Mechanism of hole propagation in the orbital compass models

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We explore the propagation of a single hole in the quantum compass model, whose nematic ground state is given by mutually decoupled antiferromagnetic chains. The compass model can be seen as the strong-coupling limit of a spinless two-band Hubbard model, which we study here using mean field theory and the variational cluster approach. Due to the symmetries of the compass model, the inherent disorder along one lattice direction turns out not to affect hole motion and doping a hole consequently does not lift the subextensive degeneracy of the nematic phase. In order to broaden and deepen understanding, we derive a generalized itinerant model and address the transition to two-dimensional Ising order. We observe coherent hole motion in both the nematic and the antiferromagnetic phases, also in the presence of quantum fluctuations away from pure Ising exchange. In addition to quantum fluctuations and interorbital hopping, three-site hopping is found to play an important role and to dominate propagation in the two-dimensional Ising limit as well as along the antiferromagnetic chains in the nematic order which forms in the compass model.

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I. INTRODUCTION

Spin-orbital physics is a very exciting and challenging field of research within the theory of strongly correlated electrons. Well known examples of Mott insulators with active orbital degrees of freedom are two-dimensional (2D) and three-dimensional (3D) cuprates, colossal magneto-resistance manganites and vanadates. These realistic models are rather complicated and difficult to investigate due to spin-orbital entanglement of exchange bonds. A common feature of spin-orbital models is intrinsic frustration of the orbital superexchange which follows from the directional nature of orbital states and their interactions. The orbital interactions are frequently considered alone, leading to orbital ordered states to valence bond crystal or to orbital pinball liquid exotic quantum states.

We concentrate below first on probably the simplest model that describes orbital-like superexchange, the so-called orbital compass model (OCM) introduced long ago by Kugel and Khomskii. This 2D model attempts to capture orbital anisotropies via couplings that are Ising-like along each bond, but where different spin components are active along different bond directions. A frequently used convention is that interactions take the form $J_z \sigma_z^i \sigma_z^j$ and $J_x \sigma_x^i \sigma_x^j$ along the $a$ and $b$ axis of the square lattice. Despite its deceptive simplicity, the compass model is challenging even for classical interactions. Recent interest in this model is motivated by its interdisciplinary character as it plays a role in the variety of phenomena beyond the correlated oxides: is also dual to recently studied models of $p + ip$ superconducting arrays namely to the Hamiltonian introduced by Xu and Moore and to the toric code model in a transverse field. Its 2D and 3D version was studied in the general framework of unified approach to classical and quantum dualities and in the 2D case it was proven to be self-dual. The OCM was also suggested as an effective description for Josephson arrays of protected qubits as realized in recent experiment. It could also describe polar molecules in optical lattices and systems of trapped ions. Recent developments on arrays of nitrogen-vacancy centers, constituting point-like defects in a diamond matrix bring a further motivation to the study of OCM, as shown in Ref. 26.

For further discussion of the properties of the 2D OCM it is helpful to recall the one-dimensional (1D) case. The 1D generalized variant of the compass model with $z$-th and $x$-th spin component interactions that alternate on even/odd exchange bonds is strongly frustrated, similar to the 2D OCM. The 1D OCM can be solved exactly by analytical methods in two different ways. We note that the 1D OCM is equivalent to the 1D anisotropic XY model, solved exactly in the seventies. An exact solution of the 1D OCM demonstrates that certain NN spin correlation functions change discontinuously at the point of a quantum phase transition (QPT) when both types of interactions have the same strength, similarly to the 2D OCM. This somewhat exotic behavior is due to the QPT occurring in this case at the multicritical point in the parameter space. The entanglement measures, together with so called quantum discord in the ground state characterizing the quantumness of the correlations, were analyzed recently to find the location of quantum critical points and to show that the correlations between two pseudospins on even bonds are essentially classical in the 1D OCM. A slight anisotropy of the interactions leads to particular short-range correlations dictated by the stronger interaction, but balanced interactions induce a QPT to a highly degenerate disordered ground state.

