Spectral properties of trapped one-dimensional ultracold fermions loaded on optical lattices

Atsushi Yamamoto,[1,2] Susumu Yamada,[1,2] Masahiko Okumura,[2,3] and Masahiko Machida[1,2]
[1]*CCSE, Japan Atomic Energy Research Institute, 6-9-3 Higashi-Ueno, Taito-ku, Tokyo 110-0015, Japan*
[2]*JST-CREST, 5 Sanbancho, Chiyoda ku, Tokyo, 102-0075, Japan*
[3]*Computational Condensed Matter Physics Laboratory, RIKEN, Wako, Saitama 351-0198, Japan*
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We examine spectral properties on one-dimensional (1D) trapped ultracold Fermi atoms loaded on optical lattices by using the dynamical density-matrix renormalization group (DDMRG) method. We find that spectra are very rich due to the interplay of free or repulsive interaction and the harmonic-trap potential. One of the rich examples is that a 1D Tomonaga-Luttinger (TL) liquid spectrum emerges beneath multiple bound-state flat levels in the Mott-plateau phase and the TL spectrum gradually disappears with a partial breakdown of the central Mott plateau by increasing the trap strength. A more striking example is the growth of a distinct low-energy broadened band from the bound-state flat levels together with the breakdown. It demonstrates a carrier doping effect into the Mott phase in optical lattice systems.

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I. INTRODUCTION

Ultracold Fermi atoms loaded on an optical lattice have recently attracted considerable interest from condensed matter physicists [1–7]. The experimental flexibility offers an excellent test bed from which to access various unsolved issues in strongly correlated materials, and the perfect nondisorder lattice makes it possible to directly compare model calculations with experiments. So far, there have been a large number of struggles with strongly correlated materials. However, problems inevitable for real materials have prevented us from gaining a clear understanding of them. Meanwhile, the optical lattice is a powerful tool to help clarify such problems.

Recent experimental techniques have succeeded in measuring a one-particle excitation spectrum (OPES) in a trapped atomic Fermi gas [8] similar to that obtained using angle-resolved photoemission spectroscopy (ARPES) [9–11] on solid state materials. This success prompted us to study OPESs in fermionic optical-lattice systems by employing the same technique. In solid-state matters, ARPES has revealed one-dimensional (1D) anomalous OPES properties, e.g., a spin-charge separation spectrum [9–11], by examining $SrCuO_2$ and accessed 2D doping effects on antiferromagnetic Mott insulators as a topological change of the Fermi surface by intensively studying high-T_c cuprate superconductors [12–17]. In this paper, we therefore examine spectral properties on 1D trapped fermions loaded on an optical lattice by using the dynamical density-matrix renormalization group (DDMRG) method [18–20] prior to experiments. The merit of the use of the DDMRG method is its high accuracy among several quantum solvers on highly correlated fermion systems. The 1D lattice fermion system is one of the most intriguing stages, in which exotic quantum many-body features such as spin-charge separation are accessible [21].

In all atomic gas experiments, the presence of the trap potential is an inevitable complexity [22–30], while it is incidentally an attractive source of novel physics. For instance, the trap potential induced spatial-modulation of the atom density is a crucial drawback in the identification of Fulde-Ferrel Larkin-Ovchinikov superfluidity [31,32]. In contrast, in strong repulsively interacting regimes, the Mott-insulating phase automatically emerges together with metallic wings as a consequence of matter concentration by the trap potential [4–7]. In this paper, we then treat the effects of the trap potential directly and clarify that the OPES becomes quite rich due to its presence. The main results in this paper are composed of two findings: one of which is a spectral change obtained by tuning the trap potential in free and weakly interacting regimes, and another of which is a nontrivial change seen in the strongly interacting regimes. The highlight in the present paper is the latter one, in which an unexpected spectral change occurs together with breakdown of a 1D local Mott phase. It is emphasized that such a change is quite difficult to observe in condensed matter systems but is easily accessible in optical lattice systems.

