Dynamical instability in the $S = 1$ Bose-Hubbard model

Rui Asaoka, Hiroki Tsuchiura, Makoto Yamashita\textsuperscript{1}, and Yuta Toga

Department of Applied Physics, Tohoku University, Sendai 980-8579, Japan
\textsuperscript{1}NTT Basic Research Laboratories, NTT Corporation, Atsugi, Kanagawa 243-0198, Japan

(Dated: April 30, 2015)

We study dynamical instabilities of current carrying superfluid states in bosonic systems with spin degrees of freedom in an optical lattice, using the $S = 1$ Bose-Hubbard model. The real-time evolution of Bose-Einstein condensates for each spin-component is described within the time-dependent Gutzwiller approximation, which can applied from weakly correlated regime to near the superfluid to Mott-insulator transition. In this calculation, superfluid flows of spin-less and spin-1 condensates with same interaction strength decay at different critical values due to spin effect. We calculate the stability phase diagrams of spin-less and spin-1 condensates, and discuss difference of the boundaries and dependence of the spin-1 diagram on the average number of particles per site. Finally, we analyze density modulation and spin modulation associated with the dynamical instability. We find that properties of spin modulation depends on presence or absence of a uniform magnetic field on a spin-1 condensate.

I. INTRODUCTION

Because of the recent development in experimental technique, there has been an emerging interest in dynamical properties of Bose-Einstein condensates (BEC) in an optical lattice \cite{1, 2}. In particular, dynamical instability for current-carrying superfluid states in BEC on a lattice is a novel instability for BEC predicted a decade ago \cite{3, 4}, and has attracted much attention both theoretically \cite{5-8} and experimentally \cite{9-13}. Beside the well-known Landau instability, the dynamical instability is caused by the interplay between nonlinearity due to the inter-particle interactions in the BEC and periodicity of the lattice in the equation of motion governing the dynamics of the system. It is known that an arbitrary small spatial fluctuation of the original superfluid flow may grow exponentially in time, resulting in decay of the original flow.

Such dynamical instability itself is indeed commonly seen in many nonlinear systems governed by classical fluid mechanics. However, by using cold atom systems, we may now approach a new question of dynamical instabilities in systems with internal degrees of freedom. It is known that multicomponent bosons \cite{14-16} and Bose-Fermi mixtures \cite{17, 18} in an optical lattice contain rich physics such as many quantum phases, and the dynamical instability of multicomponent bosons has also been studied lately \cite{19, 20}.

In such multicomponent systems, bosonic systems with unfrozen spin degrees of freedom which include spin exchange process show more complex and intriguing phenomena \cite{21}. One of the simplest of such systems is $S = 1$ bosonic systems. In continuum and weakly correlated systems, interesting instabilities of $S = 1$ BEC have been investigated using Gross-Pitaevskii equation, for instance, spin mixing instability \cite{22, 23}, counterflow instability \cite{24, 25}, and occurrence of spin domain \cite{26, 27}. Every phenomenon is the instability only for a $S = 1$ bosonic system where spin exchange process plays an important role. The effect of this spin exchange process is difficult to see in a linear stability analysis \cite{28, 29} of differential equations commonly used in analyses about current instabilities, so that one should also use methods that real-time evolution is observed.

On the other hand, properties of a $S = 1$ bosonic system in a lattice are well described by the $S = 1$ Bose-Hubbard model (BHM) \cite{30-32}. Thus far, the phase diagram and static properties of this model has been extensively studied based on several theoretical methods \cite{33-41}. It is known that Gutzwiller-type variational wavefunctions fairly well describe the superfluid to Mott-insulator transition, aside from spin correlations in the Mott phase \cite{41}. In these studies, it is intriguing that dependence of the average particle number per site strongly emerges in superfluid to Mott-insulator transition. For example, superfluid regime extends (reduces) than the spin-less case in the phase diagram with odd (even) average number of particles per site if on-site spin interactions are anti-ferromagnetic like \cite{34, 35}. This parity can naturally emerge in the dynamical instability which sensitively depends on the interparticle interaction.

In this paper, we analyze the dynamical instability, in particular the stability of spin-resolved superfluid current flows in the $S = 1$ BHM for a wide range of interaction parameter. Since we are particularly interested in the effect of spin exchange process in the real-time evolution of the BEC for each spin component, we employ the time-dependent Gutzwiller approximation, which is used by Altman et al. \cite{7, 8} to analyze the dynamical instability of SF in spin-less BHM. We first discuss dynamical decay and time development of spin components, then show the dynamical phase diagram of $S = 1$ superfluid flow discussing the dependence of the average number of particles per site on the dynamical instability. Finally, we argue the density modulation and the spin modulation associated with the dynamical instability with or without a uniform magnetic field.
II. MODEL AND METHOD

