Recent results obtained with a variational cluster approach and the method are briefly explained in the next section. II. MODEL AND METHOD

We extend the BHZ model, which is defined on a two-dimensional square lattice, to include an on-site Coulomb interaction. The Hamiltonian reads

\[ H = -t \sum_{\langle ij \rangle} c_{i \alpha}^\dagger c_{j \alpha} + U n_{i \uparrow} n_{i \downarrow} \]

where \( c_{i \alpha} \) is the annihilation operator of an electron in site \( i \) with spin \( \alpha \), \( t \) is the hopping integral, and \( U \) is the on-site Coulomb interaction.
\[ H = H_{\text{BHZ}} + U \sum_{i, \alpha} n_{i, \alpha \uparrow} n_{i, \alpha \downarrow} \]

\[ H_{\text{BHZ}} = \sum_{i, \alpha} \varepsilon_n n_{i, \alpha \sigma} - \sum_{i, j, \sigma, \alpha} t_{i,j}^\sigma \hat{c}_{i, \sigma, \alpha}^\dagger \hat{c}_{j, \sigma, \alpha}, \]

\[ -t_{i,j} = \left( t'(\text{sign}(\sigma) (\delta_{i,j+y} - \delta_{i,j-y}) + i(\delta_{i,j+z} - \delta_{i,j-z})) \right) \]

where \( n_{i, \alpha \sigma} = c_{i, \alpha \sigma}^\dagger c_{i, \alpha \sigma} \). The operator \( c_{i, \alpha \sigma}^\dagger (c_{i, \alpha \sigma}) \) creates (annihilates) an electron at site \( i \) and in orbital \( \alpha = 1, 2 \) and spin \( \sigma = \uparrow, \downarrow \) state. The off-diagonal elements of the hopping matrix \( t \) drive the system into a non-trivial band insulator at \( U = 0 \). We analyze the system using DMFT, which treats local correlations exactly and is suitable for the systematic calculation of arbitrary strength of the Coulomb interaction. In DMFT, the original lattice problem is mapped onto an effective impurity model, which is solved self-consistently\(^{11-13}\). The self-consistency equation for a paramagnetic phase is given by

\[ \hat{g}^{-1}(\omega) = \left[ \sum_k \frac{1}{(\omega + i\delta)\Pi - \hat{h}_\sigma(k) - \hat{\Sigma}(\omega)} \right]^{-1} + \hat{\Sigma}(\omega), \]

where \( \hat{h}_\sigma(k) \) is the Fourier transform of the hopping matrix. The self-energy of the lattice Green’s function \( \hat{\Sigma}(\omega) \) can be computed from the Green’s function \( \hat{g}(\omega) \) of the effective impurity model. Note that, since the orbitals are hybridized by SO coupling, the hybridization function is diagonal in the orbital index. Thus, off-diagonal elements of the self-energy \( \hat{\Sigma}(\omega) \) are supposed to vanish in our model. In this study, we employ the NRG method to solve the impurity model,\(^{14,15}\) which is a powerful method for calculations at zero-temperature. To analyze the AF phase, we divide the original square lattice into two sublattices specified by checkerboard pattern.

For simplicity, we study the particle-hole symmetric case and choose the model parameters as \( t_1 = t_2 = t \), \( t' = 0.1t \) and \( \varepsilon_1(\varepsilon_2) = -t(t) \). The hopping integral \( t \) is chosen as the energy unit.

### III. NUMERICAL RESULTS

First, let us briefly discuss the Hartree-Fock results. In Fig. 1(a), the results are shown as a function of the interaction strength \( U \). A close examination of the effective Hamiltonian in the strong coupling region elucidates that the off-diagonal elements of the hopping matrix \( t_{\sigma} \) induce a spin dependent exchange; the \( z \)-component of the exchange interaction is antiferromagnetic, while the in-plane components are ferromagnetic (antiferromagnetic) between neighbors in \( y- (x-) \) direction, respectively. This results from the fact that the phase of the intra-orbital hopping affects the spin-exchange process. Thus, the spin configuration of the AF phase is expected to be the one shown in Fig. 1(a). In this figure, the staggered moment is parallel to the \( z \)-axis, and the in-plane components are zero. Here it should be noted that this effective Hamiltonian preserves four-fold symmetry; the Hamiltonian is invariant under the \( \pi/2 \) spatial rotation combined with the rotation of the spin space \( (S_{x_1}^x \rightarrow -S_{x_1}^x) \) at every site, where \( S_{x_1}^x \) represents the \( x \) component of spin operator at site \( i \) and orbital \( 1 \), respectively.

