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Quantum Transport Model based Inelastic Scattering in Non-Equilibrium Greens Function (NEGF)

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Abstract - **In the last few decades, the function of non-equilibrium green (NEGF) formalism has been proposed for the development of nanoscale unit simulation tools because it is particularly convenient to handle open unit systems based on quantum mechanics and allows handling inelastic scattering. In particular, it may explain the inelastic effects on electrons and thermal current and voltage and energy. The non-equilibrium Green Function (NEGF) method is commonly used to predict transmission in atomically resolved nano drivers and generates enormous numerical loads when it includes inelastic scattering on phonons. This enables a solution for transporting scattered electrons on phonons in atomically dissolved nanowires with a cross section greater than 5 nm × 5 nm. Inelastic scattering is handled in a quantum transport model based on the function of non-equilibrium green (NEGF). The simulation has performed on the MATLA simulation. The first script uses a simple leader described by a (2x2) Hamilton matrix to highlight the core principles, shows how to directly extend the model to any leader described by any (NxN) Hamilton matrix. Numerical results are given in both cases, highlighting the subtle influence of inelastic scattering on quantum transfer.**

Keywords – Current, Hamilton matrix, Inelastic scattering, Nan electronics, NEGF, Temperature.

INTRODUCTION

The role of inelastic scattering in electronic transmission through mesoscopic systems is a topic of current theology and experimentation. Recent experiments have revealed the importance of electron-phonon interactions in measurement in certain mesoscopic systems. In particular, the non-dispersive results were not directly quantified in the STM (Scanning tunneling microscope) measurements of the molecular control behavior in the fuel cell. Theoretically, the effect of elastic scattering on electron transmission in mesoscopic semiconductor devices has been studied in a variety of ways, starting with the Green function technique to Fermi's rule. Some theoretical models are also proposed to explain the effect of molecular overload on the molecular electronic input associated with STM. Recent work provides a way to calculate the development of electrons with a telephone, the temperature limit of electrons passing through a one-gauge conductor. These methods have given rise to important insights into the behavior of specific systems. In the absence of inelastic scattering and electronic bonding, Landauer Theory provides a general system for the calculation of electronic waves through a mesoscopic conductor with a single conductor and a multi-channel conductor. It connects the electron current with the ability to transmit the electronic events from the lead source by spreading the elastic of the conductor and entering the drain. The transmission capability is found by solving the problem of scattering the quantity of a single electron. When we consider instability processes such as phonon emission and absorption, electron scattering has become a multi-body phenomenon, in which electrons and electronic systems are happy. [1] Proposed a non -mixed method to address the problem of dispersing a system with a mesoscopic conductor (phonon support mode) combined with the ideal conduction of a single channel as an electron source and drain. Their approach approaches the problem of multiple bodies by the problem of multiple single electronic transmissions that can be successfully solved. Here, each channel corresponds to the high-speed moving conditions of the mesoscopic conductor. Through their methods it is possible to determine the probability of transmitting and reflecting all the non-dispersive and elastic phenomena that may be felt by the electrons in the conductor from the source to the source. Drain. Hans Kosina et. al [2] It is generally believed that electron-scattering (EES) alters the high energy tailings of the energy distribution function [3][4], and therefore plays an important role in the degradation model. Physics-based heat generators. It is able to distinguish the static model by considering the equilibrium distribution of the partner electronics and the independent model that considers the weight distribution of the partner team. The latter method is suitable for determining the relationship of the hot electron tube and the cold electron pool in the water discharge area. This case is being discussed in the present work. We briefly examined the details of the reduction of the single-element scattering rate and the sensitivity of the complete parabolic and band systems in the Monte Carlo simulator. Ivan Shulepov et al. (2020) examined the effect of rotation of a Ti-6Al-4V cord at 1000 ° C on changes in elasticity and dispersive electron spectra [5]. It reveals the inequality of the elasticity and the dispersed electron spectra compared to the properties of the primary Ti-6Al-4V lead. The dependence on the energy change and the strength of the scattering electronic spectrum at the angle of inclination of the surface area was first recorded. The change in energy and shape is the result of a change in the structure of the mixed crystal with evolution. The change leads to a change in the lattice angle, a rearrangement of the position of the atom and a change in the energy intensity of the electrons in the atom. This in turn converts the value of the energy obtained from the initial charge to the scattering of plasmons.

