May 16th, 12:00 AM - 12:00 AM

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Seaman, David; Spradlin, Joshua; Leger, Janelle; and Rahmani, Armin, "Modeling current flow in nanoparticle doped polymer film systems" (2018). *Scholars Week*. 56.  

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Modeling current flow in nanoparticle doped polymer film systems

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Introduction

• Nanoparticle doped polymer films are of interest for use in organic memory systems due to their ability to exhibit electrical bistabilities like that seen in figure 1 [1-3].
• Understanding of how current flows under these conditions is desired to better understand and predict how different films will behave.
• We attempt to find a computational model of the current through a simplified system with finite lead lengths as seen in figure 2.

Calculating Current

• Working in the Heisenberg picture, we calculated current using the differential equation

\[
\frac{d\hat{O}(T)}{dt} = i[H(T-t),\hat{O}(t)]
\]

Where \( \hat{O}(T) \) is the Heisenberg operator at time T, which can be written as

\[
\hat{O} = \hat{\Psi}^\dagger O\hat{\Psi}
\]

Which in the case we can write O as the following, where k is the hopping term and c the creation operators

\[
\hat{O}(t=0) = i k (c_{j+1}^\dagger - c_{j}^\dagger c_{j+1})
\]

Where O is an LxL matrix representing the single particle Hamiltonian, and \( \hat{\Psi} \) is the many particle wave function

• We can find for \( \hat{O} \) by solving for O(t) in:

\[
\frac{d\hat{O}(T)}{dt} = i[H(T-t),\hat{O}(t)]
\]

• To find the total current over time, we solve the differential equation for each T
• The expectation value of \( \hat{O} \) can be found with the initial state, \( |0\rangle \)

\[
\langle \hat{O}(T) \rangle = \langle 0|\hat{\Psi}^\dagger \hat{O}(T)\hat{\Psi}|0\rangle
\]

• To find the above expectation value, we diagonalize \( H(0) \):

\[
H(0) = VDV^\dagger
\]

V represents the eigenstates of the system, when we multiply both sides of D with

\[
\Gamma = V^\dagger \hat{\Psi}
\]

The expectation value for our operator at a given time is calculated using

\[
\langle \hat{O}(T) \rangle = \langle 0|\Gamma^\dagger V^\dagger \hat{O}(T) VT |0\rangle
\]

• When we substitute in \( O(t) = V^\dagger \hat{O}(t)V \) the calculation reduces to a summation along the diagonal of \( \hat{O} \) or:

\[
\langle \hat{O}(T) \rangle = \sum_{i \in \text{occupied}} \hat{O}_{ii}(T)
\]

Results: Non-Constant Potential

• When the duration of the non-constant potential phase lasted half time for \( T_{\text{total}} = 1 \), we saw that the current did not return to zero with the potential (figure 3).
• When the duration of non-constant potential was restricted to one tenth of the time \( T_{\text{total}} = 10 \), the current exhibits an oscillatory behavior without damping (figure 4).

Results: Constant Potential Varying Lead Lengths

• To simulate the infinite lead limit, we considered the impact of the length of the electrode leads
• For a constant potential, the current should also remain constant, following Ohm’s law
• However, we see that our model predicts a non-constant current flow
• To isolate the cause, we examine the effect of the leads has on the oscillations
• The lead length has no noticeable impact on the current flow on the time scale we considered (figure 5).

Results: Flat Potentials

• Plotted current for different constant potentials to investigate the impact of the potential
• To determine if the oscillations are arising from setting the potential too high
• We consider a variety of constant potentials varying from \( V = 0.00001 \) to \( V = 0.1 \)
• The potential has no effect on the time scale we examine in the system (figure 6).

Conclusions

• Our results are preliminary without structure change.
• Size of the leads and current values below \( V = 0.1 \) has no effect on the current behavior in our model, with both exhibiting similar oscillatory behavior
• Next step is verifying our data with linear response by comparing to a model that treats complex current junctions as a scattering problem utilizing the Landauer method as seen in Wu et. al. [4]

Acknowledgments and Funding

• Leger Group
• WWU AMSEC SEED Grant funding

References


Figure 1: Current vs. voltage for an OMEM device produced in the Leger lab

Figure 2: Simplified schematic of the polymer system. Black bars represent the leads in the system, the blue chains are the polymers, with each of the circles representing a two spin site. The large disks are the nanoparticles the solid connections between polymer chains are the interchain connections from the polymers being near each other.

Figure 3: Corresponding current for the \( T_{\text{Total}} = 1 \) case

Figure 4: Corresponding current for the \( T_{\text{Total}} = 10 \) case

Figure 5: Current flow at constant potential (\( V=0.01 \)).

Figure 6: Current with constant leads of 600 sites