Dielectric Response of the Interacting 1D Spinless Fermions with Disorder

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Dielectric responses of the one-dimensional electron system is investigated numerically. We treat an interacting one-dimensional spinless fermion model with disorder by using the Density Matrix Renormalization Group (DMRG) method which is extended for nonuniform systems. We apply an electric field $E$ to the system and calculate dielectric responses. Dielectric response of the Mott insulator and the Anderson insulator are calculated respectively. Steplike behaviors in $P - E$ curve are obtained which corresponds to breakdown of the insulating behavior. For the Mott insulator, the steps originate from generation of kink-pairs. For the Anderson insulator on the other hand, the origin of the steps is a crossing of the localized one particle energy levels. We also treat random systems with interaction. From one parameter scaling analysis of the susceptibility $\chi$, the metal-insulator transition in attractively interacting region is confirmed and a phase diagram of the random spinless fermion model is obtained.

KEYWORDS: Anderson localization, polarization, dielectric response, density matrix renormalization group

1. Introduction

Effects of randomness and interaction in electronic systems are two major problems in condensed matter physics. These two problems have been studied intensively for several decades and a lot of fundamental results are accumulated. The presence of disorder entails a localization of electronic states due to a quantum mechanical interference of the Bloch states and this phenomenon has been well studied as the Anderson localization. According to the scaling theory, all states localize in one- or two-dimensional systems without interaction, no matter how weak the randomness is. Interaction between electrons also changes states of electrons drastically. Strong Coulomb interaction can lead a metallic system to an insulator when the filling factor is rational and attractive interaction may cause superconductivity. Although we have well established understanding of the localization of non-interacting electrons, study on the correlated electrons with randomness is still unsatisfactory. It is mainly due to lack of reliable numerical techniques for the correlated electrons with randomness.  

Today, for the one-dimensional correlated systems without randomness, a lot of numer-
ical results are collected by the Density Matrix Renormalization Group (DMRG)\(^2\) method and consistent understanding with analytical predictions has been achieved.\(^3\) Recently, the DMRG was extended to random systems and it has been applied to random spin chains.\(^4\) It brings us new possibilities to investigate correlation effects on the random system. In this paper, we concentrate on dielectric responses of one-dimensional electronic systems with both randomness and interaction. Applying a finite electric field \(E\), we calculate a polarization \(P\) as a derivative of ground state energy by the field strength \(E\). Linear susceptibility \(\chi\) is also obtained numerically as a derivative of the polarization by the electric field. The polarization \(P\) reflects deviation of mass center of electrons by the field. The dielectric response is a fundamental quantity to characterize whether the system is a metal or an insulator. It is suitably defined in open boundary conditions, while Resta and Sorella defined polarization in periodic system recently.\(^5\) Hence the DMRG is naturally applied to investigating the dielectric response. Using the conventional DMRG, Aebischer \textit{et al.} investigated the dielectric response of Hubbard model with next nearest neighbor hopping by and confirmed the metal-insulator transition of the system.\(^6\) We apply the DMRG for nonuniform system by Hida\(^4\) to random fermionic systems.

We treat an interacting one-dimensional spinless fermion model in random potential. The Hamiltonian of the \(L\) site system is given as

\[
H = -t \sum_{i=1}^{L-1} (c_i^\dagger c_{i+1} + h.c.) + V \sum_{i=1}^{L-1} n_i n_{i+1} + \sum_{i=1}^{L} \epsilon_i n_i, \tag{1}
\]

where \(n_i = c_i^\dagger c_i\) and \(\epsilon_i\) is a random potential, which distributes over an interval \([-W/2, W/2]\) uniformly. We set \(t = 1\) and consider the half-filling case and impose an open boundary condition. In the absence of disorder, the system is metallic for \(-2 < V < 2\). For half-filling case, at \(V = 2\) the system undergoes a metal-insulator transition and the system has a finite charge gap for \(V > 2\). In an 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. Then the interplay between the randomness and interaction can be interesting\(^7,8\) and possible metallic phase is expected for some range of negative \(V\). Chui and Bray, and Apel treated the effect of interplay between randomness and interaction on Tomonaga model.\(^9,10\) The former authors determined critical value of the interaction constant of localize-delocalize transition by analysis of the density autocorrelation function. The latter considered the dynamic conductivity. The spin-dependent backward scattering was also treated by Chui and Bray,\(^11\) Apel and Rice,\(^12\) and Suzumura and Fukuyama.\(^13\) Giamarchi and Schulz took into account the renormalization of interaction by the disorder and obtained a phase diagram.\(^14\) Runge and Zyman, and Bouzerar and Poilblanc estimated the size of delocalized region in random interacting spinless fermion model by the exact diagonalization.\(^15,16\) Schmitteckert \textit{et al.} used the DMRG and estimated the size
of the delocalized region from analysis of the phase sensitivity.\(^{17}\)

In sec. II, we discuss on the dielectric responses of systems. Sec. III is for results and discussion. Sec. IV is a summary.

