Spin-Orbit Driven Transitions Between Mott Insulators and Finite Momentum Superfluids of Bosons in Optical Lattices

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Synthetic spin-orbit coupling in ultracold atomic gases can be taken to extremes rarely found in solids. We study a two dimensional Hubbard model of bosons in an optical lattice in the presence of spin-orbit coupling strong enough to drive direct transitions from Mott insulators to superfluids. Here we find phase-modulated superfluids with finite momentum that are generated entirely by spin-orbit coupling. Transitions between different superfluids are also found to be first-order. We investigate the rich periodic structure of the phases of the superfluids, which may be directly probed using time-of-flight imaging of the spin-dependent momentum distribution.

PACS numbers: 03.75.Mn, 67.85.Hj, 67.25.dj

I. INTRODUCTION

The Rashba effect [1] in solids derives from the motion of an electron in a strong electric field. As the electron moves in the presence of a potential gradient, \( \nabla V \), it experiences an effective magnetic field in its frame of reference. The Rashba energy [1]:

\[
\langle \nabla V \times \vec{p} \rangle \cdot \vec{\sigma},
\]

(1)
captures the energetics of electron spin reorientation due to the effective magnetic field, where \( \vec{p} \) is the particle momentum and \( \vec{\sigma} \) are the Pauli matrices. The Rashba spin-orbit coupling (SOC) energy is well known to be particularly strong at metallic surfaces [2,3] (e.g., on Ag(111) or Au(111)) because here we find extremely strong potential gradients. As a result, studies of the impact of Rashba SOC on two-dimensional (2D) conductors have a long history [4]. But the impact of Rashba SOC on the surface states of Mott insulators has come under more careful scrutiny recently because of possible connections to topological insulators [3,6].

Mott insulators localize as a result of strong interaction and would therefore appear to exclude the possibility of SOC effects, but one can argue that this is not always the case. Small momentum in Eq. (1) (the case for localized states) does not necessarily imply low Rashba energies. In an extreme limit, Mott insulating surfaces can, in principle, experience very large potential gradients that can compensate the small momentum, i.e., \( \langle \vec{p} \rangle \to 0 \) with \( \langle \nabla V \times \vec{p} \rangle \sim E_F \), where \( E_F \) is the Fermi energy. If, in this limit, the energetics of Rashba SOC compete with the Mott gap, one could observe a transition between a Mott insulator and a conducting state driven entirely by Rashba SOC in spite of the small average momentum of particles in Mott insulators. Unfortunately, the limit where Rashba SOC competes with the Mott gap is rare in solids because it would typically be precluded by other effects, such as charge transfer between bands. But this limit can be explored in another context: using synthetic SOC in optical lattices.

Recent experimental progress [7–13] demonstrates engineering of synthetic SOC for ultracold atomic gases [14]. These experiments show that Raman beams can be used to dress atoms with a spin-dependent momentum. Rashba (and/or Dresselhaus) SOCs governing these dressed states [15] are tunable to extremes not possible in solids, see Fig. 1. Recent work shows, for example, that synthetic SOC can generate flat bands [17,18], exotic superfluidity [19], and intriguing vortex structures [16,20,21].

Recent theory work has also explored the impact of SOC on the spin structure of Mott insulators in optical lattices [22–26]. Here super-exchange coupling between sites was shown to combine with Rashba SOC to lead to rich spin structures within the Mott state [22–26]. But in these studies parameters were chosen to explore the impact of Rashba SOC on the spin physics of Mott insulators while leaving the charge structure intact.

