

Skyrmion and vortex crystals in the Hubbard model

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A mutual interplay between the charge and spin degrees of freedom in itinerant magnets leads to a plethora of topological spin textures, such as magnetic skyrmion and vortex crystals, in both centrosymmetric and noncentrosymmetric hosts. Meanwhile, their stabilization has been extensively studied in a system including classical localized spins. We here study a realization of the skyrmion crystal in a centrosymmetric triangular-lattice Hubbard model, where the itinerant nature of electrons plays a more significant role. By performing self-consistent mean-field calculations, we find that two types of skyrmion crystals with spatially nonuniform charge modulations appear in the ground state at zero magnetic field. Moreover, we obtain another noncoplanar vortex crystal phase without a net scalar chirality in the vicinity of the skyrmion crystal phase. We show that the latter vortex crystal exhibits a topological phase transition to a different skyrmion phase in an applied magnetic field. Our results provide a possibility of skyrmion and vortex crystals in itinerant magnets without localized moments.

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Itinerant magnets manifest themselves not only in various magnetic orderings but also in unusual conductive phenomena as a consequence of the synergy between charge and spin degrees of freedom in electrons. The microscopic mechanisms of magnetically ordered phases are often different from those in insulating magnets; an effective interaction through the kinetic motion of electrons as well as the Coulomb interaction plays an important role in determining optimal spin configurations. A typical example is the Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction [1–3], which leads to the instability toward helical magnetic ordering with a long period structure featured by a single- Q modulation. Furthermore, such a spin-charge entanglement brings about a comparable higher-order multiple-spin interaction to the RKKY interaction depending on the electronic band structures, which results in noncoplanar magnetic orderings characterized by a superposition of single- Q helical states, i.e., a multiple- Q state [4–13]. These nontrivial spin textures are the source of nontrivial conductive phenomena even without relativistic spin-orbit coupling, such as the topological Hall effect [14–20] and nonreciprocal transport [21–24].

Recently, it was revealed that a magnetic skyrmion crystal (SkX), which has a topologically protected noncoplanar spin texture, is also realized by the itinerant nature of electrons based on the analysis for the Kondo lattice model consisting of itinerant electrons and classical localized spins [25,26]. Subsequently, the emergence of the SkX is accounted for by an effective spin model with a positive biquadratic interaction in addition to the RKKY interaction, which originates from the Fermi-surface instability [27]. As this mechanism can be applied to any lattice structures irrespective of spatial inversion symmetry, it might provide the microscopic origin of the SkXs observed in centrosymmetric magnets, such

as Gd_2PdSi_3 [28–32]. Indeed, magnetic phase diagrams in centrosymmetric skyrmion-hosting materials have been reproduced by the effective spin model, such as GdRu_2Si_2 [33–35], $\text{Gd}_3\text{Ru}_4\text{Al}_{12}$ [36,37], and EuAl_4 [38–41].

Meanwhile, there is a natural question about whether or not the SkX remains robust when electrons show an itinerant nature rather than a localized one. In other words, it is unclear whether the instability toward the SkX occurs by the kinetic motion of electrons even without a classical spin degree of freedom. To answer this question, we investigate the Hubbard model without localized spins. Based on self-consistent mean-field calculations for the Hubbard model on a centrosymmetric triangular lattice, we show that two types of the SkX appear even without an external magnetic field, as found in the Kondo lattice model [25], although the spin amplitudes are much smaller and strongly depend on the site. In addition, we discover a triple- Q ($3Q$) vortex phase without a spin scalar chirality that was not reported as the ground state in the Kondo lattice model. We show that the magnetic field causes a topological phase transition from the $3Q$ vortex phase to another SkX phase. Our results indicate the importance of the charge degree of freedom, which will become a source of not only the SkX but also different types of vortex phases in itinerant magnets.

