Dynamical Charge Structure Factor of a One-Dimensional Ionic Hubbard Model in the Low-Energy Region

Yuhei Komaki¹, Shogo Yanagimatsu², Yoshiyuki Muta², Nobuya Maeshima³,⁴*, and Ken-ichi Hino³,⁴

¹Doctoral Program in Materials Science, Graduate School of Pure and Applied Sciences, University of Tsukuba, Tsukuba, Ibaraki 305-8573, Japan
²College of Engineering Sciences, University of Tsukuba, Tsukuba 305-8573, Japan
³Center for Computational Sciences, University of Tsukuba, Tsukuba 305-8577, Japan
⁴Division of Materials Science, University of Tsukuba, Tsukuba 305-8573, Japan

(Received November 1, 2018)

We present a numerical study of the charge dynamical structure factor \(N(k, \omega)\) of a one-dimensional (1D) ionic Hubbard model in the Mott insulator phase. We show that the low-energy spectrum of \(N(k, \omega)\) is expressed in terms of the spin operators for the spin degrees of freedom. Numerical results of \(N(k, \omega)\) for the spin degrees of freedom, obtained by the Lanczos diagonalization method, well reproduce the low-energy spectrum of \(N(k, \omega)\) of the 1D ionic Hubbard model. In addition, these dominant spectral peaks are found to probe the dispersion of the spin-singlet excitations of the system.

KEYWORDS: strongly correlated electron systems, spinon, singlet excitation, dynamical structure factor

The ionic Hubbard model, a Hubbard model with an alternating single-electron potential, has been extensively studied from several points of view in condensed matter physics, such as a quantum phase transition,¹⁻⁸ the existence of a non-trivial intermediate phase,¹⁻⁴ superconductivity,⁹,¹⁰ ferromagnetism,¹¹ ferroelectric properties of transition-metal oxides,¹² and the so-called neutral-ionic transition of mixed-stack organic complexes.¹³,¹⁴

Ground state properties of the ionic Hubbard model at half-filling are mainly governed by the competition between the on-site Coulomb interaction \(U\) and the alternating potential \(\Delta\). For \(\Delta \gg U\), the periodicity of the lattice makes the system to the band insulator (BI) phase while, for \(U \gg \Delta\), the strong on-site interaction leads the system to the Mott insulator (MI) phase. The existence of the intermediate phase between them has been established in one-dimensional (1D) systems.¹⁻⁴

Properties of excited states of this model are also governed by \(U\) and \(\Delta\). In the BI phase, excited states are described by using the particle, hole, and their pair excitations while, in the MI phase, there exist low-lying spin excitations and charge excitations with the higher energy of the order of \(U\). Focusing on 1D systems, continuous unitary transformation method is applied to study excited states of the BI phase.¹⁵⁻¹⁷ In the vicinity of the boundary between BI and MI, domain wall excitations are investigated for the 1D system related to a mixed-stack organic complex TTF-CA.¹⁴ In the MI phase, a theoretical work by Katsura et al. has analytically demonstrated that, in the optical conductivity \(\sigma(\omega)\), spin excitations have finite intensity ascribed to the finite \(\Delta\).¹⁸ Some of the authors and a coworker also have numerically confirmed that there appear spectral peaks resulting from the spin excitations in \(\sigma(\omega)\).¹⁹

Here it should be noted that, in general, excitations with the wave number \(k = 0\) are probed by \(\sigma(\omega)\) while the excitations with \(k \neq 0\) are detected by the dynamical charge structure factor \(N(k, \omega)\).²⁰ Thus the preceding studies for the MI phase imply that the spin excitations with \(k \neq 0\) can be detected by \(N(k, \omega)\). In this work, we have studied low-energy properties of \(N(k, \omega)\) of the 1D ionic Hubbard model in the MI phase. We represent the charge deviation per site and \(N(k, \omega)\) in terms of the spin operators of the spin degrees of freedom of this model, and then, numerically calculated these quantities by using the Lanczos diagonalization method. Obtained results of \(N^s(k, \omega)\), the contribution to \(N(k, \omega)\) from the spin degrees of freedom, well reproduce the low-energy component of \(N(k, \omega)\). In addition, dominant spectral peaks of \(N^s(k, \omega)\) are in good agreement to the dispersion of the two-spinon singlet excitations obtained by the Bethe ansatz for the uniform chain. Thus the spin-singlet excitations can be probed by examining \(N(k, \omega)\) in the ionic Hubbard model. This is also confirmed for the bond alternating chain.