2. Dielectric response

We focus on dielectric responses of the one dimensional system. In order to observe the dielectric response directly, we apply the electric field \(E\) to the system. As a second quantized form of the potential, \(-Ex\), the coupling term
\[
H_E = -E \sum_{i=1}^{L} \left( i - \frac{L + 1}{2} \right) e n_i,
\]
(2)
is added to the Hamiltonian, where \(e\) is the charge of the electron and we set \(e = 1\) in this paper. Then the full Hamiltonian of the system is given by \(H_T = H + H_E\). As a function of \(E\), the polarization \(P\) of the system is defined as
\[
P = -\frac{1}{L} \frac{\partial E_0}{\partial E} = -\frac{1}{L} \left. \frac{\partial H_E}{\partial E} \right|_E = \frac{1}{L} \sum_{i=1}^{L} \left( i - \frac{L + 1}{2} \right) \langle n_i \rangle_E,
\]
(3)
where \(E_0\) is the ground state energy and \(\langle n_i \rangle_E\) represents the ground state expectation value of \(n_i\).\(^6\) Here we used the Feynman's theorem to derive the expression.

In the Mott insulator, for a finite value of the electric field whose potential energy is comparable with the Mott gap, we expect a collapse of the charge gap due to the interaction. Then one can expect a gap closing which is a collapse of the Mott gap at \(E_g \sim EL\) where \(E_g\) is the Mott gap. In the Anderson insulator, reconstruction of the charge occurs by transferring electrons above the tunneling barrier. The critical field strength \(E_c\) is estimated as \(E_c \sim E_{g}^{A}/L\) where \(E_{g}^{A}\) is an energy difference between the highest occupied and the lowest empty one particle states. \(E_{g}^{A}\) is of the order of \(1/L\) on the average. In each case, we can obtain information on the charge degree of freedom above its ground state.

As for a linear response regime, \(E \rightarrow 0\), we calculate zero-field dielectric susceptibility as
\[
\chi = \frac{\partial P}{\partial E}\bigg|_{E=0} = -\frac{1}{L} \frac{\partial^2 E_0}{\partial E^2} \bigg|_{E=0}.
\]
(4)

From the susceptibility \(\chi\), we directly obtain information whether the ground state is metallic or an insulator. In the 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 calculation for the pure non-interacting system\((W = 0, V = 0)\). It is also confirmed numerically for the pure interacting systems\((W = 0, -2 < V < 0)\) by the DMRG(See later).

In order to calculate the charge distribution and the ground state energy, we use the exact diagonalization for \(V = 0\), and the DMRG for the finite \(V\). In the application of the DMRG,
we use the extended infinite-size algorithm by Hida,\textsuperscript{4}) which enables us to treat non-uniform lattice models also.

3. Results

3.1 Response of the two different insulators

3.1.1 Mott insulator

We calculate the polarization $P$ in the presence of interaction for the pure systems by the DMRG. For $V = 1.0$, where the ground state of the system is the Luttinger liquid. Then the $P - E$ curve is smooth as shown in Fig. 1.\textsuperscript{18} However for $V = 6.0$, where the system is in a Mott insulator phase, the $P - E$ curve exhibits a stepwise behavior. Since the polarization corresponds to the mass center of the electrons, these steps represent a discontinuous change of the charge configuration. These steps actually come from the generation of kink-pairs. In the inset of Fig. 1, the charge distribution at $E = E_s \pm \Delta E$ are shown, where $E_s$ is the smallest value of the electric field at which the kinks are generated. At the step, the kink-pair is generated and the electrons between the kinks are shifted by one site to the right which compensates for the collapse of the Mott gap. When the kinks are separated by length $l$, the number of electrons between kinks is $l/2$. Then the energy gain of the length $l$ kinks is estimated as $\sim EL/2$. Then the first step is due to the kinks with longest length $L$.

3.1.2 Anderson insulator

We also calculated the polarization $P$ for the Anderson insulator. Fig. 2 is the $P - E$ curve for the randomness strength $W = 5$ without interaction. In the presence of randomness, the $P - E$ curve exhibits a stepwise behavior also, which is caused by crossing of one particle localized states. Matrix elements of the Hamiltonian between arbitrary localized states are exponentially small as a function of the distance. Therefore energy repulsion between the highest occupied and the lowest unoccupied states at both ends of the system is practically negligible. Then charge reconstruction of the ground state occurs which corresponds to the electron tunneling between the localized states. The inset of Fig. 2 is the charge distributions at $E = E_s \pm \Delta E$ where $E_s$ is the field strength of the step. The charge distribution near the center of the lattice is unchanged when $E$ crosses the step, but that near the edges is modified.

