Single-particle excitation spectrum in 1D ultracold fermionic optical lattices

Atsushi Yamamoto$^{a,b}$, Susumu Yamada$^{a,b}$, and Masahiko Machida$^{a,b}$

$^a$CCSE, Japan Atomic Energy Agency 6-9-3 Higashi-Ueno, Taito-ku, Tokyo 110-0015, Japan
$^b$JST-CREST, 5, Sanbancho, Chiyoda-ku, Tokyo, 102-0075, Japan

E-mail: yamamoto.atsushi@jaea.go.jp

Abstract. We investigate the properties of fermions trapped in a one-dimensional (1D) optical lattice by using the density-matrix renormalization (DMRG) group method. Owing to a harmonic confinement potential inherent in real experiments, system becomes inhomogeneous structure. Under certain conditions for weak-repulsive interaction, we find that the single-particle excitation spectrum structure changes to band branching and discrete bound-state states as increasing the trap strength. Additionally, we consider the case of strong-repulsive interacting regimes which local density profile show coexist with central Mott-plateau phase with surrounded by metallic regions. As increasing the trap strength, we find the breakdown of 1D Tomonaga-Luttinger (TL) liquid which is alternative to an effective doping into the Mott phase. We will present the various kinds of striking spectra, show the comparison of repulsive interaction case with attractive interaction one.

Recent remarkable progress in laser operation techniques has opened multiple avenues toward various unprecedented experiments in ultracold neutral atoms. Optical lattice formed by standing wave of laser lights is a typical example which provides ideal stages for an experimental investigation of many-body problems in condensed matter physics. Indeed, it is well-known that quantum phase transition from a superfluid (SF) to a Mott-insulator (MI) occurs in bosonic atom systems loaded on three-dimensional optical lattices. Moreover, the metal-insulator transition was successfully demonstrated quite recently using fermionic atoms with optical lattices [1, 2, 3, 4].

Another key experiment is the successful observation of one-particle excitation spectrum (OPES) in trapped ultracold fermionic atoms [5]. In solid state matters, angle resolved photoemission spectroscopy (ARPES) [6, 7, 8] is a powerful probe of OPES and is one of the most successful recent experimental developments on strongly-correlated materials. In the case of trapped fermionic gases, a remarkable change of the superfluid gap associated with BCS-BEC crossover has been already examined by tuning the interaction strength, and a pseudo-gap has been clearly observed in the crossover region even above the superfluid transition temperature.

In this paper, we focus on OPES in strongly-correlated fermionic gases loaded on optical lattice. Although such a combined experiment has been not yet attempted, it will be one of the most promising experiment in the future. One of the exciting targets is a change of OPES obtained by breaking the Mott insulating state. A highlight of the present paper is just the change together with Mott phase breakdown by manipulating the trapping potential.

In this paper, we demonstrate spectral properties on 1D trapped fermionic optical lattices by using dynamical density-matrix renormalization (DDMRG) group method [9] ahead of future
Figure 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 $L = 64$, 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, respectively. The right-hand side panels display correspondent typical local density profiles $\langle n_i \rangle$. 

Experiments. DDMRG is originated from DMRG [10]. DMRG method has advantage of the high accuracy for 1D systems within quantum many-body effect. Furthermore, DDMRG method is directly obtains single particle excitation function $A(k, \omega)$:

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

(1)

Here, the parameter $\gamma$ giving the spectral peak broadening is fixed to be 0.1. Strongly correlated 1D fermionic optical lattices reveal one of the most intriguing stages.

One-dimensional fermionic optical lattices are described by the following Hubbard model with harmonic trap potential:

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

(2)

where $c_{i,\sigma}^\dagger$ ($c_{i,\sigma}$) is a creation (annihilation) operator of a fermion at the $i$-th site with spin $\sigma (=\uparrow, \downarrow)$, $J$ 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. In this paper, we consider the repulsive interaction range $U > 0$.

