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Treatment of electron viscosity in quantum conductance
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 Treatment of electron viscosity in quantum conductance

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In a recent paper Sai et al. [1] identified a correction \( R_{\text{dyn}} \) 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 \( R = R_c + R_{\text{dyn}} \) where \( R_c \) is the resistance evaluated in the absence of dynamical XC effects. In this Comment we show that the numerical estimation of \( R_{\text{dyn}} \) in example systems of the type they considered should be considerably reduced, once a more appropriate form for the shear electron viscosity \( \eta \) is used.

Sai et al.’s expression for \( R_{\text{dyn}} \), based on electron-liquid theory [2], is a one-dimensional integral between the two electrodes

\[
R_{\text{dyn}} = \frac{4}{3 \varepsilon_0^2 A_e} \int_e^b \eta (\partial n)^2 n^4 dz \tag{1}
\]

where \( A_e \) is the cross-sectional area, \( \eta \) 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 LDA.

Sai et al. used a constant shear viscosity \( \eta_c = \hbar k_F / (\pi a_0)^{3/2} / 120 \) corresponding to formula (4.7) of Ref. 2, appropriate only in the high-density weakly inhomogeneous limit, and based on the bulk electrode density. Here the quantities \( k_F = (3\pi n)^{1/3} \) and \( a_0 \) are the Fermi wavevector of the bulk electrodes and the Bohr radius respectively. We make two changes to this. First, we use Formula (4.10) of Ref. 2, \( \eta_c \sim n/(60r_S^{-3/2} + 80r_S^{-1} - 40r_S^{-2} + 62r_S^{-1/3}) \), more appropriate for realistic densities \( r_S = 0...20 \) 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 \( \eta \) reduces the dynamical resistance by a factor between 6 and 98, causing it to become

\[
\begin{array}{cccc}
d & R_c & R_{\text{dyn}} & R_{\text{dyn}}^{\eta} \\
1 & 117 & 1.71 & 0.275 \\
3 & 241 & 48.5 & 5.01 \\
5 & 712 & 530 & 29.4 \\
9 & 14900 & 59600 & 604 \\
\end{array}
\]

**TABLE I**: Non-interacting and dynamical resistances per unit area (a.u.) as a function of the separation \( d \) (a.u.). The interpolated local formulation of the viscosity, \( \eta_c \), considerably reduces the dynamical resistance \( (R_{\text{dyn}}^{\eta}) \) relative to the high-density bulk formulation of Ref. 1 \( (R_{\text{dyn}}^{\eta_c}) \).

![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) (green thick 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 \( \eta_c \).

Very small compared with the single-particle resistance in all cases studied.

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