Correlations in one-dimensional disordered electronic systems with interaction

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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. [S0163-1829(97)50912-X]

The behavior of electrons in the presence of randomness has attracted a lot of attention as one of the most fundamental problems in condensed matter physics.[1] In the absence of interactions, scaling theory gives us a criterion determining whether or not states are localized.[2] It has been shown rigorously that all the states are localized for a wide class of models in one dimension.[3] In two dimensions, it is believed that all the states are localized. Randomness induces a metal-insulator transition in three dimensions. Much theoretical and experimental work has been reported. However, the validity of describing experiments by noninteracting models is open to question, since the 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[4] and the properties have been investigated. However, including randomness in such models seems to be hopeless. In the presence of randomness and without interaction, exact results were obtained on the localization of eigenstates.[3] In this way, investigations of models with interaction or randomness alone have been successful. However, it is an extremely hard task to take account for them simultaneously. Although a few results by the perturbation method[1] or by bosonization[5–9] are known, even our qualitative understanding is far from satisfactory. Numerical investigations have limitations due to the restriction of the system size. Furthermore, one needs an enormous amount of CPU time for averaging over samples to obtain enough accuracy.

In this paper we study a special model at half-filling, allowing us to investigate the effects of randomness in a strongly correlated electron system without the numerical difficulties mentioned above. The lattice structure is shown in Fig. 1 and the Hamiltonian with the open boundary condition is given by

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

where a unit cell is labeled by i. Here $p_{i\sigma}$ is an annihilation operator with spin $\sigma=\uparrow,\downarrow$ at site i. Such a ''p site'' can 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. Such a ''d site'' can have at most one electron. $n_{i\sigma}^{\alpha}$ $(\alpha=p,\,d)$ is the electron number operator. The projection operator that represents the infinitely large on-site Coulomb repulsion on d sites is $\mathcal{P}=\Pi_i(1-n_{i\uparrow}^d n_{i\downarrow}^d)$. We denote the on-site potentials for d sites by V^d's. For simplicity we parametrize t's and V^d's by positive λ's as

$$t_i=\lambda_i, \tag{2}$$

$$V_i^d=-2\lambda_i^2+2. \tag{3}$$

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

$$|\Psi_{\mathrm{G.S.}}\rangle=\mathcal{P}\prod_{i=1}^{L}\prod_{\sigma=\uparrow,\downarrow}(p_{i\sigma}^{\dagger}+p_{i+1\sigma}^{\dagger}+\lambda_i d_{i\sigma}^{\dagger})|0\rangle. \tag{4}$$

Without randomness, namely when the λ's are uniform, the exact ground state in a restricted parameter space was obtained[10] by following the construction introduced by Brandt and Giesekus.[11] The correlation functions and the momentum distribution functions were calculated exactly.[12,13] The correlation functions are exactly represented by products of the 3×3 transfer matrices.[13,14] Therefore, the correlation functions and the correlation lengths can be obtained numerically for considerably long chains, even with randomness.

When there is neither interaction nor randomness, the ground state is a band insulator. With interaction and without

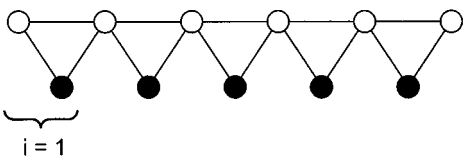

FIG. 1. The lattice structure. An open circle denotes a p site (with no interaction) and a solid circle denotes a d site (with infinitely large on-site Coulomb repulsion). A line represents hopping of electrons.

randomness, the ground state is also an insulator but of a totally different type due to the existence of a spin gap.[15] Then, the model enables us to investigate the effects of randomness on an insulating state (where the insulating behavior is due to strong correlation). Thus our results partially complement those of earlier works,[5–8] which started from metallic states. The effects of doping or other generalizations are important issues. However, it is not possible to apply our method to such cases. If one studies those cases, the numerical method can treat only very small systems. Thus one can not have reliable results that can be compared with the present ones.

We take uniform randomness with width W

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

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

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

and for $W\geqslant 2\lambda$

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

For all W, average is

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

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

Without randomness, the spin, density, singlet pair, and $\langle c_{i\sigma}^{\dagger}c_{j\sigma}\rangle$ correlation functions decay exponentially.[12,13] This suggests the existence of a finite excitation gap above the ground state, which has been confirmed numerically.[15] Of course, on d sites, the Coulomb interaction is always infinite.

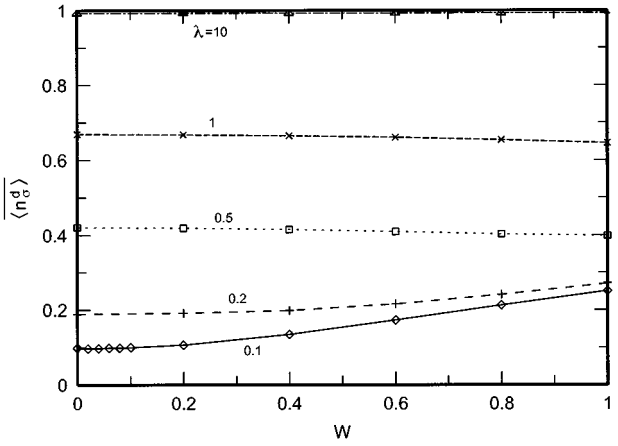

FIG. 2. The estimates of $\overline{\langle n_i^d\rangle}$ as functions of W for $\lambda=0.1$, 0.2, 0.5, 1, and 10.

