Superfluidity of one-dimensional trapped fermionic optical lattices with spatially alternating interactions

Atsushi Yamamoto and Seiji Yunoki

1 Computational Materials Science Research Team, RIKEN AICS, Kobe, Hyogo 650-0047, Japan
2 Computational Condensed Matter Physics Laboratory, RIKEN ASI, Saitama 351-0198, Japan
3 CREST, Japan Science and Technology, Kawaguchi, Saitama 332-0012, Japan
4 Computational Quantum Matter Research Team, RIKEN CEMS, Saitama 351-0198, Japan

E-mail: a-yamamoto@riken.jp

Abstract. Recent experiments have made it possible to spatially control local two-body interactions between ultracold atoms in inhomogeneous optical lattices. Motivated by this experimental progress, here we study theoretically one-dimensional trapped fermionic optical lattices with spatially modulated on-site interactions. The density matrix renormalization group method is used to examine the ground state phase diagram of a harmonically trapped Hubbard model with spatially alternating on-site repulsive interactions, \( U_1 \) and \( U_2 \). With varying the strength of the harmonic trapping potential, we find a pair correlated metallic state in the ground state phase diagram, which can be stable only when \( U_1 \neq U_2 \). We discuss the properties of this possibly new state by examining various static physical quantities.

1. Introduction

Since Bose-Einstein condensation (BEC) was observed in a \(^{87}\text{Rb}\) system [1], it has been recognized that ultracold atoms trapped in optical lattices can ideally emulate experimentally quantum models for interacting bosons or/and fermions in lattices. The most important advantage of ultracold atoms in optical lattices is high controllability of physical parameters such as interaction strength, particle number, and atomic hybridization. Therefore, these tunability enable us to simulate experimentally a wide range of quantum many body phenomena which might be difficult to observe in solid materials. In fact, many interesting phenomena including Mott insulator-metal transition [2, 3, 4] and BCS-BEC crossover [5, 6, 7] have been observed in fermionic optical lattice systems. Very recently, it has been reported that even the strength of the on-site interaction can be spatially modulated in \(^{174}\text{Yb}\) gas [8]. This system provides an interesting possibility to explore the quantum effects of spatially modulated on-site interactions, which is certainly not possible in solid materials.

In this paper, we study theoretically one-dimensional (1D) trapped fermionic optical lattices with spatially alternating on-site interactions. We use the simplest model, i.e., the 1D Hubbard model with spatially alternating on-site repulsive interactions, \( U_1 \) and \( U_2 \), for odd and even sites, respectively. We also include in the model a harmonic trapping potential and the strength of this potential is varied as one of the model parameters. Using the density matrix renormalization group (DMRG) method [9], we study static properties to establish the ground state phase diagram. Among several different states identified in the phase diagram, we find as increasing...
\[ U_1 - U_2 \] a parameter region where a charge density wave like state and a metallic like state coexist. More interestingly, we find a pair correlated metallic state close to this coexisting region. This new state is characterized with zero charge gap but with finite binding energy. We also find that the pair correlation function increases in this region. Thus, we attribute this state to a superfluid state.

The rest of this paper is organized as follows. In section 2, we describe the model Hamiltonian and give a briefly summary of the numerical methods. In section 3, we show the results of ground state phase diagram for different values of the harmonic trapping potential. We also show numerical evidence of a possible superfluid state which appears by controlling the alternating repulsive on-site interactions and the trapping potential. The summary is given in section 4.

2. Model and Method

We consider two-component spin 1/2 fermions in a harmonically trapped 1D optical lattice with spatially alternating repulsive interactions. Our model is described by the following Hamiltonian,

\[
\mathcal{H} = -J \sum_{i=1}^{L} \sum_{\sigma} \left( c_{i,\sigma}^\dagger c_{i+1,\sigma} + \text{H.c.} \right) + U_1 \sum_{i \text{ (odd)}} n_{i,\uparrow} n_{i,\downarrow} + U_2 \sum_{i \text{ (even)}} n_{i,\uparrow} n_{i,\downarrow} - V_c \left( \frac{2}{L-1} \right)^2 \sum_{i=1}^{L} \sum_{\sigma} \left( i - \frac{L+1}{2} \right)^2 n_{i,\sigma},
\]

where \( c_{i,\sigma}^\dagger \) (or \( c_{i,\sigma} \)) creates (annihilates) a fermion with spin \( \sigma (=\uparrow, \downarrow) \) at site \( i \) on a \( L \) site lattice, and \( n_{i,\sigma} = c_{i,\sigma}^\dagger c_{i,\sigma} \). The hopping parameter between the nearest neighbor sites is denoted by \( J \), the repulsive on-site interaction for odd (even) sites is denoted by \( U_1 \) (\( U_2 \)), and the strength of the harmonic trapping potential is controlled by \( V_c \).

