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Modeling current flow in nanoparticle doped polymer film systems

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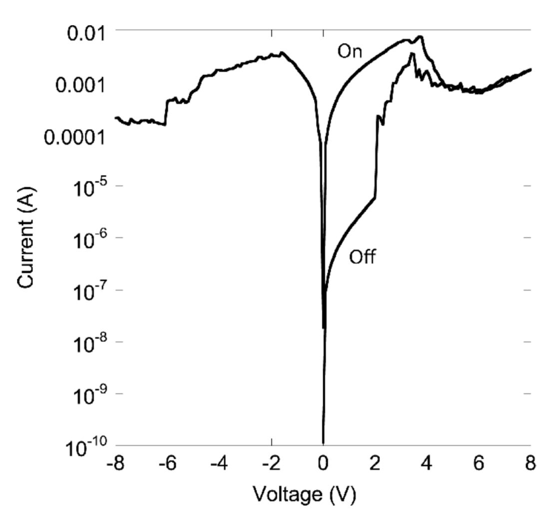
Introduction

- 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

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



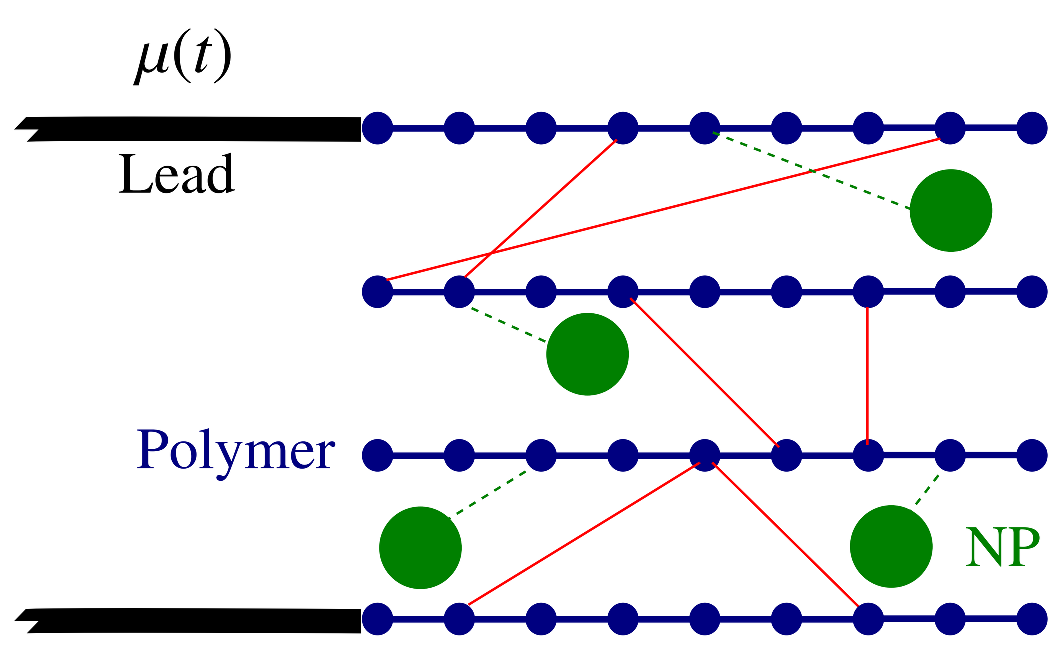


Figure 2: Simplified schematic of the polymer system. Black bars represent the leads in the system, the blue chains are the polymers, with each of the circles representing a two spin site. The large disks are the nanoparticles the solid connections between polymer chains are the interchain connections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

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

$$\hat{O} = \Psi^{\dagger} O \Psi$$

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

$$\hat{O}(t=0) = ik(c_j^{\dagger} c_{j+1} - c_{j+1}^{\dagger} c_j)$$

- Where O is an LxL matrix representing the single particle Hamiltonian, and Ψ is the many particle wave function
- We can find for $\hat{O}$ by solving for O(T) in:

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

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

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

- 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

$$\Gamma = V^{\dagger} \Psi$$

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

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

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

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

Results: Non-Constant Potential

- When the duration of the non-constant potential phase lasted half time for T_{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_{total} = 10, the current exhibits an oscillatory behavior without damping (figure 4).

