Anderson Localization and Polarization

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1. Introduction

Effects of randomness have supplied fundamental problems in condensed matter physics and localization due to interference of quantum mechanical electrons are well studied as the Anderson localization. Although we have well established understanding of the localization of non-interacting electrons, information of the correlated electrons with randomness is still missing. It was mainly due to lack of reliable numerical techniques for the correlated electrons. Today, for the one dimensional correlated systems without randomness, lots of numerical results are collected by the Density Matrix Renormalization Group (DMRG)$^{1,2}$ method and consistent understanding with analytical predictions has been achieved. In this paper, we plan to apply DMRG for the random electron systems by calculating direct responses of the system with electric field.$^2$ At first, random systems without interaction are carefully investigated. Then we try to treat both of interaction and randomness in one dimensional systems.

2. Model and Dielectric response

We investigate a one-dimensional spinless fermion model with nearest neighbor electron-electron interaction in the presence of random potential. The Hamiltonian is given as

$$H = -t \sum_{i=1}^{L-1} (c_{i+1}^\dagger c_i + c_i^\dagger c_{i+1}) + V \sum_{i=1}^{L-1} n_i n_{i+1} + \sum_{i=1}^{L} \epsilon_i c_i^\dagger c_i,$$

where $n_i = c_i^\dagger c_i$ and $\epsilon_i$ is random potential, which distributes over the interval $[-W/2, W/2]$ uniformly. We set $t = 1$ for simplicity and consider the half-filling case and impose an open boundary condition. In the absence of disorder, the system is metallic for $-2 < V < 2$. But for half-filling case, at $V = 2$ the system undergoes a metal-insulator transition and for $V > 2$ the system has a finite charge gap. In attractive interaction region at $V = -2$, the system becomes unstable due to phase separation. When the randomness is present, the system is always insulating due to the Anderson localization without interaction. The interplay between the randomness and interaction can be interesting and possible metallic phase is expected for some range of negative $V$.$^{3-5}$

In this paper, we focus on the dielectric response of the system. In order to observe the dielectric response, we apply the electric field $E$ to the system. As the second quantized form of the potential, $-{\partial E \over \partial x}$, the coupling term $H_E$ is added to the Hamiltonian. Then full Hamiltonian of the system is given by $H_T = H + H_E$ where

$$H_E = -E \sum_{i=1}^{L} \left( i - {L \over 2} \right) n_i.$$

As a function of $E$, the polarization $P$ of the system is defined by

$$P = -{1 \over L} \frac{\partial E_0}{\partial E} = -{1 \over L} \frac{\partial}{\partial E} \langle H_T \rangle_E = {1 \over L} \sum_{i=1}^{L} \left( i - {L \over 2} \right) \langle n_i \rangle_E (3)$$

where $E_0$ is a ground state energy and $\langle n_i \rangle_E$ represents the ground state expectation value of $n_i$. Here we used the Feynman’s theorem to derive the last equation.

For a finite value of the electric field, which is comparable to the Mott gap, we expect a collapse of the local charge gap due to the interaction. Also in the Anderson insulator, reconstruction of the charge by transferring electrons above the tunneling barrier could occur. In each case, we can obtain information of the charge degree of freedom above its ground state.

We turn next to the linear response regime. In this regime, we calculate zero-field dielectric susceptibility as

$$\chi = \frac{\partial P}{\partial E} \bigg|_{E=0} = -{1 \over L} \frac{\partial^2 E_0}{\partial E^2} \bigg|_{E=0}. (4)$$

From the susceptibility $\chi$, we directly obtain information whether the ground state is metallic or an insulator. In thermodynamic limit, $\chi$ is diverging if the system is metallic, but converging to a finite value if it is an insulator. Indeed $\chi \sim L^2$ is expected by the perturbation for the pure non-interacting system($W = 0, V = 0$).

In order to calculate the charge distribution and the ground state energy, we use the exact diagonalization for $V = 0$, and DMRG for finite $V$. For the application of DMRG, we use the extended infinite-size algorithm by Hida,$^6$ which enables us to treat also non-uniform lattice models. We perform three or four finite lattice sweep for the convergence. The retained states for the block is 60-100 to keep the truncation error to be less...
3. Results and Discussion

At first using exact diagonalization, we calculate the polarization $P$ as a function of the applied electric field $E$ in the absence of electron-electron interaction. The typical $P - E$ curve is shown in Fig. 1 and Fig. 2. The polarization $P$ is a smooth function of $E$ without randomness. As we increase the electric field from zero, $P$ is almost linearly increasing and approaches to a finite value, at which all electrons are collected to one side. Then at the critical field $E_s \sim 1/L$, $P$ saturates as $P \sim L$.

In Fig. 2, we plot the $P - E$ curve for finite randomness strength $W$. In the presence of randomness, the $P - E$ curve exhibits a stepwise behavior. This step is caused by crossing of the one particle energy levels. Namely, at some critical $E$, level crossing between the highest occupied state and the lowest unoccupied state occurs. By this process, the charge reconstruction of the ground state occurs which corresponds to the electron tunneling between localized states.

Using DMRG, we study also the systems with electron correlation. In Fig. 4, $\log \chi$ versus $\log 1/L$ for $V = -1.4$ is plotted. We averaged over 64 realizations of the disorder potential. When the randomness is sufficiently strong, we observe the saturation, which implies the localized ground state. However, we need more extensive analysis to obtain conclusive results. The detail analysis with finite size scaling will be given elsewhere.

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