Because of finite \( V_c \), the system becomes inhomogeneous. Indeed, when \( U_1 = U_2 \), it is known that the ground state show a coexisting state of a Mott insulating like state and a metallic like state with increasing the trap strength \( V_c \) [10]. Recently, the homogeneous system with \( V_c = 0 \) but with \( U_1 \neq U_2 \) has been also studied, revealing an unexpected metallic state [11]. Here, we focus on the effects of \( V_c \) on the ground state phase diagram. We employ the DMRG method [9] to study static properties such as local density distribution and binding energy. The number of states kept in DMRG calculations is 512 and we have checked that the results are well converged with this number of states. In the following, we set \( J = 1 \) as the energy unit.

3. Results

We first discuss the local density profile with varying \( V_c \). The results are summarized in Fig. 1 for five different values of \( V_c \). Here, we set \( L = 90 \), the numbers of up and down fermions \( n_\uparrow = n_\downarrow = 45 \) (i.e., half-filling), and the alternating repulsive interactions \( U_1 = 2 \) and \( U_2 = 10 \).

In the case of \( U_1 = U_2 \), it has been known that a coexisting phase appears, consisting of a Mott insulating state and a metallic like state, with increasing \( V_c \) [10]. Even when \( U_1 \neq U_2 \), we expect the similar coexisting phase appears with increasing \( V_c \). As we can see in Fig. 1, this is indeed what happens in the case of \( U_1 = 2 \) and \( U_2 = 10 \). The local density distribution \( \langle n_i \rangle \) gradually changes with increasing \( V_c \) and becomes nonuniform. We can clearly see in Fig. 1 (d) and (e) that for large values of \( V_c \) the local density in the central region of the system has its value of either 1 or 2, i.e., \( \langle n_i \rangle \approx 1 \) for even sites with \( U_2 = 10 \) and \( \langle n_i \rangle \approx 2 \) for odd sites with \( U_1 = 2 \), strongly indicating a charge density wave (CDW) like state in the central region. Thus, when the trapping potential and the difference of the on-site interactions are both large, a CDW
like state and a metallic like state coexist. Although this coexisting states are interesting, in this paper we focus on a parameter region of smaller values of $V_c$ [Figs. 1 (b) and (c)], where an intriguing phase may also appear such as a possible superfluid state as discussed below.

$$E_B = E(n_\uparrow + 1, n_\downarrow + 1) + E(n_\uparrow, n_\downarrow) - 2E(n_\uparrow, n_\downarrow + 1),$$

where $E(n_\uparrow, n_\downarrow)$ is the ground state energy for $n_\uparrow$ up and $n_\downarrow$ down fermions [12, 13]. As shown in Fig. 2 (a), we find that the binding energy becomes large for a region where $U_1$ and $U_2$ are very different when $V_c = 0$. The binding energy reaches its maximum value in a parameter region of $U_1 >> U_2 \approx 2$ (also equivalently $U_2 >> U_1 \approx 2$). Introducing the harmonic trapping potential, the parameter region where the binding energy becomes maximum moves to $U_1 >> U_2 \approx 2.5$ (also equivalently $U_2 >> U_1 \approx 2.5$) for $V_c = 2$ and $U_1 >> U_2 \approx 4$ (also equivalently $U_2 >> U_1 \approx 4$) for $V_c = 5$, as shown in Figs. 2 (b) and (c), respectively. The most interesting and important observation here is that with increasing $V_c$, the binding energy become negative in a region around $U_1 >> U_2 \approx 2 - 3$ (and $U_2 >> U_1 \approx 2 - 3$), as clearly seen in Fig. 2 (c). The negative binding energy is strong indication of a possible superfluid state. It should be noted here that as opposed to the cases for $V_c = 10$ and 20, these values of $V_c$ where the negative binding energy is found are not large enough to induce the coexisting states, as already discussed in Fig. 1.

