Exploration of the Coulomb Gap

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Abstract

The competition between disorder and Coulomb interaction leads to the depletion of the single-particle density of states in the Anderson insulators near the Fermi energy known as the Coulomb gap. The Coulomb gap is a thoroughly studied phenomena in solid state physics. It was conventionally believed that in order to observe such a gap numerically, one must enforce first-order stability criterion to generate a pseudo ground state, which corresponds to ensuring that the ground state energy is minimized with respect to the single-particle hopping. We believe that only the zeroth-order stability, which ensures all occupied single-particle levels are below the Fermi level, more or less reproduces the depletion of DOS near Fermi level. We propose a probabilistic argument regarding the algorithm used for the simulation and compare our proposed theory with the conventional Efros' self-consistent theory. We also explore the validity of our arguments in power-law interactions outside of the Coulomb interaction.

I Introduction

The effects of long-range Coulomb interaction in highly disordered systems are observed in the diminishing of the single particle density of states near the Fermi level.[1][2][3][4] This phenomena is the Coulomb gap which is a soft gap in the single particle density of states for localized states. The term Coulomb gap was coined by Efros and Shlovskii; however, there were studies before by Pollak[5], Srinivasan[6] and Ambegaokar that documented and explored the diminishing of the density of states near the Fermi level due to electron-electron interaction. The Efros model, designed to simulate the Coulomb gap, is a lattice half-filled with electrons in which on-site potentials are randomly assigned and electrons are subsequently filled in sites below the Fermi level[1]. The dominance of long-range Coulomb interaction leads to similar energies being unable to be close to each other near the Fermi level[4].

These effects have been documented by many experimentalists and can be shown in numerical simulation of the Coulomb gap. The total energy of the system given by Efros is:
[2][3]

$$H = \sum_{i}^{N} \phi_i n_i + \sum_{i \neq j}^{N} \frac{q_i q_j}{r_{ij}} \tag{1}$$

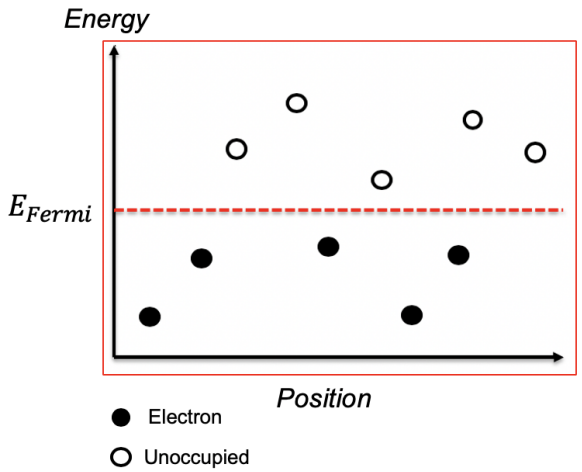

Figure 1: Efros Model Initial Lattice

Here ϕ_i is the on-site potential of site i, n_i is one if there is an electron at site i and zero if there is not an electron, q_i and q_j are the charges of sites i and j given by

$$q_{i,j} = \frac{1}{2} - n_{i,j} \tag{2}$$

Finally, r_{ij} is the distance between site i and site j. From the Hamiltonian we can derive the single particle energy as
[1]

$$E_i = \phi_i + \sum_{i \neq j}^{N} \frac{q_i}{r_{ij}} \tag{3}$$

This is the energy to bring an electron from infinity to an unoccupied site i within the lattice. Efros assumed random ordering of particles in the system and predicted the density of states of the Coulomb gap to follow

$$g(E)_{Efros} = \frac{\alpha}{1-\alpha} \mid E \mid^{\frac{d}{\alpha}-1} \tag{4}$$

Here α is the power of r in the Coulomb potential, and d is the dimension of the system. The Coulomb gap can be shown numerically by enforcing two criterion, zeroth and first-order, in the energy minimization process.[1] Zeroth-order criterion ensures that all electrons in the system are below the Fermi level. First-order criterion requires zeroth-order stability to be satisfied and that the energy to move an electron from below the Fermi level to a site above the Fermi level is a positive value. We believe the zeroth-order criterion is sufficient to simulate the Coulomb gap based on a probabilistic approach. We assume the electrons in the initial state are randomly positioned. We then argue that in order for zeroth-order stability criterion to be satisfied, all electrons must be below the Fermi level. In this case it is probabilistically favorable that the number of sites disordered to the wrong side of the Fermi level on the last step of the zeroth-order criterion is small. This number is given by

$$N \cong ln[(\frac{L}{a})^d] \tag{5}$$

Here L is the linear length of the system, and a is the distance between each site in the lattice.

