Correlations in one-dimensional disordered electronic systems with interaction

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Abstract

We investigate the effects of randomness in a strongly correlated electron model in one-dimension at half-filling. The ground state correlation functions are exactly written by products of 3×3 transfer matrices and are evaluated numerically. The correlation lengths depend on randomness when the interaction is effectively weak. On the contrary, they are completely insensitive to randomness when the interaction is effectively strong.
The behavior of electrons in the presence of randomness has attracted a lot of attentions as one of the most fundamental problems in condensed matter physics \cite{1}. In the absence of interaction, the scaling theory gives us a criterion whether states are localized or not \cite{2}. It was shown rigorously that all the states are localized for wide class of models in one dimension \cite{3}. In two dimensions, it is believed that all the states are localized. Randomness induces a metal-insulator transition in three dimensions. So far, a lot of theoretical and experimental works have been reported. However, the validity to describe the experiments by non-interacting models is an open question, since Coulomb interaction between electrons is always present.

In one dimension, some interacting models without randomness can be solved exactly by the Bethe ansatz technique or bosonization \cite{4} and the properties have been investigated. However, approaches of including randomness to such models seem to be hopeless. In the presence of randomness and without interaction, exact results were obtained on the localization of eigenstates \cite{3}. In this way, the individual investigations of models with interaction or randomness have been succeeded considerablcgly. However, it is extremely hard task to take into account them simultaneously and we have no reliable method to analyze. Although a few results by the perturbation method \cite{1} or by bosonization \cite{5} are known, even the qualitative understandings are far from satisfactory. Numerical investigations have difficulty due to the restriction of the system size. Furthermore, one needs enormous amount of CPU time for averaging over samples to obtain enough accuracy.

In this paper, we study a special model at half-filling to avoid the numerical difficulties mentioned above to investigate the effect of randomness in the strongly correlated electron model. The lattice structure is shown in Fig.\,1 and the Hamiltonian with the open boundary condition is given by

\[ H = \mathcal{P} \sum_{\sigma = \uparrow, \downarrow} \left\{ \sum_{i=1}^{L} \left[ \left( -p_{i\sigma}^\dagger p_{i\sigma} - t_{i} p_{i\sigma}^\dagger d_{i\sigma} - t_{i} p_{i+1\sigma}^\dagger d_{i\sigma} + h.c. \right) + V_{i}^d n_{i\sigma}^d \right] + n_{1\sigma}^p + n_{L+1\sigma}^p \right\} \mathcal{P}, \tag{1} \]

where a unit cell is labeled by \( i \). Here \( p_{i\sigma} \) is the annihilation operator with spin \( \sigma = \uparrow, \downarrow \) at site \( i \) with no interaction (a \( p \)-site) which have at most two electrons with opposite spins, \( d_{i\sigma} \) is the the annihilation operator at a site with infinitely large on-site Coulomb repulsion (a \( d \)-site) which can have at most one electron, and \( n_{i\sigma}^\alpha \) (\( \alpha = p, d \)) is the electron number operator. The projection operator which represents the infinitely large on-site Coulomb repulsion on \( d \)-sites is \( \mathcal{P} = \prod_{i} (1 - n_{i\uparrow}^d n_{i\downarrow}^d) \). We denote the on-site potentials for \( d \)-sites by \( V^d \)'s. For simplicity we parametrize \( t^d \)'s and \( V^d \)'s by positive \( \lambda \)'s as

\[ t_{i} = \lambda_{i}, \quad V_{i}^d = -2\lambda_{i}^2 + 2. \tag{2} \]

Then the on-site potentials at \( p \)-sites are set to be zero except at the boundaries. We shall take \( \lambda \)'s to be independent random variable. The advantages of the model (1) is that the exact and unique ground state (at half-filling) is explicitly written as

\[ |\Psi_0\rangle = \mathcal{P} \prod_{i=1}^{L} \prod_{\sigma = \uparrow, \downarrow} \left( p_{i\sigma}^\dagger + p_{i+1\sigma}^\dagger + \lambda_{i} d_{i\sigma}^\dagger \right) |0\rangle. \tag{4} \]
Without randomness, namely when λ’s are uniform, the exact ground state in a restricted parameter space was obtained [6] by following the construction introduced by Brandt and Giesekus [7]. The correlation functions and the momentum distribution functions were calculated exactly [8,9]. The correlation functions are exactly represented by products of the 3×3 transfer matrices [9,10]. Therefore, the correlation functions and the correlation lengths can be numerically obtained for considerably long chains even for random chains.