The 2D OCM is similarly characterized by both classical correlations on ordered bonds and by large ground

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state degeneracy. Balanced interactions \( J_x = J_z \) define here a QPT between competing types of 1D nematic orders: for \( J_x > J_z \) (\( J_x < J_z \)), antiferromagnetic (AF) chains form along a \((b)\) that are — in the thermodynamic limit — not coupled along b \((a)\). When going through the QPT, nearest neighbor (NN) spin correlations are discontinuous. This picture is supported by high-order perturbation theory, a rigorous mathematical approach, mean field (MF) theory on the Jordan-Wigner fermions, and a sophisticated infinite projected entangled-pair state (PEPS) algorithm.

At the isotropic point \( J_x = J_z \), the nematic order with its highly degenerate ground state manifold persists. It has been shown by quantum Monte-Carlo methods to remain stable at finite temperature up to \( T_c = 0.055 J \) and the phase transition to the fully disordered (paramagnetic) phase is in the Ising universality class. This resembles periodic frustrated Ising models, where also a phase transition at finite temperature is found. The ground state degeneracy was found to be exponential in the linear size of the system implying subextensive entropy at zero temperature. As shown by Doucot et al., the eigenstates of the OCM are twofold degenerate and the number of low energy excitations scales as linear size of the system. It has also been shown that the isotropic OCM is not critical in the sense that the spin waves remain gapful in the ground state, confirming that the order in the 2D OCM is not of magnetic type.

While the compass model is used to describe a variety of systems, see above, it represents a generic simplified concept of the orbital physics. Modifications that bring it closer to specific systems have been suggested, which allow one on one hand to assess how robust the features of the OCM are, and on the other lead to insights about the OCM itself. It was proven by exact diagonalization of small systems that the low energy excitations of the OCM correspond to the spin flips of whole rows or columns of the 2D lattice and that these characteristic excitations survive when a small admixture of the Heisenberg interactions is included into the compass Hamiltonian. A second generalization interpolates between the OCM and an isotropic Ising model, this will be here referred to as the generalized compass model (GCM). The elaborated multiscale entanglement-renormalization ansatz (MERA) calculations, together with high-order spin-wave expansion showed that the 2D GCM undergoes a second order QPT between the generic OCM and the Ising model.

Recent progress in the 2D OCM was achieved by making use of its symmetries. It has been shown that the symmetry allows one to reduce the original \( L \times L \) compass cluster to a smaller \((L - 1) \times (L - 1)\) one with modified interactions which made it possible to obtain exact eigenspectra for larger clusters and investigate the specific heat up to a \(6 \times 6\) system. The spin transformations that provided this reduction were also used to uncover a hidden order in the ground state of OCM manifested by the exact identities in the four-spin correlation function valid despite imposed anisotropy. It has been shown numerically that site dilution reduces ordering temperatures, but keeps the nematic character intact. Electron itinerancy has been addressed in the weak-coupling limit at temperatures above the ordering transition.

The purpose of this paper is to characterize the motion of a single hole in the ordered phases of both the OCM and the GCM, by obtaining the spectral functions of the itinerant models that reproduce both compass models in the strong coupling regime. A great advantage of using the itinerant models is that a variational cluster approach (VCA) could be used to obtain unbiased results for both weak and strong coupling regime. The VCA was introduced to study strongly correlated electrons in models with local interactions. Recently the VCA was used for the description of the excitonic insulator state in the two-orbital Hubbard model appearing in the broad parameter range between band and Mott insulator phases. This method was successfully applied to investigate hole propagation in the \(t_2g\) orbital model. We will compare its results here with MF results valid for weak coupling.

Since superexchange interactions are here Ising-like, quantum fluctuations are suppressed and the paradigm for hole propagation known from the spin \(t-J\) model, i.e., via coupling to such fluctuations may no longer apply. Indeed, it has been recognized that the Ising-like superexchange arising for \(t_2g\) electrons in \(ab\) planes of \(Sr_2VO_4\) implies that holes move mostly via three-site terms instead. In the case of \(e_g\) electrons, describing ferromagnetic (FM) \(LaMnO_3\) planes, inter-orbital hopping becomes an additional possibility.