Let us consider the Hubbard model on a two-dimensional triangular lattice, which is given by

$$\mathcal{H} = - \sum_{ij\sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} - B \sum_i S_i^z, \quad (1)$$

where the operator $c_{i\sigma}^\dagger$ ($c_{i\sigma}$) is a creation (annihilation) operator for an electron with spin σ at site i . The first term describes the kinetic energy of the electrons with the transfer

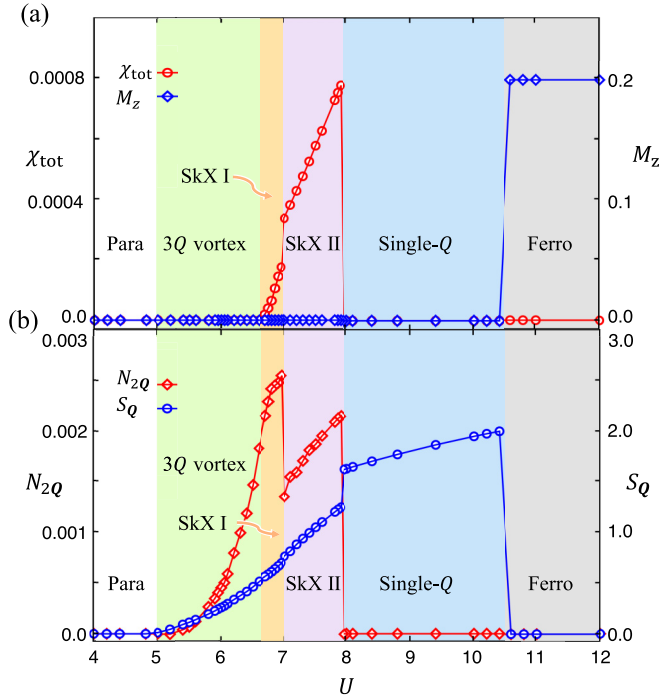


FIG. 1. U dependence of (a) the total scalar chirality χ_{tot} and the magnetization M_z , and (b) the charge structure factor N_{2Q} and the spin structure factor S_Q summed over $2\mathbf{Q}_\mu$ and \mathbf{Q}_μ , respectively. The different colors in the background represent the different phases.

integral between sites i and j , t_{ij} , that typically take around 10^0 – 10^2 meV depending on the itinerancy of the electrons. The second term represents the on-site Coulomb interaction with the coupling constant U where $n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}$. The third term represents the Zeeman coupling to an external field along the z direction: $S_i^z = \frac{1}{2}(c_{i\uparrow}^\dagger c_{i\uparrow} - c_{i\downarrow}^\dagger c_{i\downarrow})$.

In the following calculations, we consider the nearest-neighbor hopping, $t_1 = 1$ (energy unit of the model), and third-neighbor hopping, $t_3 = -0.85$, since these hopping parameters lead to a Fermi-surface instability at the commensurate wave vectors, $\mathbf{Q}_1 = (\pi/3, 0)$, $\mathbf{Q}_2 = (-\pi/6, \sqrt{3}\pi/6)$, and $\mathbf{Q}_3 = (-\pi/6, -\sqrt{3}\pi/6)$ for the electron filling $n_i \equiv \sum_\sigma n_{i\sigma} \simeq 0.398$ [27] (the lattice constant of the triangular lattice is set as unity); the instability toward the SkX with $3Q$ modulation at \mathbf{Q}_1 – \mathbf{Q}_3 has been found in the Kondo lattice model with classical localized spins [25].

For the model in Eq. (1), we perform self-consistent mean-field calculations at zero temperature based on the Hartree-Fock approximation for the Coulomb interaction: $\sum_i n_{i\uparrow} n_{i\downarrow} \simeq \langle n_{i\downarrow} \rangle n_{i\uparrow} + \langle n_{i\uparrow} \rangle n_{i\downarrow} - \langle n_{i\uparrow} \rangle \langle n_{i\downarrow} \rangle - \langle c_{i\downarrow}^\dagger c_{i\uparrow} \rangle c_{i\uparrow}^\dagger c_{i\downarrow} - \langle c_{i\uparrow}^\dagger c_{i\downarrow} \rangle c_{i\downarrow}^\dagger c_{i\uparrow} + \langle c_{i\uparrow}^\dagger c_{i\downarrow} \rangle \langle c_{i\downarrow}^\dagger c_{i\uparrow} \rangle$.