PROPOSED MODEL

We model the simplest structure that can have inelastic scattering. This structure is a conductor with two energy levels. In addition, to specifically examine the effects of inelastic transport, we assume that these levels are only associated with the dispersion process, and each level is connected to only one contact, as shown in Figure 1.
The Hamiltonian for the two-level model is given as:

$$H=\begin{matrix} \varepsilon_1 & 0 \\ 0 & \varepsilon_2 \end{matrix}$$

ε Are the two energy levels of the system? This models a 1-D conductor with two points at two different energies as in fig.3.The off diagonal elements are 0 because they are not connected. Therefore the current can only flow due to inelastic scattering between the two points. The transport equations are based on the NEGF formalism as described in [6]. Self-consistent born approximation was used to incorporate scattering in the model.

$$U_S = \begin{bmatrix} 0 & A \\ A^* & 0 \end{bmatrix}$$

Where A is determined by parameters of a specific problem and dependent on specific scattering mechanism and is in general complex. The product AA* gives the magnitude of the interaction A0 (N+1) and A0 (N) for emission and absorption respectively. In this model it is assumed that the scatterers are of a single energy and are described by a Bose Einstein distribution. The tensor D is given by kronecker product of Us and Us* followed by average over the random phase of the scattering potential. Therefore:

$$D = Us_{ikjl} \otimes Us_{ikj}$$

The in-scattering and out-scattering for emission and absorption and the self energy due to scattering for the two-level model.

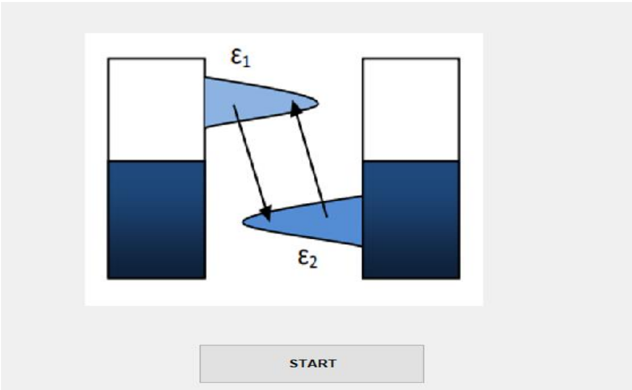

FIG. 1
TWO ELECTRONIC LEVEL MODEL IN THE ZERO BIAS CONDITION

The shaded area of the switch represents the electrochemical potential of the switch. Assume that the conductor is immersed in a spreading bath with a specific temperature Ts, which may be different from the temperature T in the switch. We can also apply a voltage difference to the contacts. The transmission equation is based on the NEGF form described in [7]. The rate of spread between energy levels is based on Fermi's golden rule, which is described in detail in [8].

The transport equations developed are independent of the basis in which the Hamiltonian and Self energy matrices are written [9-12]. The scripts developed work with any basis and size of the Hamiltonian. The method considers all the elements of the D during the calculation of the scattering rates [13]. This ensures generality in the various scattering processes that can be handled [14]. Different scattering mechanism may have different shapes for the scattering potential depending on the basis chosen for the Hamiltonian. Therefore it is important to consider all the elements of the tensor D while calculating in-scattering and out-scattering terms. To test the validity of calculation under basis independence, all the matrices were transformed to different bases generated by random unitary matrices and calculated with original Hamiltonian as described before [15-19]. The transformation matrices are set to Identity matrices in the scripts and the generation steps for the random unitary matrices are observation elsewhere. While running the scripts, to test the basis independence of the final results uncomment the generation steps and run the scripts. Check the H and D matrix from the Array Editor in MATLAB to view different basis transformed matrices [20].