Now, it is highly interesting to calculate pair correlation functions. The pair correlation function $\Delta i|\Delta j$ is defined by

$$\Delta i|\Delta j = \langle \Psi_0 | c^\dagger_i c^\dagger_j c_j c_i | \Psi_0 \rangle,$$
Figure 2. (Color online). Contour plots of the binding energy $E_B$ as functions of $U_1$ and $U_2$ for (a) $V_c = 0$, (b) $V_c = 2$, and (c) $V_c = 5$. The system size is $L = 90$ and the numbers of up and down fermions are $n_\uparrow = 45$ and $n_\downarrow = 45$, respectively.

where $|\Psi_0\rangle$ is the ground state. The results are summarized in Fig. 3 for different values of $V_c$ and $L = 90$. The pair correlation function $\Delta_i^\dagger \Delta_j$ is calculated for a given site $j$, i.e., for $j = 15$ [Fig. 3 (a)] and for $j = 29$ [Fig. 3 (b)]. Notice that, as shown in Fig. 1, the local state at site $j = 15$ is always within a metallic like state for all values of $V_c$ studied here, while the local state at site $j = 29$ changes gradually from a metallic like state to a CDW like state with increasing $V_c$. Figure 3 clearly show that the pair correlation functions decay exponentially for large vales of $V_c \geq 10$. However, for small values of $V_c$, we notice that the long range tail of the pair correlation function increases with increasing $V_c$ from 0 up to 5 as compared with the results for $V_c = 0$. The enhancement of the pair correlations strongly indicates that a state with the negative binding energy is indeed superfluid.

Figure 3. (Color online). Pair correlation function $\Delta_i^\dagger \Delta_j$ as a function of $i$ for (a) $j = 15$ and for (b) $j = 29$ with different $V_c$ indicated in the figures. The system size is $L = 90$ and the numbers of up and down fermions are $n_\uparrow = 45$ and $n_\downarrow = 45$, respectively. Here, we set $U_1 = 2$ and $U_2 = 10$.

4. Summary
We have studied the harmonically trapped 1D fermionic optical lattice with the spatially alternating on-site repulsive interactions. Using the DMRG method, we have obtained the ground state phase diagram and found that the ground state phase diagram is affected strongly by the harmonic trapping potential. We have found that a possible superfluid state can be stable in the phase diagram by tuning both the spatially modulated on-site interactions and the
harmonic trapping potential. It is highly interesting to study whether a similar superfluid state appears in two spatial dimensions as well.

Acknowledgments
We wish to thank A. Koga, T. Saito, T. Shirakawa, H. Watanabe, M. Machida, and S. Yamada for valuable discussions. The calculations were performed mostly using the RIKEN Integrated Cluster of Clusters (RICC).

References
[1] Anderson M H, Ensher J R, Matthews M R, Wieman C E and Cornell E A 1995 Science 269, 198
[2] Greiner M, Mandel O, Esslinger T, Hänsch T W and Bloch I 2002 Nature 415 39
[3] Jördens R, Strohmaier N, Günter K, Moritz H and Esslinger T 2008 Nature 455 204
[4] Schneider U, Hackermüller L, Will S, Best Th, Bloch I, Costi T A, Helmes R W, Rasch D and Rosch A 2008 Science 322 1520
[5] Jochim S, Bartenstein M, Altmeyer A, Hendl G, Riedl S, Chin C, Hecker Denschlag J and Grimm R 2003 Science 302 2101
[6] Zwierlein M W, Stan C A, Schunck C H, Raupach S M F, Gupta S, Hadzibabic Z and Ketterle W 2003 Phys. Rev. Lett. 91 250401
[7] Bourdel T, Khaykovich L, Cubizolles J, Zhang J, Chevy F, Teichmann M, Tarruell L, Kokkelmans S J J M F and Salomon C 2004 Phys. Rev. Lett. 93 050401
[8] Yamazaki R, Taie S, Sugawa S and Takahashi Y 2010 Phys. Rev. Lett. 105, 050405
[9] White S R 1992 Phys. Rev. Lett. 69 2863; 1993 Phys. Rev. B 48 10345
[10] Rigol M, Muramatsu A, Batrouni G G and Scalettar R T 2003 Phys. Rev. Lett. 91 130403; Rigol M and Muramatsu A 2004 Phys. Rev. A 69 053612
[11] Yamamoto A, Yamada S and Machida M 2012 (unpublished).
[12] Noack R M, White S R and Scalapino D J 1994 Phys. Rev. Lett. 73 882; 1995 Europhys. Lett. 30 163; 1996 Physica C 270 281
[13] Hayward C A, Poilblanc D, Noack R M, Scalapino D J and Hanke W 1995 Phys. Rev. Lett. 75 926