The Hamiltonian of the $S = 1$ BHM is given as [31]

$$
\mathcal{H} = -t \sum_{\langle i,j \rangle} \sum_{\gamma} \left( \hat{a}_{i,\gamma}^\dagger \hat{a}_{j,\gamma} + \hat{a}_{j,\gamma}^\dagger \hat{a}_{i,\gamma} \right) - \mu \sum_i \hat{n}_i + \frac{U_0}{2} \sum_i \hat{n}_i (\hat{n}_i - 1) + \frac{U_2}{2} \sum_i \left( \hat{S}_i^2 - 2 \hat{n}_i \right),
$$

(1)

where $t$ is the hopping amplitude of bosons, $\langle i,j \rangle$ in the summation denotes the pairs of nearest neighbors, $\mu$ is the chemical potential, $U_0(>0)$ is the on-site spin-independent repulsion, and $U_2$ is the on-site spin-dependent interaction. In cold atom systems, the value of $U_2$ depends on the characteristic of $s$-wave scattering length that is specific to atom species; for example, $U_2 > 0$ ($< 0$) for Na (Rb) atoms. $\hat{a}_{i,\gamma}$ is an annihilation operator of a boson on site $i$ with a spin state $\gamma (= 0, \pm 1)$, the local particle number operator $\hat{n}_i = \sum_{\gamma} \hat{a}_{i,\gamma}^\dagger \hat{a}_{i,\gamma}$, and $\hat{S}_i = \sum_{\gamma,\gamma'} \hat{a}_{i,\gamma}^\dagger \hat{a}_{i,\gamma'}$ is the spin operator on site $i$ where $S_{\gamma,\gamma'}$ corresponds to the spin-1 matrices. The square of the local spin operator $\hat{S}_i^2$ is represented in a more convenient formula:

$$
\hat{S}_i^2 = (\hat{S}_{i,-1} \hat{S}_{i,1} + \hat{S}_{i,1} \hat{S}_{i,-1})/2 + \hat{S}_i^2,
$$

(2)

where the ladder operators are defined by $\hat{S}_{i,-1} = \sqrt{2} (\hat{a}_{i,0}^\dagger \hat{a}_{i,1} - \hat{a}_{i,1}^\dagger \hat{a}_{i,0})$ and $\hat{S}_{i,1} = \hat{S}_i^\dagger$, correspondingly. This formula also reads in terms of creation and annihilation operators, $\hat{S}_i^2 = (\hat{n}_{i,1} - \hat{n}_{i,-1})^2 + \hat{n}_i + \hat{n}_{i,0} + 2 \hat{n}_{i,1} \hat{n}_{i,-1} + 2 \hat{n}_{i,0} \hat{n}_{i,-1} + 2 \hat{n}_{i,0} \hat{n}_{i,1} \hat{n}_{i,-1}$. The last two terms in Eq. (2) induce spin mixing between $S_z = \pm 1$ and $S_z = 0$ states, which enriches the physics of this model as compared with spinless models or multi-component models without mixing of components.

We first investigate the quantum dynamics of this model within the dynamical Gutzwiller scheme [7,8]. The variational wave function for the $S = 1$ BHM can be written as the direct product of superposition states at each lattice site

$$
|\Psi_G\rangle = \prod_i \sum_{n_{i,0}, n_{i,\pm 1}} f_i(n_{i,1}, n_{i,0}, n_{i,-1}) |n_{i,1}, n_{i,0}, n_{i,-1}\rangle,
$$

where $|n_{i,1}, n_{i,0}, n_{i,-1}\rangle$ denotes the local Fock state determined by the local number of atoms for each spin component on site $i$. Here the Gutzwiller parameters are normalized as $\sum_{n_{i,\pm 1}} f_i(n_{i,1}, n_{i,0}, n_{i,-1})^2 = 1$. Minimizing $\langle \Psi_G \vert \hat{H}^2 - \mathcal{H} \vert \Psi_G \rangle$ on the basis of the time-dependent variational principle, we derive equations of motion with respect to these Gutzwiller parameters. The equations are explicitly shown in Appendix A. Note that $p(t)$ in Eq. (A2) corresponds to the relative momentum between a condensate and a lattice for a condensate on a moving lattice or a moving condensate on a stationary lattice. We introduce $p(t)$ as the phase difference of particles between adjacent sites using the transformation: $\hat{a}_{i,\gamma} \rightarrow \hat{a}_{i,\gamma} e^{i p(t)}$ (note that, $t$ represents time here). In the time-evolution calculations, we assume $p = 0$ at the initial time and the system stays in the ground state initially for given $U_0$ and $U_2$. The momentum is then increased linearly with time at the acceleration rate $\alpha$: $p(t) = \alpha t$. We perform this procedure almost adiabatically by choosing a very small rate $\alpha = 0.005$. Since loss of atoms is neglected in our study, the total number of particles should be conserved during time evolution. We ensure the number conservation from the fact that the filling $n = n_1 + n_0 + n_{-1}$ (i.e., the average particle number per site) is kept constant within the numerical precision. The calculated system is a two dimensional lattice of the unit size $L = 40 \times 2$ with the periodic boundary conditions, and we set the hopping amplitude $t = 1$ as a unit of energy. In our calculation, the sum of the wavefunction (3) is limited to a finite number of states for reducing of computational tasks. We confirmed that the truncation does not produce noticeable differences in the numerical results.

