Stripe Formation in Fermionic Atoms on 2-D Optical Lattice inside a Box Trap: DMRG Studies for Repulsive Hubbard Model with Open Boundary Condition

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We suggest that box shape trap enables to observe intrinsic properties of the repulsive Hubbard model in a fixed doping in contrast to the conventional harmonic trap bringing about spatial variations of atom density profiles. In order to predict atomic density profile under the box trap, we apply the directly-extended density-matrix renormalization group method to 4-leg repulsive Hubbard model with the open boundary condition. Consequently, we find that stripe formation is universal in a low hole doping range and the stripe sensitively changes its structure with variations of $U/t$ and the doping rate. A remarkable change is that a stripe formed by a hole pair turns to one by a bi-hole pair when entering a limited strong $U/t$ range. Furthermore, a systematic calculation reveals that the Hubbard model shows a change from the stripe to the Friedel like oscillation with increasing the doping rate.

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Ultra-cold atomic Fermi-gas [1, 2] has attracted not only atomic gas community but also several physicists studying strongly-correlated electron systems. The reason is that the so-called “optical lattice” [3] formed by counter laser beams creates a periodical lattice potential described by the tight-binding model and the “Feshbach resonance” enables to access to the Hubbard model with the repulsive on-site interaction. Thus, a research goal in the optical lattice with the Feshbach tuning is to directly observe several controversial issues due to strong correlation as seen in High-$T_c$ cuprate superconductors and other metal oxides in controllable manners [4].

Generally, ultra-cold Bose and Fermi gases are trapped inside a harmonic trap to avoid the free expansion of atoms. The optical lattice is created inside the trap potential by utilizing the field modulation in the standing waves of lasers. Then, the model Hamiltonian on Fermi atoms (e.g., in 1-dimensional (1-D) case) is described by a Hubbard model with a harmonic trap potential [2, 6] given by

$$H_{\text{Hubbard}} = -t \sum_{i,j,\sigma} (a_{i\sigma}^\dagger a_{j\sigma} + \text{H.c.}) + U \sum_{i} n_{i\uparrow} n_{i\downarrow} + V \left( \frac{2}{N-1} \right)^2 \sum_{i,\sigma} n_{i\sigma} \left( i - \frac{N+1}{2} \right)^2, \quad (1)$$

where, a two-component Fermi gas is assumed, $a_{i\sigma}^\dagger$ is the creation operator of a Fermi atom with pseudo-spin $\sigma = \uparrow$ or $\downarrow$, $n_{i\sigma} = a_{i\sigma}^\dagger a_{i\sigma}$ is the density operator of the $i$-th site, $N$ is the total number of sites, and the summation $(i,j)$ in the first term describing the tunneling between lattice site is usually taken over the nearest neighbor sites. The on-site repulsive interaction $U$ is controllable via Feshbach resonance, and the presence of the harmonic trap potential is characterized by the last term including $V$. In the model Hamiltonian [1], it is well-known that the atomic density profile gives spatial variation, whose typical one is composed of the central Mott domain ($\sum_{i} n_{i\sigma} \sim 1$) and the periphery metallic edges ($\sum_{i} n_{i\sigma} < 1$) in a large repulsive $U/t$ range. Such a variation is universal irrespective of the space dimension as long as the harmonic well type of trap is employed. Actually, an example of 2-dimensional (2-D) case is shown in Fig. 1 (a), in which the harmonic potential is applied only along the $x$ axis. The result of Fig. 1 (a) is obtained in 4-leg Hubbard model by using the directly-extended density-matrix renormalization group (dex-DMRG) method [7, 8, 9] to 2-D systems. See Ref. [3] for other characteristic variations of 1-D system in different parameter ranges.

Such specific spatial-patterns have their own novel interests, e.g., how the spin correlation structures change from the Mott domain to metallic edges and whether the holes in the metallic edges form Cooper pairs or not [10, 11]. However, one clearly notices that intrinsic properties of the Hubbard model under a fixed doping are not directly observable. Although the system is quite clean and controllable, there is no direct relationship with solid state physics except for a few artificial cases [12]. In this paper, we therefore suggest that an alternative trap, whose shape is box (see the right hand side panel in Fig. 1 (b)), enables to experimentally study the Hubbard model with the open boundary condition. A typical dex-DMRG result in the case is shown in Fig. 1 (b), which displays atomic density profile in the half-filled case. This result clearly shows that the Mott domain ($\sum_{i} n_{i\sigma} \sim 1$) extends over all region. By using such a trap shape, we can fully examine the Hubbard model under a fixed doping and an interaction.