3.2 Linear Response Regime

3.2.1 Susceptibility of non-interacting systems

In this section we focus on the linear response region($E \ll t/L$). We calculate the susceptibility $\chi$ as a function of $L$ by numerically differentiating the ground state energy. At first, we consider the non-interacting case($V = 0$). In order to calculate $\chi$, we apply small electric field $\pm \Delta E$. $L\Delta E \sim 10^{-3}$. We need to avoid the occurrence of the step in $\pm \Delta E$. When the step occurs near $E = 0$ accidentally, we do not use the data. The number of occurrence of
such step is typically $1 \sim 2$ in 100 samples when $W$ is large ($W \sim 5$). The calculations are always carried out in the localized region except $W = 0$, then we expect $\chi \sim e^{-\xi/L}$ when the system size is sufficiently large. Therefore we take an average of $\log \chi$ as is shown in Fig. 3. We averaged over 500 realizations of the disorder potentials. For $W = 0$, $\chi$ increases as $\chi \sim L^2$ and $\chi$ seems to diverge. This implies the system is metallic. On the other hand, for $W = 3$, $\chi$ is convergent to a finite value which is consistent with the insulating ground state. For intermediate $W$, saturation of $\chi$ is not clearly observed up to $L = 500$ and only deviation from $\chi \sim L^2$ is observed. This is because the localization length $\xi$ is larger than the system length we used.

Therefore we need a finite-size scaling analysis to determine localization length $\xi$. We perform the finite-size scaling analysis by assuming

$$\frac{\chi(L)}{L^2} = g\left(\frac{\xi(W)}{L}\right),$$

where $\xi(W)$ is a localization length and $g(x)$ is a scaling function. If $L$ is much larger than $\xi$, $\chi$ becomes constant. Therefore the scaling function $g$ behaves as $g(x) \sim x^2$ for $x \to 0$. On the other hand, when $L$ is much smaller than $\xi$ ($L \ll \xi$), the wavefunction spread over entire system and the system looks like metallic. Then, $\chi \sim L^2$ is expected and the scaling function $g$ behaves as $g(x) \sim \text{const.}$ for $x \to \infty$. The scaling function $g$ we obtained for $V = 0$ is shown in Fig. 3. It shows the above-mentioned one parameter scaling hypothesis works quite well in the model.

### 3.2.2 Metal-insulator transition in attractive $V$

Using the random DMRG, we study the systems with attractive electron-electron interaction. In our implementation of the DMRG, three or four finite lattice sweeps are performed to get the convergence of the ground state energy and the number of retained states for each block is 60-100 to keep the truncation error to be less than $10^{-9}$. The susceptibility $\chi$ is calculated for various values of $V$ and $W$. The calculations are carried out up to the system size $L = 100$. We take an average over 128 realizations of the disorder potentials for $V = -1.4$ and over 64 realizations of the disorder potentials for $V = -0.5, -0.8, -1.0, -1.1, -1.2, -1.3, -1.5, -1.6$ and $-1.8$. The steps in $P - E$ curve become smoother when interaction is introduced. When $\log \chi$ is larger than 5, we consider this as an influence of the step and we do not use the data. Then we perform the finite-size scaling analysis similarly to the noninteracting case assuming the same one parameter scaling hypothesis. In order to avoid finite size effect, we use the data for $L \geq 20$ to determine the localization length $\xi$. The obtained scaling function $g$ for $V = -1.4$ is shown in Fig. 4. The scaling hypothesis for the interacting case also seems to work well in the present model. For $V = -1.8$ the $L$ dependence of $\chi$ deviates from $\chi \sim L^2$ in $L < 50$ even for $W = 0$. We could only treat systems $V \geq -1.6$ due to the finite size effects.

In Fig. 5, $W$ dependence of the localization length $\xi$ is shown for various value of $V$. 

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Note that the localization length $\xi$ is normalized by $\xi(W = 3)$. For $V = 0$, it seems that $\xi$ is divergent at $W = 0$, but for $V = -1.4$, $\xi$ increases rapidly with decreasing $W$ and diverge around $W \sim 1$.