The Hamiltonian of the 1D ionic Hubbard model reads

\[
\mathcal{H} = -\sum_{ij\sigma} t_{ij} c_{i\sigma}^{\dagger} c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} + \sum_i \varepsilon_i (n_i - 1), \quad (1)
\]

where \(c_{i\sigma}^{\dagger} (c_{i\sigma})\) is the creation (annihilation) operator of an electron with spin \(\sigma\) at site \(i\), \(n_{i\sigma} = c_{i\sigma}^{\dagger} c_{i\sigma}\), and \(n_i = n_{i\uparrow} + n_{i\downarrow}\). The parameter \(t_{ij}\) denotes the transfer

*maeshima@ims.tsukuba.ac.jp
The dynamical charge structure factor of this system is given by

\[ N(k, \omega) = \frac{1}{N} \sum_{\alpha} \left| \langle \alpha | n_k | 0 \rangle \right|^2 \delta(\omega - E_\alpha + E_0), \]

(2)

where \( n_k = \sum_i e^{-ikl} n_l \) and \( k = 2\pi n/N(n = 0, 1, \ldots, N-1) \) is the wave number. We note that \( n_l \) is replaced by the charge deviation from the unity integral and we set \( t_{ij} = 0 \) for \( j \neq i \pm 1 \) for describing the 1D system with only the nearest-neighbor hopping. The on-site Coulomb interaction is represented by \( U \) and the site-dependent potential at site \( i \) is defined by \( e_i = (-1)^i \Delta/2 + \phi_i \), where \( \Delta \) is the strength of the alternating potential and \( \phi_i \) represents an external scalar field. We focus on the case of the half-filling and thus the total number of the electron is equivalent to the system size \( N \).

Fig. 1. (Color online) The charge deviation \( \delta n_l \) and \( \delta n_l^s \) for the uniform chain with \( U/t = 20 \) and \( N = 12 \).

By using these results, \( \delta n_k^s \) is derived as

\[ \delta n_k^s = \sum_{l,j} e^{-i(k+\pi)\eta} \sum_{l,j} \left( S_i \cdot S_j - \frac{1}{4} \right), \]

(8)

which suggests that the state \( \delta n_k^s | 0 \rangle^s \) has the wave number \( k + \pi \). Then the \( \alpha \)-th eigenstate \( | \alpha \rangle^s \) of the model (3), having finite matrix element \( \langle \alpha | \delta n_k^s | 0 \rangle^s \), also has the wave number \( k + \pi \) within the Hilbert space of the model. That is, \( N^*(k, \omega) \) probes excited states with the wave number \( k + \pi \), and therefore, when \( N^*(k, \omega) \) is plotted below, the wave number is shifted by \( \pi \).

In actual calculations, we use the Lanczos diagonalization to calculate eigenstates including the ground state \( |0\rangle \) and other quantities. Here it should be also noted that we impose the periodic boundary condition. As for the dynamical charge structure factor the \( \delta \)-function is replaced by the Lorentzian with finite broadening \( \epsilon = 0.01t \).

First, we deal with the uniform chain. Before analyzing the charge dynamical structure factor, we confirm that the charge deviation (6) gives valid results. Figure 1 shows \( \delta n_l \) of the ionic Hubbard chain and \( \delta n_l^s \) of the Heisenberg chain for even site (\( l = 0 \)) and odd site (\( l = 1 \)) in an \( N = 12 \) system with \( U/t = 20 \). It can be seen that the results of \( \delta n_l \) and \( \delta n_l^s \) are in good agreement, showing that the formula (6) works well.

