Nature of carriers in one-dimensional correlated electron systems

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Electron densities at the edge site in one-dimensional Hubbard model and \textit{t-J} model are studied by using the Bethe ansatz solutions and exact diagonalization method. It is found that the boundary is electron-attractive, or equivalently hole-repulsive, near half-filling. We propose a new criterion to determine whether the carriers in a strongly correlated system are electron-like or hole-like depending on the electronic behavior at the boundary.

A suitably substituted impurity atom in condensed matter systems can play a role as an atomic scale probe for local response of the system. In particular in strongly correlated electron systems, the response to an impurity offers a key to understand the nontrivial properties of the system. Therefore, a large number of studies have been carried out on the impurity effects in the strongly correlated electron systems, especially in high-\textit{T}_\text{c} superconductors. One of the most important findings concerning the impurity effects in high-\textit{T}_\text{c} superconductors is the appearance of local magnetic moments around a non-magnetic impurity, such as Zn or Li atom, substituted for Cu in the CuO\textsubscript{2} plane in underdoped compounds. \textsuperscript{1,2,3,4,5}

Recently, we have pointed out that whether the impurity in the CuO\textsubscript{2} plane tends to expel electrons or holes is crucial for the appearance of induced moments or the local enhancement of antiferromagnetic (AF) correlation \textsuperscript{6}. If the system is in the overdoped region, it has been shown that electrons are expelled from the neighborhood of the impurity and thus a hole-rich region is locally formed around the impurity. As a result, AF correlation is collapsed because the effective exchange coupling between electrons is locally suppressed. Conversely, if the nature of the carriers is hole-like in the underdoped region or close to half-filling, we expect that the holes are scattered by the impurity and then an electron-rich region is formed around the impurity. If this is the case, it is natural to consider that local magnetic moments appear near the impurity since the local region approaches half-filling. Therefore, it is very important to clarify the nature of carriers in correlated electron systems, on which the local magnetism around an impurity strongly depends.

In the two-dimensional systems, however, it is difficult to determine the nature of carriers doped in the Mott insulator. Slave-boson mean-field theory suggests that the charge degrees of freedom can be represented as a small number of holons, however this naive picture is uncertain because there exists the large Gauge fluctuation. In this paper, we investigate the nature of carriers in one-dimensional (1D) systems where the essence of strong correlation can be clarified in exact solutions.

It is worthwhile noting here that even in 1D systems, the nature of carriers has not been understood because there is no Hall effect. Thermopower was suggested to clarify the charge of the carriers, but its calculation is only phenomenological \textsuperscript{7}. Instead of these quantities we propose that the local electron density near the impurity gives a good quantity for determining whether the carriers are hole-like or electron-like. When the impurity is repulsive, it scatters the mobile carrier. Near half-filling, we expect that the holes are scattered and the hole density should decrease around the impurity. Using this criterion we determine the phase diagram in the 1D Hubbard model.

When we assume the impurity scattering is in the unitarity limit, the impurity is equivalent to the boundary in 1D systems. We calculate the electron density at the edge site of the 1D Hubbard model and \textit{t-J} model with boundary by using the Bethe ansatz solutions\textsuperscript{8,9,10,11,12,13} and the exact diagonalization method.

The Hamiltonian of the open Hubbard chain with boundary fields, \( p_1 \) and \( p_L \), is given as

\[
\mathcal{H}_{\text{Hub}} = - \sum_{j=1}^{L-1} \left( c_{j\sigma}^\dagger c_{j+1\sigma} + \text{h.c.} \right) + U \sum_{j=1}^{L} n_{j\uparrow} n_{j\downarrow} \\
+ \mu \sum_{j=1}^{L} (n_{j\uparrow} + n_{j\downarrow}) \\
- p_1 (n_{1\uparrow} + n_{1\downarrow}) - p_L (n_{L\uparrow} + n_{L\downarrow}),
\]