In Fig. 1(c), we show that for \( U < 3.3 \) \( (U > 3.8) \), the system is in a paramagnetic phase (AF phase) respectively. Accordingly, the Brillouin zone is reduced (Fig. 1(b)), since the ordering vector is \( (\pi, \pi) \). In this figure, for \( 3.5 < U < 3.78 \), a hysteresis behavior is observed, and in the region of \( 3.3 < U < 3.5 \), the paramagnetic (AF) solution is stable (unstable). Corresponding to the magnetic transition, in Fig. 1(d), we observe that the topological property changes at \( U = 3.8 \) \( (U = 3.5) \) with increasing (decreasing) interaction. As a result, a non-trivial AF phase is not found. This is attributed to the large Hartree shift induced in the AF phase. Recall that in our model, the origin of the gap depends on the energy splitting \( \varepsilon'_2 - \varepsilon'_1 \), where \( \varepsilon'_\alpha,\sigma \) is the energy level of each orbital including the Hartree shift, and if it becomes zero, the gap closing occurs. In the region of \( \varepsilon'_1 - \varepsilon'_2 < 0 \), the gap is induced by the SO interaction. Moreover, in this region, we can confirm that the system possesses non-trivial topology (see Fig. 1(d)). If the Green’s function has no anomaly (gap closing or zeros of it), the topological properties are never changed.\(^{16,17}\) We thus conclude that for \( \varepsilon'_1 < \varepsilon'_2 \) the system is driven into the non-trivial phase. Keeping this in mind, we plot the energy levels in Fig. 1(e). In this figure, a region satisfying the non-trivial condition is not found within the AF phase. We have also checked other choices of parameters, but could only find a topological-trivial AF phase in the physically sensible parameter regions.

Let us now discuss the results obtained with DMFT, and clarify what happens when electron correlations are taken into account. In Fig. 2(a), the AF moment is plotted as a function of interaction strength. We can clearly observe a jump at \( U = 4.5 \) \( (U = 4.2) \) with increasing (decreasing) interaction strength, respectively. In order to clarify the topological properties, we calculate the spin...
The coexistence region inherent in the first-order transition, can be found. The energy of each phase crosses at $U_0$, which determines the phase transition point for the thermodynamically stable phase diagram. Note that in this figure, no non-trivial AF phase is found.

We note again that the AFTI phase can be stabilized in our model, since the electronic structure of this system becomes trivial. In this trivial magnetic phase, the spectral functions of each spin state are identical. In the AFTI phase ($U = 4.4$), the spectral functions for $(\alpha, \sigma) = (1, \downarrow)$ and $(2, \uparrow)$ have peaks near the Fermi energy, while those for $(\alpha, \sigma) = (1, \uparrow)$ and $(2, \downarrow)$ have a hump structure around the Fermi energy.

For further insights into the AFTI phase, the momentum-resolved spectral functions are plotted in Fig. 2(b). In this figure, we find that the system has a bulk gap for each phase, as discussed momentarily below. In this figure, we observe a bulk gap in both phases. In the paramagnetic phase, the spectral functions of each spin state are identical. In the AFTI phase ($U = 4.4$), the spectral functions for $(\alpha, \sigma) = (1, \downarrow)$ and $(2, \uparrow)$ have peaks near the Fermi energy, while those for $(\alpha, \sigma) = (1, \uparrow)$ and $(2, \downarrow)$ have a hump structure around $\omega \sim \pm U/2$. With further increasing the interaction strength, the topological structure of this system becomes trivial. In this trivial AF phase, we can see that the electronic structure near the Fermi energy is changed; the peak just below (above) the Fermi energy is mainly composed of the state $(\alpha, \sigma) = (2, \uparrow)$ $(1, \downarrow)$ respectively.

For further insights into the AFTI phase, the momentum-resolved spectral functions are plotted in Figs. 3 and 4. In these figures, it is shown that states near the Fermi energy can be well labeled by the momentum (correlated band insulator). As seen in Fig 4(a) and (b), in the region

$$N_{\text{SChN}} = \frac{\epsilon_{\mu \rho}}{48\pi^2} \int d^3p \sum_{\sigma} \text{sign}(\sigma) 
\text{tr}\left[ G_{\sigma}^{-1}(p) \frac{\partial}{\partial \mu} G_{\sigma}(p) \frac{\partial}{\partial \mu} G_{\sigma}(p) G_{\sigma}^{-1}(p) \frac{\partial}{\partial \rho} G_{\sigma}(p) \right].$$