However, all these models show truly 2D magnetic order in the ground state. While propagation along the 1D ordered chains of the OCM may be expected to show features characteristic of Ising-like order, the second and disordered direction presents a qualitatively new challenge. Concerning magnetism (resp. orbital superexchange), these bonds are inactive in the thermodynamic limit and do not contribute to the energy. A hole can, in contrast, still hop on these bonds and might thus in principle mediate couplings between ordered chains. As we are going to show, the symmetries of the OCM imply that this does not happen: The kinetic Hamiltonian of the hole turns out not to depend on the relative orientation of neighboring chains. We are also going to see that propagation in one of the two orbitals reveals the signatures of Ising-like order, namely it depends crucially on three-site hopping processes allowing for coherent propagation along the ordered chains.

The paper is organized as follows: In Sec. 11 we present both compass models and their itinerant counterparts. In Sec. 111 we discuss the symmetries specific for the OCM in the context of its itinerant version, and in Sec. 1V we solve the itinerant models in the MF approximation assuming two possible orders of the GCM (from Ref. 99). In Sec. 1V we present the VCA spectral functions of the OCM at different \(U\), starting from the weak coupling, metallic regime and ending in the insulating phase. Fi-
nally, in Sec. [VI] we present analogical results for the GCM at the strong coupling at different values of the control parameter \( \theta \), starting from the classical limit at \( \theta = 0 \) and ending at the critical value \( \theta_c \), where the GCM becomes very similar to the OCM. Summary and conclusions are presented in Sec. [VII]. The paper is supplemented by three appendices with more technical details: in Appendix A we show the form of the three-site hopping Hamiltonians for the OCM and the GCM, in Appendix B we show how the GCM and the OCM can be related to each other by the rotation in the space of fermion operators at the level of their itinerant models, and in Appendix C we derive the form of the hopping Hamiltonian after the transformation that changes the sign of coupling in the OCM.

II. HUBBARD HAMILTONIANS FOR THE COMPASS MODELS

The quantum compass model (OCM) on a square lattice is defined as (we consider here AF interactions with \( J > 0 \)),

\[
\mathcal{H}_J^0 = J \sum_i \{ \sigma_i^x \sigma_{i+a}^x + \sigma_i^y \sigma_{i+b}^y \},
\]

where \( \{ \sigma_i^x, \sigma_i^z \} \) are \( S = 1/2 \) pseudospin operators and \( (i+a(b)) \) is a shorthand notation for the nearest neighbor of site \( i \) in the direction \( a(b) \). Similarly, the generalized compass model (GCM) considered here can be written as

\[
\mathcal{H}_J^0 = J \sum_i \{ \bar{\sigma}_i(\theta) \bar{\sigma}_{i+a}(\theta) + \bar{\sigma}_i(-\theta) \bar{\sigma}_{i+b}(-\theta) \},
\]

where

\[
\bar{\sigma}_i(\theta) = \cos(\theta/2)\sigma_i^x + \sin(\theta/2)\sigma_i^z
\]

are the composed pseudospins interpolating between \( \sigma_i^x \) for \( \theta = 0 \) and \( (\sigma_i^x \pm \sigma_i^z)/\sqrt{2} \) for \( \theta = \pi/2 \). For \( \theta = 0 \), this corresponds to the usual Ising model coupling the x components of spin on all bonds. In the opposite limit \( \theta = \pi/2 \), it describes the OCM in a rotated spin space: bonds along \( a \) couple the spin component \( S^x + S^z \) and bonds along \( b \) the orthogonal \( S^x - S^z \). For \( 0 < \theta < \pi/2 \), the GCM interpolates between Ising and compass models. The rotation of the compass model provides an additional convenient way to detect the phase transition between 2D-Ising and nematic compass order: In the former, moments lie along \( x \) while they lie along either \( x + z \) (in the following identified with lattice axis \( a \)) or \( x - z \) in the latter.

