

They confirm the above finding, namely that the size-independence is indeed very weak. In addition, the conductance for $J = 4$ can be compared with that for the noninteracting level ($J = 0$) (thin dashed line in Fig. 2b); the substantial difference between them indicates a significant electron correlation effect on the electric transport. To exemplify, we note that this Coulomb interaction diminishes the half-width of the curve $G = G(\alpha)$ roughly by a factor two (from $\Gamma = 2$ to 0.8). At $\alpha = \varepsilon_F \pm \Gamma$ ($\Gamma = 2\beta^2/\xi = 2$), i. e. at the half maximum in the uncorrelated case, the electron correlations suppress the conductance by a factor ~ 5 . Importantly, for situations even farther away from resonance (and this is the usual case, including also that of the recent experiments of Ref. 41), Fig. 2b shows that the suppression factor becomes considerably larger.

On the basis of the results presented in this subsection, we claim that the correlated electron transport through a molecule attached to organic electrodes can be accurately obtained by carrying out microscopic calculations for small extended molecules; besides the (true) molecule of interest, they should only include a reduced number of electrode layers.

B. Case of metallic electrodes

In comparison with organic electrodes, metallic electrodes are characterized by a larger bandwidth (4ξ). To model (physisorbed) molecules weakly coupled to metallic electrodes within the framework of the present paper, one should consider values of ξ larger than in Sect. V A.

In Fig. 3, we present numerical results on resonance for two values of the molecule-electrode resonance integral, $\xi = 10$ ($\Gamma = 0.2$) and $\xi = 5$ ($\Gamma = 0.4$), and several sizes N of the extended molecule. The trend that, as the extended molecule becomes larger, the linear conductance approaches the unitary limit ($G \rightarrow G_0$) can be seen in both panels of Fig. 3. So, the basic physical argument behind the approximation of a sufficiently large extended molecule is also confirmed by these numerical results. However, unlike in Fig. 2a, the deviations of the numerical values of G from the exact value G_0 visible in Fig. 3a and b are significant and deserve further analysis.

Figs. 3a and b show that the departure from the unitary limit is larger for a stronger Coulomb contact strength J . This behavior can be easily understood. The stronger the electron-electron interaction, the more important is the renormalization of the contact self-