In this work we explore Rashba SOC that is strong enough to cause the breakdown of charge ordering in Mott insulators. This extreme limit is of direct relevance to optical lattice experiments with synthetic SOC. We study, in particular, a 2D lattice model of two-component interacting bosons in the presence of tunable Rashba coupling. We find that strong Rashba SOC can cause the breakdown of the Mott insulating state and drive a direct transition between the Mott insulator and a superfluid state, even in the absence of single particle tunneling between sites of the lattice. This limit is the lattice version of the limit discussed above, \( \langle \vec{p} \rangle \to 0 \) with \( \langle \nabla V \times \vec{p} \rangle \sim E_F \), where vanishing kinetics leaves Rashba SOC to generate its own conducting state. For the case of lattice bosons studied here, we find that Rashba SOC generates finite momentum superfluids. We show that these superfluids are characterized by staggered phase patterns. We also find that distinct superfluid states are
FIG. 1: Comparison of SOC strengths in solids and cold atoms. $h$, $\alpha$, and $E_F$ denote the Zeeman energy, SOC coefficient, and Fermi energy, respectively. For GaAs, the effective mass is $m^* = 0.067m_0$ [28], where $m_0$ is the electron mass, the Rashba SOC strength is $\alpha = (0.04-0.06) \times 10^{-11}$ eV-m [28], and the $g$-factor is $g^* = -0.45$ [29]. For InAs the parameters are: $m^* = 0.026m_0$ [21], $\alpha = (0.28-1.4) \times 10^{-11}$ eV-m [30], and $g^* = -15.1$ [31]. For InSb the parameters are: $m^* = 0.0135m_0$ [27], $\alpha K_F = (1.0-1.2) \times 10^{-11}$ eV-m [32], and $g^* = -51$ [31]. And for the metallic surfaces: $m^* \approx 0.255m_0$ [23], where the $g$-factor is assumed to be $g^* = 2$. The parameters for these four different examples are plotted at an external magnetic field of 5 Tesla. A high carrier density, $n = 10^{11}$ cm$^{-2}$, is used for the semiconductors. For SrTiO$_3$/LaAlO$_3$ oxide interfaces, the data are taken from Ref. 33. Additional feasible parameter regimes are plotted as horizontal and vertical bars.

The paper is organized as follows: In Sec. II we construct a Bose-Hubbard model of two-component atoms in the presence of Rashba SOC. We also discuss two complimentary mean field approaches that allow us to compute the phase diagram, transition properties, and the momentum distribution. In Sec. III we present results on finite lattice sizes. We use Gutzwiller mean field theory to show that Rashba SOC causes the Bosonic Mott insulator to give way to finite momentum superfluids. We also explore inter-superfluid transitions. We find that first order transitions separate distinct phase patterns of finite momentum superfluids. We demonstrate in Sec. IV that these different finite momentum phases can indeed be observed in experiments with a trapping potential. In Sec. V we present analytic arguments that the first order transitions depend critically on boundary effects, akin to effects found in Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) superconductors [34, 37]. We show that analytic mean field calculations in the infinite system size limit do not show these first order transitions. We summarize in Sec. VI.

II. MODEL AND METHODS

We consider a 2D square optical lattice containing bosonic atoms with two hyperfine levels. States with two hyperfine levels act as a pseudo-spin 1/2 state. We also assume the presence of Raman beams that couple the atomic momentum to the spin to generate synthetic SOC [7–11, 13]. The interaction between alkali atoms is governed by a short-range (s-wave) repulsion. For a deep optical lattice, the problem can be accurately described in the single-band, tight-binding limit [42] where the s-wave interaction becomes an on-site Hubbard interaction and the SOC is discretized.

To study this system we construct a Hubbard model of two-component bosons in the presence of Rashba SOC on a square lattice. We allow the on-site Hubbard interaction to have a spin-dependent interaction:

$$H = -t \sum_{\langle ij \rangle} \Psi_i^\dagger \Psi_j + \frac{U}{2} \sum_{\sigma} n_{i\sigma}(n_{i\sigma} - 1) + U_{t\uparrow\downarrow} \sum_{i} n_{i\uparrow} n_{i\downarrow} - \mu \sum_{\sigma} n_{i\sigma} + i\lambda \sum_{\langle ij \rangle} \Psi_i^\dagger \vec{e}_z \cdot (\vec{\sigma} \times \vec{d}_{ij}) \Psi_j + H.c.,$$