II. MODEL AND METHOD

Let us describe a theoretical model to examine a trapped 1D two-component Fermi gas on an optical lattice. The system with the trap potential is given by the following Hubbard Hamiltonian including the harmonic potential,

$$\mathcal{H} = -J\sum_{i=1,\sigma}^{L}(c_{i,\sigma}^{\dagger}c_{i+1,\sigma} + \text{H.c.}) + U\sum_{i=1}^{L} n_{i,\uparrow}n_{i,\downarrow} - V_c\left(\frac{2}{L-1}\right)^2\sum_{i=1,\sigma}^{L}\left(i - \frac{L+1}{2}\right)^2 n_{i,\sigma}, \quad (1)$$

where $c_{i,\sigma}^{\dagger}$ ($c_{i,\sigma}$) is a creation (annihilation) operator of a fermion at the ith site with spin σ ($=\uparrow,\downarrow$), J is the nearest-neighbor hopping integral, L is the total number of lattice sites, U is the on-site interaction, and V_c is the potential height of the harmonic trap at both side lattice edges. Throughout this paper, we confine ourselves to the repulsive interaction range, $U > 0$. The attractive case will be published elsewhere [33].

In order to obtain a OPES in the model, Eq. (1), we use the DDMRG method. Using the local-density approximation (LDA) method [34,35] may be another choice. However, since our interest is in strongly interacting fermions, we employ the

DDMRG method, which is the most highly accurate tool for calculating OPES as well as the exact diagonalization scheme [36,37].

The DDMRG method follows the original idea of the DMRG method [38] and directly obtains $A(k,\omega)$:

$$A(k,\omega) = -\frac{1}{\pi}\mathrm{Im}\langle 0|\, c^{\dagger}_{k,\sigma}\, \frac{1}{E_0 - \omega - \mathcal{H} + i\gamma} c_{k,\sigma}\, |0\rangle. \qquad (2)$$

In the present paper, the number of states kept, i.e., m, is taken to be 256 except for benchmark tests on accuracy, and the parameter γ giving the spectral peak broadening is fixed to be 0.1. The numerical precision is confirmed by a comparison with the exact diagonalization method, and the number $m = 256$ is proved to be enough.

III. RESULTS

Now, let us present numerical calculation results. Before going to OPES results, we briefly revisit a phase diagram of 1D trapped lattice fermions as a function of the repulsive interaction U and the harmonic trap potential strength V_c. Figure 1 is U-V_c phase diagram, in which the size $L = 64$ and the trapped fermion number $N_f = 48$. The atomic-density distribution profile in each phase is, respectively, displayed on the right-hand side of Fig. 1, where all the main central phases are characterized by (a) metal, (b) Mott insulator, and (c) band insulator. We emphasize that all these phases are experimentally accessible because the variation range of the parameters (U and V_c) in Fig. 1 is fully within the present experimental technique. In the rest of this paper, we clarify OPES in each phase.

Let us present the calculation results of OPESs for each phase. The first result, Fig. 2(a), is $A(k,\omega)$ at $U = 0$ and $V_c = 7.5$. The case is a free trapped lattice-fermion system. The correspondent atomic-density profile is given in the upper panel of Fig. 2(a). In such a confined case, the wave number k is not a good quantum number in contrast to the periodical

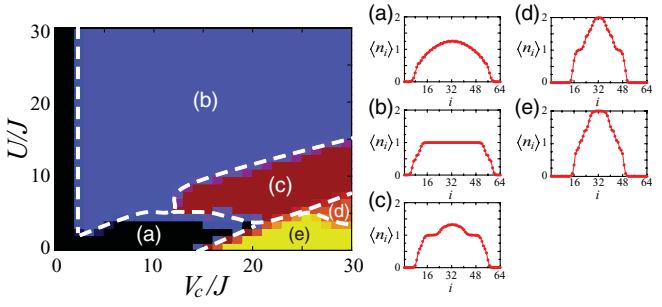

FIG. 1. (Color online) A phase diagram of the trapped 1D Fermi atoms loaded on optical lattices as a function of the repulsive interaction U and the trap potential strength V_c. The employed parameters are as follows: $L = 64$ and $N_f = 48$ ($N_\uparrow = 24$, $N_\downarrow = 24$). The phases painted by different colors correspond to (a) an all metallic phase, (b) a Mott one surrounded by the metallic wings, (c) a small metallic one emerging on the central Mott one with metallic wings, (d) a band-insulating one surrounded by the Mott one with metallic wings, and (e) a band insulating one with metallic wings. The right-hand side panels display correspondent typical local-density profiles $\langle n_i \rangle$.

