

Critical Voltages and Coulomb Blockade in Single-molecule Transistors

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The Hamiltonian of 1M2-system

$$H = H_e + H_m + H_{int} + H_f(t)$$

$$H_e = \sum_{r\mathbf{k}\sigma} E_{r\mathbf{k}} a_{r\mathbf{k}\sigma}^\dagger a_{r\mathbf{k}\sigma} \quad \text{-- electrode's Hamiltonian}$$

$$H_m = \sum_{M(N)} E_{M(N)} |M(N)\rangle \langle M(N)| \quad \text{-- molecular Hamiltonian}$$

$$H_{int} = \sum_{r\mathbf{k}\sigma} \sum_{N,MM'} [V_{M'(N+1);r\mathbf{k}\sigma M(N)} \times |M'(N+1)\rangle \langle M(N) a_{r\mathbf{k}\sigma}| + h.c.]$$

-- Hamiltonian of interaction between electrodes and molecule

$$H_f(t) = -\mathbf{E}(t) \sum_{MM'} \mathbf{d}_{MM'} |M'(N)\rangle \langle M(N)|$$

-- Hamiltonian of interaction with electromagnetic field