In this paper, we discuss the instability of superfluid flow by introducing two characteristic momenta: a decay momentum $p_d$ and a critical momentum $p_c$. $p_d$ corresponds to the momentum at which a superfluid flow actually starts to decay drastically owing to the dynamical instability during time evolution. We obtain $p_d$ based on the dynamical Gutzwiller method mentioned above by numerically solving Eq. (A1). On the other hand, $p_c$ is the minimum momentum at which a superfluid flow can dynamically collapse, which is evaluated on the assumption that a superfluid flows steadily. It should be noted that, as we will see later, $p_d$ becomes larger than $p_c$ because of the small nonadiabaticity in the process of ramping up the momentum and agrees with $p_c$ in the limit of $\alpha \rightarrow 0$ [43].

Here we briefly explain the way to calculate $p_c$ for the spinless case as a simple example [7,43]. The critical momentum $p_c$ is determined from the (non-dimensional) group velocity $v(p) = p \rho(p) \sin(p)$ where $\rho(p)$ is the density of a steady superfluid flowing with momentum $p$. The periodicity of $v(p)$ reflects the structure of the lowest Bloch band in an optical lattice. Here the density $\rho(p)(\propto t'/U_0)$ is a monotonically decreasing function of $p$ according to the effective hopping amplitude $t'$ given by $t' = (d + \cos(p-1))/d$ where $d$ corresponds to the dimension of the system. The group velocity $v(p)$ has a maximum at a certain momentum $p = p_c(< \pi/2)$ as $p$ is increased, indicating that, beyond this $p_c$, the effective mass changes its sign and the superfluidity becomes unstable. We evaluate the superfluid density variationally on the basis of the conventional (i.e., not the dynamical) Gutzwiller approximation. In this framework [43], the density $\rho(p)$ is equivalent to the condensate fraction $n_{k=p} = \langle \hat{a}_{k=p}^\dagger \hat{a}_{k=p} \rangle = |\langle \hat{a}_{k=p} \rangle|^2$ defined as the population of the state with momentum $p$, where $k$ is the quasi-momentum of a condensate in an optical lattice. Finally, the critical momentum $p_c$ is obtained self-consistently under the condition that the group velocity becomes maximum:

$$
p_c = \arctan \left( \frac{n_{k=p=p_c}}{\frac{dn_{k=p}}{dp}} \right).
$$

(3)

Note that this equation is also applicable to the $S = 1$ BHM. In this paper, we determine the phase boundary of dynamical instability using this $p_c$ to remove the influence of momentum acceleration rate $\alpha$, while the previous work employed $p_d$ [7].
III. RESULTS AND DISCUSSION

A. Dynamics of superfluid flow

Figure 1 shows the time-evolution of condensate fractions \( n_{k=p} \) for the spin-1 \((S=1)\) and the spinless \((S=0)\) BHM with filling \( n = 1 \) and on-site repulsion \( U_0 = 10 \), as functions of increasing momentum in time as \( p(t) = 0.005 t \). In the \( S=1 \) BHM, we set \( U_2/U_0 = -0.3 \) (ferromagnetic) and \( U_2/U_0 = 0.3 \) (antiferromagnetic). At time \( t = 0 \), we choose the ground state as the initial state for corresponding \( U_0 \) and \( U_2 \) values. Note that the total \( S_z = \sum_{i,z} S_i \) in the system is conserved during time evolution. From Fig. 1, \( n_{k=p} \) gradually decreases as the momentum \( p(t) \) is increased, and then suddenly decays owing to the dynamical instability. The decay momenta are correspondingly \( p_d = 0.44 \) for \( U_2/U_0 = -0.3 \) and \( 0.45 \) for \( U_2/U_0 = 0.3 \) in the \( S = 1 \) BHM, and \( 0.38 \) in the \( S = 0 \) BHM. We find that the \( S = 1 \) condensate persists to larger \( p(t) \) than the \( S = 0 \) condensate, indicating some influences of the spin-dependent interaction included in the Hamiltonian Eq. (1). Interestingly, the initial condensate fraction at \( p(0) = 0 \) in the \( S = 1 \) BHM with \( U_2/U_0 = 0.3 \) is almost the same as that in the \( S = 0 \) model. Moreover, even in the \( S = 1 \) BHM, \( p_d \) for \( U_2/U_0 = 0.3 \) is slightly larger than that for \( U_2/U_0 = -0.3 \), while the condensate fraction around \( p = p_d \) for \( U_2/U_0 = 0.3 \) is apparently smaller than that for \( U_2/U_0 = -0.3 \). These results suggest that the amplitude of condensate fraction does not solely determine \( p_d \), which is very consistent with the fact that the derivative \( \frac{dn_{k=p}}{dp} \) is also included in Eq. (3) for determining \( p_c \).