(1)

following the notation in ref. \textsuperscript{9}. The hopping integral, \( t \), has been taken as a unit of energy (\( t = 1 \)). We describe the length of the chain by \( L \), which is assumed to be an even integer. The average number of electrons at the edge site \( \langle n_1 \rangle \) taken with respect to the ground state \( |\Phi_0\rangle \) is obtained from

\[
n_1 = - \frac{\partial}{\partial p_1} \langle \Phi_0 | \mathcal{H}_{\text{Hub}} | \Phi_0 \rangle.
\]

(2)

The Bethe ansatz equations for the above Hamiltonian
where \( n = U/4, N \) is the total number of electrons and \( M \) is the number of down spins \( \mathbf{4} \). In this letter, we only discuss the repulsive Hubbard model. For this case it is useful to denote the negative \( k_j \)'s and \( \lambda \)'s as \( k_j = -k_{-j}, \lambda_{-\lambda} = -\lambda \). Using standard procedures, the Bethe ansatz equations for the ground state can be rewritten as the following linear integral equations for \( \sigma^c_L(k) \) and \( \sigma^s_L(\lambda) \), which represent the densities of solutions for the real quasimomenta \( k_j \) and spin rapidities \( \lambda \):

\[
\begin{align*}
\sigma^c_L(k|k^+, \lambda^+) &= \frac{1}{\pi} + \frac{1}{\pi L} \frac{dp_0}{dk} \\
+ \frac{\cos k}{2\pi} \int_{-\lambda^+}^{\lambda^+} d\lambda' K_1(\sin k - \lambda') \sigma^s_L(\lambda'|k^+, \lambda^+) ,
\end{align*}
\]

\[
\sigma^s_L(\lambda|k^+, \lambda^+) = \frac{1}{\pi} \frac{dg_0}{dk}
+ \frac{1}{2\pi} \int_{-k^+}^{k^+} dk' K_2(\lambda - \sin k') \sigma^c_L(k'|k^+, \lambda^+)
- \frac{1}{2\pi} \int_{-\lambda^+}^{\lambda^+} d\lambda' K_2(\lambda' - \lambda) \sigma^s_L(\lambda'|k^+, \lambda^+),
\]

where

\[
K_1(x) = \frac{2u}{u^2 + x^2}, \quad K_2(x) = \frac{4u}{4u^2 + x^2},
\]

are the standard kernel for the Hubbard model, and

\[
p_0(k) = k + \frac{1}{2} \theta_0(k, p_1) + \frac{1}{2} \theta_0(k, p_L) - \tan^{-1} \frac{\sin k}{u},
\]

\[
q_0(\lambda) = -\tan^{-1} \frac{\sin \lambda}{2u}, \quad \theta_0(k, p) = 2\tan^{-1} \left( \frac{p \sin k}{1 - p \cos k} \right).
\]

The values of \( k^+ \) and \( \lambda^+ \) are determined from the conditions

\[
\int_{-k^+}^{k^+} d\sigma^c_L(k|k^+, \lambda^+) = \frac{2N + 1}{L}, \\
\int_{-\lambda^+}^{\lambda^+} d\sigma^s_L(\lambda|k^+, \lambda^+) = \frac{2M + 1}{L}.
\]

In one-dimensional systems with open boundaries, the first finite-size correction for the ground state energy \( E_L \) is of order \( L^0 \), which is the contributions from the boundary. Thus the ground state energy of the present model can be written as

\[
E_L = L e_\infty(k^+, \lambda^+) + e_1(k^+, \lambda^+) + O(1/L)
\]

with

\[
e_\infty(k^+, \lambda^+) = \frac{1}{2\pi} \int_{-k^+}^{k^+} dk \varepsilon_c(k),
\]

\[
e_1(k^+, \lambda^+) = \frac{1}{2\pi} \int_{-k^+}^{k^+} dk \varepsilon_c(k) \frac{dp_0}{dk}
+ \frac{1}{2\pi} \int_{-\lambda^+}^{\lambda^+} d\lambda \varepsilon_s(\lambda) \frac{dp_0}{d\lambda} + 1 - \frac{\mu}{\mathbf{2}}.
\]