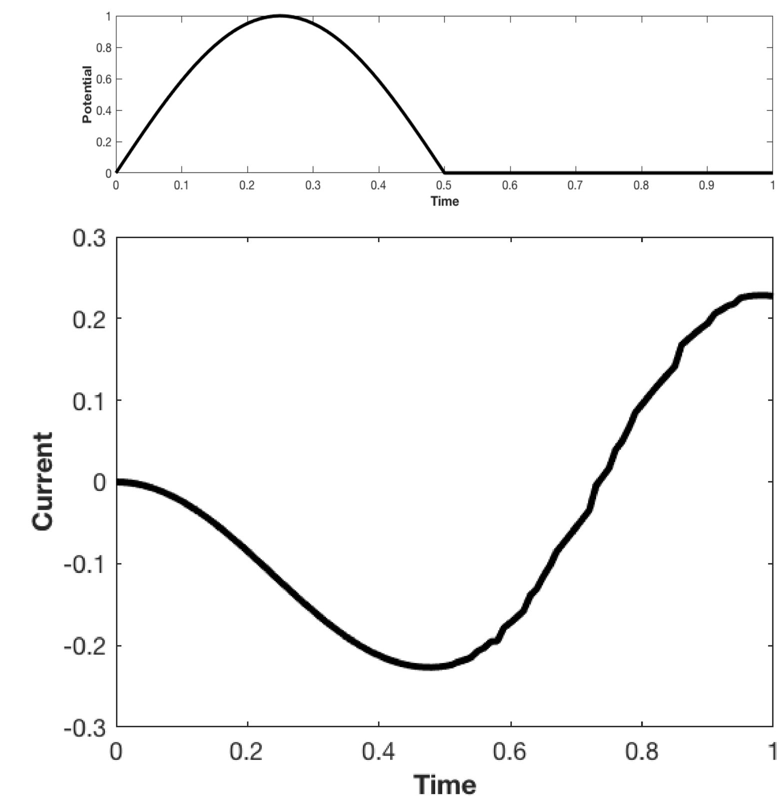


Figure 3: Corresponding current for the T_{total} = 1 case

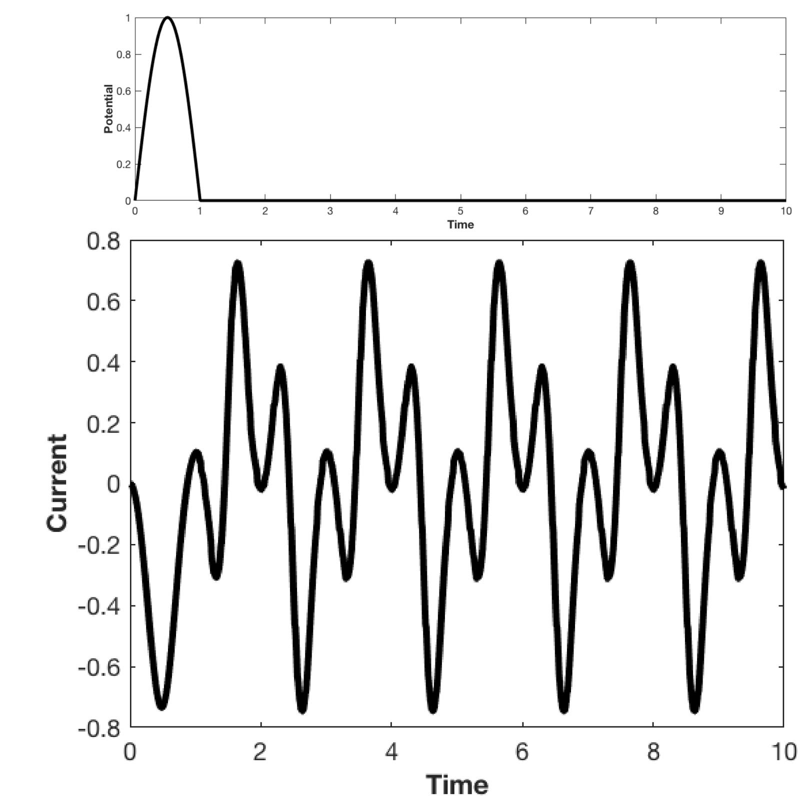


Figure 4: Corresponding current for the T_{total} = 10 case

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)

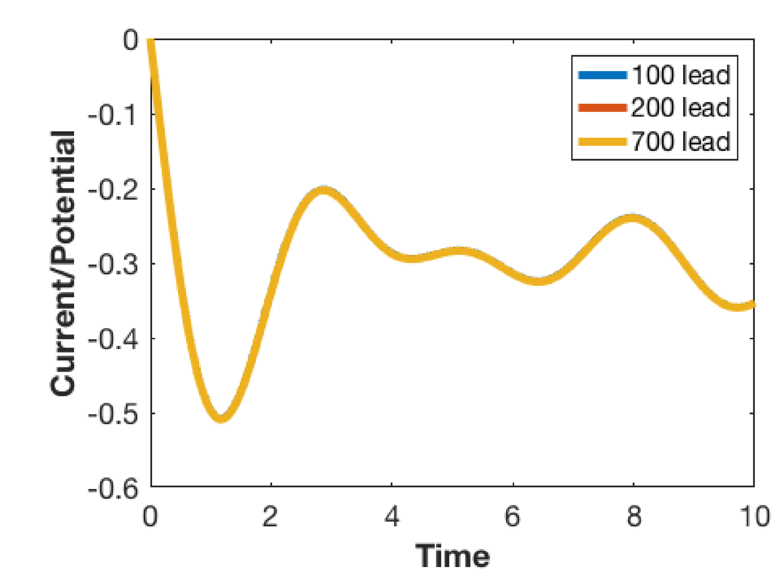


