Effect of external field on the I-V characteristics through the molecular nano-junction

Lu Niu

The University of Sydney

luke.niu@sydney.edu.au

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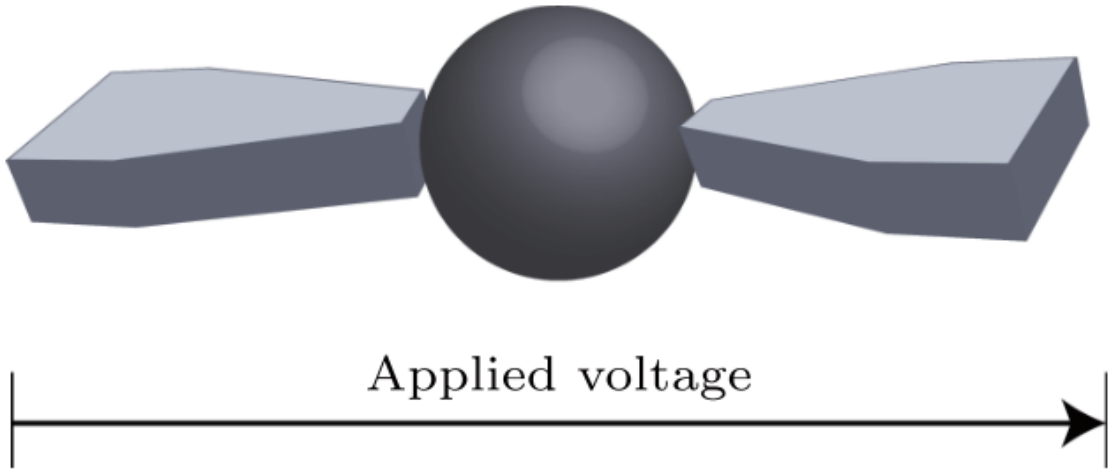
Overview

Background

As the basic functional unit of molecular electronics, the structure of single molecular nano-junction sandwiched between Nano-electrodes has been attracted many interests in molecular science. The charge transmission dynamics problems received increasing attention and have been subsequently studied extensively, in particular, its current voltage (IV) characteristics induced by an external field.



Method Section

In the system of molecular nano-junction which composed by a molecule between a pair of leads, with the method of extended General Master Equation, the characteristic curves of stationary and transient current have been computed and explained theoretically. It is found that the current can be evidently controlled via some factors adjustments, such as external field, the relaxation of molecules, intra-molecular vibration energy redistribution, and others.

Theoretical Model Description

The introduced electron-vibrational states, are used for an expansion of the overall molecular junction Hamiltonian:

$$H = H_{mol} + H_{lead} + H_{mol-lead} + H_{mol-field} \tag{1}$$

The Hamiltonian of the molecular part:

$$H_{mol} = \sum_{\alpha} \hbar\varepsilon_{\alpha} |\psi_{\alpha}\rangle \langle\psi_{\alpha}| + \sum_{\alpha\beta} W_{\alpha\beta} |\psi_{\alpha}\rangle \langle\psi_{\beta}| \tag{2}$$

The quadratic quantized form of the Hamiltonian of leads:

$$H_{lead} = \sum_{X=L,R} H^{X}_{lead} = \sum_{X=L,R} \sum_{k,s} \hbar\omega_{Xks} \alpha^{\dagger}_{Xks} \alpha_{Xks} \tag{3}$$

Theoretical Model Description: Hamiltonian

The Hamiltonian of the interaction between the leads and the molecule:

$$\begin{aligned} H_{mol-lead} = & \sum_{X=L,R} \sum_{k,s} T_X(N+1a, Nb, ks) \times \alpha_{Xks} \left|\varphi_{N+1a}\right\rangle \left\langle\varphi_{Nb}\right| \\ & + \sum_{X=L,R} \sum_{k,s} T_X(Na, N+1b, ks) \times \alpha_{Xks} \left|\varphi_{Na}\right\rangle \left\langle\varphi_{N+1b}\right| \end{aligned} \tag{4}$$