We consider the magnetically ordered states in an $N_m = 48$ -site magnetic unit cell under periodic boundary conditions to accommodate the SkX with \mathbf{Q}_1 – \mathbf{Q}_3 [see also Fig. 2(a) for the definition of the magnetic unit cell]. In order to reduce the finite-size effect, we introduce supercells made of $N_k = 60 \times 60$ magnetic unit cells. Almost the same results are obtained for $N_k = 32 \times 32$, which indicates the size dependence is almost negligible. The convergent condition is determined by $\Delta(\langle c_{i\sigma}^\dagger c_{i\sigma'} \rangle) < 10^{-8}$ for each site i and spin σ .

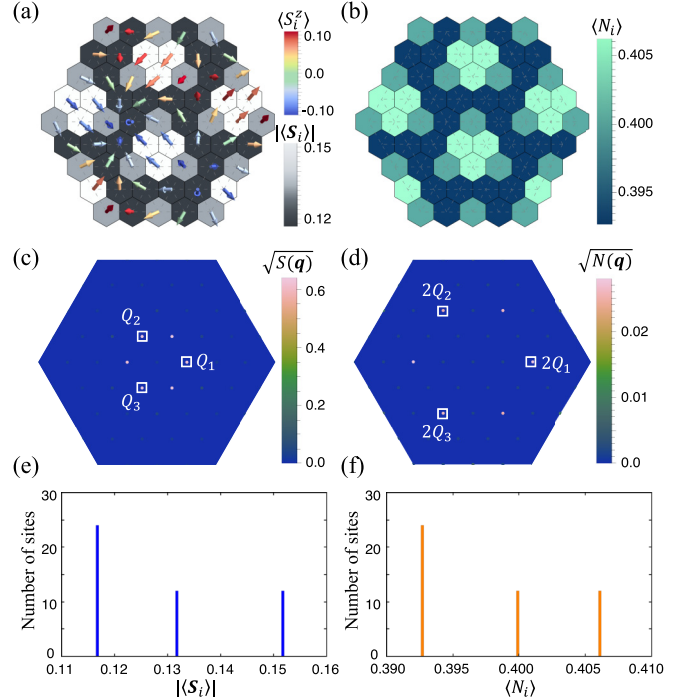


FIG. 2. (a) Real-space spin configuration in the SkX II phase at $U = 7.8$. The arrows represent the spins, their colors display the z -spin component, and the contour shows the spin norm $|\langle \mathbf{S}_i \rangle|$. (b) The contour plot for the charge density. (c), (d) The intensity plot of the square root of (c) the spin structure factor $S(\mathbf{q})$ and (d) the charge structure factor $N(\mathbf{q})$. (e) The histogram of $|\langle \mathbf{S}_i \rangle|$ with a bin width of 0.0005. (f) The histogram of $\langle N_i \rangle$ with a bin width of 0.0002.

Once the convergent spin configurations are obtained, we examine the spin and charge properties by calculating the spin and charge structure factors, $S(\mathbf{q})$ and $N(\mathbf{q})$, respectively, which are given by

$$S(\mathbf{q}) = \frac{1}{N} \sum_{ij} \langle \mathbf{S}_i \rangle \cdot \langle \mathbf{S}_j \rangle e^{i\mathbf{q} \cdot (\mathbf{r}_i - \mathbf{r}_j)}, \quad (2)$$

$$N(\mathbf{q}) = \frac{1}{N} \sum_{ij} \Delta n_i \Delta n_j e^{i\mathbf{q} \cdot (\mathbf{r}_i - \mathbf{r}_j)}, \quad (3)$$