(2)

where, $\Psi_i = (b_{i\uparrow}, b_{i\downarrow})^T$ is a two-component bosonic annihilation operator at the site $i$, $n_{i\sigma} = b_{i\sigma}^\dagger b_{i\sigma}$, $t$ is the spin-independent nearest neighbor tunneling, $U (U_{t\uparrow\downarrow})$ is the on-site interaction between bosons of the same (different) spin $\sigma$, and $\mu$ is the chemical potential. In the last term $\lambda$ is the Rashba SOC strength, $\vec{d}_{ij}$ is the unit vector between the neighboring sites $i$ and $j$, and $\vec{e}_z$ is the unit vector along the $z$ direction. In the following we use $U = 1$ to set the energy scale.
The tunneling and Rashba terms induce two different types of superfluidity. To see this we plot the spin-independent tunneling and spin-dependent tunneling in Fig. 2. The left panel shows that the spin-independent tunneling favors phase uniformity since $t$ is real. But in the right panel we see that SOC has two effects: It induces tunneling between neighboring sites with two different spin states and it imposes phase variation.

The phase variation depends strongly on the direction of the neighboring sites. SOC therefore favors highly anisotropic superfluid states. Without SOC the system has at least an $U(1)$ symmetry, which means that the total number of each species is conserved; however, SOC introduces spin flips between two neighboring sites, thus the system only respects $U(1)$ symmetry and, as a result, the phase difference between the neighboring sites cannot be gauged out. The competition between spin-independent tunneling and spin-dependent tunneling tunes the transition between these different superfluids and can therefore be a first order process.

In the weakly interacting limit the model exhibits three different superfluid phases: In the regime when spin-independent tunneling dominates ($t \gg \lambda$), the uniform superfluid is preferred and the total momentum of the superfluid is zero; in the opposite regime, a staggered superfluid phase is preferred; and in the intermediate regime, $t \sim \lambda$, the strong competition between the two tunnelings gives rise to superfluids with phase patterns that depend strongly on boundary effects.

Strong interactions add competing Mott insulating phases and complicates estimates of the phase diagram. To study the competition between all ground states we use two complimentary mean field approaches. We apply the Gutzwiller mean field method to finite system sizes (relevant to experiments) and compare with an otherwise equivalent mean field limit applied to infinite system sizes.

We now discuss the Gutzwiller mean field method \cite{42, 43}. The method assumes a product ground state of the form: $|G\rangle = \prod_n \langle n_1^{\dagger} n_\downarrow | n_2^{\dagger} n_\uparrow | \cdots | n_N^{\dagger} n_{\downarrow} \rangle$. This form for the wavefunction has been extensively applied to bosons in optical lattices \cite{42}, even in the presence of complex hopping amplitudes \cite{14}. It generally gives quantitatively reliable results in 2D and 3D, (for comparisons, see, e.g., Ref. \cite{15}), and is a particularly excellent approximation when computing local correlation functions (See, e.g., Ref. \cite{16}). The variational parameters $f$ are obtained by minimizing the total energy:

\begin{equation}
E = \frac{\langle G | H | G \rangle}{\langle G | G \rangle}.
\end{equation}

We minimize the total ground state energy with the gradient descent algorithm \cite{47, 48}. The ground state energy is reached when the energy variation is less than $10^{-5}U$, which is sufficient to distinguish the energy difference between different phases.

We supplement the finite system size Gutzwiller method with an equivalent mean field limit applied to infinite system sizes. We assume $\langle b_{i\sigma} \rangle = \psi e^{i\theta_{\sigma}}$, where $\psi$ is a real number. This assumption is equivalent to the assumed form for $|G\rangle$ but works best on infinite system sizes. The total energy then becomes:

\begin{equation}
E_\psi = (U + U_{\uparrow\downarrow}) \psi^4 - (U + 2\mu + tA + \lambda B)\psi^2,
\end{equation}

where $N$ is the total number of sites and the coefficients are:

\begin{equation}
A \equiv N^{-1} \sum_{\langle ij \rangle} \left[ e^{i(\theta_{j\uparrow} - \theta_{i\uparrow})} + e^ {i(\theta_{j\downarrow} - \theta_{i\downarrow})} + H.c. \right],
\end{equation}