Theoretical Model Description

The coupling to the external optical field:

$$H_{mol-field}(t) = -\sum_{\alpha,\beta} |\alpha\rangle \langle\beta| \, \vec{d}_{\alpha\beta} \cdot \vec{E}(t) \tag{5}$$

The filed form:

$$\vec{E}(t) = \vec{n} \cdot E(t) e^{-i\omega t} + c.c. \tag{6}$$

The general form of rate equation:

$$\frac{\partial}{\partial t} P_\alpha(t) = -\sum_{\beta} [P_\alpha(t) K_{\alpha\to\beta}(t) - P_\beta(t) K_{\beta\to\alpha}(t)] \tag{7}$$

Numerical Simulation

Due to the strong electronic-vibrational coupling, the IV curves have the inelastic character in the molecular nanojunction and the stationary current increase as steps with the applied bias voltage. The Franck-Condon blockage can be effectively removed by the application of coupled external field. Applying Gaussian pulse widths of different orders of magnitude, the stationary current in the molecule needs different time period has been revealed on our work. Thought system described and computed, we got results of current curves with varying voltages applied as shown in Fig.1, and different magnitudes of pulse width as shown in Fig.2.

Numerical Simulation

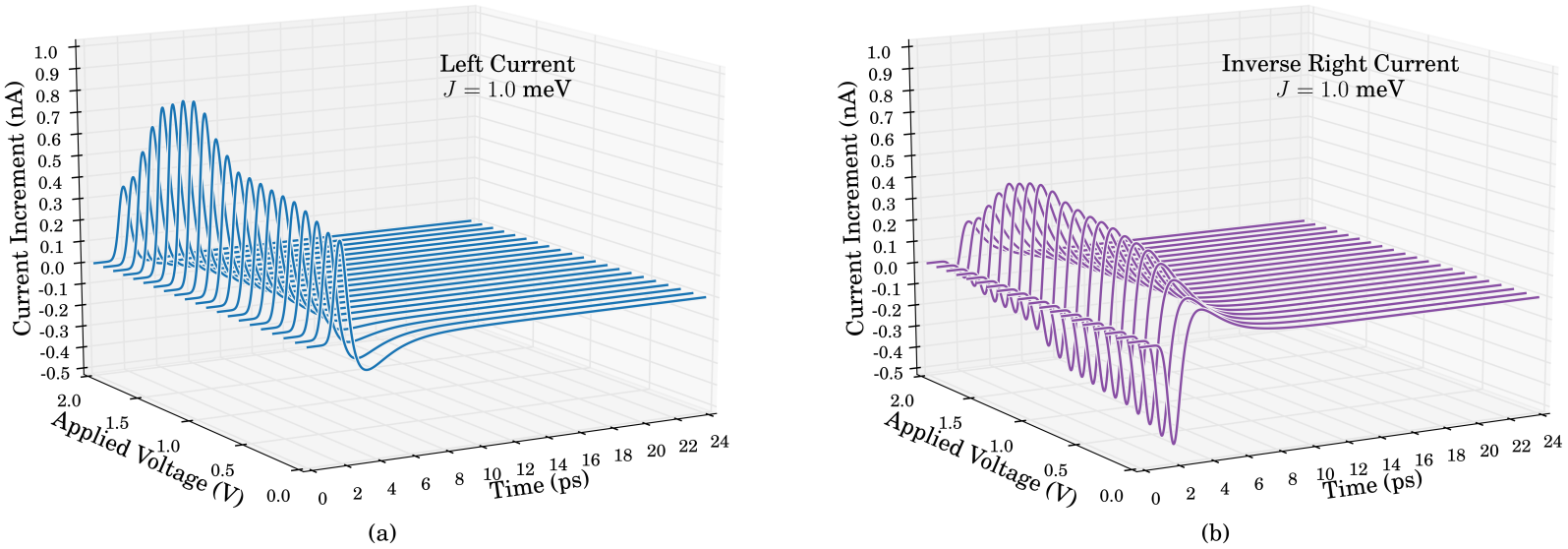


Fig.1: Applied a Gaussian external field and the bias voltage between 0-2V with the coefficient of IVR at 1.0meV, the transient IV characteristic curves are demonstrated: (a) the transient current from left lead to molecule; (b) the transient current from the right lead to molecule.