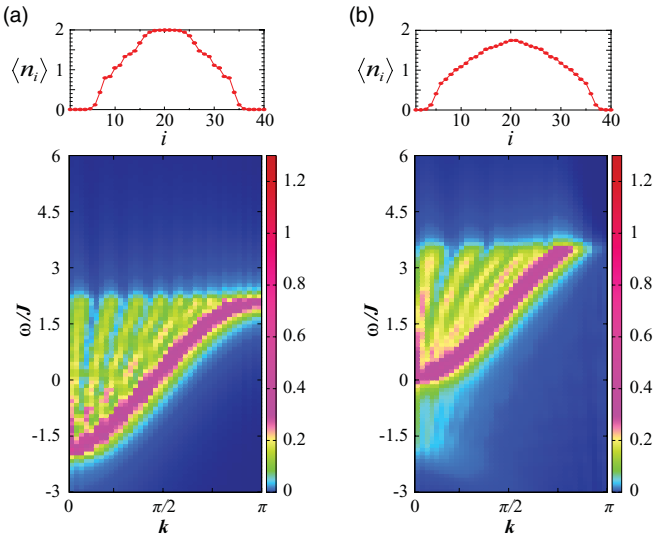

FIG. 2. (Color online) The density profiles, $\langle n_i \rangle$, and OPES's, $A(k,\omega)$, for (a) $U = 0$ and $V_c = 7.5$ and (b) $U = 2$ and $V_c = 7.5$, respectively. In both cases, the number of total sites $L = 40$ and the number of total fermions $N_f = 40$.

system, where $A(k,\omega)$ is characterized by only a single Hubbard band. Thus, the Hubbard band in the trapped case branches into several multiple bands as seen in Fig. 2(a), which demonstrates the existence of multiple periodical structures. In fact, one finds that the density profile is not a simple smooth one but includes fine multiple stepwise structures. It is noted that such fine structures are intrinsic to lattice systems.

Next, we turn on a weak repulsive interaction in the presence of the same trap potential. The result of a OPES at $U = 2$ is presented in Fig. 2(b), where whole the spectrum is found to shift toward a high-energy range without major spectrum changes expect for interaction-induced spectrum broadening. This result indicates that switching on such a weak interaction is mainly characterized by a simple energy shift as expected from the mean-field level approximation.

We further increase only the trap potential strength on the results in $U = 0$ [Fig. 2(a)] and $U = 2$ [Fig. 2(b)]. Here, it is noted that the increased strength is still within an experimentally realistic level. The results are, respectively, presented in Figs. 3(a) and 3(b), which correspond to the noninteracting case ($U = 0$) and the weakly interacting case ($U = 2$), respectively. It is found from both the profiles of the matter density that their phases are composed of the central band-insulator and metallic wings. In both the OPES figures, we notice that the dispersive feature partly remains in a deep ω range of the spectrum while the flat discrete levels are clearly dominant in the energy shallow range. Such features are kept except for the energy shift and broadening even when turning on a weakly repulsive interaction $U(= 2)$ as seen in Fig. 3(b). These results clearly demonstrate that the metallic wing region is not a simple metal but is characterized by distinct discrete flat excitations. From these structures, it is found that a resonant-type excitation is observable at the wing region when a frequency of the external oscillation coincides with the energy distance between the discrete levels. In fact, the time-dependent DMRG calculations horizontally shaking