At zero bias and with same temperature of the electrons and scatterers (equilibrium condition) there should be no current [21-23]. If the bias is kept zero, but the temperature of the scattered bath and the contacts are different, the electron+scatterer system is no more in equilibrium and we should expect to see a current flow [24]. This is evidenced in real systems like solar cells where the scatterers (photons) have the temperature of the surface of the sun during the day and therefore we can get a current from the device [25]. However in the dark the solar cells do not work due the equilibrium between photon bath and contacts. If a bias is applied between two contacts we expect a current to flow. If we can obtain currents that are emission or absorption limited, i.e.

primarily due to the emission or absorption of the scatterers, we should expect the currents to be in the ratio of N+1:N, where N is the number of scatterers given by the distribution function of the scattered bath. There is extra broadening of the two levels due to scattering (this is additional broadening over the broadening introduced by the contacts). This should be observable in the magnitude of current as well

RESULT AND DISCUSSION

Initial the Developed a MATLAB script to simulate the transport through a two-level conductor with inelastic scattering. If both the levels (in the two-level model) are connected to the contacts, what is the effect of scattering at zero bias but with scattered and electrons at different temperatures.

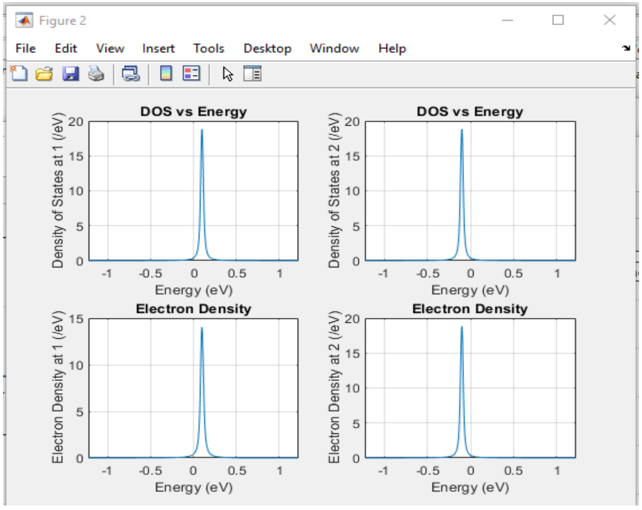

FIG. 2
ELECTRON DENSITY VS ENERGY (EV)

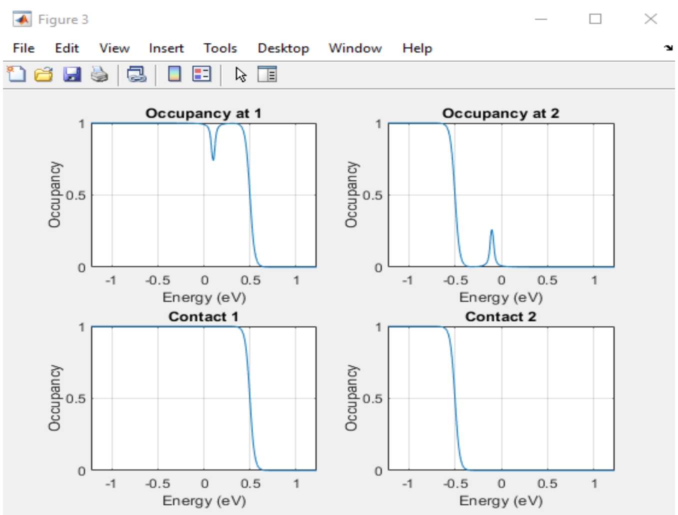

FIG. 3
ENERGY LEVEL EXTRA BROADENING OF THE TWO LEVELS DUE TO SCATTERING

Current-voltage characteristic- The current using a varying voltage difference between the contacts. It is assumed that the energy level does not change due to the bias used. Under high positive bias, the left contact is full, and under high negative bias, the right contact is full. Therefore, the current is emitted under high positive bias mainly. while the current is mainly absorbed under high negative bias. The ratio of emissivity to absorption is given by N + 1: N, which is also reflected in the ratio of saturation current. At zero voltage, the current is zero. Show in fig 4.