Here, the notation $p = (\omega, \mathbf{p})$ is used. Note that even in the interacting case, this quantity is proportional to the spin-Hall conductivity. In Fig. 2(b), the SChN is plotted as a function of interaction strength.
FIG. 3: (Color Online) Spectral functions for an up-spin dominant sublattice \((\alpha, \sigma)(\omega)\) for several values of interaction strength. At \(U = 3\), (4.4, 4.8), the system is in the TBI (non-trivial AF, trivial AF) phase respectively. Solid red (solid blue, dashed red, dashed blue) line represents that of the state \((\alpha, \sigma) = (1, \uparrow)\) ((1, \downarrow), (2, \uparrow), (2, \downarrow)) respectively. Inset (left): the total spectral functions \((\Sigma_{\alpha, \sigma} A_{\alpha, \sigma})\) near the Fermi energy \((\omega = 0)\). Inset (right): the spectral function near the Fermi energy around \(\omega = 0\). Between \((k_x, k_y) = (3\pi/4, 0)\) and \((\pi/2, \pi/2)\), each orbital contributes to the coherence peaks, which is consistent with the behavior of the LDOS (see Fig. 3). Thus, we can conclude that the gap is generated by the SO interaction in this region, while as seen in Fig. 4(c) and (d), in the trivial AF phase, the peaks below the Fermi energy are mainly contributed by the state \((\alpha, \sigma) = (2, \uparrow)\), and thus, the gap is induced by the AF order. This confirms that the topological AF phase is induced by the electron correlation.

Since the system behaves as a correlated band insulator in the non-trivial AF region, as mentioned above, we expand the self-energies around \(\omega = 0\) and plot the renormalized energy level of each orbital defined by \(\varepsilon_{\alpha, \sigma}^* = z_{\alpha, \sigma}(\varepsilon_{\alpha, \sigma} + \Sigma_{\alpha, \sigma}(\omega = 0))\), where \(z_{\alpha, \sigma}\) is the renormalization factor of each orbital in Fig. 5. Note that as long as the system is recognized as a correlated band insulator, the relation \(\varepsilon_{2, \uparrow}^* > \varepsilon_{1, \downarrow}^*\) is the condition required for existence of the SO induced gap. In this figure, we can see that for \(4.2 < U < 4.6\), the state \((\alpha, \sigma) = (1, \downarrow)\) is
located below the Fermi energy, implying that the energy gap is dominated by the SO interaction. Since such an SO induced energy gap in the AF phase is not observed at the Hartree-Fock level, we conclude that correlation effects renormalize each band and thus suppress the energy shifts resulting from the spin polarization. This kind of renormalization should commonly occur in TBIs.

Before summarizing this paper, the effects of spatial fluctuations, which are neglected in the DMFT framework, should be mentioned. Spatial fluctuations generally suppress the magnetic order and have a tendency to shift the transition point to the strongly correlated region. Therefore, such fluctuations would usually cause substantial effects on magnetic transitions, so we have to carefully examine our results on the non-trivial magnetic phase. Although we cannot draw a definite conclusion beyond the DMFT results in this paper, we expect that the non-trivial phase found here can persist even when such spatial fluctuations are incorporated. First, we should note that while the magnetic transition point is shifted to the correlated region, the topological properties also remain up to, at least, antiferromagnetic transition point as long as singularities in the Green’s function are absent. Furthermore, as demonstrated in this paper, the band renormalization effects, which mainly originate from the local fluctuations, are essential for stabilizing the non-trivial magnetic phase. We thus expect that the essential properties of the non-trivial magnetic phase can be captured with the DMFT treatment, and the qualitative properties may not be changed even in the presence of spatial fluctuations. To confirm this point, however, the microscopic analysis taking into account spatial fluctuations properly (e.g. with cluster extension of DMFT, variational cluster approach, etc.) should be necessary, which is left for our future work.

Finally, we comment on the edge states. The nonzero spin Hall conductivity in the AFTI phase implies the existence of gapless spin excitations on open edges, which carries the spin Hall current, when the system has open boundaries. Thus one can deduce that the AF order is suppressed at the edges, and the helical edge states are topologically protected against magnetic instability, in spite of the existence of the bulk AF order.

IV. SUMMARY

In summary, we have studied topological properties of the AF phases in the extended BHZ model including local Coulomb interaction. The DMFT+NRG calculation of the magnetic moment and the spin Chern number has suggested the existence of a topologically non-trivial antiferromagnetic phase, where one can observe both the quantized spin Hall conductivity and the magnetic order, even if the Hartree-Fock treatment does not support it. We have demonstrated that the correlation effects are essential to realize the non-trivial AF magnetic phase; the correlation effects strongly renormalize the energy-level shift induced by the AF ordering, keeping the system still in the band-inversion regime. Although the detailed situations should depend on the system under consideration, this kind of renormalization effect is inherent in the TBI caused by the band-inversion mechanism, which encourages us to look for topologically non-trivial phases in the strong correlation regime.

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In the coexistence region, which is inherent in the first-order transition, the solution depends on the initial condition imposed for solving the self-consistent mean field equation. The stable phase is determined by examining the internal energy of each solution. That is, both the paramagnetic phase and the AF phase can be the self-consistent solutions in the coexistence region. 

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