In order to determine the critical disorder strength $W_c$, we fit the localization length $\xi$ as

$$\xi(W) = (A + B(W - W_c))(W - W_c)\beta, \quad (6)$$

where $A, B$ and $\beta$ are fitting parameters. For $V = 0$, we obtained $W_c = 0.02 \pm 0.09$ and $\beta = -2.1 \pm 0.3$, which is consistent with expected value $W_c = 0$ and $\beta = -2$.

In Fig. 6, the obtained phase diagram is shown. The vertical lines represent errorbars. This phase diagram is consistent with the one obtained from the analysis of the phase sensitivity.\textsuperscript{17}

4. Summary

In the present paper we have studied the dielectric response of the one-dimensional spinless fermion model with interaction and disorder by using the random DMRG. At first, we have calculated the polarization of the Mott insulator and the Anderson insulator. In the $P - E$ curve we observed stepwise behaviors both for the Mott insulators and the Anderson insulators. From the change of the charge distribution, we could understand the stepwise behaviors. For the Mott insulator the steps come from the generation of kink-pair and occur at $E \sim 1/L$. On the other hand, the steps for the Anderson insulator represent the crossing of the energy levels and the steps occur at $E \sim 1/L^2$. From the zero field susceptibility, we performed the finite-size scaling and determined the localization length $\xi$. Also we confirmed the existence of the metallic region in attractive interacting regime.

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References

1) P. A. Lee and T. V. Ramakrishnan: Rev. Mod. Phys. 57 (1985) 287.
2) S. R. White: Phys. Rev. Lett. 69 (1992) 2863; Phys. Rev. B 48 (1993) 10345.
3) Density-Matrix Renormalization: A New Numerical Method in Physics, edited by I. Peschel et al.
   (Springer-Verlag, Berlin, 1999).
4) K. Hida: J. Phys. Soc. Jpn. 65 (1996) 895.
5) R. Resta and S. Sorella, Phys. Rev. Lett. 82 (1992) 370.
6) C. Aebischer, D. Baeriswyl and R. M. Noack: Phys. Rev. Lett. 86 (2001) 468.
7) S. Fujimoto, N. Kawakami: Phys. Rev. B 54 (1996) R11018.
8) Y. Otsuka and Y. Hatsugai: J. Phys. Condens. Matter 12 (2000) 9317.
9) S. T. Chui and J. W. Bray: Phys. Rev. B 16 (1977) 1329.
10) W. Apel: J. Phys. C 15 (1982) 1973.
11) S. T. Chui and J. W. Bray: Phys. Rev. B 19 (1979) 4020.
12) W. Apel and T. M. Rice: Phys. Rev. B 26 (1982) 7063.
13) Y. Suzumura and H. Fukuyama: J. Phys. Soc. Jpn. 52 (1983) 2870.
14) T. Giamarchi and H. J. Schulz: Phys. Rev. B 37 (1988) 325.
15) K. J. Runge and G. T. Zimanyi: Phys. Rev. B 49 (1994) 15212.
16) G. Bouzerar and D. Poilblanc: J. Phys. I (France) 4 (1994) 1699.
17) P. Schmitteckert et al.: Phys. Rev. Lett. 80 (1998) 560.
18) M. Kishi and Y. Hatsugai: J. Phys. Soc. Jpn. 72 (2003) Suppl. A pp.147.

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Fig. 1. Polarization $P$ as a function of the applied electric field $E$. (a) For the pure system ($W = 0$).
The Luttinger liquid regime ($V = 1.0$) and the Mott insulator regime ($V = 6.0$). The system size is $L = 30$. (b) The charge distribution at each site, solid line $:E = E_s - \Delta E$, broken line $:E = E_s + \Delta E$ where $E_s$ is the value of the electric field where the stepwise behavior is observed.
Fig. 2. The polarization $P$ as a function of the applied electric field $E$, non-interacting system ($V = 0, W = 5, L = 20$). Inset: the charge distribution at $E = E_s + \Delta E$ (broken line) and $E = E_s - \Delta E$ (solid line).

Fig. 3. Left: Average log $\chi$ as a function of log 1/L. The system sizes are between 10 and 500. $V = 0$. $W = 0, 0.5, 1.5, 3.0$ and 5.0. We averaged over 500 realizations of the disorder potentials. Right: The scaling function $g$ for $V = 0$ is shown.
Fig. 4. Scaling plots of $\chi/L^2$ vs $\xi/L$ in a log-log scale. $V = -1.4$.

Fig. 5. $\xi$ vs $W$. $V = 0$ and $-1.4$. $\xi$ is scaled by the value at $W = 3$. The dashed lines show fitting curves by eq (6).

Fig. 6. Phase diagram of the half-filled spinless fermion model. The vertical lines are errorbars.