Comment on "Dynamical Corrections to the DFT-LDA Electron Conductance in Nanoscale Systems"

In a recent Letter, Sai *et al.* [1] identified a correction R^{dyn} to the dc conductance of nanoscale junctions arising from dynamical exchange-correlation (XC) effects within time-dependent density functional theory. This quantity contributes to the total resistance through $R = R_s + R^{\mathrm{dyn}}$, where R_s is the resistance evaluated in the absence of dynamical XC effects. In this Comment, we show that the numerical estimation of R^{dyn} in example systems of the type they considered should be considerably reduced, once a more appropriate form for the shear electron viscosity η is used.

Sai *et al.*'s expression for R^{dyn}, based on electron-liquid theory [2], is a one-dimensional integral between the two electrodes

$$R^{\mathrm{dyn}} = \frac{4}{3e^2 A_c} \int_a^b \eta \frac{(\partial_z n)^2}{n^4} dz, \tag{1}$$

where A_c is the cross-sectional area, η is the shear viscosity of the electron liquid, and n is the electron density. The example system we have considered is the metal-vacuum-metal (MVM) junction that can be formed by two jellium surfaces separated by a distance d [3]. Since this system is translationally invariant parallel to the surface, the electron density $n(z)$ is defined unambiguously. We have chosen $r_S = 3$ for the jellium electrodes, to allow comparison with the gold-electrode systems presented in Ref. [1]. The density is calculated within the local-density approximation.

Sai *et al.* used a *constant* shear viscosity $\eta_c = \hbar(k_F/\pi a_0)^{3/2}/120$ corresponding to Eq. (4.7) of Ref. [2], appropriate only in the high-density weakly inhomogeneous limit and based on the bulk electrode density. Here the quantities $k_F = (3\pi^2 n)^{1/3}$ and a_0 are the Fermi wave vector of the bulk electrodes and the Bohr radius, respectively. We make two changes to this. First, we use Eq. (4.10) of Ref. [2], $\eta_v \simeq n/(60r_S^{-3/2} + 80r_S^{-1} - 40r_S^{-2/3} + 62r_S^{-1/3})$, which is more appropriate for realistic densities ($r_s = 0 \ldots 20$ a.u.), [2] in recognition of the fact that $r_S = 3$ is not a high density. This alone reduces the dynamical resistance by a factor of 5.37 for a density corresponding to $r_S = 3$. Second, in Eq. (1) we evaluate this viscosity at the *local* density rather than taking the bulk viscosity to apply outside the bulk region. This further reduces the dynamical resistance by a d-dependent factor of 1.16–18.4 (see Table I), particularly for larger d when the dominant contribution to the integral in Eq. (1) comes from the low-density region in the vacuum (see Fig. 1). Thus, a more appropriate choice of the shear electron viscosity η reduces the dynamical resistance by a factor between 6 and 98, causing it to become very small compared with the single-particle resistance in all cases studied.

TABLE I. Noninteracting and dynamical resistances per unit area (a.u.) as a function of the separation d (a.u.). The interpolated local formulation of the viscosity η_v considerably reduces the dynamical resistance (R_v^{dyn}) relative to the high-density bulk formulation of Ref. [1] (R_c^{dyn}).

d	R_s	R_c^{dyn}	R_v^{dyn}
1	117	1.71	0.275
3	241	48.5	5.01
5	712	530	29.4
9	14 900	59 600	604

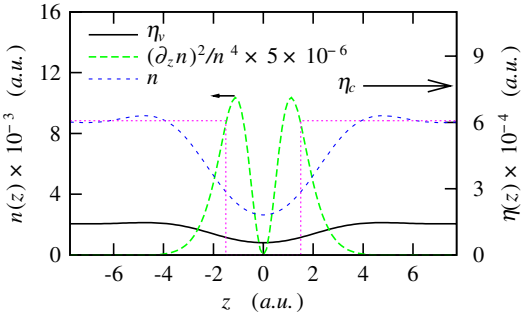

FIG. 1 (color online). MVM junction separated at $d = 3$ a.u. The electron charge density and the background positive charge density are represented by thin discontinuous lines. Important contributions to the integral of Eq. (1) (thick green dashed line) arise within the vacuum junction, where the electronic viscosity (solid line) is lower, tending to reduce the dynamical resistance. The value of viscosity used in Ref. [1] is indicated by η_c.

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