Hopping in a Molecular Wire

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We utilize the Hubbard model approach in analyzing the effect of the hopping parameter in the transport properties of a two-atom molecular device (Kostyrko & Bulka, 2003). The system consists of a molecule with two identical atoms connecting two metal electrodes. In this model, two important and realistic energy parameters are considered which affects the transport properties. The first is the kinetic energy required to "hop" from one atomic site to the next. We call this parameter the hopping term denoted by t, in arbitrary units of energy. The next is an on-site Coulombic repulsion, U, between two electrons on the same atomic site.

The molecular wire is represented by the Hubbard Hamiltonian

$$H_{mol} = \sum_{i,j}{}' \sum_{\sigma} \left(E_i \delta_{i,j} + t \right) c^{\dagger}_{i,\sigma} c_{j,\sigma} + U \sum_{i} n_{i,\uparrow} n_{i,\downarrow} \quad . \quad (1)$$

We then used the nonequilibrium Green's function formalism (Datta, 2000) to obtain the transport equations for the system. These transport equations are solved self-consistently. We utilized a root finding method to implement such calculations. Our results for the current at t = 1.0 agree with that in the literature (Kostyrko & Bulka, 2003).

The behavior of the current-voltage characteristics was shown to depend on the position of the molecular self-consistent energy levels with respect to the Fermi energy levels. For $U > 0$, the molecular levels are pinned between the Fermi levels of the source and drain electrode for values of $t \leq 0.5$. The threshold voltage is fixed for these values of t (Fig. 1) and continuous to increase for values to $t < 0.5$. For $U = 0$, the molecular levels continue to decrease as t decreases. The threshold

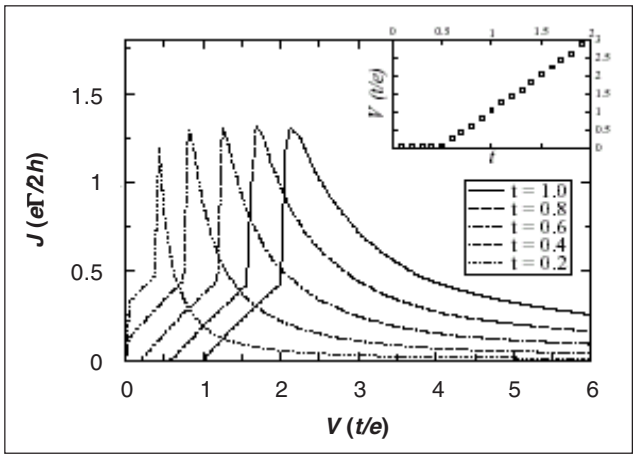

Fig. 1. Current-voltage characteristics for U = 4 for different values of t.

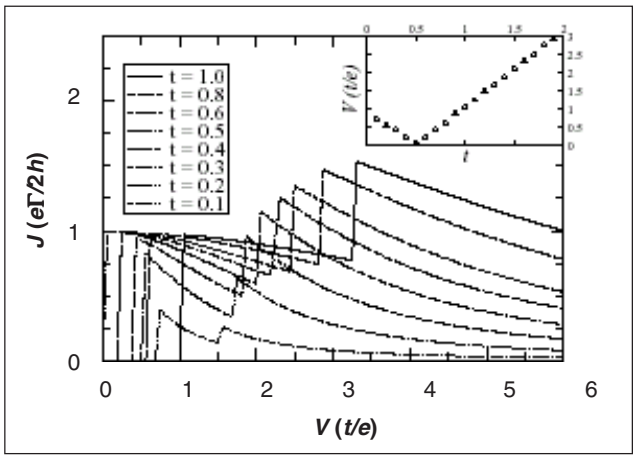

Fig. 2. Current-voltage characteristics for U = 0 for different values of t.

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voltage reaches its minimum at $t = 0.5$ (Fig. 2) corresponding to the point where the antibonding energy levels at $V = 0$ are located between the Fermi level of the source and drain. When both molecular levels are below the Fermi level of the drain, transport does not occur.

REFERENCES

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