Results of \( N(k, \omega) \) and \( N^*(k, \omega) \) for the uniform chain with \( U/t = 20, \Delta/t = 2, \) and \( N = 16 \) are displayed in Fig. 2. We can see that \( N^*(k, \omega) \) shows almost the same peak structure as \( N(k, \omega) \). It is also found that the dominant spectral peaks are located around \( k = \pi/2 \) and \( 3\pi/2 \), which are clearly different from those of the spin structure factor

\[ S(k, \omega) = \frac{1}{N} \sum\sum_{\alpha} \left| \langle \alpha | S_k^\alpha | 0 \rangle \right|^2 \delta(\omega - E_\alpha + E_0), \]

(9)

where \( S_k^\alpha = \sum l e^{-ikl} S_l^\alpha \) (see Fig. 3). However, the region where the peaks of \( N(k, \omega) \) exist is almost the same.
as that of \( S(k, \omega) \); both are inside the upper and lower bounds of the two-spinon excitation in the thermodynamic limit,\(^{21,22}\) suggesting that \( N(k, \omega) \) mainly probes the two-spinon excitations similar to \( S(k, \omega) \).\(^{21,24}\) To further examine excited states contributing to \( N(k, \omega) \) we calculate the two-spinon singlet and triplet excitations of the 1D Heisenberg model with \( N = 16 \) using the Bethe ansatz following Ref. 25. It can be found that the main spectral peaks of \( N(k, \omega) \) are coincident with the two-spinon singlet excitations while those of \( S(k, \omega) \) are coincident with the two-spinon triplet excitations. Thus our results suggest that by probing \( N(k, \omega) \) we obtain the dispersion relation of the two-spinon singlet excitations. This is consistent with that \( \delta n^\sigma \) commutes with the total spin \( S_{\text{tot}} = \sum_i S_i \) and that \( \sigma(\omega) \) of the 1D ionic Hubbard model detects the singlet excitations.\(^{18}\)

Our results, of course, do not deny the possibility that \( N(k, \omega) \) may have a finite contribution from the multi-spinon state as \( S(k, \omega) \) does.\(^{26}\) Investigating that point is, however, beyond the scope of this letter.

In the thermodynamic limit of the uniform chain, the dispersion of the two-spinon singlet is coincident with that of the two-spinon triplet.\(^{25}\) Now, we turn our attention to properties of the bond-alternating chain, where the dispersion of the singlet excitations is clearly separated from that of the triplet excitations. Figure 4 shows numerical results of \( N^\sigma(k, \omega) \) and \( S^\sigma(k, \omega) \) for the 28-site chain with \( U/t = 20, \Delta/t = 2 \) and the alternating transfer integral \( t_{i+1} = t[1 + u(-1)^i] \), where \( u = 0.2 \) gives the strength of the bond alternation. It is well-known that in the bond-alternating chain the lowest singlet states have higher energy than the lowest triplet bound states having the dominant contribution to \( S(k, \omega) \).\(^{27}\) Obtained results of \( S(k, \omega) \) clearly show dominant peaks corresponding to the dispersion of the lowest triplet states while the \( N(k, \omega) \) shows small numerous peaks around \( k = \pi/2 \), whose energies are higher than the lowest triplet excitations.

As we can see from these results, \( N^\sigma(k, \omega) \) detects low-lying spin-singlet excitations of the 1D ionic Hubbard model. However, it should be noted that the intensity of \( N^\sigma(k, \omega) \) is much smaller than the contribution from the charge degrees of freedom. Figure 5 (a) shows the ratio of the integrated intensity \( I_s/I_{\text{tot}} \), where \( I_{\text{tot}} = \int d\omega N(k = \pi/2, \omega) \) is the total contribution of the 1D ionic Hubbard model and \( I_s = \int d\omega N^\sigma(k = \pi/2, \omega) \) gives the contribution from the spin degrees of freedom. Obtained results suggest that the ratio \( I_s/I_{\text{tot}} \) is at most the order of \( 10^{-2} \) within the MI phase, which is distinguished from the BI phase by the jump of the charge.
Fig. 5. (Color online) (a) The ratio of the integrated intensity $I_s/I_{\text{tot}}$ and (b) the charge transfer $\rho$ of the 1D ionic Hubbard model with $N = 12$.

The charge transfer $\rho$ defined as

$$ \rho = 1 - \frac{1}{N} \sum_i (-1)^i \langle n_i \rangle $$

(10)

for finite systems [see Fig. 5 (b)].

The reason why $I_s/I_{\text{tot}}$ increases with $\Delta$ is because $I_s$ is proportional to $\eta$ defined by Eq. (7) and $\eta$ increases with $\Delta$.