This number is so small because only the last step of the zeroth-order stability criterion relaxation could push surrounding electrons to the wrong side of the Fermi level and be unaccounted for. The probability that zero sites will be pushed to the wrong side of the Fermi level is given by

$$P_{NoSites} = e^{-N} = (\frac{L}{a})^d \tag{6}$$

From this argument, we propose the single particle density of states in localized states in the system are given by

$$g(E)_{Proposed} = \frac{d^2\Gamma(\frac{d}{2})}{2\alpha\pi^{\frac{d}{2}}} \mid E \mid^{\frac{d}{\alpha}-1} \tag{7}$$

From equation 6, we expect as dimension increases there will be less variation between zeroth and first-order stability since the probability of no sites being disordered exponentially grows with dimension. In this project, we attempt to accurately simulate the Coulomb gap satisfying only zeroth-order criterion. We test the effectiveness of zeroth and first-order stability criterion in 1D, 2D, and 3D systems. We also compare the success of Efros' conventional theory to our proposed theory.

II Method

In this experiment we simulated the Coulomb gap in a highly disordered system. The gap forms when the highly disordered system is in its ground state.[4] Finding the ground state of a highly disordered system is, however, a difficult problem. Numerically, a pseudo ground state is obtained by relaxing the electrons in the lattice by two criterion. The highly disordered system was simulated by creating a virtual lattice in which positive charge $q = \frac{1}{2}$ was applied to every state. On-site energies were then randomly assigned positions with energy between a range of values $(-w, w)$. In our experiment the on-site potential spanned randomly from $(-1, 1)$. The probability distribution is given by [2]

$$P(\phi_i) = \begin{cases} \frac{1}{2w} & -w \leq \phi_i \leq w \\ 0 & (-\infty, -w) \cup (w, \infty) \end{cases}$$

The sites in the lattice below the Fermi level were occupied with an electron with charge $q = -1$ which leaves each occupied site with net charge $q = -\frac{1}{2}$, while the sites above the Fermi level were left unoccupied with net charge $q = \frac{1}{2}$. This process ideally will lead to a system in which the total charge is zero. In our simulation, there was usually minuscule net charge which was small enough that it negligibly affected our results. After the non-interacting lattice was populated with electrons, the Coulomb interaction was calculated for each electron and subsequently the single particle energy of each site. The Coulomb interaction leads to some occupied sites being excited above the Fermi level and some unoccupied sites to have energy below the Fermi level. The algorithm then searches the lattice for the electron furthest above the Fermi level and the unoccupied site furthest below the Fermi level. The occupancy of these two minimum and maximum sites are swapped. The Coulomb interaction is then recalculated for each site in the new configuration of the lattice. This process continues until there are zero occupied sites above the Fermi level and zero unoccupied sites below the Fermi level. This is the zeroth-order stability criterion of the simulation in which we believe is the only necessary criterion. First-order criterion goes a step further after the completion of zeroth-order stability criterion. The first-order stability criterion is satisfied by enforcing the following inequality when $E_i > 0$ and $E_j < 0$

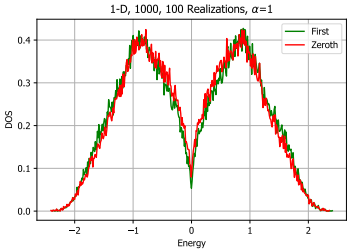

Figure 2: One Dimension

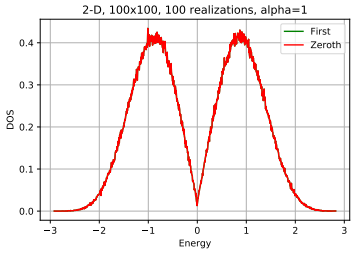

Figure 3: Two Dimensions

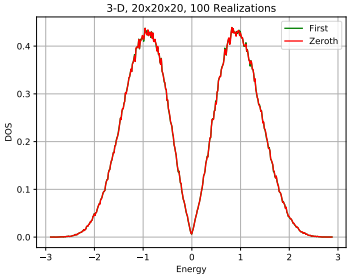

Figure 4: Three Dimensions

$$E_i - E_j - \frac{e^2}{r^\alpha} > 0 \tag{8}$$

This means that the energy to move any electron from below the Fermi level to a site above the Fermi level is greater than zero. If all of these energies are greater than zero, the system has reached the first-order criterion pseudo ground state. If the energy required to swap an electron to an unoccupied site is less than zero, then the system is not in the most energetically favorable configuration. In this case, the algorithm moves the electron to the more energetically favorable unoccupied site and relaxes the lattice by enforcing zeroth-order criterion. First order criterion is then once again enforced. This process continues until both criterion are satisfied. The single particle energies ϕ_i in the zeroth-order pseudo ground state and first-order pseudo ground state are recorded when the corresponding criterion are satisfied. The simulations of the Coulomb gap were created for 1D, 2D, and 3D lattices. The code allowed us to experiment with various parameters including the potential, the parameter for the range of on-site potentials,w, and the number of realizations in each run.