where \mathbf{r}_i is the position vector at site i in the larger magnetic unit cell for $N = 12 \times 12 = 3N_m$ sites corresponding to a modulation period of $\pi/6$; $\Delta n_i \equiv \sum_\alpha \langle c_{i\alpha}^\dagger c_{i\alpha} \rangle - n_{\text{ave}}$ with the average charge density n_{ave} . We also calculate the total magnetization per site $M_z = \sum_i \langle S_i^z \rangle / N_m$. In addition, to identify whether or not the obtained states are topologically trivial, we compute the scalar spin chirality per triangle in the magnetic unit cell, $\chi_{\text{tot}} = \sum_{\langle ijk \rangle} \langle \mathbf{S}_i \rangle \cdot (\langle \mathbf{S}_j \rangle \times \langle \mathbf{S}_k \rangle) / 2N_m$. The nonzero value of χ_{tot} becomes the origin of the topological Hall effect [14].

Figure 1 shows the ground-state phase diagram against U at a zero field, i.e., $B = 0$. There are six phases characterized by different spin, charge, and chirality quantities. We show the U dependence of χ_{tot} and M_z in Fig. 1(a) and the sum of the structure factors at the commensurate wave vectors \mathbf{Q}_μ and $2\mathbf{Q}_\mu$, $N_{2Q} \equiv \sum_\mu N(2\mathbf{Q}_\mu)$ and $S_Q \equiv \sum_\mu S(\mathbf{Q}_\mu)$, in Fig. 1(b). In the weak(strong)-correlation regime, the paramagnetic (ferromagnetic) state is realized, whose tendency

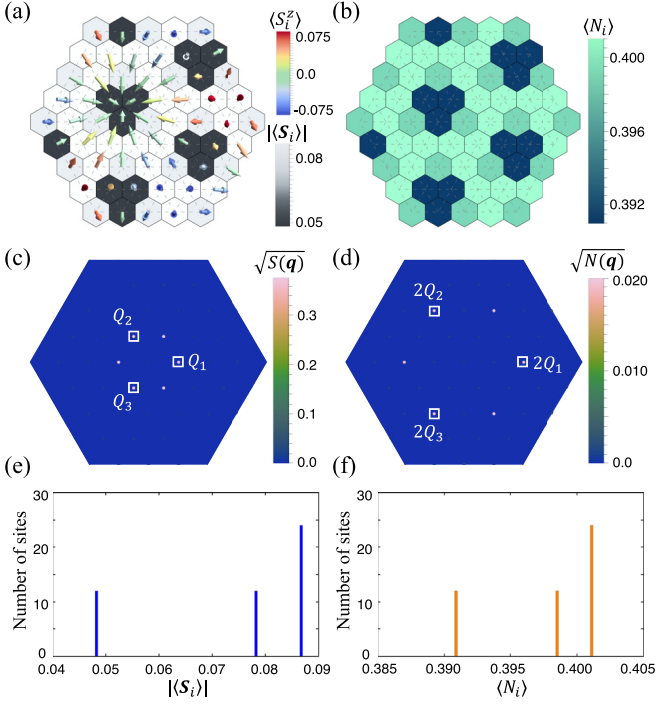


FIG. 3. The same plots as in Fig. 2 in the $3Q$ vortex phase at $U = 6.4$.

has been found in the Hubbard model [42,43]. Meanwhile, in the intermediate-correlation regime, we obtain four magnetic phases. Among them, three out of the four are characterized by multiple- Q states: the $3Q$ vortex phase, SkX I, and SkX II. The remaining single- Q state next to the ferromagnetic state is characterized by the single- Q spiral state with S_Q but without χ_{tot} , M_z , and N_{2Q} .