To summarize, we have studied the low-energy spectrum of the charge dynamical structure factor $N(k, \omega)$ of the 1D ionic Hubbard model in the MI phase. We represent the charge deviation per site and $N(k, \omega)$ in terms of the spin operators and then, numerically calculated these quantities by using the Lanczos diagonalization. Obtained results of $N_s(k, \omega)$ well reproduce the low-energy component of $N(k, \omega)$. In addition, dominant spectral peaks of $N_s(k, \omega)$ are in good agreement to the dispersion of the two-spinon singlet excitations obtained by the Bethe ansatz. Thus the spin-singlet excitations can be probed by examining $N_s(k, \omega)$ in the ionic Hubbard model. This is also confirmed in the system with the bond alternation, where the spin-singlet excitations are clearly separated from spin-triplet excitations. We have also shown that, although the spectral intensity of $N_s^*(k, \omega)$ basically small, it rapidly increases with $\Delta$ owing to increasing $\eta$. Therefore, in order to observe $N_s^*(k, \omega)$, it would be appropriate to use the system corresponding to the vicinity of the boundary between the MI phase and the BI phase.

acknowledgment This work was supported by JSPS KAKENHI Grant Number 26800163 from the Ministry of Education, Culture, Sports, Science and Technology (MEXT), Japan.

1) G. Ortiz, P. Ordejón, R. M. Martin, and G. Chiappe, Phys. Rev. B 54, 13515 (1996).
2) R. Resta and S. Sorella, Phys. Rev. Lett. 82, 370 (1999).
3) M. Fabrizio, A. O. Gogolin, and A. A. Nersesyan, Phys. Rev. Lett. 83, 2014 (1999).
4) M. E. Torio, A. A. Aligia, and H. A. Ceccatto, Phys. Rev. B 64, 121105 (2001).
5) S. R. Manmana, V. Meden, R. M. Noack, and K. Schönhammer, Phys. Rev. B 70, 155115 (2004).
6) H. Otsuka and M. Nakamura, Phys. Rev. B 71, 155105 (2005).
7) Ö. Legeza, K. Buchta, and J. Sólyom, Phys. Rev. B 73, 165124 (2006).
8) A. P. Kampf, M. Sekania, G. I. Japaridze, and P. Brune, J. Phys.: Condens. Matter 15, 5895 (2003).
9) K. Kuroki, Phys. Rev. B 81, 104502 (2010).
10) T. Watanabe and S. Ishihara, J. Phys. Soc. Jpn. 82, 034704 (2013).
11) H.-F. Lin, H.-D. Liu, H.-S. Tao, and W.-M. Liu, Sci. Rep. 5, 9810 (2015).
12) S. Ishihara, T. Egami, and M. Tachiki, Phys. Rev. B 49, 8944 (1994).
13) N. Nagaosa and J. Takimoto, J. Phys. Soc. Jpn. 55, 2735 (1986).
14) N. Nagaosa and Takimoto, J. Phys. Soc. Jpn. 55, 2745 (1986).
15) M. Hafez and S. A. Jafari, Eur. Phys. J. B 78, 323 (2010).
16) M. Hafez and M. R. Abolhassani, J. Phys.: Condens. Matter 23, 245602 (2011).
17) M. Hafez Torbati, Nils A. Drescher, and Götz Uhrig, Phys Rev. B 89, 245126 (2014).
18) H. Katsura, M. Sato, T. Furuta, and N. Nagaosa, Phys. Rev. Lett. 103, 177402 (2009).
19) K. Yokoi, N. Maeshima, and K. Hino, J. Phys. Soc. Jpn. 86, 104708 (2017).
20) W. Stephan and K. Penc, Phys. Rev. B 54, R17269 (1996).
21) J. des Cloizeaux and J. J. Pearson, Phys. Rev. 128, 2131 (1962).
22) T. Yamada, Prog. Theor. Phys. 41, 880 (1969).
23) A. H. Bougourzi, M. Couture, and M. Kacir, Phys. Rev. B 54, R12669 (1996).
24) M. Karbach, G. Müller, A. H. Bougourzi, A. Flederjohann, and K.-H. Mütter, Phys. Rev. B 55, 12510 (1997).
25) M. Karbach, K. Hu, and G. Müller, arXiv:9809163.
26) J.-S. Caux and R. Hagemans, J. Stat. Mech.: Theory Exp. P12013 (2006).
27) E. Sørensen, I. Affleck, D. Augier, and D. Poilblanc, Phys. Rev. B 58, R14701 (1998).