Recently, the 1-D box-shape confinement potential was...
actually created, and the system was successfully condensed to Bose-Einstein condensate inside the box [13]. According to Ref. [13], 1-D array of several small optical wells is also available inside the box trap in a controllable manner. Thus, 1-D fermion Hubbard model with the open boundary condition is accessible if bosons are replaced by fermions. Although the box trap dimension is now still one, the extension to 2-D box is expected to be straightforward. Our expecting potential shape is described in Fig. 2, where 2-D box is created inside the \( x-y \) plane with a narrow confinement along \( z \)-axis, and 2-D optical lattice is loaded inside the box plane by adding the Gaussian walls [13] as shown in Fig. 2 or a standing wave light fields with shallow Gaussian envelope curve. Such a stage is just described by 2-D Hubbard model with the open boundary condition. We emphasize that the system becomes the best playground for simulating controversial phenomena of High-\( T_c \) superconductors and other layered metal oxides. Furthermore, we would like to point out that ladder type models with the open boundary are recently good targets for advanced DMRG methods [14, 17, 18] and direct comparative studies are possible. However, it should be noted that the box shape is just the first step to remove the spatially dependent features of the filling. The temperature reduction in such a trap remains as the next step.

A key issue in the repulsive 2-D Hubbard model with the open boundary is the stripe formation, i.e., which types of stripes are formed with variation of doping and \( U/t \) still remains controversial. Although the stripe formation have been also examined in \( t-J \) model [14], we focus on solely the Hubbard model in this paper. The reason is because \( t-J \) model requires more specific conditions in realizing its equivalent situation on atomic Fermi gases. Therefore, our research priority is the Hubbard model. In addition, we note that the Hubbard model requires much more efforts in numerically exploring the ground state than \( t-J \) model since the degree of freedom is much bigger than that of \( t-J \) model [15] and therefore the stripe formation and its profile in the ground state of the Hubbard model is the present-day numerically challenging issue.

Let us briefly review DMRG studies for the stripe formation of the Hubbard model. After an early DMRG work on 3-leg Hubbard ladder [16], White and Scalapino applied the multichain algorithm of DMRG to 6-leg Hubbard model and found the appearance of hole stripes [17]. Afterwards, Hager et al. re-examined it in a more systematic manner [18]. However, their results do not reach to the ground state because the observed stripes still include the spin polarized modulation contrary to the Lieb-Mattis theorem as mentioned by themselves [16, 17, 18]. Although these pioneering works lacked final confirmations, they judged the stripe states as the ground state from the convergent tendencies. Thus, the accurate stripe profile in the ground-state are still unknown and \( U/t \) and filling dependence of the profile are also unsolved. On the other hand, the authors have recently developed dex-DMRG and confirmed that the hole stripe is really the ground state. The results converge and satisfy the Lieb-Mattis theorem. This indicates that the present results give the first accurate profile of the stripe in the Hubbard model. The extension to 2-D (ladder) is achieved by parallelizing the diagonalization of the superblock Hamiltonian. See Ref. [17] for its methodological details, performance, and accuracy. This method gives us a chance of direct analysis on the ground-state. In this paper, we confine ourselves 4-leg ladder \((20 \times 4)\) Hubbard-model because the present dex-DMRG easily reaches its ground state and enables to do systematic calculations varying \( U/t \) and the doping rate within our computational resources. When using the present dex-DMRG, the 4-leg case \((20 \times 4)\) almost converges within
3 times sweeps, which take about 3-hours under the use of
128 CPU’s on Altix 3700Bx2 in JAEA. We obtain the
ground state in a doping range from $p = 0.025$ to 0.350
with $U/t = 1 \sim 15$.

Let us present numerical calculation results. At first,
we focus on a case when a hole pair (↑, ↓) is doped into
the half-filling. The doping rate is $p(\equiv 1 - \frac{1}{N} \sum_{i,\sigma} n_{i,\sigma}) = 0.025$, which corresponds to a heavily underdoped region
in High-$T_c$ cuprate superconductors. The interest in
the region is how the doped holes distribute, i.e., whether
the two holes form a pair or not. If yes, then how the
pair localizes (or delocalizes)? Such a fundamental
question is deeply relevant to unsolved issues in heavily-
deroped High-$T_c$ superconductors [19]. An alterna-
tive experimental-stage is provided by the 2-D optical
lattice inside a 2-D box trap. Figure 3 displays $U/t$ de-
pendence of the hole distribution profiles. In all cases,
the spin-polarization completely drops to zero everywhere
according to the Lieb-Mattis theorem. One finds for all
the three cases (a)–(c) that the doped two holes form a stripe,
called a hole-pair stripe. The area of the hole-pair stripe
is much more compact than that of the single hole (↑ or ↓) doped case (not shown). This means that an
attractive interaction effectively works between two holes.
In addition, the dex-DMRG results show that the stripe
shape changes from the oval to the complete stripe one
with increasing $U/t$ (see 2-D projected contour maps of
(a) to (c)). This means that the shape is affected by
the boundary edge along the ladder leg ($x$) direction.