and:

\begin{equation}
B \equiv N^{-1} \sum_{\langle ij \rangle} \left[ Z_{ij} e^{i(\theta_{j\uparrow} - \theta_{i\uparrow})} - Z^*_{ij} e^{i(\theta_{j\downarrow} - \theta_{i\downarrow})} + H.c. \right],
\end{equation}

with $Z_{ij} \equiv d_{ij}^* + i d_{ij}^\prime$. An important point here is that the total energy depends not only on the magnitude of the order parameter $\psi$, but also on the phase difference between neighboring sites. We see that the minimal energy $E_\psi$ corresponds to a maximal value of $A$ and $B$ when $U$, $U_{\uparrow\downarrow}$, $\lambda$, and $t$ assume positive values (the case studied in this paper). Here $A$ depends only on the phase difference between the same spin states, while $B$ depends strongly on the phase difference between spin up and spin down states in the neighboring sites. The competition between $A$ and $B$ governs competition between superfluids.

FIG. 3: (Color online) Phase diagrams of 2D optical lattices with bosons obtained from Gutzwiller variational simulations for a $4 \times 4$ lattice with periodic boundary condition at (a) $U_{\uparrow\downarrow} = 0, \lambda = 0$, (b) $U_{\uparrow\downarrow} = 0, \lambda = 0.04U$, (c) $U_{\uparrow\downarrow} = 0.5U, \lambda = 0$, and (d) $U_{\uparrow\downarrow} = 0.5U, \lambda = 0.04U$. The phase diagrams are determined by the amplitude of the spin-up superfluid order parameter. The spin-down superfluid order parameter produces similar results.
with distinct phase patterns. Obviously, when \( \lambda = 0 \), \( A \) takes its maximum value when all of the sites have the same phase, which corresponds to the uniform superfluid phase.

III. QUANTUM PHASES IN FINITE LATTICES WITH PERIODIC BOUNDARIES

We now discuss results that demonstrate the competition between various Mott and superfluid phases in the presence of SOC. We first present our results on small system sizes with periodic boundaries. These system sizes are consistent with mesoscopic states formed in the center of traps in experiments.

Fig. 3 shows the phase diagram for four different limits of the model, Eq. (2). Fig. 3a plots the Bose-Hubbard phase diagram \([19]\) that results from setting the SOC term and the inter-spin interaction term to zero in Eq. (2), i.e., \( \lambda = U_{\uparrow \downarrow} = 0 \). The absence of inter-spin interactions allows two identical copies of the Mott insulator to form a conducting state (in this case, a superfluid). Below we show that the precise nature of the re-}

Fig. 3c then corresponds to \( \lambda = 0 \) superfluids found on this part of the phase diagram \( \lambda = 0 \), SOC actually supplanted by SOC-generated superfluids. The upper and lower small Mott lobes exhibit degeneracies (for \( t = 0 \)) and correspond to \( \langle n_{i\uparrow} \rangle = 2, \langle n_{i\downarrow} \rangle = 0 \). The upper and lower small Mott lobes exhibit degeneracies (for \( t = 0 \)) and correspond to \( \langle n_{i\uparrow} \rangle = 3, \langle n_{i\downarrow} \rangle = \pm 1 \) and \( \langle n_{i\uparrow} \rangle = 1, \langle n_{i\downarrow} \rangle = \pm 1 \), respectively. Here we exclude super exchange effects, \( O(t^2/U) \), discussed in other work \([22, 24, 26]\).

