Research Plan

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1 Problems of Molecular Systems

The exploration into electron transport of molecular systems has become an active topic in the world of quantum physics and electronics [4]. This research plays heavily into both the future development of new technologies such as photovoltaic, thermo-electrics, and molecular electronics, and raises fundamental questions into the differences of conventional electronics versus quantum electronics. These quantum systems are vastly different from conventional electronics because when on the quantum scale, there are discreet channels and limits to the conductance [5].

Currently, when scientists run experiments on these nano-scale conductors, it is not known how to hold the microscopic details constant in order to evaluate the outcomes of these tests. Between each test, the way the molecule channel links to the electrode can vary. These uncontrollable variables make the tests highly irreproducible and difficult to analyze[3]. This also raises the question of how to measure these physical details that, to date, cannot be controlled. Likewise, the properties that influence these channels and create optimal conductors are very hard to measure and hold constant. In order to get around the problems raised by this process, scientists order the outcomes in histograms, and have concluded that these conductances organize into single-channel peaks.

When these conductances are arranged into histograms, they sometimes form a single-channel peak[3]. Scientists currently know that the shape of these peaks say something about the chemistry of the system, but very little research into the area has been done. Presently, no one has done any analysis over the data or line shapes. The farthest tests or analysis done has been over empirical models that were used to describe the data. So the model devised must be able to estimate what values and physical information are affecting the line shapes of single-channel peak histograms. Therefore the primary point of this method is to understand what fundamental physics is affecting the outcome of these conductances. If it is possible to understand these fundamental processes, then new, groundbreaking work can be done into fields dealing with quantum electron transport.

2 Goals

The goals of this project is to gain some new insight into what physical parameters affect the conductance of molecular systems. In order to address this problem, it is necessary to determine a way to best address the line shapes created by the conductance histograms. This project would effectively predict the different individual aspects of the system affecting conductance histograms by simulating the histogram and preforming an inverse function to extract the best fitting values for the histogram.

3 Procedure

In order to first start the analysis of conductance histograms, a model was created using probability theory. The model gave the integral,

$$\hat{G}(g) = \int_{-\infty}^{\infty} d\epsilon \int_{0}^{\infty} d\Gamma \hat{P}_{\epsilon} \hat{P}_{\Gamma}(\Gamma) \delta \left(\frac{\Gamma^2}{(E_F - \epsilon)^2 + \Gamma^2} - g \right) \tag{1}$$

and this integral will be evaluated to derive the different equations pertaining to different cases of the molecular system[2][1] .

In order to validate that the equations used to model the histograms are valid, a control experiment must be devised. First a program will be written that simulates control histograms where the input values of $\Gamma_L, \Gamma_R, \epsilon$, and E_F are all known. This program had to use a random number generator in order to simulate the experimental uncertainty. This program simulated several hundred data points, and from here this data was then sent to a binning program that organized the simulated data points into a conductance histogram in which the input values were known. From here, the fitting program was fitted to the histogram. Then the input values will be compared to the extracted values given by the program created. Finally a python script will be created to re-run these tests multiple times in order to validate our equations and program. Our results will be organized in graphs comparing the input values to the extracted values. This will show that the program created for simulating and modeling these histograms is accurate and effective.

References

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