Here, \( \varepsilon_c(k) \) and \( \varepsilon_s(\lambda) \) are the dressed energies defined as

\[
\varepsilon_c(k) = -2\cos k + \mu
+ \frac{1}{2\pi} \int_{-\lambda^+}^{\lambda^+} d\lambda K_1(\sin k - \lambda) \varepsilon_s(\lambda),
\]

\[
\varepsilon_s(\lambda) = \frac{1}{2\pi} \int_{-k^+}^{k^+} dk' \cos k' K_1(\lambda - \sin k') \varepsilon_c(k')
- \frac{1}{2\pi} \int_{-\lambda^+}^{\lambda^+} d\lambda K_2(\lambda - \lambda') \varepsilon_s(\lambda').
\]

If the energy \( E_L \) in the thermodynamic limit is minimized for \( k^+ = k_0 \) and \( \lambda^+ = \lambda_0 \), the parameters \( k_0 \) and \( \lambda_0 \) are obtained by

\[
\frac{\partial e_\infty}{\partial k^+} \bigg|_{k^+ = k_0} = 0, \quad \frac{\partial e_\infty}{\partial \lambda^+} \bigg|_{\lambda^+ = \lambda_0} = 0.
\]

These conditions are equivalent to

\[
\varepsilon_c(k_0) = 0, \quad \varepsilon_s(\lambda_0) = 0,
\]

which are the same as in the periodic-boundary case.

Now we expand \( e_\infty \) and \( e_1 \) up to the second order in \( \Delta k = k^+ - k_0 \) and \( \Delta \lambda = \lambda^+ - \lambda_0 \). As far as the conditions eq. \( \mathbf{1} \) are satisfied, we find \( \Delta k \) and \( \Delta \lambda \) are of the order of \( 1/L \), and \( k^+ \) and \( \lambda^+ \) in eq. \( \mathbf{1} \) can be replaced by \( k_0 \) and \( \lambda_0 \), whose values are determined from the conditions

\[
\int_{-k_0}^{k_0} d\sigma^c_L(k) = \frac{2N}{L}, \quad \int_{-\lambda_0}^{\lambda_0} d\sigma^s_L(\lambda) = \frac{2M}{L}.
\]
Here $\sigma_0^\infty(k)$ and $\sigma_0^\infty(\lambda)$ are obtained by taking the limit of $L \rightarrow \infty$ in eqs. 12 and 13. Since $\lambda_0 = \infty$ for the case of $N = 2M$, $\sigma_0^\infty(\lambda)$ can be solved from the Fourier transformation. Substituting $\sigma_0^\infty(\lambda)$ into the integral equation for $\sigma_0^\infty(k)$, we obtain

$$\sigma_0^\infty(k) = \frac{1}{\pi} + \cos k \int_{-k_0}^{k_0} dk' R_k R(k - \sin k') \sigma_0^\infty(k')$$

with

$$R_k(k) = \frac{1}{2\pi} \int_{-k_0}^{k_0} dx \frac{e^{-ikx}}{1 + e^{2aNx}}.$$  

Finally to obtain $e_1(k_0, \lambda_0)$, we need $\varepsilon_c(k)$ and $\varepsilon_s(\lambda)$. In the same way as $\sigma_0^\infty(k)$, we have

$$\varepsilon_c(k) = -\cos k + \mu + \int_{-k_0}^{k_0} dk' R_k R(k - \sin k') \cos k' \varepsilon_c(k').$$

As a result, the electron density at the edge site is given by

$$n_1 = \frac{\partial e_1}{\partial p_1} \bigg|_{p_1=0} = -\frac{1}{2\pi} \int_{-k_0}^{k_0} dk \varepsilon_c(k) \cos k.$$  

In the actual calculation, we solve eqs. 13 and 14 to obtain $k_0$ and $\sigma_0^\infty(k)$ for each value of $U/t$ and $N/L$. Then using the obtained $k_0$, we solve $\varepsilon_c(k)$ in eq. 16 to calculate $n_1$.