For $7.0 \lesssim U \lesssim 7.9$, we find that the SkX II with nonzero χ_{tot} but zero M_z becomes the ground state, as shown in Fig. 1(a). This state has triple- Q charge and spin modulations, as shown in Fig. 1(b). Indeed, almost the same intensities at Q_μ ($2Q_\mu$) are observed in the spin (charge) structure factor, as shown in Figs. 2(c) and 2(d). It is noted that the triple- Q peak structure in $N(q)$ is driven by the triple- Q spin density waves. The peak position at $2Q_\mu$ indicates that the constituent spin density waves propagate in an orthogonal way in spin space [44,45]. The equal triple- Q intensities in $S(q)$ and $N(q)$ appear in the real-space spin and charge distributions in Figs. 2(a) and 2(b), respectively; both $|\langle S_i \rangle|$ and $\langle N_i \rangle$ are distributed in a threefold-symmetric way. In addition, we find that both of them exhibit three discrete values, as shown in Figs. 2(e) and 2(f), which means that there are three independent environments in the SkX II phase. This phase presumably corresponds to the SkX stabilized in the Kondo lattice model [25].

On the other hand, for $5.0 \lesssim U \lesssim 6.6$, the $3Q$ vortex phase is stabilized, which also exhibits triple- Q charge and spin modulations [Figs. 1(b), 3(c), and 3(d)] but no χ_{tot} and M_z [Fig. 1(a)]; the charge modulation at $2Q_\mu$ indicates a similar multiple- Q superposition to the SkX II. In addition, the absence of χ_{tot} suggests the occurrence of the phase shift among the constituent waves from the SkX II [46–48], which

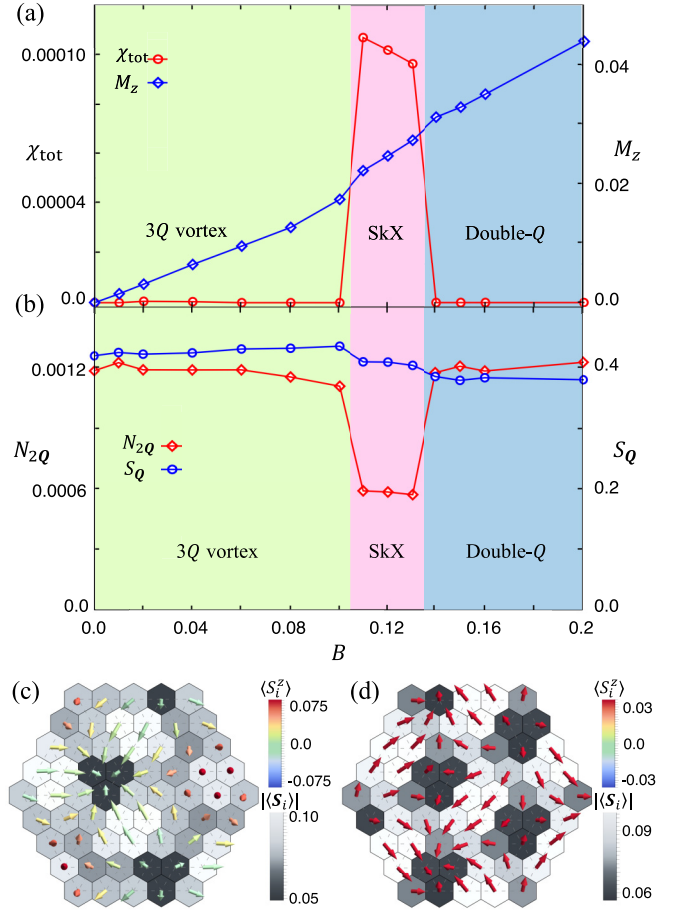


FIG. 4. B dependence of (a) χ_{tot} and M_z , and (b) N_{2Q} and S_Q . (c), (d) The spin configurations in (c) the SkX phase at $B = 0.12$ and (d) the double- Q phase at $B = 0.16$.

