**Examining the Information Content of Voltage-Dependent, Two-Dimensional Conductance Histograms**

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1. **Introduction**

In nanometer-scale systems in which quantum mechanical effects are crucial, the study of the conductance of a single molecule is a topic that has undergone several significant recent advances and has garnered excitement due to its potential applications in areas such as molecular electronics, photovoltaic technologies, and thermo-electrics. It is popularly hoped that a better understanding into the currently murky realm of molecular conductance properties will lead to the replacement of electronic components with small molecules, allowing for dramatic size reduction. As an example, smaller parts would mean more efficient placement of transistors in chips and far more procession power, possibly past the outlook of Moore’s law. However, current challenges lie in finding the most efficient way to measure the conductance, and also in the analysis of the actual factors contributing to the property.

In contrast with conventional electronics, molecular systems do not have precisely-measurable properties. The workings of quantum electron transport as well as small changes in particular parameters contribute to variation in tests. The molecule can be thought of as a collection of channels: there are a finite number of channels within the molecular system that can be used for transmission of electron charges, and these channels have varying states of conductance ranging from closed (conductance of zero, no transport) to open (conductance of one, certain transport). The channels do not ensure transmission, and in such small systems, the variability of the relatively limited channels due to physical changes creates significant uncertainty when trying to state a faithful value. Therefore, conductance histograms are a common way for experimental studies to characterize the conductance through the system. Experimental techniques are performed thousands of times to generate large amounts of conductance data, and the properties must then be determined statistically. After compiling the data into the histogram, there is much debate on how analysis should be done on it, but in general, the peak is interpreted as the “expected” conductance.

With recent developments of experimental technique by S. Guo et al. and analysis fitting model by M. G. Reuter and P. D. Williams, the field is ready for in-depth study on the effects of an applied voltage, or *bias*, to the system. In contrast to traditional conductance histograms which use an axis of conductance values versus an axis of number of times observed, the two-dimensional histograms proposed here relate voltage to conductance while preserving the frequency of the conductance using contour shading. We attempt to relate this additional physical parameter to its effects on changes in conductance data, along with the other meaningful physical information previously studied by Reuter and Williams such as *E*, the energy of the electron, ε, the channel energy, Γ, the channel-electrode coupling, and *EF*, the Fermi level. Our model is based on derivations from the Landauer-Büttiker-Imry theory of transmission.

**References**

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