Figure 1 shows the obtained $n_1$ as a function of the electron density, $n = N/L$, of the whole system. In the noninteracting case ($U/t = 0$), $n_1$ is always smaller than $n$ in less-than-half-filling case ($n < 1$), which means that the carriers are electrons. For $n > 1$, $n_1$ can be easily obtained from the electron-hole symmetry and is larger than $n$, indicating that the carriers are hole-like. As $U/t$ increases, the crossover point from $n_1 > n$ to $n_1 < n$ approaches $n = 0.5$ from $n = 1$. If we take the limit of $U/t \rightarrow \infty$, the $n_1-n$ relation is just half-size of that for $U/t = 0$, i.e., $n = 2$ for $U/t = 0$ corresponds to $n = 1$ for $U/t \rightarrow \infty$. This can be easily understood because the charge degrees of freedom are expressed as a Slater determinant of spinless fermions [14]. Thus, $n = 0.5$ means the half-filled band of the spinless fermions.

Figure 2 shows the crossover points as a function of $t/U$. Apparently, in the region of $n \sim 1$ and large $U/t$, $n_1$ is larger than $n$. From these results, we interpret that the holes are scattered by the impurity (in this case, by the boundary) and thus the nature of carriers in this region is hole-like. This is one of the typical effects of strong correlation in the doped Mott insulator.

Next we study the same problem in the $t$-$J$ model. The Hamiltonian of the open $t$-$J$ chain with boundary fields is given as

$$\mathcal{H}_{t-J} = -t \sum_{j=1}^{L-1} \sum_{\sigma} P_G \left( c_{j,\sigma}^\dagger c_{j+1,\sigma} + \text{h.c.} \right) P_G$$

following the notation in ref. 13. The Bethe ansatz equations for the open $t$-$J$ model are available only when $J/t = 2$ under periodic [13] and open boundary conditions [12, 13]. Following the same procedure as for the Hubbard model, we obtain the electron density at the edge site. For the other values of $J/t$, we calculate $n_1$ in the exact diagonalization of the system with 16 sites.

Figure 3 shows the results of the $t$-$J$ model in the same manner as in Fig. 1. Note that $J/t = 0$ corresponds to $U/t \rightarrow \infty$ in the Hubbard model. The exact diagonalization (ED) results show that, as $J/t$ increases, $n_1$ decreases for any values of $n$ and hole-like region shrinks. This behavior is consistent with that of the Hubbard model in the large $U$ region. For $J/t = 2$, the ED results slightly overestimate the value of $n_1$ compared to the Bethe ansatz (BA) results. This is the finite size ef-
fect, i.e., there is no enough space where electrons escape from the boundary in small systems.

It is interesting to compare the results for the $t$-$J$ model with that for the Hubbard model. For $J/t = 2$, the BA result shows that $n_1 < n$ for any values of $n$, which means that the carrier is always electron-like. Actually, the result for $J/t = 2$ is very close to that for the free fermion case ($U/t = 0$ in Fig. 1). The reason is as follows. When $J/t = 2$, the electron motions driven by the hopping term and by the exchange term have the same amplitude $t = J/2$. Therefore, electrons can move almost independently with each other and thus a free electron-like behavior can be seen for $J/t = 2$. Furthermore the result for $J/t = 1$ is close to that for $U/t = 4$, which is consistent with the relation between $J$ and $U$, i.e., $J = 4t^2/U$. Even though the so-called three-site terms, which appear in the perturbation theory with respect to $t/U$, are neglected in eq. (18), we can see that the nature of carriers has a strong correspondence between the Hubbard model and the $t$-$J$ model when $J/t \lesssim 1$.

In summary, we have investigated the electron number at the edge site of the one-dimensional Hubbard model and $t$-$J$ model by using the Bethe ansatz solutions and the exact diagonalization method. We propose a new criterion to determine whether the carriers in strong correlated systems are electron-like or hole-like, which is usually difficult in 1D because of the lack of the Hall effect. We expect the similar behavior in 2D Hubbard model or $t$-$J$ model. Although reliable estimation of the crossover point will be difficult, it is natural to expect that the carriers are hole-like (or holons) near half-filling, which causes the local magnetic moments around impurities. As the system approaches half-filling, the number of the hole-like carriers decreases leading to the metal-insulator transition.

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