As we briefly mentioned in the former section, the decay momentum \( p_d \) inevitably becomes larger than the critical momentum \( p_c \) of Eq. (4) under the condition that the system parameters are equal, i.e., the same interaction strength, filling, and lattice geometry. Our previous work in Ref. [43] elucidated that a superfluid can flow stably beyond the critical momentum \( p_c \) until the unstable mode casing dynamical instability fully grows. This retardation effect always exists as long as a finite acceleration of a condensate in calculations or experiments. We confirmed in Fig. 1 that \( p_d \) approaches \( p_c \) in the both BHMUs using a smaller coefficient \( \alpha (< 0.005) \) for \( p(t) = \alpha t \).

Next we discuss how the spin-exchange processes play a role during time evolution in the \( S = 1 \) BHM, which is governed by the third and the forth terms on the right-hand side of Eq. (A1) in Appendix A. We focus on the antiferromagnetic case with \( U_2/U_0 = 0.3 \), in which spin degrees of freedom are unfrozen. In our calculations, all particles are in the \( S = 1 \) state and spins are completely frozen in the ferromagnetic case of \( U_2 < 0 \). Figure 2 shows the time-evolution of the condensate fraction \( n_{k=p} \) and the population of each spin component \( n_{\gamma}/n(\gamma = 0, \pm 1) \) for two interaction strengths: (a) \( U_0/U_{0c} = 0.2 \) and (b) \( U_0/U_{0c} = 0.8 \), respectively. Here \( U_{0c} \) denotes the critical interaction strength at the Mott-insulator transition point in the \( S = 1 \) BHM and \( U_{0c} = 37.9 \) in the case of \( U_2/U_0 = 0.3 \). Note that in Fig. 2 both \( n_1 \) and \( n_{-1} \) are equal all the time owing to the initial state we choose and the conservation of total \( S_z \). For \( U_0/U_{0c} = 0.2 \) shown in Fig. 2(a), the populations of the \( S_z = \pm 1 \) states gradually decrease and that of the \( S_z = 0 \) state increases with increasing momentum, and finally all the spin components mix chaotically, which is accompanied by the decay of a superfluid flow. We also find the similar chaotic mixing of spin components in the case of \( U_0/U_{0c} = 0.8 \) in Fig. 2(b) after the populations of the \( S_z = \pm 1 \) states slightly increase and that of the \( S_z = 0 \) state decreases. However, the variation in spin populations is quite small during the time evolution, suggesting that spins are almost frozen in this case. We can naturally understand these results by noting that the third and the forth terms in Eq. (A1) contribute more largely to spin-mixing in the region where \( U_0 \) is small enough and correspondingly the amplitude of the Gutzwiller parameters \( |f_i(n_i \geq 2)|^2 \) becomes larger. Furthermore, it should be also noted here that we can not find any novel magnetic instabilities in the time evolution shown in Fig. 2.

B. Phase diagram at unit filling

Figures 3(a) shows the dynamical phase diagram of the \( S = 1 \) BHM with ferromagnetic interaction \( U_2/U_0 = -0.3 \) along with the results of the \( S = 0 \) BHM. Each line represents the critical momentum \( p_c \) as a function of interaction strength \( U_0 \) and corresponds to the phase boundary which separates between a stable and an unstable phase. The dynamical instability occurs in the upper unstable region. Note that these phase boundaries are determined via the maximum of group velocity as is explained in Sec. II. From Fig. 3(a), it is found that the critical momentum of dynamical instability smoothly changes from \( p_c = \pi/2 \) at \( U_0 = 0 \) to \( p_c = 0 \) at \( U = U_{0c} \) (i.e., the interaction strength at the MI transition point in thermal equilibrium). The critical interactions are \( U_{0c} = 33.3 \) for the \( S = 1 \) BHM and \( U_{0c} = 23.3 \) for the \( S = 0 \) BHM, respectively. The cross mark at about \( p/\pi = 0.44 \) in Fig. 3(a)
Hamiltonian (1) becomes equivalent to the spin-less case. Next, we view the phase diagram for ferromagnetic ($U_2 < 0$) case. The situation is relatively simple in this case. The lowest energy state, in our calculation, is the state in which all particles are in the $S_z = 1$ state. Therefore, the spin dependent $U_2$ term in the Hamiltonian (1) becomes equivalent to