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, no electrons can be added. 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, λ, is infinitesimal compared with V^d, one has $\langle n^d\rangle\to 0$. Thus the effective interaction is weak, since no electron occupies a d site.

The occupation and the correlation functions are exactly written[13]

$$\langle n_i^{\alpha}\rangle=\frac{\langle\Phi_{\text{G.S.}}|n_i^{\alpha}|\Phi_{\text{G.S.}}\rangle}{\langle\Phi_{\text{G.S.}}|\Phi_{\text{G.S.}}\rangle}=\frac{\vec{I}^t\left(\prod_{k=1}^{i-1}T_k\right)N_i^{\alpha}\left(\prod_{k=i+1}^{L}T_k\right)\vec{F}}{\vec{I}^t\left(\prod_{k=1}^{L}T_k\right)\vec{F}}, \tag{9}$$

where $|\Phi_{\text{G.S.}}\rangle$ is the ground state wave function given by (4), and

$$\begin{aligned}\langle\mathcal{O}_i^{\alpha}\mathcal{O}_j^{\beta}\rangle&=\frac{\langle\Phi_{\text{G.S.}}|\mathcal{O}_i^{\alpha}\mathcal{O}_j^{\beta}|\Phi_{\text{G.S.}}\rangle}{\langle\Phi_{\text{G.S.}}|\Phi_{\text{G.S.}}\rangle}-\langle\mathcal{O}_i^{\alpha}\rangle\langle\mathcal{O}_j^{\beta}\rangle\\&=\frac{\vec{I}^t\left(\prod_{k=1}^{i-1}T_k\right)O_i^{\alpha}\left(\prod_{k=i+1}^{j-1}M_k\right)O_j^{\beta}\left(\prod_{k=j+1}^{L}T_k\right)\vec{F}}{\vec{I}^t\left(\prod_{k=1}^{L}T_k\right)\vec{F}}\\&\quad-\langle\mathcal{O}_i^{\alpha}\rangle\langle\mathcal{O}_j^{\beta}\rangle,\end{aligned} \tag{10}$$

where

$$\vec{I}=\begin{bmatrix}1\\2\\1\end{bmatrix}, \quad \vec{F}=\begin{bmatrix}1\\0\\0\end{bmatrix}. \tag{11}$$

Here $\mathcal{O}^{\alpha}$'s are the number, spin, creation (annihilation) of singlet pair, or creation (annihilation) operators, and α, $\beta = p$ or d. The matrices T, M, and O are the corresponding transfer matrices given by

$$T_n=\begin{bmatrix}2\lambda_i^2+1 & \lambda_i^2+1 & 1\\ 2\lambda_i^2 & 2\lambda_i^2+1 & 2\\ 0 & \lambda_i^2 & 1\end{bmatrix}, \tag{12}$$

$$\begin{cases} M_k=-\begin{bmatrix}\lambda_i^2+1 & \lambda_i^2\\ 1 & 1\end{bmatrix} \\ O_i^p=\begin{bmatrix}\lambda_i^2 & \lambda_i^2+\frac{1}{2} & 1\\ 0 & \lambda_i^2 & 1\end{bmatrix} \quad O_j^p=-\begin{bmatrix}\lambda_i^2+\lambda_i^4 & \lambda_i^2\\ \lambda_i^4 & \lambda_i^2\\ 0 & 0\end{bmatrix} \quad \text{for the correlation functions } \langle c_{i\sigma}^{\dagger}c_{j\sigma}\rangle, \\ \mathcal{O}_i^d=-\begin{bmatrix}\lambda_i & \frac{1}{2}\lambda_i & 0\\ 0 & \frac{1}{2}\lambda_i & 0\end{bmatrix} \quad O_j^d=-\begin{bmatrix}\lambda_i & \lambda_i\\ \lambda_i & 2\lambda_i\\ 0 & \lambda_i\end{bmatrix}, \end{cases} \tag{13}$$

$$\begin{cases} M_i=1, \\ O_i^p=[0 \quad -\lambda_i^2 \quad -1] \quad O_j^p=\begin{bmatrix}\frac{1}{2}\\0\\0\end{bmatrix} \text{ for the spin correlation functions,} \\ O_i^d=[-\lambda_i^2 \quad 0 \quad 0] \quad O_j^d=\begin{bmatrix}\frac{1}{2}\lambda_i^2\\ \lambda_i^2\\ \frac{1}{2}\lambda_i^2\end{bmatrix}, \end{cases} \tag{14}$$