We calculate the phase diagram of the local density as a function of $V_c$ and $U$ by choosing the parameters as $L = 64$, $N_f = 48$ as shown in Fig. 1. The local density profile in each phase is displayed in the right side of Fig. 1, where all the main central phases are characterized by metal, Mott insulator, and band insulator, respectively. We clarify that all phases are experimentally accessible owing to the tuning of the several parameters ($U$ and $V_c$). We focus on kinds of phases as shown in Fig. 1, we clarify the OPES in each phase.

We present calculation results of OPES’s on each phase as shown in Fig. 2, and we also show the local density profile at the upper panel of Fig. 2. First result, Fig. 2(a) is $A(k, \omega)$ at
Figure 2. (color online). The local density profiles $\langle n_i \rangle$ and single particle excitation $A(k, \omega)$, (a) $U = 0$ and $V_c = 7.5$, (b) $U = 2$ and $V_c = 7.5$, (c) $U = 2$ and $V_c = 30$, respectively. Parameters are fixed the number of total sites $L = 40$ and the number of total fermions $N_f = 40$. And (d) $V_c = 0$ (no trap potential), (e) $V_c = 12$, (f) $V_c = 15$, (g) $V_c = 20$, and (h) $V_c = 35$, respectively. The number of total sites $L = 64$, the number of total fermions $N_f = 52$, and the on-site interaction $U = 10$.

$U = 0$ and $V_c = 7.5$ and it is a free trapped lattice-fermion system. In the inhomogeneous case, the wave number $k$ is not a good quantum number for the periodical system. And $A(k, \omega)$ is characterized by only a single Hubbard band. We can find not only the single Hubbard band but also branches of several multiple bands in Fig. 2(a). It is notable fine structures as intrinsic inhomogeneous systems. Next, we consider a weak repulsive interaction in the presence of the same trap potential. As shown in Fig. 2(b), the spectrum is found to shift for higher energy range, and spectrum changes to broadening structure. This result indicates that switching on such a weak interaction is mainly characterized by a simple energy shift as just expected from the mean-field level approximation. We further increase the trap potential strength on the results in Fig. 2(c). We can see the profiles of the local density that their phases are composed by the central band-insulator with metallic wings. We find 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.

We consider the strongly-interacting regime. To compare with inhomogeneous systems, Fig. 2(d) is a spectrum in a homogeneous case as half filling within demonstrated by the upper panel of Fig. 2(d). On the other hand, we show the inhomogeneous case as Mott-insulator phase surrounded by metallic wings as shown in Fig. 2(e). The lower panel of Fig. 2(e) shows the characteristic spectrum. We can find multiple flat discrete-levels above the dispersive part. Furthermore, owing to the spectrum is a typical spin-charge separation within the comparison between Fig. 2(d) and (e) clearly indicates that the spectrum beneath the multiple bound-state levels in the trapped case is characterized by the spin-charge separation. Next we examine spectral change obtained by partly breaking the Mott phase and discuss the change in a context of doped Mott insulators case. Figure 2(f)-(h) is a typical spectral change, and we only increasing only the trap potential strength without any other parameters. As seen in upper panels of Fig 2(f)-(h), the central Mott phase is found to be partially broken as a function of the applied potential strength. We find that a new dispersive and broadened band grows from the flat bound-state levels while the anomalous spectrum owing to an 1D confinement instead disappears as shown in Fig 2(f) and (g). Bound-state discrete levels on the metallic wings change into a strongly-correlated metallic band. And this regions become relevant to an emergence of low-energy states extended over all sites. Such breakdown of the Mott insulating structure is not specific to the trapped system, however it is found in High-$T_c$ cuprate materials with doping.
In summary, we studied dynamical properties of 1D fermionic optical lattices as a function of on-site repulsive interaction and trap potential strength. As increasing the trap potential, single particle spectra crossover from band-like dispersive spectra to discrete bound-state levels in the presence of free or weakly repulsive interaction. In strongly interacting case, we find the coexistence of spin-charge separated exotic spectrum and with bound-state discrete levels in the Mott insulating region at trap center and metallic regions at around sites. Furthermore, we present the results of directly confirmed by JILA’s group technique and dynamical features predicted. Such studies will predict a future experiment, and show the systematically understand the doped Mott insulator or unsolved phases including unconventional superfluidity.

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