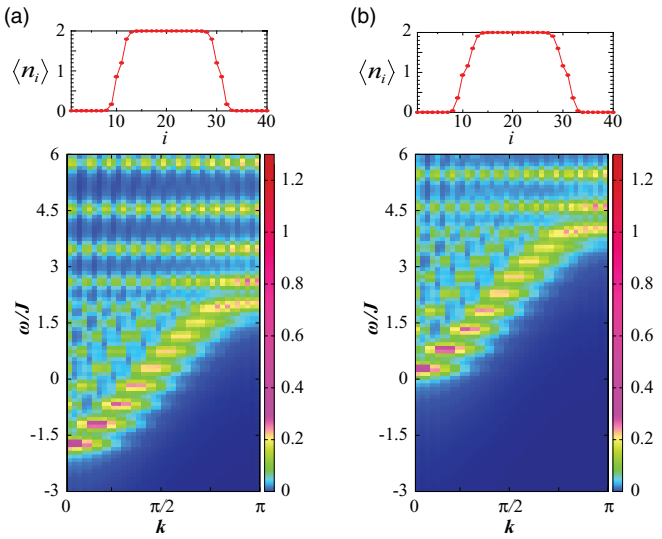

FIG. 3. (Color online) The density profiles, $\langle n_i \rangle$, and OPESs, $A(k,\omega)$, for (a) $U = 0$ and $V_c = 30$ and (b) $U = 2$ and $V_c = 30$, respectively. The other parameters are the same as in Fig. 2.

the trap [39] demonstrated that the resonance occurs and the density profile heavily vibrates when the shaking frequency coincides with the energy level distance. This indicates that the present many-body system is a controllable quantized system. More details of the time-dependent behaviors will be published elsewhere [39].

Let us turn to a strongly interacting regime. One of the most intriguing issues in the regime is a spectrum in a typical phase, i.e., a Mott-insulator phase surrounded by metallic wings as shown in Fig. 4(a). The lower panel of Fig. 4(a) shows the notable spectrum, in which one finds a characteristic anomalously dispersive spectrum deep beneath the chemical potential together with multiple flat, discrete levels above the dispersive part. For comparison, Fig. 4(b) is a spectrum in a uniform nontrapped case whose occupation is $\langle n_i \rangle = 1.0$, i.e., half filling as demonstrated by the upper panel of Fig. 4(b). Since the spectrum is a typical spin-charge separated one, then the comparison between Figs. 4(a) and 4(b) clearly indicates that the spectrum beneath the multiple bound-state levels in the trapped case is characterized by the spin-charge separation. Moreover, this spectral structure indicates that shallow discrete levels are ascribed to the metallic wings. In other words, the excitation energy to excite the Mott phase is so deep (high) that the Mott phase is highly protected on any low-energy perturbations. This explains why one does not need to significantly lower the temperature in observing the central Mott phase [4–7].

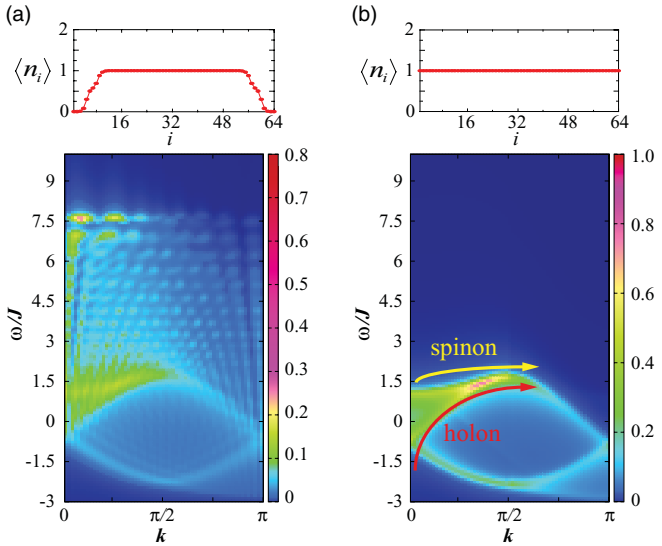

FIG. 4. (Color online) The density profiles, $\langle n_i \rangle$, and OPESs $A(k,\omega)$, for (a) $U = 10$ and $V_c = 12$ and (b) $U = 10$ and $V_c = 0$ (no trap potential), respectively. The number of total sites is $L = 64$ for both cases, and the number of total fermions is (a) $N_f = 52$ and (b) $N_f = 64$, respectively.