As $U/t$ increases, the edge depression is considered to
be defeated by the energy cost-down due to the stripe-
formation. Figure 3 (d), which is $U/t$ dependence of the
distribution profile of the hole density along the ladder
rung ($y$) direction at the center ($x = 10$), shows that
there is a qualitative difference between $U/t = 5$ and 7
in the stripe shape. Next, in order to check the stability
of the hole-pair stripe, we examine its leg-length de-
pendence and confirm that the stripe keeps the same shape
up to 40 × 4 sites model. Although the maximum limit of
the leg-length is presently 40, any shape changes in the
distribution profiles are not observable. Thus, one finds
that two holes are bound and the pair sits in the most
stable location (the center) as a stripe.

Next, let us study interaction between the hole-pair
stripes. The motivation comes from a question whether
they simply merge or repel each other as multiple hole-
pair stripes closely stay. Such a situation shows up
when holes are sufficiently doped. If two hole-pair stripes
merge, it means that the system prefers the hole segrega-
tion [19] or the stripe formation of a bi-hole pair [20]. On
the other hand, if they are separated, then it indicates
that the hole-pair stripe is more stable. Here, we note
that although such a study should include the size depen-
dence check, we concentrate on results only in a finite size
system ($20 \times 4$) due to lack of computational resources
in this paper. The size dependence will be reported else-
where [21]. Figure 4 shows $U/t$ dependence of the hole
distribution profile. The number of the doped holes is 8
and the doping rate is $p = 0.10$, which corresponds to an
underdoped region in High-$T_c$ superconductors [10].
In Fig. 3 (a) ($U/t = 3$), one finds 4 hole pair stripes, whose
distance is almost equivalent. It is found in this case that
the stripes repel each other. The surprising thing occurs
at $U/t = 5$, in which two stripes merge in the central area
and a large stripe appears. Moreover, the merged stripe
shows a stronger 1-D anisotropic feature (see and com-
pare the 2-D projected contour plots), because the hole
density does not relatively drop at the edges along the
ladder leg ($x$) direction. This stripe just corresponds to a
bi-hole pair stripe, which extends over about 4 site. Such
a stripe structure characterized by 4 holes was predicted
by Chang and Affleck [20]. As $U/t$ increases further, the
merged stripe starts to split into two hole-pair stripes
at $U/t = 10$, again, and the split becomes complete at
$U/t = 13$. The bi-hole pair stripe is observable only for
$5 \leq U/t < 10$. These behaviors indicate that the stripe
formation occurs in not only a simple manner but also
multiple manners depending on the doping rate and the
interaction. The transition between these multiple struc-
tures may be too difficult to clearly identify in solid state
systems. Therefore, more controllable optical lattice with
the box shape trap is promising.

Finally, let us show a systematic result of the doping-
rate dependence of the hole distribution profiles. The
doping rate varies from $p = 0.025$ to 0.350, and $U/t$ is
fixed to be 10. In High-$T_c$ superconductors, the heav-
iest doped rate ($p = 0.350$) is in an overdoped range, in
which the materials almost show metallic behaviors. Fig-
ure 5 shows a doping rate dependence on $x$-directional
profiles of hole distributions at $y = 2$. It is found in
Fig. 5 that there are two characteristic profiles in the
Before closing, let us discuss finite temperature effects on all the present results. In atomic gases, the temperature reduction is always one of difficulties in exploring the ground-state properties of many-body interacting systems. The present results are static modulations of holes in the ground-state, which are expected to fluctuate in non-zero temperature. However, in sufficiently low temperature, the resultant tiny fluctuation does not matter for the static local-density probe. On the other hand, in relatively high temperature, the static modulations become fluctuating stripes, which can be observed by not local but density correlation probes \[22\]. Actually, dynamical stripe like fluctuations have been reported in High-Tc superconductors \[10\], in which charge and spin fluctuations are detectable much above the superconducting transition temperature by various probes. Thus, the present stripe structures can be also identified by using suitable correlation probes \[23\] in finite temperature.

In conclusion, we suggested in atomic Fermi gases that the box shape trap is essential for studies on intrinsic properties of the Hubbard model with a fixed doping rate and an interaction. We applied the dex-DMRG method to the 4-leg Hubbard model with the open boundary condition in order to predict rich varieties of hole profiles including stripe formations due to strong correlation. Consequently, we observed the hole-pair stripe, the bi-hole pair stripe, and other stripe structures including more than 4 holes in the overdoped region. These structures merge and split with the variation of $U/t$ and the doping rate. On the other hand, such characteristic features disappear and only a monotonic oscillation pattern emerges in the overdoped one. These results can be directly confirmed in atomic Fermi gases, and moreover, more systematic studies are possible in experiments of atomic Fermi gases. We believe that the optical lattice inside the box shape trap can solve significant controversial issues like the stripe formation in High-Tc superconductors and other metal oxides.

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