



FIG. 5: Normalized conductance G/G_0 plotted versus J/Γ for $\xi = 10, 5, 3.33, 2$. All the curves were computed for the out-of-resonance situation $|\alpha - \varepsilon_F| = \Gamma/2$, which corresponds to $G/G_0 = 0.8$ at $J = 0$. Notice that, the smaller the ξ -value, the stronger the size-dependence of thin curves computed from Eq. (24), and the larger the departure from the practically N -independent renormalized curves, depicted by thin lines.

$\hat{\mathbf{G}}|_{DFT} = \left(\hat{\mathbf{G}}_i^{-1}|_{DFT} - \hat{\mathbf{\Sigma}}_{0,L} - \hat{\mathbf{\Sigma}}_{0,R} \right)^{-1}$ of the extended molecule coupled to electrodes, those approaches employ the bare self-energies $\hat{\mathbf{\Sigma}}_{0,L}$ and $\hat{\mathbf{\Sigma}}_{0,R}$. Because the isolated extended molecule is modeled by an effective Kohn-Sham effective Hamiltonian, the underlying picture is a one-particle picture, and therefore the Landauer-type formulae (16) and (24) with $\hat{\mathbf{G}}^r$ replaced by $\hat{\mathbf{G}}^r|_{DFT}$ follow as “exact” results (i. e., without any other approximation as the DFT-approximation itself).

We emphasize that Landauer-type expressions like those Eqs. (16) and (24) are *not* valid in general for correlated electron systems. As explained in Sect. II, they represent justified approximations in the correlated case *only* when sufficiently large extended molecules are considered. The advantage of the approach based on this concept is its clear physical content. Eqs. (16) and (24) hold for electron correlations that can be strong within the molecule but are negligible at the ends of a sufficiently large extended molecule. This is the reason we employed in the Dyson equation (14) the bare self-energies $\hat{\mathbf{\Sigma}}_{0,L}$ and $\hat{\mathbf{\Sigma}}_{0,R}$, as in the NEGF-DFT approach. However, at variance with the latter, our approach accurately