$$ U_2 \sum_i \hat{n}_i (\hat{n}_i - 1). \tag{4} $$

Since this form is equal to the form of the $U_0$ term in the Hamiltonian (1), the $U_2$ term gives just the shift of $U_0 \rightarrow U_0 + U_2$; in the present case of $U_2 = -0.3U_0$, $U_0$ is effectively reduced to 0.7$U_0$. The phase boundaries in the spin-less case and the $S = 1$ case hence match when $U_0$ is normalized with each $U_{0c}$ as is shown in Fig. 2(b). So this case is essentially equivalent to the spin-less case. Next, we view the phase diagram for $U_2 > 0$, anti-ferromagnetic case. In Fig. 2(b), we find that the phase boundaries are quite close together for $U_0 \lesssim 5$ ($S = 1$ boundary is slightly below), and gradually diverge for $U_0 \gtrsim 5$. This divergence of the phase boundaries for $U_0 \gtrsim 5$ basically originates from the difference of the Mott-transition points of $S = 0$ and $S = 1$. In the strongly correlated system, the probability of double occupation $n_j = 2$ at each site in the $S = 1$ system is much larger than in the $S = 0$ system for an equal interaction strength $U_0$ owing to the formation of local spin singlet state $|n_i, S_i, S_{i,z}⟩ = |2, 0, 0⟩$ (this formulation is defined by formula (23) in the reference [44]), which has the energy gain $-2U_2$ in the $U_2$ term. This larger fluctuation of the number of particles prevents the Mott-transition in the $S = 1$ system with unit filling. The critical interaction strength in the Mott-transition of the $S = 1$ system, consequently, is larger than that of the $S = 0$ system. The stable area of the $S = 1$ system in the phase diagram expands compared with the $S = 0$ system with this larger critical interaction strength.

Figure 2(b) shows the phase diagram with normalized horizontal axis with $U_{0c}$ for $U_2 = 0.3U_0$. The phase boundaries are quite close together for $U_0/U_{0c} \gtrsim 0.6$, gradually diverge $U_0/U_{0c} \lesssim 0.6$, and both reach $p = \pi/2$ at $U_0/= 0$. In the anti-ferromagnetic case, the spin dependent term does not become a plain form such as the formula (4) specially due to the spin exchange terms, the last two terms of right hand in Eq. (3) (an expectation value of these spin exchange terms vanishes in the ferromagnetic case). The spin dependent $U_2$ term, therefore, does not work as just the shift of $U_0$, and the divergence of the boundaries for $U_0/U_{0c} \lesssim 0.6$ occurs. We examine this phase diagram dividing it into the two regime, the strongly correlated regime in which the phase boundaries are close ($U_0/U_{0c} > 0.6$, region 1) and the weaker correlated regime in which the boundaries diverge ($U_0/U_{0c} < 0.6$, region 2).

First, we show that the phase boundaries match in region 1. We suppose a system where the maximum number of particles per site is $n_{\text{max}} = 2$ because the probability of the $n_i \geq 3$ states is tiny due to the slight number fluctuations in the strongly correlated regime. In this case, only the states, $|n_i, S_i, S_{i,z}⟩ = |2, 0, 0⟩$, $|2, 2, \eta⟩$ ($\eta = 0, \pm 1, \pm 2$) have the non-zero energies corresponding to the

FIG. 2. Time evolutions of condensate fractions $n_{\text{cond}}$ and populations of each spin components $n_{\gamma}/n_{\text{tot}}$ ($\gamma = 0, \pm 1$) in the $S = 1$ BHM for $U_2/U_0 = 0.3$: $U_0/U_{0c} = 0.2$ (a), $U_0/U_{0c} = 0.8$ (b) where $U_{0c} (= 37.9)$ is the repulsive interaction strength at the Mott-insulator transition point.

FIG. 3. (Color online) Dynamical phase diagrams using $U_0$ (a) and $U_0/U_{0c}$ (b) axes for $U_2/U_0 = -0.3$. Superfluids can dynamically collapse in the upsides to the phase boundaries. The arrow in figure (a) indicates the horizontal axis in the Fig 4(a) and the cross mark indicates the collapse point in Fig 4(b). Phase boundaries of $S = 0$ and $S = 1$ are completely identical in figure (b).
U₂ term. The energy expectation values of the U₂ term is \(-2U₂\) for \([2,0,0]\) and \(U₂\) for \([2,2,\eta]\). \([2,2,\eta]\) states degenerate because of no magnetic field. As this, the energy by the U₂ term has only the two values. Then, we write \(|S_i = 0\rangle \equiv [2,0,0]\) and \(|S_i = 2\rangle \equiv \sum_\eta [2,2,\eta]\). The population of \(|S_i = 0\rangle\) state in \(n_i = 2\) states \(P₀ = \sum \sqrt{f_i(0,2,0) - \sqrt{2}f_i(1,0,1)}^2 / \sum f_i(n_i,0,n_i-1)\) at \(p = 0, p_c\) is shown in Fig. 4 (b) (the population of \(|S_i = 2\rangle\) state is \(P₂ = 1 - P₀\)). Here \(\sum n_i,n_i,0,n_i-1\) denotes the summation under the condition \(n_i, + n_i,0 + n_i, -1 = 2\). Note that, in region 1, the spin state becomes stationary irrespective of interaction strength and the superfluid momentum. This result is consistent with the slight spin variation seen in Fig. 2 (b). In this region, the spin exchange process does not occur and consequently the spin dependent U₂ term leads to a shift of \(U₀\). We can thus understand that the phase boundaries of both the \(S = 0\) and the \(S = 1\) BH models match when \(U₀\) is normalized by the corresponding \(U₀c\) as in Fig. 4 (b).

