concern the authors is unimportant.

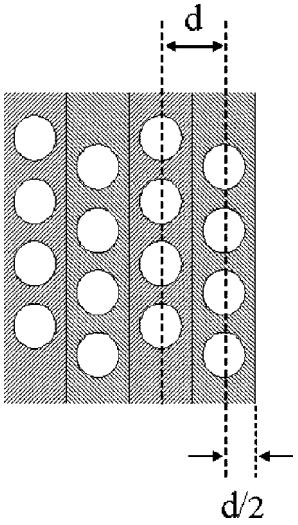

FIG. 1. Schematic of the construction of the jellium model out of an ionic lattice. The electrode is built up symmetrically slab by slab so that the positive-background edge of the jellium is half an interplanar spacing d in front of the outermost lattice plane. Circles represent the ions and the jellium edge is on the right.

The essence of the construction of the jellium model is that *each* lattice plane of the ions of the metal electrode is smeared out *symmetrically* into a uniform slab of positive charge (see Fig. 1). Thus the plane of ions is at the center of the slab which replaces it, and the edge of the positive background is half an interplanar spacing *in front* of the outermost lattice plane (see Fig. 1).

In thinking about this construction, it is useful to consider the difference $\delta V(\mathbf{r})$ between the potential due to the ionic lattice and that due to the semi-infinite positive background which represents it. This $\delta V(\mathbf{r})$, which can be used to perturbatively reintroduce the discrete lattice as done, e.g., in Ref. 2, can only be viewed as a small perturbation if the sheet of ions is at the slab center, since otherwise $\delta V(\mathbf{r})$ will not vanish at $\pm\infty$ (see footnote 25 of Ref. 3). These issues are also discussed in Ref. 4.

Since for Au(100), discussed in Ref. 1, the interplanar spacing is $(1/2)a_0$, the distance between the jellium surface and a gold layer put down on it will be half of this, i.e., $(1/4)a_0$. This spacing, as noted before, gives the correct conductance. Similar conclusions can be drawn for other systems as well. For instance, it was shown in Ref. 5 that the conductance of an organic molecule between two jellium electrodes is quite similar whether the molecule makes contact directly with the jellium surface or with a plane of gold atoms adjacent to the jellium surface.

One of us (M.D.) acknowledges support from the NSF Grant Nos. DMR-01-02277 and DMR-01-33075, and Carilion Biomedical Institute.

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