Emergence of Quantum Nonmagnetic Insulating Phase in Spin-Orbit Coupled Square Lattices

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We investigate the metal-insulator transition (MIT) and phase diagram of the half-filled Fermi Hubbard model with Rashba-type spin-orbit coupling (SOC) on a square optical lattice. The interplay between the atomic interactions and SOC results in distinctive features of the MIT. Significantly, in addition to the diverse spin ordered phases, a nonmagnetic insulating phase emerges in a considerably large regime of parameters near the Mott transition. This phase has a finite single-particle gap but vanishing magnetization and spin correlation exhibits a power-law scaling, suggesting a potential algebraic spin-liquid ground state. These results are confirmed by the non-perturbative cluster dynamical mean-field theory.

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The study of quantum many-body effects and new exotic states of matter are currently amongst the main topics in condensed-matter physics [1, 2]. During the last few years, the successful manipulation of ultracold atoms in optical lattices [3–8] and the experimental progress in the spin-orbit coupling (SOC) of degenerate atomic gases [9–13] have made it possible to explore diverse quantum phases [14–21]. More recently, optical lattices combined with SOC have attracted enormous interests. It was shown that SOC plays prominent roles in many fascinating phenomena, such as non-Abelian interferometry [22] and magnetic monopole [23, 24], topological phase transitions [25–27], non-Abelian localization [28], or emerging relativistic fermions [29].

When further competing with strong atomic interactions, SOC introduces additional degrees of quantum fluctuation, giving rise to remarkable many-body ground states. For example, the study of the superfluid to Mott insulator transition in the Bose-Hubbard model with synthetic SOC has demonstrated that, Rashba-type SOC can induce intriguing magnetism in the deep Mott regime [30–38], as well as an exotic superfluid phase with magnetic textures near the Mott transition [31, 37]. Despite this, the essential properties of the metal-insulator transition (MIT) of interacting fermion systems have been less achieved.

In this Letter, we show that SOC can stabilize a quantum nonmagnetic insulating (NMI) phase in a strongly correlated fermion system. Such a system described by the spin-orbit (SO) coupled Fermi Hubbard model (see Eq. (1)) has strong implications for realistic electronic materials [39]. Our main results are summarized in Fig. 1 which displays a rich phase diagram. First, the SOC tends to destroy the conventional antiferromagnetic fluctuations. This results in the distinctive features of the MIT with diverse spin ordered phases occurring on the side of Mott insulator. Significantly, a NMI phase emerges in the vicinity of the Mott transition for \( \alpha > \alpha_c \) (\( \alpha \) is the strength of SOC). This phase possesses a finite single particle energy gap with vanishing magnetic orders and the spin correlation function exhibits a power-law scaling, suggesting a potential algebraic spin-liquid ground state. Recently, enormous attentions have been paid to the search for the quantum disordered phase in

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**FIG. 1:** (color online). Phase diagram of the half-filled Fermi Hubbard model with Rashba-type SOC obtained by the cluster dynamical mean-field theory with a 2 \( \times \) 2 cluster at \( T = 0.05t \). The solid line with dots is the phase boundary of the MIT. The purple-colored regions denote the diverse spin ordered phases of \( xy \)-antiferromagnet (\( xy \)-AFM), spiral (the green and red arrows indicate the spins have up or down \( z \)-components), stripe, and spin vortex (SV) in the Mott insulating regime. For \( \alpha > \alpha_c \), there exhibits a nonmagnetic insulating (NMI) phase in the vicinity of the MIT.
the interacting fermion systems [40, 43]. Our results formulate a promising new route to achieve this intriguing quantum state through the SO coupled fermions.