On the other hand, in region 2, spin configurations become complex because the population of \(n_i \geq 3\) states increases and the spin exchange in the U₂ term plays a role (Fig. 5 (b)). Here we examine how the spin degrees of freedom influences the value of critical momentum \(p_c\) and discuss the origin of the divergence of phase boundaries in region 2 seen in Fig. 4 (b). First, it follows from Eq. (3) that \(p_c\) is monotonically proportional to \(n_{k = p,p_c}/|dn_{k,p} / dp|\). It is generally known that the effective hopping amplitude of a condensate carrying the momentum \(p\) becomes \(t' = t \cos(p)\). The increment of momentum hence diminishes the condensate fraction \(n_{k = p}\) as shown in Fig. 1 which reduces the number fluctuations of a condensate at the same time. In the \(S = 1\) Bose-Hubbard model, this effect becomes more prominent thanks to the Hamiltonian. From Fig. 5, the population of \(|S_i = 0\rangle\) state increases with increasing momentum in the weakly correlated regime, while the population \(n_i \geq 3\) states decreases. This suggests that the number fluctuations in the \(S = 1\) system are further suppressed in order to energetically gain the spin dependent interactions. Therefore, \(|dn_{k,p} / dp|\) is generally larger than \(|dn_{k,p} / dp|\) in the weakly correlated regime. We can confirm this fact numerically from our result present: \(\delta n_{k,p} = n_{k,p} - n_{k,p}\) is 0.045 for the S=1 case with \(U₂/U₀ = 0.3\), which is nearly two times higher than 0.025 for the S=0 case. Going back to Fig. 4 (a), the difference of phase boundaries between \(S = 1\) and \(S = 0\) is very small in the weakly correlated regime owing to the small \(U₂\) values there. However, the normalized phase diagram in Fig. 4 (b) successfully extracts the existence of the spin effect on the dynamical instability of superfluid flow.

C. Phase diagrams at other fillings

1. commensurate case

It is generally known that the SF-MI transition in the BHM strongly depends on fillings (i.e., the average number of particles per site). Especially, in the \(S = 1\) BHM with anti-ferromagnetic interactions, the critical interaction strength at the transition \(U₀c\) shows a clear dependence on the parity of fillings: \(U₀c\) at odd fillings is larger than that in the \(S = 0\) BHM system, while it becomes smaller at even fillings [34, 35]. This property is easily understood from the fact that the formation of the local singlet-state for gaining the energy of \(-2U₂\) in the U₂ term in the Hamiltonian Eq. (1) enhances (suppresses) the density fluctuations at odd (even) fillings. Here we discuss how the parity affects the dynamical instability in the \(S = 1\) BHM.

In Fig. 6(a)-(c), the dynamical phase diagrams of the \(S = 1\) BHM for \(U₂/U₀ = 0.3\) are given at the several different fillings (i.e., \(n = 2, 3,\) and 4) along with the results of the \(S = 0\) model. From these figures and Fig. 4 (a), we find that the influence of the parity clearly appears in the dynamical phase diagrams. The stable area of the \(S = 1\) model basically expand (shrink) at even (odd) fillings in comparison with the \(S = 0\) model, which reflects to the corresponding increase (decrease) of \(U₀c\). In the case of \(n = 3\) shown in Fig. 6 (c), however, the stable area obviously decreases in the weakly correlated regime. As we pointed out for the unit filling in
FIG. 5. (a): Populations of the local spin singlet state |\(S_z = 0\) at \(p = 0\) (dashed line) and \(p = p_c\) (solid line). (b): Population of \(n_j \geq 3\) states within our truncated Fock space at \(p = 0\) (dashed line) and \(p = p_c\) (solid line).

In the previous subsection, the unfrozen spins that prefer to form the local singlet state highly suppress the density fluctuations and make a superfluid flow unstable in the weakly correlated regime. We have confirmed this effect more clearly in the case of \(n = 3\) filling.

On the other hand, in Fig. 6(d), we plot the dynamical phase diagram for the \(n = 2\) filling as a function of the normalized interaction \(U_0/U_{0c}\). The \(S = 1\) phase boundary is located above the \(S = 0\) curve in the entire range of interactions, which is in contrast to the phase diagram at the unit filling shown in Fig. 4(b). This suggests that the unfrozen spins prefering the local singlet states stabilize a superfluid flow. We have found this tendency also in the case of \(n = 4\) filling as a characteristic of the dynamical instability at even fillings. Moreover, the stable area expands more widely for this \(n = 4\) case in comparison with Fig. 5(d). It can be concluded that spins have a greater influence on the dynamical property of a superfluid flow at larger fillings.

2. Incommensurate case

In the system with incommensurate fillings, the SF-MI transition does not occur owing to extra particles deviating from commensurate fillings. Polkovnikov et al. calculated the dynamical phase diagram of the \(S = 0\) BHM with incommensurate fillings based on the Gutzwiller approximation in Ref. [8]. They clarified that the critical momentum \(p_c\) has a minimum at a certain interaction strength and then asymptotically approaches \(\pi/2\) with increase in interaction strength. The superfluidity of extra particles becomes highly robust in the strongly interacting regime, i.e., the recovery of superfluidity due to the repulsive interaction. Here we analyze this tendency in the \(S = 1\) BHM with the anti-ferromagnetic interaction \(U_2/U_0 = 0.3\).

