write the part H_M that specifies the extended molecule

$$\begin{aligned} H &= H_L + H_R + H_{LM} + H_{MR} + H_M \ , \\ H_L &= \mu_L \sum_{l=-M_L-1}^{-\infty} a_l^\dagger a_l - \xi_L \sum_{l=-M_L-1}^{-\infty} \left(a_l^\dagger a_{l-1} + h.c. \right) \ , \\ H_R &= \mu_R \sum_{r=M_R+1}^{+\infty} a_r^\dagger a_r - \xi_R \sum_{r=M_R+1}^{+\infty} \left(a_r^\dagger a_{r+1} + h.c. \right) \ , \\ H_{LM} &= -\xi_L \left(a_{-M_L}^\dagger a_{-M_L-1} + h.c. \right) \ , \\ H_{MR} &= -\xi_R \left(a_{M_R}^\dagger a_{M_R+1} + h.c. \right) \ , \end{aligned} \tag{19}$$

and

$$\begin{aligned} H_M = \ & \mu_L \sum_{l=-1}^{-M_L} a_l^\dagger a_l - \xi_L \sum_{l=-1}^{-M_L+1} \left(a_l^\dagger a_{l-1} + h.c. \right) \\ & + \mu_R \sum_{r=1}^{M_R} a_r^\dagger a_r - \xi_R \sum_{r=1}^{M_R-1} \left(a_r^\dagger a_{r+1} + h.c. \right) \\ & - \beta_L \left(a_{-1}^\dagger a_0 + h.c. \right) - \beta_R \left(a_{+1}^\dagger a_0 + h.c. \right) \\ & + J_L \left(a_0^\dagger a_0 - \frac{1}{2} \right) \left(a_{-1}^\dagger a_{-1} - \frac{1}{2} \right) + J_R \left(a_0^\dagger a_0 - \frac{1}{2} \right) \left(a_{+1}^\dagger a_{+1} - \frac{1}{2} \right) + \alpha a_0^\dagger a_0 \ . \end{aligned} \tag{20}$$

In the above equation, the extended molecule comprises, besides the "molecule" itself, represented by a single site (labeled by 0), parts of the left and right electrodes (sites $-M_L, \ldots, -1$ and $1, \ldots, M_R$, respectively). Importantly, the energy of the molecular level α can be tuned by direct molecular orbital gating, as demonstrated by a remarkable very recent experiment [41], or electrochemical gating [42–45] in a way that is similar to the usage of a "plunger" gate electrode in quantum-dot nanoelectronic devices [46, 47]. Unlike in quantum-dot based single-electron transistors, where the relevant α-range is of the order of a few meV [46, 47], in the aforementioned experiment [41] the energy of the molecular level α could be varied, remarkably, within much broader ranges: $1.1\,eV \lesssim \varepsilon_F - \alpha \lesssim 1.9\,eV$ for single-electron transistors based on 1,8-octanedithiol and $0.4\,eV \lesssim \varepsilon_F - \alpha \lesssim 1.8\,eV$ for those based on 1,4-benzenedithiole by varying the gate potential V_G within $-3.3\,V < V_G < 0$ and $-3\,V < V_G < 3\,V$, respectively. In the presently considered case of half filling, the number of sites of the extended molecule $N = M_L + M_R + 1$ must be even. This implies that M_L is odd and M_R is even or vice versa, and therefore it is impossible to consider perfectly symmetrical extended molecules. The numerical results presented below correspond to the