has been found at finite temperatures in the Kondo lattice model [46]. The real-space spin configuration is characterized by four different spin vortices where the spin norm $|\langle S_i \rangle|$ becomes small, as shown in Fig. 3(a). Accordingly, the charge distribution is also threefold symmetric around the vortices with small $|\langle N_i \rangle|$, as shown in Fig. 3(b). The histograms of $|\langle S_i \rangle|$ [Fig. 3(e)] and $\langle N_i \rangle$ [Fig. 3(f)] show the opposite tendency to the SkX II in Figs. 2(e) and 2(f); the sites with larger $|\langle S_i \rangle|$ and $\langle N_i \rangle$ are preferred in the $3Q$ vortex. The ratio of maximum and minimum values of $|\langle S_i \rangle|$ is around 0.56, which is much smaller than that of the SkX II phase 0.77, while the ratio in terms of $\langle N_i \rangle$ takes similar values: 0.975 for the $3Q$ vortex and 0.967 for the SkX II. This result implies that the site-dependent moment reduction due to the kinetic motion of electrons, i.e., the charge degree of freedom, is important for the realization of the $3Q$ vortex as the ground state [49].

In the narrow region sandwiched by the $3Q$ vortex and the SkX II, the SkX I appears. Although this state shows a nonzero scalar chirality as the SkX II, its spin and charge structure factors appear to be continuously connected from the $3Q$ vortex phase, as shown in Figs. 1(a) and 1(b). In addition, the spin norm and charge density take four discrete values, which suggests the SkX I phase has a lower symmetry than the $3Q$ vortex and SkX II phases with three independent

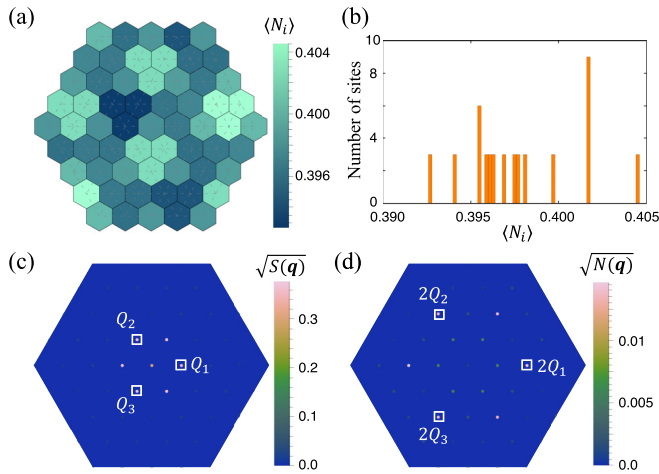


FIG. 5. The data of the SkX phase at $B = 0.12$. (a) The charge density distribution in real space. (b) The histogram of $\langle N_i \rangle$ with a bin width of 0.0002. (c), (d) The intensity plot of the square root of (c) $S(\mathbf{q})$ and (d) $N(\mathbf{q})$.

environments. Thus, the SkX I is regarded as the intermediate state between the $3Q$ vortex and SkX II.

Let us compare the present results with those in the Kondo lattice model [25]. In both models, the SkXs characterized by the triple- Q structures in $S(\mathbf{q})$ and $N(\mathbf{q})$ are stabilized at zero field, but a distinct difference between them is found in the spin norm. The SkX II in the Hubbard model shows a strong spatial dependence of $|\langle S_i^z \rangle|$ [Fig. 2(a)] in contrast to the case of the Kondo lattice model with fixed-length classical spins. This indicates that the itinerant character appears more clearly in the Hubbard model. Such a qualitative difference might be the origin of another triple- Q vortex phase in Fig. 3(a), which is not stabilized as the ground state in the Kondo lattice model due to the constraint in terms of the spin norm. Thus, the interplay between the charge and spin degrees of freedom plays an important role in inducing noncoplanar multiple- Q states, which will bring about further exotic spin-charge entangled topological spin textures.