Figure 7 shows the dynamical phase diagrams of the \(S = 1\) BHM with the filling factors deviating slightly from \(n = 1\) and \(n = 2\), along with the diagrams of the \(S = 0\) BHM. From these figures, the dynamical phase diagrams of the \(S = 1\) BHM at incommensurate fillings qualitatively agree with those of the spin-less \(S = 0\) model. However, we still find the influence of the parity which we have seen in the phase boundaries for the commensurate cases. In Fig. 7(a) and (b) where the fillings are close to \(n = 1\), the critical momentum reaches a minimum at larger interaction strength in the \(S = 1\) BHM when we compare with the \(S = 0\) BHM. On the other hand, in Fig. 7(c) and (d) where the fillings are close to \(n = 2\), the minimum for \(S = 1\) is apparently smaller than that for \(S = 0\). This behavior can be roughly understood from whether the formation of the local spin singlet-state conceals or accentuates the extra particles. As mentioned in the commensurate case, the formation of the local singlet-state enhances (suppresses) the density fluctuation of a condensate with the odd (even) fillings. The intense density fluctuation of a condensate conceals the effect of the extra particles in the left side from the minimum points while the suppressed density fluctuation accentuates the extra particles in the right side. Therefore, in the cases of the fillings close to \(n = 1\), the extra particles are more concealed due to the formation of the local spin singlet-state and the minimum point for \(S = 1\) slides to the right compared to that of \(S = 0\), while the extra particles are more accentuated due to the formation of the local spin singlet-state and the minimum point for \(S = 1\) slides to the left compared to that of \(S = 0\). Furthermore, there exits the particle-hole symmetry in the dynamical phase diagrams with incommensurate fillings by noting the consistency be-
physical information, is significant to understand the dynamical instability. This collective excitation, which involves much more than the density modulation associated with the dynamical instability. It is known that a spin-less superfluid flow in an optical lattice shows the population modulation as a precursor phenomenon of the dynamical instability. Whether the spin modulation of a superfluid flow occurs in the $S_z = 0$ component while the total density modulation develops intensely. This reflects the consistent develop of the modulations of $S_z$ components above. Therefore, the spin modulation occurs only within the $xy$ plane.

Next, let us examine the spin modulation in the system with a uniform magnetic field in the $z$ direction. In this case, the populations of $S_z = \pm 1$ components develop independently, namely, small spatial fluctuations in a condensate grow independently in $S_z = 1$ and $S_z = 0$ components. This result indicates that $S_z = \pm 1$ components seemly equivalent decay independently if only there is difference between the populations of the components. As a result, spin modulation of $S_z$ component occurs as is shown in Fig. 9 (b).

IV. SUMMARY

In this work, we have analyzed the dynamics of a spin-1 superfluid in the $S = 1$ Bose-Hubbard model assuming that the dynamical instability is significant to understand the dynamical instability. This calculation involving the spin degrees of freedom clarified that the dynamical phase diagram of the spin-1 system shifts to that of spin-less one. This shift fundamentally differ for the on-site ferromagnetic interaction and anti-ferromagnetic interaction. In the case of $U_2 > 0$, anti-ferromagnetic case, as obviously shown notably in the $n = 3$ phase diagram, the difference of the Mott-insulator transition points does not entirely decide the difference of phase boundaries between $S = 1$ and $S = 0$ although that difference affects as a main cause in the strong correlated regime. We also shows the dependence of the phase diagram on the average number of particles per site, in particular, the parity. Finally argued the density modulation and the spin modulation associated with the dynamical instability. We found that the anisotropy of the spin modulation depending on with or without a uniform magnetic field. It is intriguing that properties of
FIG. 8. (Color online) Density modulation associated with the dynamical instability with no magnetic field. (a): Density distributions of $S_z = 1$ (triangle), $S_z = 0$ (circle), and $S_z = -1$ (square) components in real space. The density distributions of $S_z = \pm 1$ are fully consistent. (b): Vertical axis represents for the deviation from the positional mean value of particle number (light line) and magnetization (dark line). The parameters are settled as $n = 1$, $U_0 = 10$, and $U_2/U_0 = 0.3$. These results are at $p/\pi = 0.46$, after the decay at $p\pi/\pi = 0.45$.

ACKNOWLEDGMENTS

Some of the numerical computations were carried out at the Yukawa Institute Computer Facility and at the Cyberscience Center, Tohoku University. This work was partly supported by JSPS KAKENHI Grant Number 25287104.