The model.—The Hamiltonian of a two-component Fermi gas subject to an optical square lattice is given by

\[ \hat{H} = -t \sum_{<ij>} \sum_{\sigma\sigma'} (\hat{c}_{i\sigma}^\dagger R_{ij} \hat{c}_{j\sigma'} + H.c.) + U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} + \mu \sum_i \hat{n}_i, \]

where \( t \) is the overall tunneling matrix element and \( c_{i\sigma} (c_{i\sigma}^\dagger) \) denotes fermionic annihilation (creation) operator for a fermion of spin \( \sigma = \uparrow, \downarrow \) on the lattice site \( i \). The first term describes the nearest-neighboring hoppings with the hopping matrices given by \( R_{ij} \equiv \exp[i \mathbf{A} \cdot (\mathbf{r}_i - \mathbf{r}_j)] \), where \( \mathbf{A} = (\beta \sigma_y, \alpha \sigma_x, 0) \) denotes a non-Abelian gauge field which can be generated by the laser-induced spin-flipped tunneling [22, 23]. In this Letter we set \( \beta = -\alpha \), which implies that the SOC is of Rashba type [34, 38]. In this case, the spin-conserved hopping term is proportional to \( t \cos \alpha \), and the spin-flipped term is in proportion to \( t \sin \alpha \). \( U \) is the on-site atomic repulsion and \( \mu \) is the chemical potential. The particle number operator is \( \hat{n}_i = \hat{n}_{i\uparrow} + \hat{n}_{i\downarrow} \) with \( \hat{n}_{i\sigma} = \hat{c}_{i\sigma}^\dagger \hat{c}_{i\sigma} \).

Method.—We study the physical properties of Hamiltonian (1) with the non-perturbative cluster dynamical mean-field theory (CDMFT), using Hirsch-Fye Quantum Monte Carlo algorithm as the impurity solver [44, 45]. In the presence of SOC, we can map the square lattice onto two sets of sublattices for spin up (down) respectively, as shown in Fig. 2a. The \( 2 \times 2 \) clusters are embedded in a self-consistent medium with the Weiss function of the cluster represented by \( g(i\omega) = \begin{pmatrix} g_{\uparrow\uparrow} & g_{\uparrow\downarrow} \\ g_{\downarrow\uparrow} & g_{\downarrow\downarrow} \end{pmatrix} \), where \( g_{\uparrow\downarrow} \) and \( g_{\downarrow\uparrow} \) are the \( 4 \times 4 \) matrix corresponding to spin conserved and spin flipped Weiss functions. Due to the presence of the spin-flipping term in Eq. (1), \( g_{\uparrow\downarrow} \) and \( g_{\downarrow\uparrow} \) are generally nonzero. The CDMFT incorporates spatial correlations and has been shown to be successful in the study of MIT and magnetic orders [46–48]. In this work, we shall investigate the phase diagram on the half-filled square lattice with full range of strength of atomic interactions and SOC.

Before proceeding, we first examine the case with \( \alpha = 0 \) in Hamiltonian (1), which recovers the Hubbard model on a conventional square lattice. At half filling, the Fermi surface for non-interacting fermions is perfectly nested and the antiferromagnetic (AF) fluctuations can drive the system into an insulator with infinitesimal atomic interaction [43]. In the approach of CDMFT, it was demonstrated that without AF fluctuations, the MIT between the paramagnetic metal and the paramagnetic Mott insulator occurs at \( U_c/t \approx 6.05 \) [50]. Here in our simulations, we allow magnetic orders to set in and find that \( U_c/t \) is greatly reduced as shown in Fig. 1. Further, we perform a scaling analysis in Fig. 3a, showing that the interaction strength \( U_c/t \) at zero temperature would approach to much smaller values in larger clusters.

MIT.—Now, we turn to the effects of the SOC on the MIT. We concentrate on the basic region given by \( \alpha \in [0, \pi/2] \) since the relevant physical results are not affected in other regions. First, the single-particle spectrum is split into two bands [see Fig. 2b)], with the zero energy Fermi surface possessing a particle and hole Fermi-pocket around the center and corner of the Brilloin zone. The corresponding Density of states (DOS) for non-interacting fermions is shown in Fig. 2c), where the zero energy DOS is suppressed and the bandwidth shrinks gradually with increasing \( \alpha \). The suppressed zero energy DOS reduce the correlation effects on Fermi sur-
face and hence enhance $U_c/t$ of the MIT, whereas the shrinking bandwidth tends to make the Mott insulator happen at smaller $U_c/t$. The two effects compete with each other, leading to the drastic changes of the MIT boundary in the phase diagram. In Fig. 1 we show that, away from $\alpha = 0$ the value of $U_c/t$ is rapidly increased due to the suppression of the conventional AF fluctuation on square lattices. Subsequently, the MIT exhibits a nonmonotonic behavior as a function of $\alpha$. Specially at $\alpha = \pi/2$, the MIT occurs at a finite atomic interaction with $U_c/t = 4.1$.