When there is neither interaction nor randomness, the ground state is a band insulator. With interaction and without randomness, the ground state is also an insulator but totally different type due to the existence of a spin gap [11]. Then the model enables us to investigate the effect of randomness to an insulating state (where the insulating behavior is due to the strong correlation). The extension of the method to other parametrizations of the model and other models of similar type is straightforward.

We take uniform randomness with width $W$

$$\lambda - \frac{W}{2} \leq \lambda_i(= t_i) \leq \lambda + \frac{W}{2}. \quad (5)$$

The probability density function for $W \leq 2\lambda$ is

$$\rho(x = V_i^d) = \begin{cases} \frac{1}{W\sqrt{8(2-x)}} & \text{for } -2\left(\lambda + \frac{W}{2}\right)^2 + 2 \leq x \leq -2\left(\lambda - \frac{W}{2}\right)^2 + 2 \\ 0 & \text{otherwise} \end{cases} \quad (6)$$

and for $W \geq 2\lambda$

$$\rho(x = V_i^d) = \begin{cases} \frac{1}{W\sqrt{8(2-x)}} & \text{for } -2\left(\lambda + \frac{W}{2}\right)^2 + 2 \leq x \leq -2\left(\lambda - \frac{W}{2}\right)^2 + 2 \\ \frac{1}{W\sqrt{2(2-x)}} & \text{for } -2\left(\lambda - \frac{W}{2}\right)^2 + 2 \leq x < 2 \\ 0 & \text{otherwise} \end{cases} \quad (7)$$

For all $W$, average is

$$\overline{V_i^d} = -2\left(\lambda^2 + \frac{W^2}{12}\right) + 2. \quad (8)$$

The difference of the on-site potentials between $p$- and $d$-sites depends both on $\lambda$ and $W$.

Without randomness, the spin, density, singlet-pair, and $\langle c_i^\dagger \sigma c_j \sigma \rangle$ correlation functions decay exponentially [6,8]. This suggests the existence of a finite excitation gap above the ground state and it was numerically confirmed [11]. Of course, on $d$-sites Coulomb interaction is always infinity. However, by choosing on-site potential $V^d$, the model interpolates between the following two limits: (i) $\lambda \to \infty$. In this limit $V^d \to -\infty$ and $\langle n^d \rangle \to 1$. Since each $d$-site is occupied by one electron, they forbid to have additional electrons. In this sense the effective interaction is strong. (ii) $\lambda \to 0$. In this limit $V^d \to 2$. Since the hopping matrix elements between $p$- and $d$-sites, $\lambda$, is infinitesimal comparing with $V^d$, one has $\langle n^d \rangle \to 0$. Thus the effective interaction is weak since no electron is in $d$-sites.

The occupation and the correlation functions are exactly written [6]
\[
\langle n_i^\alpha \rangle = \frac{\langle \Phi_{G.S.} | n_i^\alpha | \Phi_{G.S.} \rangle}{\langle \Phi_{G.S.} | \Phi_{G.S.} \rangle}
\]
\[
= \frac{\tilde{I}^\dagger \left( \prod_{k=1}^{L-k} T_k \right) N_i^\alpha \left( \prod_{k=j+1}^{L} T_k \right) \tilde{F}}{\tilde{I} \left( \prod_{k=1}^{L} T_k \right) \tilde{F}}
\]
(9)