Figure 5: Current flow at constant potential (V=0.01).

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)

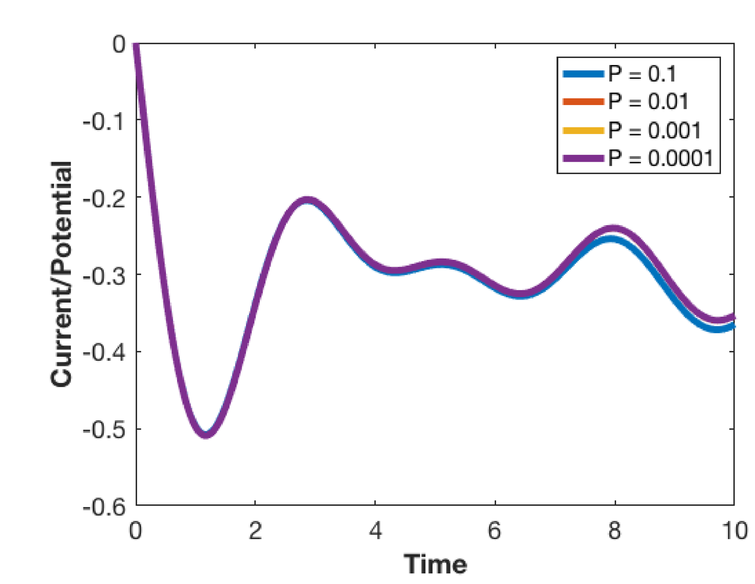


Figure 6: Current with constant leads of 600 sites

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]

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