In order to feature the MIT in the presence of SOC, Fig. 3(b) plots the evolution of DOS at different atomic interactions for $\alpha = 1.0$. We show that, compared to $\alpha = 0$ case, the zero energy spectral peak in the metal phase (red line) is largely suppressed by the SOC. Simultaneously, two satellite peaks appear corresponding to the Van Hove singularity shown in Fig. 2(c). Then, the zero energy peaks are gradually reduced and a gap opens with the increase of atomic interactions.

Fig. 4(a) plots the corresponding single-particle gap $\Delta$ and magnetization $m$ as functions of $U/t$ for $\alpha = 1.0$. The insulating phase characterized by a non-zero $\Delta$ is accompanied by a finite $m$ simultaneously, indicating a magnetic order arises. The specific magnetic phases in Fig. 4 can be determined by identifying the spin configurations on the cluster, see the Supplementary material for more details. Fig. 4 shows that, as $\alpha$ increases the system transits from $xy$-antiferromagnet ($xy$-AFM) to spiral, stripe, and spin vortex (SV) phases. Qualitatively, this can be understood from an effective spin model, where the induced DM-type super-exchange term competes with the Heisenberg coupling, tending to form diverse spin phases. However, the effective spin model works only for the deep Mott regime with the atomic kinetic energies being treated perturbatively. In close proximity to the more interested Mott transition, such a perturbative description breaks down and the strong fluctuations arising from SOC may destroy the magnetic orders and trigger an order to disorder transition. To address this issue, one needs to implement a non-perturbative method such as CDMFT to explore in detail the phase diagram as in Fig. 4.

**NMI phase.**—To our surprise, despite the robustness of the diverse spin phases in the Mott insulating regime with up to modest values of SOC, a NMI phase is found to emerge in the vicinity of the MIT for $\alpha > \alpha_c$ ($\alpha_c \simeq 1.43$). The NMI phase is characterized in Fig. 4(b), where the single-particle gap $\Delta$ and magnetization $m$ occur for different atomic interactions $U_{c_1}$ and $U_{c_2}$. Specifically in the intermediate region $U_{c_1} \leq U \leq U_{c_2}$, the system enters into an insulating state but with no long-range magnetic order. This is a unique feature of the SO coupled square lattice for $\alpha$ being close to $\pi/2$, where the single-particle hopping becomes nearly spin-flipped and the DOS is almost suppressed at zero energy.

The emergence of the NMI phase is further confirmed on a $4 \times 4$ cluster. The larger size of cluster incorporate more spin correlations and thus, a better description of the atomic correlations and SOC induced fluctuations can be expected. Fig. 5 plots the phase diagram for $\alpha$ being close to $\pi/2$. We found that, in the $4 \times 4$ cluster, the regime of the NMI phase is slightly expanded, demonstrating that the NMI is robust in this system. We further show, in the inset of Fig. 5 the temperature dependence of the NMI phase. The interval between the metallic and SV phases enlarge with decreasing temperature. It demonstrates that the NMI phase is more stable at low temperatures by the suppression of thermal fluctuations.

The NMI phase breaks neither spin nor lattice symmetry, suggesting a potential spin-liquid (SL) ground state. Such a fundamental state was first proposed by Anderson and has long been sought in the frustrated spin systems. Recently, interacting fermion models have attracted wide attentions, and it was reported that a SL state can be identified on honeycomb lattice between semimetal and AF insulator with $3.5t \leq U \leq 4.3t$ for $\alpha = 1.0$.
Despite this, its presence has been challenged since the interval of the SL phase is small, which may vanishes under the size scaling [54, 55]. The latest results using large-scale quantum Monte Carlo (QMC) showed that, if the SL state exists, the possible regime reduces substantially to a small interval $3.8t \leq U \leq 3.9t$ [56]. Similar situations have been encountered for the staggered-flux model on a square lattice [59, 60]. Here, the essential feature characterizing the present system is the considerably large space of parameters, where the NMI phase emerges. This is in sharp contrast to the limited phase space ($3.4t \leq U \leq 3.9t$) obtained in the interacting fermions on honeycomb lattices [61]. Specially, the predicted NMI phase occurs until $\alpha > \alpha_c$, showing that it is a strong field effect of the SOC.