We now discuss the phase diagram that results from adding SOC. Figs. 3b and 3c plot the phase diagrams that result from adding SOC to the states depicted in Figs. 3a and 3d, respectively. In both figures we see that the Mott insulators at higher \( \mu \) vanish. Increasing \( \mu \) causes a direct transition from a Mott insulator to a SOC-generated superfluid. At \( t = 0 \), SOC alone drives the formation of a superfluid. We find that the Mott insulators that normally persist at \( t = 0 \) for all \( \mu \) are actually supplanted by SOC-generated superfluids. The \( t = 0 \) superfluids found on this part of the phase diagram derive kinetics purely from the spin-dependent tunneling in SOC. We therefore find that even in the limit of vanishing kinetics, the Rashba effect drives the Mott insulator into a conducting state (in this case, a superfluid state). Below we show that the precise nature of the resulting superfluid depends on the relative strengths of \( \lambda \) and \( t \), as well as boundary effects. Figs. 3b and 3c also show first order jumps in the superfluid order parameter. Here we see that the phase of the superfluid is at first staggered but then completely reorients across the transition. These jumps derive from finite size effects that vanish in the thermodynamic limit (see below).

Fig. 4 shows the first order nature of these transitions. The left column shows the order parameters at \( \mu = U \), where the transition from the Mott phase to the phase-uniform superfluid is shown. But the right column shows results in a different regime, when \( \mu = 1.3U \). Here SOC dominates and the nonzero order parameters
are unchanged for $t \leq 0.01U$. At $t \sim 0.01U$, there is a sudden change of the order parameter and the total energy $E$. This explicitly shows the first order quantum phase transition between different superfluids. A similar phase transition also takes place at $t = 0.032U$ for these parameters.

The first order transitions between superfluids correspond to transitions between superfluids with different momenta. To see this we compute the spin-dependent momentum distribution at wavevector $k$:

$$
\langle \rho_{\uparrow,\downarrow}(K) \rangle = N^{-2} \sum_{i,j} \langle b_{i\uparrow}^\dagger b_{j\downarrow} \rangle e^{iK(R_i-R_j)},
$$

where the lattice spacing is chosen as the unit of distance and $R_j$ is the location of the lattice site $j$. Fig. 5 plots $\langle G | \rho_{\uparrow,\downarrow}(K) | G \rangle / \langle G | G \rangle$ for three different superfluids. Here we see that these three different states have qualitatively distinct momentum distributions. Here we have also verified that in these different phases, the magnitude of the order parameter is uniform over the whole lattice, indicating that only the phase pattern changes during the first order transition. Note that the peak in the momentum distribution for the first two phases depends strongly on the ratio between $\lambda$ and $t$. It is therefore possible to directly infer their ratio from the position of the peaks. We also note that the results presented in Fig. 5 relate directly to time-of-flight imaging that can measure momentum distribution of distinct hyperfine states.

The bottom panels in Fig. 5 show distinct symmetries in the phase of the superfluid order parameter. Fig. 5a shows the limit where the system has only $U(1)$ symmetry, thus the superfluid only has one phase degree of freedom defined by the angle $\alpha$. However, in the small $t$ limit, Fig. 5b, the phase pattern is mainly determined by the SOC term. Here we find phase patterns defined by two degrees of freedom, the angles $\alpha$ and $\beta$. In this limit the spin up in one site primarily couples to the spin down in the nearest neighbor sites. As a result, the $4 \times 4$ lattice decouples into two lattices, each of which contributes one phase degree of freedom. We find similar features in Fig. 5b where $\lambda \sim t$. This regime is different from Fig. 5a and c. It depends strongly on the lattice size. For instance, in a $5 \times 5$ and $6 \times 6$ periodic lattice (not shown here), the phase pattern only has one phase degree of freedom.

**IV. QUANTUM PHASES IN A TRAPPING POTENTIAL**

We now consider the effects of realistic confinement on the superfluid transitions. The finite momentum superfluids considered here are akin to the FFLO phase discussed in the context of trapped atomic Fermi gases. The FFLO state depends strongly on lattice geometry. Finite size effects are normally not considered to be relevant in solids because system sizes are typically much larger than correlation lengths. But cold atomic gases can be put into mesoscopic regimes where the system size is on the order of superfluid correlation lengths.