Next, we consider the effect of the magnetic field B on the $3Q$ vortex phase. Figure 4(a) shows the B dependence of χ_{tot} and M_z , while Fig. 4(b) shows that of N_{2Q} and S_Q at $U = 6.4$. When introducing B , M_z becomes nonzero and linearly increases in the $3Q$ vortex phase in Fig. 4(a). While increasing B , χ_{tot} jumps to nonzero values at $B = 0.11$, which implies the appearance of the SkX phase. The obtained SkX spin configuration is shown in Fig. 4(c). Compared with the SkX II in Fig. 2(a), the spatial distributions of $|\langle S_i^z \rangle|$ in Fig. 4(c) and $\langle N_i \rangle$ in Fig. 5(a) are more complicated; indeed, the histogram of $\langle N_i \rangle$ exhibits multiple values, as shown in Fig. 5(b). Accordingly, additional intensities appear at Q_μ and $Q_\mu - Q_{\mu'}$ in $N(\mathbf{q})$ in Fig. 5(d). Owing to the multiple peak structures in $N(\mathbf{q})$, the intensity of N_{2Q} becomes small compared to that of the $3Q$ vortex, as shown in Fig. 4(b). In addition, this state exhibits a nonzero net magnetization owing to the magnetic field; see also the $\mathbf{q} = \mathbf{0}$ component

in the spin structure factor in Fig. 5(c). Thus, this SkX phase induced by the magnetic field is qualitatively different from the SkX I and SkX II obtained at zero field, where only the former SkX exhibits nonzero net magnetization and nonzero $N(Q_\mu)$. Since a further increase of B suppresses the z -spin modulation in the SkX, the spin state turns into the double- Q state with the in-plane double- Q modulated spin structure shown in Fig. 4(d). In the double- Q state, $N(\mathbf{q})$ shows peaks at two out of three $2Q_\mu$ as does the $3Q$ vortex, whose amplitude is comparable to each other [Fig. 4(b)].

Meanwhile, there is no instability toward such a field-induced SkX in the case of SkX II. In this case, the SkX II phase turns into another vortex phase with a skyrmion number of 0 at $B = 0.065$, whose spin and charge modulations are similar to those found in the Kondo lattice model at high fields [25].

It is noteworthy to mention that the obtained SkX under the magnetic field in Fig. 5 is qualitatively different from the SkX found in the Kondo lattice model [25] and other spin models. By closely looking into the spin configuration of the SkX phase in Fig. 4(c), one finds that almost all the spins have a positive $\langle S_i^z \rangle$ and only a few spins around the two skyrmion cores where $|\langle S_i^z \rangle|$ becomes small have a slight negative $\langle S_i^z \rangle$. These two skyrmion cores yield a winding number of +1, i.e., a skyrmion number of -0.5 , which reflects the slight negative $\langle S_i^z \rangle$ at the core. Intriguingly, in this phase, there is another vortex core, where the spin is almost parallel to the $+z$ direction in the middle right-hand side of the spin configuration. This vortex accompanies the winding number of -2 , i.e., the skyrmion number of -1 . In the end, the total skyrmion number in the magnetic unit cell is given by -2 . This is in contrast to the SkX in the Kondo lattice model, where the z -spin component of the skyrmion core points along $S_i^z = -1$ and the spin configuration possesses a skyrmion number of -1 [25]. Reflecting such a difference, an intriguing excitation spectrum, such as the separation of spin and charge excitations [45,50], might be expected in the present SkX phases, which is left for future study.

To summarize, we have studied the ground-state spin configurations in the Hubbard model on a centrosymmetric triangular lattice with an emphasis on the itinerant nature of electrons. Based on the mean-field analysis, we have discovered several multiple- Q phases including the SkX and vortex phases in the presence of strong spin-charge entanglement. Our discovery indicates that itinerant magnets provide a variety of topological spin crystals even without the classical localized spins, and suggests the experimental feasibility of multiple- Q states in centrosymmetric materials consisting of d and $5f$ electrons with an itinerant character. This result provides a further possibility to search for exotic topological magnetism.

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