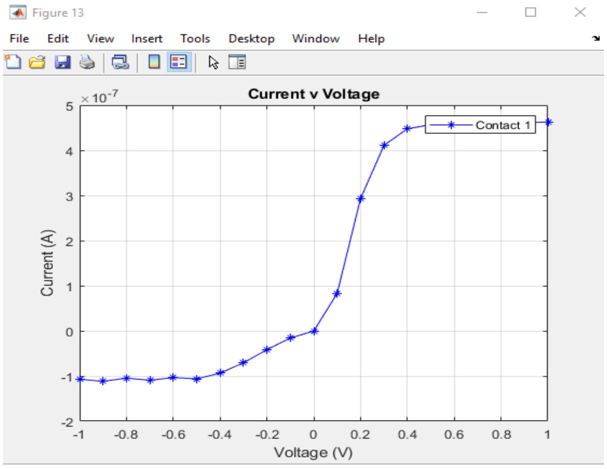

FIG. 4
CURRENT AT LEFT CONTACT

If we change the temperature Ts in the diffuser (Figure 4), we can see that the current is no longer zero below zero bias voltage, so due to the imbalance between the electron and the scattering, we get a limited short-circuit current. We also see that the current ratio due to the change in the number of diffusers N is different.

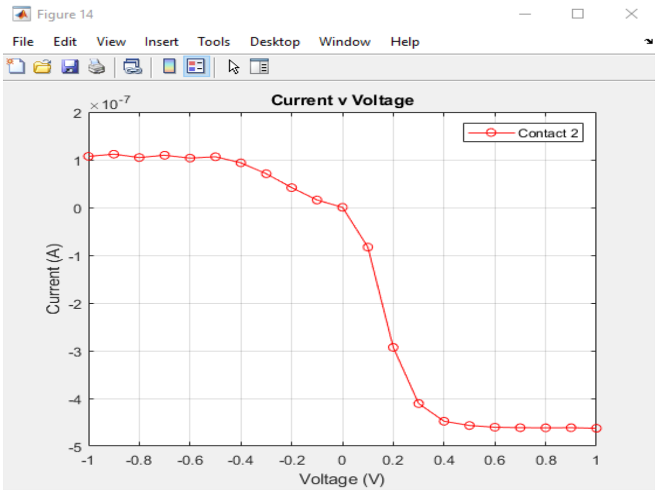

FIG. 5
CURRENT AT LEFT CONTACT

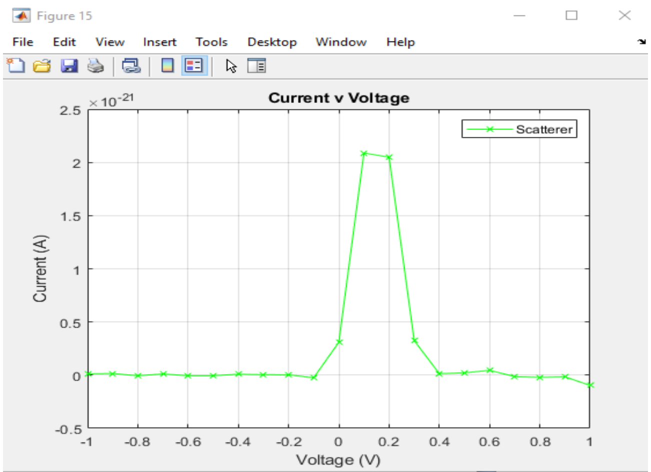

FIG. 6
CURRENT AT RIGHT CONTACT WITH CHANGE IN SCATTERER TEMPERATURE

Current at a Single Bias: To calculates the current at a given bias. It is assumed that the bias used does not change the energy level in the device, but will change the Fermi energy level in the switch. Figure 7 shows the energy dissolution current from the left and right contacts and the current due to the scatter. When the left switch is full and the right switch enables the energy levels ε1 and ε2, respectively, this is a bias (1V). In this case, the current is due to the emission of the scatter because ε1 is at the selected higher energy. That scattering acts as the third point of contact in the device; it absorbs electrons from higher energy and injects them back at lower energy. Due to the current conservation, the total current generated by the spread is zero.