Small magneto-optical trapping potentials can be created in cold atom systems. We add a spatially varying chemical potential term to Eq. (2) to model confinement: $\sum_i V(\vec{R}_i)(n_{i,\uparrow} + n_{i,\downarrow})$. The trapping potentials are well approximated by a parabolic potential. We consider:

$$
V(\vec{R}_i) = 0.025U \left[ \left( R_i^x - \frac{L_x - 1}{2} \right)^2 + \left( R_i^y - \frac{L_y - 1}{2} \right)^2 \right]^{\frac{1}{2}}
$$

where $R_i^x (R_i^y)$ is the $x (y)$ coordinate of site $i$ and $L_x (L_y)$ is the lattice size along the $x$ ($y$) direction. The trap coefficient is chosen to ensure that the trapped atom density vanishes before the edge of the lattice is reached.

We now show that the sudden phase change, discussed in periodic systems above, also manifests in trapped systems. Fig. 6 shows a typical example obtained from solving Eq. (2) in the presence of parabolic trapping using the Gutzwiller ansatz. Here we see that small changes in kinetic energy induce totally different phase patterns. The top two panels show that the phase of the super-
fluid order parameter completely reorients with small changes in the hopping. The bottom four panels show that these changes do not reveal themselves in other correlation functions. The effects predicted here are observable in measurements sensitive to the phase of the superfluid order parameter (e.g., the momentum distribution function). This calculation shows that realistic trapping potentials lead to finite sized systems that harbor the first order transitions found in periodic systems discussed above.

V. QUANTUM PHASES IN INFINITE LATTICES

So far our study has been limited to finite-sized lattices. Here boundary effects put a strong constraint on the superfluid phase patterns that can be realized. But we can use Eq. (4) to study infinite lattices. We find a general solution for the lowest-energy state, \( \alpha \), above.

We now study infinite lattice sizes. In the infinite system size limit we find: \( E_k \rightarrow -4\sqrt{2}\lambda \sin(\alpha) - 8t \cos(\alpha) \). This implies that the energy will change smoothly as the period of the finite momentum superfluids changes dramatically. Fig. 7 shows that the energy computed on the infinite system size is in fact smooth. We therefore conclude that infinite lattice sizes will eliminate the first order transitions observed in finite sized systems. A similar result was found in studies of FFLO superfluids where periodic boundaries also constrain the FFLO momentum to select certain values [50, 51]. But we note that realistic experiments are actually trapped finite sized systems with \( N \sim 10^2 - 10^3 \). We therefore conclude that the first order transitions between distinct superfluids found here should be observable in the small system limit defined by the trap center.

VI. SUMMARY

We have studied the interplay of strong interaction and Rashba SOC in a model motivated by optical lattice experiments: a 2D Hubbard model of two-component bosons. We used mean field theory to map out the phase diagram and study transitions. We find that strong Rashba SOC can completely destroy the Mott insulator state, even in the absence of spin-independent tunneling in the lattice. The Rashba SOC leads to superfluids with complex phase patterns and finite momentum. We identified first order transitions between distinct superfluids, e.g., the transition between superfluids with two different staggered phase patterns, that can be identified in the spin-dependent momentum distribution. The spin-dependent momentum could be accessed in time-of-flight measurements on optical lattices. We expect these transitions to occur in finite sized systems but the phase patterns and precise momenta depend strongly on the boundaries. We checked that these first order transitions become smooth in infinite system sizes.

Our work relates to the nature of Mott insulator states in solids. Our study of a 2D lattice finds that it is in principle possible for strong Rashba SOC to convert a Mott insulator into a conducting state even in the limit of vanishing kinetics \( t \rightarrow 0 \) with \( \lambda \sim 1 \) in the lattice model or \( \langle p \rangle \rightarrow 0 \) with \( \langle \vec{V} \times \vec{p} \rangle \sim E_F \) in the continuum. This limit could have bearing on the nature of 3D Mott insulator surface states that experience very weak kinetics but strong electric fields.

Acknowledgements Y. Q., V. S., and C. Z. are supported by ARO (W911NF-12-1-0335, W911NF-12-1-0334), AFOSR (FA9550-11-1-0313), NSF-PHY (1249293), and DARPA-YFA. M.G is supported in part by Hong Kong RGC/GRF Project 401512, the Hong Kong Scholars Program (Grant No. XJ2011027) and the Hong Kong GRF Project 2130352.