Finally, let us examine a spectral change obtained by partly breaking the Mott phase and discuss the change in a context of doped Mott insulators. One of the most important issues in condensed matters is carrier doping into Mott insulators, in which slight doping still keeps strongly correlated features while full doping brings about metallic ones. High-T_c superconductivity in cuprate compounds emerges in a range from slightly doped to moderately doped and disappears in a full doping range [40–43]. Thus, our interests are OPESs observable in such a highly correlated region. Although there have been so far a tremendous number of theoretical works on the region, it is still far from clear understanding. On the other hand, ARPES measurements have revealed several anomalous features such as pseudogaps, hole pockets, Fermi arcs, etc. [44–49]. Figure 5 is a typical spectral change, which can be obtained by increasing only the trap potential strength without any other changes. In this case, the central Mott phase is found to be partially broken depending on the applied potential strength. As seen in Figs. 5(a) to 5(b), one finds that a new dispersive but considerably broadened band grows from the flat bound-state levels while the anomalous spectrum due to 1D confinement instead disappears. This indicates that the bound-state discrete levels on the metallic wings change into a strongly correlated metallic band which is relevant to

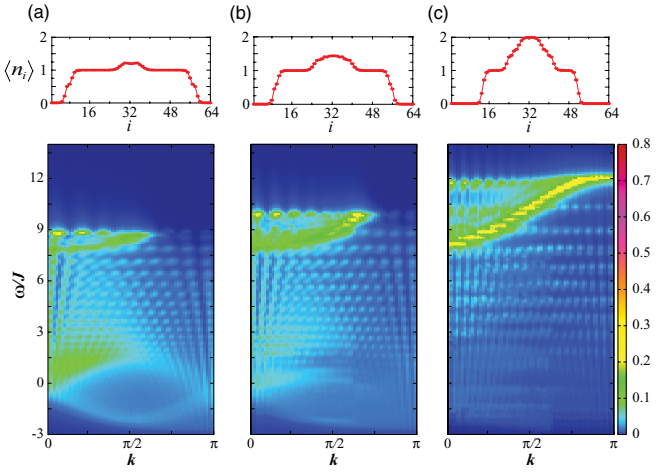

FIG. 5. (Color online) The density profiles, $\langle n_i \rangle$, and OPESs, $A(k,\omega)$, for (a) $V_c = 15$, (b) $V_c = 20$, and (c) $V_c = 35$. The number of total sites $L = 64$, the number of total fermions $N_f = 52$, and the on-site interaction $U = 10$, respectively.

an emergence of low-energy states extended over all sites. Namely, such an effective doping into the central Mott phase in trapped cases [see the upper panels of Fig. 5(a)] creates a nonlocalized (mobile) low-energy excitation characterized by the emergent dispersive band. In a more explicit and dynamical image, these results suggest that the doped region, i.e., a small hill-like region on the Mott phase as observed in Figs. 5(a) and 5(b) can move over the Mott phase as a density excitation. Such a breakdown of the insulating nature is not specific to the trapped system but also is found in high-T_c cuprate materials with doping [50,51]. As we compare the present cases with those obtained by doping into homogeneous Mott insulators, we notice that the present doping does not correspond to hole doping but rather to electron doping. It is noted that hole doping may be difficult to realize within the present setups. With the electron doping, we find that the specific change is the spectral weight transfer from the 1D characteristic spectrum to the emergent metallic band around the chemical potential. The weight transfer occurs between widely distant energy levels. Such a drastic feature is a sign of the phase change from Mott insulator created by a large U parameter to a correlated metal. In higher dimensions, it is of great interest to examine whether such an emerging metallic part in the Mott phase shows unconventional superfluidity or not. This is because any symmetry-breaking phenomena like superfluidity are strongly suppressed in 1D cases while such an ordering is stabilized in higher dimensions.

IV. SUMMARY

In summary, we clarified spectral properties of atomic Fermi gases on 1D optical lattice in a wide range of the repulsive interaction and the trap potential strength. The control of the trap potential brings about a change from bandlike dispersive spectra to discrete bound-state levels in the presence of free or weakly repulsive interaction. On the other hand, the spin-charge separated exotic spectrum is observable together with bound-state discrete levels in a strongly interacting regime as the Mott phase emerges in the trap center. Furthermore, we find that the potential control can mimic doping into the Mott phase and creates a strongly correlated metallic-band spectrum with a partial breakdown of the Mott phase. We propose that the present results are directly confirmed by JILA's group technique and dynamical features predicted from the excitation spectrum are also observable in nonequilibrium experiments. Such studies will open a new avenue to systematically understand the Mott phase and its unsolved vicinity phases including unconventional superfluidity.

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