The absence of magnetic orders in the NMI phase implies strong short-range spin correlation. However, it may decay as a power-law or exponentially. To explore this issue, we calculate the staggered spin-spin correlation function

$$C(r) = (-1)^r \langle S^z_{\text{0,0}} S^z_{r,r} + S^x_{\text{0,0}} S^x_{r,r} + S^y_{\text{0,0}} S^y_{r,r} \rangle,$$

(2)
as shown in Fig. 6 where the spin correlation functions are fitted to a power-law as $C(r) \sim 1/r^\alpha$. In NMI phase, we find that the exponent $\alpha$ is less than 2 with $\alpha \sim 1.6$ in our simulations. Whereas in the deep Mott insulating regime where spin is ordered, $\alpha$ becomes much smaller. Therefore, the NMI phase seems to suggest a candidate of algebraic SL. Further studies would be implemented by QMC calculations in the future.

The above phenomena of the intriguing MIT and exotic matter states can be investigated in experiments. In optical lattices, the Mott insulating phase can be detected by site-resolved imaging of single atoms [62, 63], and the spin textures occurring in the Mott phase can be observed via in situ microscopy [61] or through spin-resolved time-of-flight measurements [64]. On the other hand, the spin correlation can be measured by the spin structure factors in optical Bragg scattering [65], which may present the signatures of the spin ordered phases and the power-law scaling of the NMI phase. In addition, an extremely low-temperature has been recently realized to approach the superexchange energy scales [70].

In summary, we have investigated the half-filled Fermi Hubbard model with Rashba-type SOC on a square lattice. We show that this system displays a rich phase diagram. The interplay between the atomic interactions and SOC results in distinctive features of the MIT with diverse spin ordered phases occurring on the side of Mott insulator. Near the Mott transition, a quantum NMI phase is found to emerge in a considerably large regime of parameters due to the strong field effect of the SOC, formulating a new avenue to achieve the intriguing quantum disordered state beyond the spin systems.

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Supplementary Material
Emergence of Quantum Nonmagnetic Insulating Phase in Spin-Orbit Coupled Square Lattices
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In this Supplementary Material, we describe how to determine the diverse spin phases and the corresponding magnetization. First, in the approach of CDMFT, the Weiss function of the N-site cluster embedded in a self-consistent medium is determined by the cluster self-energy Σ(ιω) via the coarse-grained Dyson equation \[ g^{-1}(ιω) = \left[ \sum_K \frac{ιω + μ - t(K) - Σ(ιω)}{iω} \right]^{-1} + Σ(ιω), \] (1)

where t(K) is the Fourier-transformed hopping matrix with wave vector K in the cluster reduced Brillouin zone of the superlattice. Note that, in the presence of SOC both the above Weiss function and the self-energy of the cluster in Eq. (1) become \[ g(ιω) = \begin{pmatrix} g_{↑↑}(ιω) & g_{↑↓}(ιω) \\ g_{↓↑}(ιω) & g_{↓↓}(ιω) \end{pmatrix} \] and \[ Σ(ιω) = \begin{pmatrix} Σ_{↑↑} & Σ_{↑↓} \\ Σ_{↓↑} & Σ_{↓↓} \end{pmatrix}. \] In this case, we introduce two-component row and column fermionic field operators: \( \hat{Ψ}^† = [c_{↑}^†, c_{↓}^†]^T \) and \( \hat{Ψ} = [c_{↑}, c_{↓}]^T \), and define the cluster Green’s function as \( G_{σσ}(τ) = \langle \hat{Ψ}(τ)\hat{Ψ}^†(0) \rangle = \begin{pmatrix} G_{↑↑}(τ) & G_{↑↓}(τ) \\ G_{↓↑}(τ) & G_{↓↓}(τ) \end{pmatrix} \).