Numerical Simulation

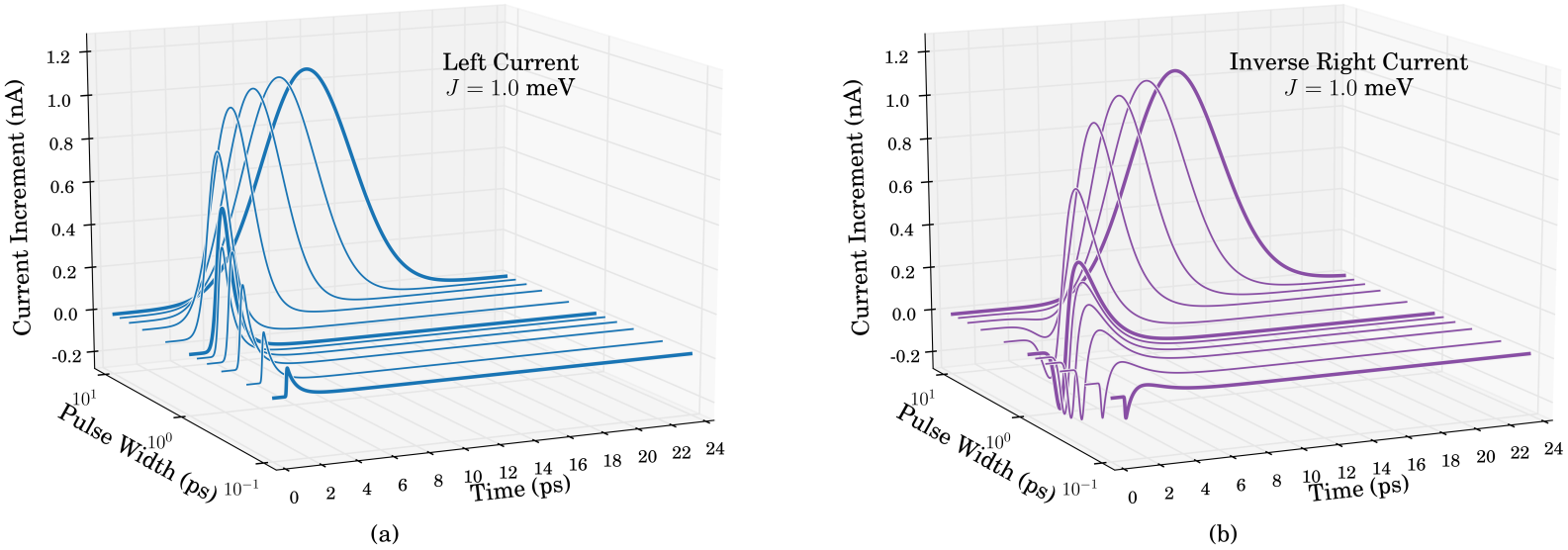


Fig.2: With the applied bias voltage of 1V and the coefficient of IVR at 1.0meV, the left and right transient current curves are plotted for various pulse widths of Gaussian external field. From the front to back, pulse widths are 0.1ps(bold), 0.2ps, 0.4ps, 0.6ps, 0.8ps, 1.0ps(bold), 2ps, 4ps, 6ps, 8ps, 10ps(bold) respectively.

Result Analysis

It is obviously that the transient current with its left part different with the right part is very significant for the 1ps width pulse excitation. In this case, the system stays in the state of non-equilibrium. However, with pulse width and applied voltage increasing, the current through the molecular nanojunction tends to be equilibrium.

Thank You