

results from the fact that (irrespective of the values of  $\xi$ ,  $\beta$ , and  $J$ ) for  $\mu_L = \alpha = \mu_R$  all sites are half occupied,  $n_j \equiv \langle 0|a_j^\dagger a_j|0\rangle = 1/2$ , and this yields, via Friedel's rule  $G = G_0 \sin^2(\pi n_0)$  [38], a perfect transmission ( $G = G_0$ ). Numerically, the result  $G = G_0$  on resonance was obtained by means of time-dependent density matrix renormalization group calculations [37].

Our results for the on-resonance case at  $\beta = \xi$  are presented in Fig. 2a. As visible there, even the smallest possible extended molecule ( $N = 4$ ) represents a “sufficiently large” extended molecule, enabling to accurately reproduce the exact result. Indeed, even for the strongest coupling shown in Fig. 2a ( $J = 10$ , which is in fact unrealistically strong), the numerical results deviate from the exact value  $G = G_0$  by  $\simeq 13\%$ . As expected from the physical analysis backing the approximation of a sufficiently large extended molecule, Fig. 2 reveals that the deviation from the exact result diminishes with increasing sizes; for the next smallest size ( $N = 6$ ), the error is at most 5%.

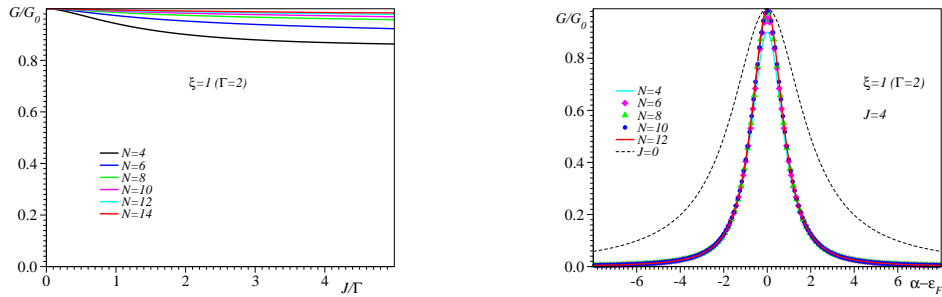


FIG. 2: Conductance  $G$  computed numerically from Eq. (24) for several sizes  $N$  in units of quantum conductance  $G_0 = e^2/h$  plotted versus: (a) Coulomb contact repulsion  $J$  at resonance ( $\alpha = \epsilon_F$ ), and (b) molecular level energy  $\alpha$  for  $\xi = 1$ ,  $J = 4$ . The sizes  $N$  of the extended molecules are given in the legend. The thin dashed line in panel (b) corresponds to a vanishing Coulomb interaction ( $J = 0$ ).

Because  $G = G_0$  holds on resonance even for the uncorrelated case ( $J = 0$ ), where the results are anyway independent on the size of the extended molecule (cf. Sect. I), one might suspect that the very weak size-independence displayed in Fig. 2a does not demonstrate the validity of the approximation of a sufficiently large extended molecule, but rather that the electron correlations themselves are weak. To illustrate that this is not the case, we present in Fig. 2b results for the conductance out of resonance ( $\alpha \neq \epsilon_F$ ) and realistic, moderately strong Coulomb strength  $J = 2\Gamma = 4$  (and equal to the electrode bandwidth  $4\xi = 4$ ).