Once \( g(ιω) \) is determined, the impurity solver can be used to compute the cluster Green’s function \( G(ιω) \). Eventually, by using the Dyson equation \( Σ(ιω) = g^{-1}(ιω) - G^{-1}(ιω) \), the self-consistent iterative \( G(ιω) \) is obtained.

The energy gap \( Δ \) can be derived by the local density of states (LDOS). By implementing the analytic extension of the imaginary time cluster Green’s function \( G(ιω) \) via the maximum entropy method \[ ² \], we have

\[ ρ(ω) = \sum_k A(k, ω) \approx -\frac{1}{π} \text{Im}[G_{ii}(ω)]. \] (3)

Then in the spectrum of LDOS, we can obtain the energy gap \( Δ \) by the energy width of zero density of states.

The different spin phases in the Mott insulating regime can be characterized by the spin structure factor \( S_q = |\sum_i S_i e^{iπ⋅q⋅r_i}| \) with q the 2D wave vector. Here, \( S_i = \langle \hat{S}_i \rangle \) denotes local magnetic order parameter on site \( i \) of the cluster, with three components given by

\[ S_q^x = \frac{1}{2}(c_{i↑}^† c_{i↓} + c_{i↓}^† c_{i↑}) = \frac{1}{2} \text{Re}[G_{i↑↓}(0^+) + G_{i↓↑}(0^+)], \] (4)

\[ S_q^y = -\frac{1}{2}(c_{i↑}^† c_{i↓} - c_{i↓}^† c_{i↑}) = -\frac{1}{2} \text{Im}[G_{i↑↓}(0^+) - G_{i↓↑}(0^+)], \] (5)

\[ S_q^z = \frac{1}{2}(c_{i↑}^† c_{i↑} - c_{i↓}^† c_{i↓}) = \frac{1}{2} \text{Re}[G_{i↑↑}(0^+) - G_{i↓↓}(0^+)]. \] (6)

The spin ordered phases in Fig. 1 of the main text are derived on 2 × 2 cluster, where the structure factor of the xy-AFM has a peak at \( q = (π, π) \), the stripe phase at \( q = (0, π) \), and the SV phase at \( q = (π, 0) \) and \( q = (0, π) \). Between the xy-AFM and stripe phases, spiral phases where the spins spiral in the z-q plane with \( q = (q, π) \) the in-plane wave vector may appear. However, the spiral phase is hard to be explicitly identified on 2 × 2 cluster. To overcome this difficulty, we explore on a larger 4 × 4 cluster, and a spiral-4 phase with spatial period of 4 × 2 lattice sites is clearly identified in the following FIG. 1.

Finally, we present the definition of magnetization. In the spin ordered phases, we can rotate the local magnetic order parameter \( S_i \) on each cluster site to a global coordinate system: \( S_i^ρ = U(φ_i)S_i \), with \( φ_i \) the angle between the local
and global coordinates. Then we can define \( \mathbf{m} = \frac{1}{N} \sum_{i=1}^{N} \mathbf{S}_i' \) with the magnetization given by \( m^2 = \sum_{a=x,y,z} m_a^2 \). For example, in the \( xy \)-AFM shown in Fig. 1, there are two sublattices \( \phi_{i \in A} = 0, \phi_{i \in B} = \pi \), we have \( \mathbf{m} = \frac{1}{N} \sum_{i=1}^{N} \epsilon_i \mathbf{S}_i \), where \( \epsilon_i = \pm 1 \) is for sites belonging to sublattice \( A(B) \) respectively. This general definition of magnetization is also applied to other spin phases throughout this paper.

FIG. 1: (color online). Spin phase diagram in the Mott insulating regime with \( U/t = 7.5 \) on the \( 4 \times 4 \) cluster. The intervals of the \( xy \)-AFM, SV and stripe phases agree well with those on \( 2 \times 2 \) cluster. Specifically, a spiral-4 phase with spatial period of \( 4 \times 2 \) lattice sites (the green and red arrows indicate the spins have up or down \( z \)-components) is explicitly identified between the \( xy \)-AFM and stripe phases. The shaded area indicate other commensurate or non-commensurate spiral phases.

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