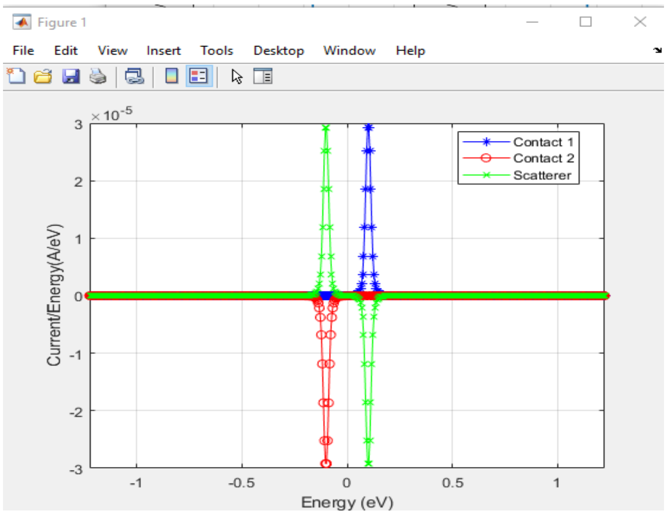

FIG. 7
PLOT OF ENERGY RESOLVED CURRENT AT CONTACTS (LEFT) FOR LOW BIAS TRANSPORT WITH INELASTIC SCATTERING THROUGH A 1-D NANOWIRE

Current-Temperature characteristics: The spreading temperature changes and keeps the voltage difference between the contacts zero. In this case at high diffuser temperature (Ts), since the left contact is almost empty and the right contact almost full at energy ε1 and ε2, the current is mainly absorbed. The number of diffusers is given by the Bose-Einstein distribution, which increases exponentially at high temperatures, giving an exponentially increasing current. Since the number of electrons in left contact with energy ε1 is small but limited, a small current will be generated at low temperatures. In this case, N is close to zero, but since the current is mainly emission and the spreading rate is proportional to N + 1, there is still a small amount of current. When T = Ts, the current is exactly zero. Shown in fig 8

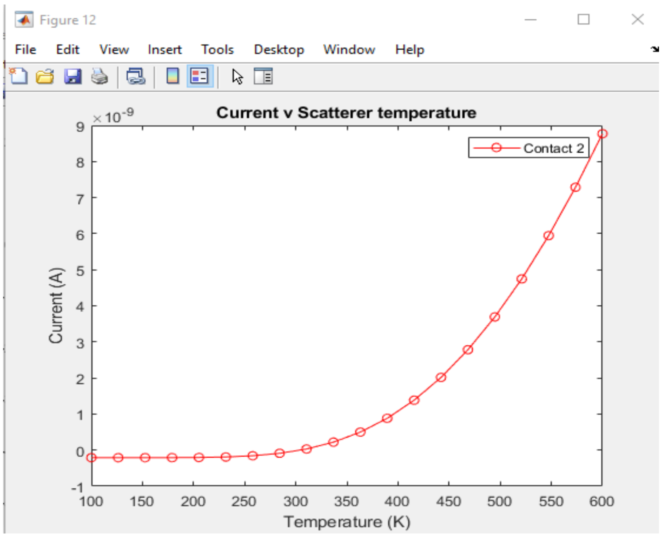

FIG. 8
CURRENT AT RIGHT CONTACT WITH CHANGE IN SCATTERED TEMPERATURE

CONCLUSION

This result show explain recent inelastic electron scattering observations with different temperature and different energy level and the effects obtained using inelastically scattered electrons, and also shows that such inelastic scattering for quantum transport model based on the function of non-equilibrium green (NEGF). The equations developed are independent of the basis in which the Hamiltonian and Self energy matrices are written. The scripts developed work with any basis and size of the Hamiltonian. The method considers all the elements of the D during the calculation of the scattering rates. This ensures generality in the various scattering processes that can be handled. Different scattering mechanism may have different shapes for the scattering potential depending on the basis chosen for the Hamiltonian and simulate the transport through a two-level conductor with inelastic scattering. If both the levels in the two-level model are connected to the contacts, what is the effect of scattering at zero bias but with scattered and electrons at different temperatures.

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