\[
\langle O_i^\alpha O_j^\beta \rangle = \frac{\langle \Phi_{G.S.} | O_i^\alpha O_j^\beta | \Phi_{G.S.} \rangle - \langle O_i^\alpha \rangle \langle O_j^\beta \rangle}{\langle \Phi_{G.S.} | \Phi_{G.S.} \rangle}
\]
\[
= \frac{\tilde{I}^\dagger \left( \prod_{k=1}^{L-k} T_k \right) O_i^\alpha \left( \prod_{k=j+1}^{L} M_k \right) O_j^\beta \left( \prod_{k=j+1}^{L} T_k \right) \tilde{F}}{\tilde{I} \left( \prod_{k=1}^{L} T_k \right) \tilde{F}} - \langle O_i^\alpha \rangle \langle O_j^\beta \rangle,
\]
(10)

where
\[
\tilde{I} = \begin{bmatrix} 1 \\ 2 \\ 1 \end{bmatrix}, \quad \tilde{F} = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}.
\]
(11)

Here \( O^\alpha \)'s are the number, spin, creation (annihilation) of singlet-pair, or creation (annihilation) operators, and \( \alpha, \beta = p \) or \( d \). The matrices \( T \)'s, \( M \)'s, and \( O \)'s are the corresponding transfer matrices is given by
\[
T_n = \begin{bmatrix} 2\lambda_i^2 + 1 & \lambda_i^2 + 1 & 1 \\ 2\lambda_i^2 & 2\lambda_i^2 + 1 & 2 \\ 0 & \lambda_i^2 & 1 \end{bmatrix},
\]
(12)

\[
O_i^p = \begin{bmatrix} \lambda_i^2 & \lambda_i^2 + \frac{1}{2} & 1 \\ 0 & \lambda_i^2 & 1 \end{bmatrix}, \quad O_j^p = -\begin{bmatrix} \lambda_i^2 + \lambda_i^4 & \lambda_i^2 \\ \lambda_i^4 & \lambda_i^2 \\ 0 & 0 \end{bmatrix}
\]
for the correlation functions \( \langle c_i^{\sigma} c_j^{\sigma} \rangle \) (13)

\[
M_i = 1,
\]

\[
O_i^p = \begin{bmatrix} 0 & -\lambda_i^2 & -1 \end{bmatrix}, \quad O_j^p = \begin{bmatrix} 1/2 \\ 0 \\ 0 \end{bmatrix}
\]
for the spin correlation functions
(14)

\[
O_i^d = \begin{bmatrix} -\lambda_i^2 & 0 & 0 \end{bmatrix}, \quad O_j^d = \begin{bmatrix} 1/2 \lambda_i^2 \\ \lambda_i^2 \\ \lambda_i^2 \end{bmatrix}
\]

\[
M_k = T_k,
\]

\[
O_i^p = O_j^p = \begin{bmatrix} \lambda_i^2 + 1 & 1/2 & 0 \\ 2\lambda_i^2 & \lambda_i^2 + 1 & 1 \\ 0 & \lambda_i^2 & 0 \end{bmatrix}
\]
for the density correlation functions
(15)
\[
\left\{
\begin{align*}
M_i &= 1, \\
O^p_i = \begin{bmatrix} 0 & \lambda_i^2 & 1 \end{bmatrix} & O^p_j = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} & \text{for the singlet-pair correlation functions} \\
O^d_i = \begin{bmatrix} 0 & \lambda_i & 0 \end{bmatrix} & O^d_j = \begin{bmatrix} 2\lambda_i \\ 2\lambda_i \\ 0 \end{bmatrix}
\end{align*}
\]

The correlation lengths of the correlation functions between \(p\)-sites and between \(d\)-sites are the same up to order \(O(1/L)\), since only the matrices at \(i\) and \(j\) sites are different in the representation (10). Due to the same reason, the correlation lengths of the spin and the singlet-pair correlation functions are the same up to order \(O(1/L)\). For a fixed set \(\{\lambda_i\}\), we numerically evaluate the quantities

\[
\langle n^\alpha_i \rangle \equiv \frac{1}{N} \sum_{i=L_B}^{L_B+N} \langle n_i \rangle \\
\langle O^\alpha_i O^\beta_j \rangle_{m=j-i} \equiv \frac{1}{N} \sum_{i=L_B}^{L_B+N} \langle O^\alpha_i O^\beta_{i+m} \rangle,
\]

