A HOPPING MODEL FOR THE C-60 SINGLE MOLECULAR TRANSISTOR WITH QUADRATIC COUPLING

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The pioneering fabrication of a single molecular transistor has inspired experimentalists and theorists alike in the study of phonon assisted tunneling of electrons through molecules [1,2]. We have formulated a hopping model for the current across a C-60 molecular transistor, in which we demonstrate that linear coupling of the vibrational modes of the molecule's centre of mass to the electronic motion is not sufficient to model this system. However, with the inclusion of quadratic coupling we obtain results that are in very good agreement with experimental data.

The data that was published in 2000 by Park et al. showed I/V curves for various gate voltages for a C-60 single molecular transistor [figure 1]. As of yet, several notable features of these curves are not completely understood. Although it is agreed upon that the step structure in the current arises from vibrational coupling, other features of the data have yet to be explained. In particular, there is a glaring asymmetry in the forward and reverse bias curves. The forward bias current appears to increase much quicker with applied source-drain voltage than the reverse bias current, and the step structure is only distinct for low forward bias voltages.

We model the current across the transistor using a hopping model [3] and are able to reproduce the general structure of the observed I/V curves using a simple linear coupling Hamiltonian. However, to characterize the irregularities in the data it is necessary to account for the distortion of the molecular potential when it is in its charged state, as compared to when it is in its uncharged state. This is accomplished by changing the width of the harmonic potential for the two charge states, which amounts to adding quadratic coupling of the electronic motion to the molecular vibrational modes. With both linear and quadratic coupling incorporated into the hopping model, we are able to obtain a reasonable fit to the experimental data, and clarify the origins of the asymmetries in the I/V curves [figure 2].

References:

[1] H. Park et al., Nature, **407** (2000) 57.
[2] A. Nitzan and M.A. Ratner, Science, **300** (2003) 1384.
[3] S. Braig and K. Flensberg, Phys. Rev. B, **68** (2003) 205324.

Figures:

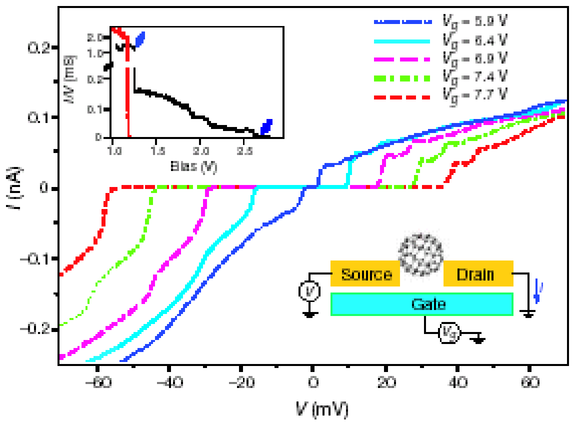

Figure 1

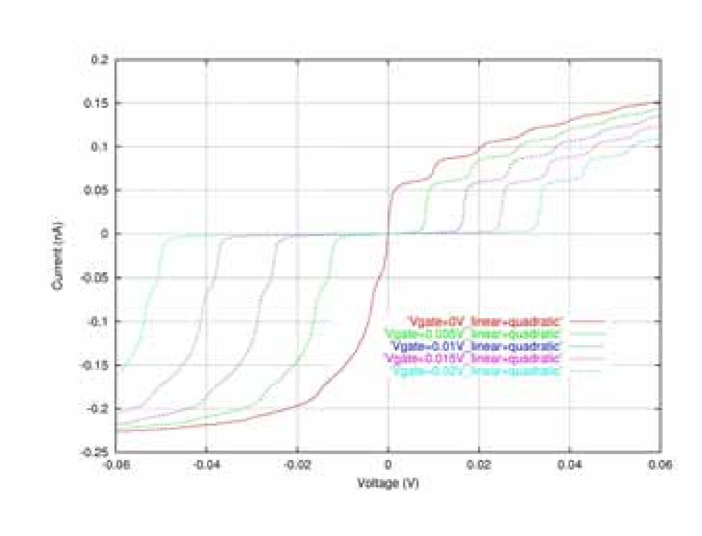

Figure 2