Appendix A: The equations of spin-1 Gutzwiller parameters

The equations of motion for Gutzwiller parameters in the $S=1$ BHM is given as

$$i\dot{f}_j(n_{j,-1}, n_{j,0}, n_{j,1}) = \frac{U_0}{2} n(n-1)f_j(n_{j,-1}, n_{j,0}, n_{j,1})$$

$$+ \frac{U_2}{2} (n_{j,0}^2 - 2n_{j,1}n_{j,-1} + n_{j,-1}^2 - n_{j,1} - n_{j,-1} + 2n_{j,1}n_{j,0} + 2n_{j,0}n_{j,-1})f_j(n_{j,-1}, n_{j,0}, n_{j,1})$$

$$+ U_2 \sqrt{n_{j,1}(n_0 + 1)(n_0 + 2)n_{j,-1}f_j(n_{j,-1} - 1, n_{j,0}, + 2, n_{j,1} - 1)}$$

$$+ U_2 \sqrt{(n_{j,1} + 1)n_0(n_0 - 1)(n_{j,-1} + 1)f_j(n_{j,-1} + 1, n_{j,0} - 2, n_{j,1} + 1)}$$

$$- t z \left( \sqrt{n_{j,0}f_j(n_{j,-1} - 1, n_{j,0}, n_{j,1})\psi_j,-1 + \sqrt{n_{j,-1} + 1}f_j(n_{j,-1} + 1, n_{j,0}, n_{j,1})\psi^*_j,-1} \right)$$

$$- t z \left( \sqrt{n_{j,0}f_j(n_{j,-1} - 1, n_{j,0}, n_{j,1})\psi_j,0 + \sqrt{n_{j,-1} + 1}f_j(n_{j,-1} + 1, n_{j,0}, n_{j,1})\psi^*_j,0} \right)$$

$$- t z \left( \sqrt{n_{j,1}f_j(n_{j,-1} - 1, n_{j,0}, n_{j,1})\psi_j,1 + \sqrt{n_{j,1} + 1}f_j(n_{j,-1} + 1, n_{j,0}, n_{j,1} + 1)\psi^*_j,1} \right),$$

(A1)

where

$$\psi_{j,1} = \frac{1}{2} \sum_{\{n_{j,-}\}} \sqrt{n_{j+1,1} + 1} f_{j+1}^* (n_{j+1,-1}, n_{j+1,0}, n_{j+1,1}) f_{j+1} (n_{j+1,-1}, n_{j+1,0}, n_{j+1,1} + 1) e^{ip(t)}$$

$$+ \frac{1}{2} \sum_{\{n_{j,-}\}} \sqrt{n_{j-1,1} + 1} f_{j-1}^* (n_{j-1,-1}, n_{j-1,0}, n_{j-1,1}) f_{j-1} (n_{j-1,-1}, n_{j-1,0}, n_{j-1,1} + 1) e^{-ip(t)}$$

$$+ \frac{1}{2} \sum_{\tau} \sum_{\{n_{j+\tau,-}\}} \sqrt{n_{j+\tau,1} + 1} f_{j+\tau}^* (n_{j+\tau,-1}, n_{j+\tau,0}, n_{j+\tau,1}) f_{j+\tau} (n_{j+\tau,-1}, n_{j+\tau,0}, n_{j+\tau,1} + 1).$$
FIG. 9. (Color online) Density modulation associated with the dynamical instability with uniform magnetic field. The parameters are \( n = 1, U_0 = 10, \) and \( U_2/U_0 = 0.3 \) as well as Fig 8. Uniform magnetic field is applied to adjust the populations of spin components to \( n_1 : n_{-1} \sim 7:3 \) only at initial state \( p = 0 \) along \( z \) direction. These results are at \( p/\pi = 0.44 \) after the decay at \( p_d/\pi = 0.427 \).

\[
\psi_{j,0} = \frac{1}{z} \sum_{\{n_j, \tau\}} \sqrt{n_j+1,0} + \frac{1}{z} \sum_{\{n_j, \tau\}} \sqrt{n_j-1,0} + \frac{1}{z} \sum_{\{n_j, \tau\}} \sqrt{n_j+\tau,0} + \frac{1}{z} \sum_{\{n_j, \tau\}} \sqrt{n_j-\tau,0} \cdot \frac{1}{z} \sum_{\{n_j, \tau\}} \sqrt{n_j+1,1} + \frac{1}{z} \sum_{\{n_j, \tau\}} \sqrt{n_j-1,1} + \frac{1}{z} \sum_{\{n_j, \tau\}} \sqrt{n_j+\tau,1} + \frac{1}{z} \sum_{\{n_j, \tau\}} \sqrt{n_j-\tau,1}.
\]

(A2)

Here \( j+1, j-1, \) and \( j+\tau \) denotes \((j_1+1, j_2), (j_1-1, j_2), \) and \((j_1, j_2+\tau)\) respectively, where \( j_1 \) is the site index of the flow direction and \( j_2 \) is that of the orthogonal direction. The summation \( \sum_{\tau} \) runs over the nearest neighbors of site \( j \) in the orthogonal direction, and \( z \) is the number of adjacent sites in the lattice.

[1] I. Bloch, Nat. Phys. 1, 23 (2005).

[2] O. Morsch and M. Oberthaler, Rev. Mod. Phys. 78, 179 (2006).