where \(N\) is the number of sites which are used for the averaging in a sample and \(L_B\) is the number of sites which is ignored to exclude contributions form the boundary. We choose \(L = 10000\), \(L_B = 2500\), and \(N = 5000\). The occupations of \(d\)-sites are shown in Fig. 2. The sizes of the error bars are smaller than those of the plotted points. Note that \(\langle n^p_i \rangle = 2 - \langle n^d_i \rangle\), since the system is half-filled. We confirmed that the correlation functions decay exponentially. The correlation lengths are given from \(\langle O^\alpha_i O^\beta_j \rangle_{m=j-i} \propto \exp\left[-m/\xi_O\right]\), where \(O = S\) for the spin and \(O = c\) for the correlation function \(\langle c_i^\dagger c_j \rangle\). The correlation lengths are estimated by least square fit for the values \(\log \langle O^\alpha_i O^\beta_j \rangle_{m=j-i} \rangle\). The estimates of \(\xi_c\) and \(\xi_S\) are shown in Figs. 3 and 4, respectively. The size of the error bars is smaller than that of the plotted points.

The behavior of the correlation lengths depends on the occupation of \(d\)-sites, namely the effective interaction. For the parameter regime \(\lambda \ll 1\) where the effective interaction is weak, the correlation lengths become short as \(W\) increases. This behavior seems to be similar to the non-interacting cases. For \(\lambda \gg 1\) where the effective interaction is strong, the correlation lengths are independent of the strength of the randomness. We obtained similar behaviors for the density and the singlet-pair correlation functions.

For the non-interacting cases, spin degree of freedom has nothing to do with the properties of the systems. For the interacting cases, on the other hand, spin degree of freedom plays an important role and the effects of randomness are likely to be different from those for the non-interacting cases. The ground state (4) is given by superpositions of spin singlet states. Within the analysis of this model, the results suggest that the states where the effective interaction is strong have a tendency to have local nature and the overlappings do not contribute much to the expectation values of the correlations. Thus their properties are stable against randomness.

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REFERENCES

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[1] For reviews, see P.A. Lee and T.V. Ramakrishnan, Rev. Mod. Phys. 57, 287 (1985); D. Belitz and T.R. Kirkpatrick, Rev. Mod. Phys. 66, 261 (1994).

[2] E. Abrahams, P.W. Anderson, D.C. Licciardello, and T.V. Ramakrishnan, Phys. Rev. Lett. 42, 673 (1979).

[3] For a review, see K. Ishii, Prog. Theo. Phys. Suppl. No. 53, 77 (1973).

[4] See, for example, The Many-Body Problem, edited by D.C. Mattis (World Scientific, Singapore, 1993).

[5] S. Fujimoto and N. Kawakami, Phys. Rev. B54, 24640 (1996).

[6] R. Strack, Phys. Rev. Lett. 70, 833 (1993).

[7] U. Brandt and A. Giesekus, Phys. Rev. Lett. 68, 2648 (1992).

[8] P.-A. Bares and P.A. Lee, Phys. Rev. B49, 8882 (1993).

[9] M. Yamanaka, S. Honjo, Y. Hatsugai, and M. Kohmoto, J. Stat. Phys. 84, 1133 (1996).

[10] H. Tasaki, Phys. Rev. Lett. 70, 3303 (1993); Phys. Rev. B49, 7763 (1993).

[11] K. Kimura, Y. Hatsugai, and M. Kohmoto, unpublished.
FIGURES

FIG. 1. The lattice structure. An open circle denotes a $p$-site (with no interaction) and a solid circle denotes a $d$-site (with infinitely large on-site Coulomb repulsion). A line represents hopping of electrons.

FIG. 2. The estimates of $\langle n^d_i \rangle$ as functions of $W$ for $\lambda = 0.1, 0.2, 0.5, 1,$ and 10.

FIG. 3. The estimates of $\xi^c$ as functions of $W$ for $\lambda = 0.1, 0.2, 0.5, 1,$ and 10.

FIG. 4. The estimates of $\xi^S$ as functions of $W$ for $\lambda = 0.1, 0.2, 0.5, 1,$ and 10.