Quantum Transport in Two Dimensions

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by

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Abstract

Bilayer graphene is a material of interest due to its novel electronic properties. Throughout the course of this project, we will investigate the metal-insulator transition in bilayer graphene through the use of a simulation run on the SciClone cluster. Past research has investigated this transition from a classical perspective using percolation calculations [4]. Our simulation builds on past work by considering the effects of quantum tunnelling as well. By analyzing the relationship between the conductance and adjustable parameters within the simulation, we can learn more about the metal-insulator transition in bilayer graphene.

Motivation and Background

The electronic properties associated with bilayer graphene have generated public interest because of interest in novel industrial applications [1]. However, more research needs to be done to investigate the metal-insulator transition in bilayer graphene.

Figure 1: Mock experimental setup of bilayer graphene sample. From [2]

Figure 1 depicts what a physical version of our bilayer graphene sample would look like. A gap voltage is created across the bilayer graphene sample (the red slice), creating a band...
gap. The presence of impurities in the white layer, separated from the bilayer graphene sample by a thin slice of SiO$_2$, creates potentials within the graphene–this is the disorder parameter within our simulation.

From an industrial standpoint, the metal-insulator transition is important for future production of transistors. An ideal transistor is a perfect conductor when turned on and a perfect insulator when turned off [4]. To fabricate an effective bilayer graphene-based transistor, its metal-insulator transition needs to be investigated. This would help determine which parameters can be adjusted to improve conductance when the transistor is on and improve resistance when the transistor is off. Single layer bilayer graphene has no band gap, but an electric field induced across a bilayer graphene sheet, known as the gate voltage, can create a band gap [5]. The application of this gate voltage allows bilayer graphene to be considered for applications within the semiconductor industry.

$$h(k) = \frac{\Delta}{2} \tau_z + \hbar v_F (k_x \sigma_x + k_y \sigma_y) - \frac{\gamma_1}{2} (\sigma_x \tau_x + \sigma_y \tau_y)$$ (from [6]) (1)

Formula 1 shows the Hamiltonian used to describe the system. The $\tau$ and $\sigma$ variables both represent Pauli matrices, where the $\tau$ variables represent layer degrees of freedom and the $\sigma$ variables represent sublattice degrees of freedom. The $\frac{\Delta}{2}$ term shows the effect of the band gap. The second term is the bilayer graphene Hamiltonian, while the $\frac{\gamma_1}{2}$ term is the correlation factor for electrons hopping between the two sheets in the bilayer system.

In a two dimensional lattice, there are a variety of factors that influence the transport of electrons through the lattice. Potentials within the lattice arising from external sources, as well as the application of an electric field perpendicular to the bilayer graphene sheets, are two such factors. According to Rossi and Sarma [3], the potentials manifest themselves as electron-hole puddles in a disorder-induced inhomogeneous density landscape. The creation
of this landscape affects the band structure of bilayer graphene, but the effects are not as straightforward as those caused by the application of an electric field.

Rossi and Sarma [4] used a classical percolation treatment of the system to determine information about the metal-insulator transitions. From the classical results, conductance increased as disorder increased within the system. Conductance also increased with a higher applied voltage. This project aims to build on the 2011 paper by using a quantum treatment of electron transport to investigate the metal-insulator transitions. By tuning the external potentials in terms of both strength and configuration, we hope to gain a better understanding of the nature of the metal insulator transition within a bilayer graphene system.

Methodology

Our simulation used a transfer matrix approach to determine conductivity within the bilayer graphene sample. Given a particular graphene sample, we divided it up along its length into \( N \) subintervals of equal width. This allows us to use the Born approximation to create a transfer matrix for each subinterval. As \( N \) approaches infinity, the approximation becomes exact, so it is beneficial to have a large number of subintervals [2]. Various properties of bilayer graphene were investigated by running the simulation on the SciClone cluster here at William and Mary.

There is a tradeoff between high accuracy of the simulation and practical run times. The importance of efficiency is compounded by the fact that, for each set of parameters, a large number of randomized impurity distributions need to be tested through the simulation. Much of the work on this project was focused on tuning different parameters within the simulation to attain desired accuracy alongside reasonable run times.
Figure 2: Curves are plotted with various charge_dis_rms values, which measure the density of impurities which create electron-hole puddles within the bilayer graphene. As the size of the system increases, the conductivity value \( g \) tends to decrease.

One parameter we tuned was the size of the graphene sample. Figure 2 shows that as the size of the sample increases, the conductance value \( g \) decreases. This holds true regardless of the charge_dis_rms value. At very large sample sizes, the conductance eventually hits a saturation point where it doesn’t decrease significantly. We are interested in this saturated value, so a large enough sample needs to be simulated to obtain these values. The simulation is valid for sample sizes where the width of the sample is bigger than the length–optimally, the width would be infinite, but a factor of 2 is typically sufficient. Thus, increasing the length of the sample comes with quadratic time cost scaling, and a balance had to be found between the accuracy and runtime of this simulation.

In the simulation, Fourier transforms are calculated along the width of the bilayer graphene sample. This means the number of Fourier modes must be tuned as well–fewer modes means shorter run time, but more modes means more accuracy. As shown in Figure 3, there doesn’t seem to be much of a difference between the two curves when the band gap is set to 0.08, as shown in Figure 3 (the band gap parameter is referred to as ”mass”).
All the curves seem to have converged to one curve, even with relatively few Fourier modes (referred to in the plot as ”Msamples”). When band gap = 0.095, which was the case in Figure 4, there were clear differences between the curves, which indicates that more Fourier modes are necessary to obtain accurate results.

This shows the importance of tuning the accuracy and resolution of the simulation depending on the input parameters. In order for our simulations to give accurate results, we must also tailor the number of necessary Fourier modes in the calculation in accordance with the values of other parameters.

Figure 3: There is little to no difference between curves calculated using different numbers of Fourier modes.
Figure 4: The curves calculated for various numbers of Fourier modes seem to be further apart relative to lower band gap simulations. However, there seems to be a trend of convergence towards a single curve as the number of Fourier modes is increased, with diminishing returns at very high values.

Results

From the classical simulation, we expected the presence of a band gap created by an electric field to cause the conductance to increase with respect to disorder [4]. Figures 5 and 6 show the difference in the relationship between conductance and disorder for samples without and with a bandgap, respectively.
Figure 5: In this figure, there is no bandgap in the bilayer graphene sample. In this case, conductance (g value) goes down as the disorder (charge_dis_rms or charge concentration value) increases. Two curves with different numbers of Fourier modes (MSAMPLES) were plotted here to confirm convergence of the curves with respect to the number of modes.

Figure 6: In this figure, a bandgap has been opened in the bilayer graphene sample. Conductance (g value) increases as the disorder (charge_dis_rms or charge concentration value) increases.

We see that increasing disorder without the presence of a band gap decreases the con-
ductivity. In contrast, the presence of a band gap causes conductance to increase with disorder. Our results agree qualitatively with the classical treatment of the system, which is encouraging.

**Conclusion**

Within the simulation, the gate voltage and the strength of the potential "puddles" are parameters that affect the conductance of bilayer graphene. We found that both classical and quantum treatment of the system demonstrate that increasing disorder in a gapped bilayer graphene sample increases conductance. Varying gap size and disorder simultaneously allows us to determine zones where the bilayer graphene sample acts as a conductor, insulator, or some form of semiconductor. Since there are two independent variables being tuned, searching for this behavior requires many simulations to be run. Investigating the values used for each of these zones would help determine how to tune a bilayer graphene system to exhibit better semiconducting behavior.

**References**