III Results and Discussion

We have found that there is obvious diminishing of the single particle density of states for localized states while only enforcing zeroth-order stability, and zeroth and first-order stability criterion behave differently in various potential and dimension.

We began our experiment by testing the effectiveness of zeroth and first-order stability criterion in one, two, and three dimensions. We noticed that as dimension increases there is less variation between zeroth and first-order stability criterion. This effect can be seen in Figure 1, Figure 2 and Figure 3. This result was expected from equation five which exponentially relates the probability of no sites being excited to the wrong side of the Fermi level to the dimension of the simulated lattice.

We explored various potentials in order to observe how first-order and zeroth-order stability criterion differ while modelling systems which are not highly disordered. For this reason we tested the simulation of many potentials. We chose to explore various potentials for a one-dimensional lattice for computational efficiency. The findings in the one-dimensional toy model can be easily generalized to more complex higher dimensional arguments. We found that in potential closer to $\alpha = 1$, α being the power of the separation,r, in the denominator of Coulomb potential, zeroth and first-order stability have more agreement. This can be shown in Figure 1 and Figures 4-8. As alpha decreases to $\alpha = 0.1$, zeroth and first-order stability become increasingly distinct from one another.

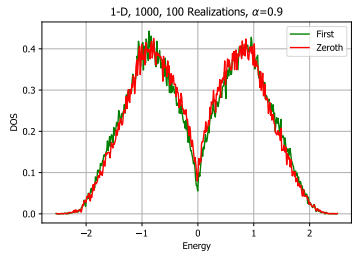

Figure 5

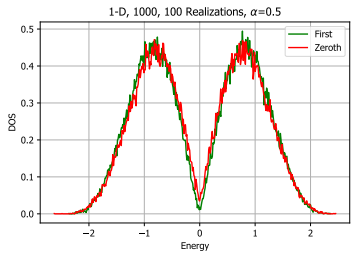

Figure 6

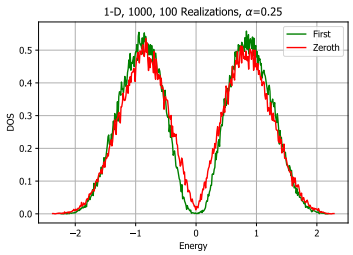

Figure 7

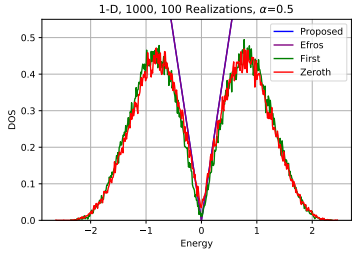

Figure 8

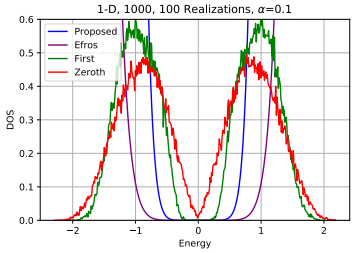

Figure 9

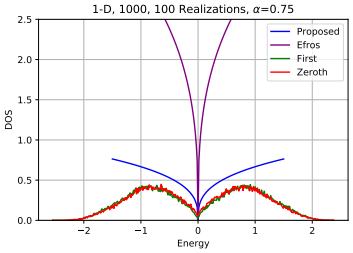

Figure 10

Theory

After evaluating how the two criterion differed in various potentials we wanted to compare our results to the Efros' original prediction for the density of states and to our new proposed prediction. Efros' prediction and our proposed prediction are in complete agreement and successful predicting the density of states for $\alpha = 0.5$. For that reason the blue proposed curve can not be seen in Figure 7. As alpha increases and decreases from this case, however, Efros' theory begins to drastically fail compared to our proposed theory as shown in Figure 8 and Figure 9. In all cases, our proposed theory either matches or exceeds the prediction by Efros' theory.

IV Conclusions

We have found explicit evidence that both zeroth and first-order stability criterion lead to a diminishing of the single particle density of states for localized states near the Fermi level. There is less variation between zeroth and first-order stability criterion in higher dimension, and as the power of the distance in Coulomb interaction decreases first and zeroth-order stability become less alike. We have also proposed a new prediction for the Coulomb gap in various potentials which fits with our data as well or better than Efros' conventional prediction in every case. Finally, we have found that the enforcement of zeroth and first-order stability criterion in multiple potentials successfully finds a configuration of the system close to the ground state. The first and zeroth-order pseudo ground state are approximations to the true ground state. The algorithm we implemented can be utilized to determine complex ground states.

V Acknowledgements

This project was conducted during the Ohio State University center for emergent materials (CEM) REU as part of NSF Materials Research Science and Engineering Center (MRSEC) with NSF Award Number DMR-1420451.

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