$$\begin{cases} M_k=T_k, \\ O_i^p=O_j^p=\begin{bmatrix}\lambda_i^2+1 & \frac{1}{2} & 0\\ 2\lambda_i^2 & \lambda_i^2+1 & 1\\ 0 & \lambda_i^2 & 0\end{bmatrix} \text{ for the density correlation functions,} \\ O_i^d=O_j^d=\begin{bmatrix}\lambda_i^2 & \lambda_i^2 & 0\\ \frac{1}{2}\lambda_i^2 & \lambda_i^2 & \frac{1}{2}\lambda_i^2\\ 0 & 0 & 0\end{bmatrix}, \end{cases} \tag{15}$$

$$\begin{cases} M_i=1, \\ O_i^p=[0 \quad \lambda_i^2 \quad 1] \quad O_j^p=\begin{bmatrix}1\\0\\0\end{bmatrix} \text{ for the singlet-pair correlation functions,} \\ O_i^d=[0 \quad \lambda_i \quad 0] \quad O_j^d=\begin{bmatrix}2\lambda_i\\ 2\lambda_i\\ 0\end{bmatrix}. \end{cases} \tag{16}$$

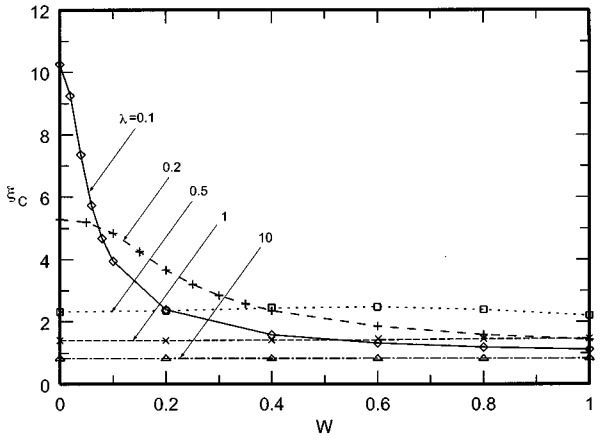

FIG. 3. The estimates of ξ_c as functions of W for $\lambda = 0.1$, 0.2, 0.5, 1, and 10.

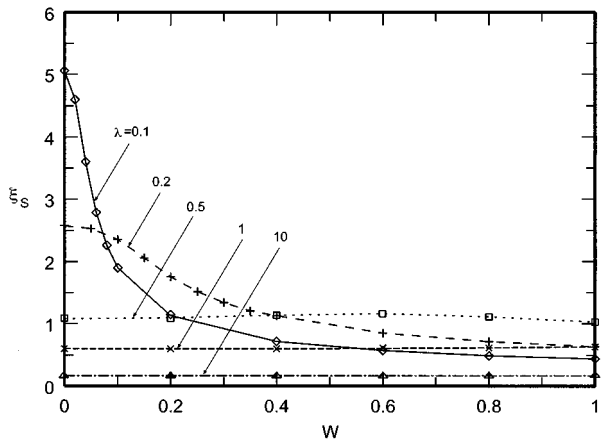

FIG. 4. The estimates of ξ_S as functions of W for $\lambda = 0.1$, 0.2, 0.5, 1, and 10.

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

$$\overline{\langle n_i^\alpha \rangle} \equiv \frac{1}{N} \sum_{i=L_B}^{L_B+N} \langle n_i \rangle,$$

$$\overline{\langle \mathcal{O}_i^\alpha \mathcal{O}_j^\beta \rangle}_{m=j-i} \equiv \frac{1}{N} \sum_{i=L_B}^{L_B+N} \langle \mathcal{O}_i^\alpha \mathcal{O}_{i+m}^\beta \rangle, \tag{21}$$

where N is the number of sites that are used for the averaging in a sample and L_B is the number of sites that are ignored to exclude contributions from 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 $\langle n_i^p \rangle = 2 - \langle n_i^d \rangle$, since the system is half-filled. We confirmed that the correlation functions decay exponentially. The correlation lengths are given from $\overline{\langle \mathcal{O}_i^\alpha \mathcal{O}_j^\beta \rangle}_{m=j-i} \propto \exp[-m/\xi_O]$, where $O=S$ for the spin and $O=c$ for the correlation function $\langle c_{i\sigma}^\dagger c_{j\sigma} \rangle$. The correlation lengths are estimated by least-squares fit for the values $\log_{10}[\overline{\langle \mathcal{O}_i^\alpha \mathcal{O}_j^\beta \rangle}_{m=j-i}]$. The estimates of ξ_c and ξ_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 noninteracting 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 noninteracting cases, the spin degree of freedom has nothing to do with the properties of the systems. For the interacting cases, on the other hand, the spin degree of freedom plays an important role and the effects of randomness are likely to be different from those for the noninteracting 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 local nature, with overlappings contributing negligibly to the expectation values of the correlations. Thus their properties are stable against randomness.

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