Both models can be derived as a large–U limit of the two-orbital Hubbard model of the form

\[
\mathcal{H}_{t-U} = t \sum_i \sum_{\mu,\nu=\alpha,\beta} \left\{ A_{\mu\nu} c_{i,\mu}^\dagger c_{i+\alpha,\nu} + B_{\mu\nu} c_{i,\mu}^\dagger c_{i+\beta,\nu} \right\} + \text{H.c.}
\]

\[+
U \sum_i n_{i,\alpha} n_{i,\beta},
\]
Hamiltonian $\mathcal{H}_i^0$ of Eq. (1) commutes with $P_i$ and $Q_i$ operators defined as,

$$P_i = \prod_n \sigma^z_{i+n,b}, \quad Q_i = \prod_n \sigma^x_{i+n,a}.$$  \hspace{1cm} (13)

How does it work for the $t$-$U$ compass model Eq. (4)? The operator $Q_i$ should be first generalized to the case of double and zero occupancy of site $i$. This can be done by modifying $\sigma^z_i$ as follows,

$$\sigma^z_i \rightarrow \tilde{\sigma}^z_i = (1 - n_i)^2 + \sigma^z_i,$$  \hspace{1cm} (14)

so that $(\tilde{\sigma}^z)^2 = 1$. Now we can produce new $\tilde{Q}_i$ operators in the same way as before and see its action on the fermion operators, which is

$$\tilde{Q}_i \left(c_{j,\alpha(\beta)}\right) \tilde{Q}_i = c_{j,\beta(\alpha)},$$  \hspace{1cm} (15)

for all $c_{j,\mu}$ lying on the line of $\tilde{Q}_i$ and unity for the others. Under this change the interaction part of the $\mathcal{H}_i^0$ remains unchanged, i.e.,

$$\tilde{Q}_i \mathcal{H}_i^0 \tilde{Q}_i = U \sum_i n_{i,\alpha} n_{i,\beta}.$$  \hspace{1cm} (16)

In the hopping part the hopping matrices $A_0$ and $B_0$ transform by the anti-diagonal transposition, i.e.,

$$A_0 = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \rightarrow \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix},$$  \hspace{1cm} (17)

for the $a$-bonds overlapping with $\tilde{Q}_i$ and unity for the others. For $b$-bonds incoming to and outgoing from the line of $\tilde{Q}_i$ the same transformation acts as identity,

$$B_0 = \begin{pmatrix} 1/2 & 1/2 \\ 1/2 & 1/2 \end{pmatrix} \rightarrow \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix},$$  \hspace{1cm} (18)

so all the $b$-bonds remain unchanged. This brings us to the conclusion that $\mathcal{H}_i^0$ is covariant under the action of the $\tilde{Q}_i$; the exact form of the Hamiltonian changes, but the change is such that the properties of the new Hamiltonian are the same as before — only the orbitals along one line are renamed which is not relevant for the physics. Also the the pseudospin part $\mathcal{H}_i^0$ derived out of such a Hamiltonian is the same as before.

We discuss here the AF GCM/OCM model, but it should be noted that all physical properties remain valid for the FM variants. The equivalence of FM and AF couplings is of course well known for the Ising limit $\theta = 0$, but since the compass limit $\theta = \pi/2$ is characterized by frustration, one may wonder whether it is lifted in the FM variant. This is not the case, as one can see by explicitly carrying out the transformation. This is done in Appendix [C] by use of an (anti)symmetry operator that anticommutes with $\mathcal{H}_i^0$, which we call $Y$ operator. The $Y$ transformation transforms the AF OCM into a FM model, but — as can be seen from the $Y$-transformed hopping in Appendix [C] — hole motion remains frustrated in exactly the same way as in the AF case.

IV. MEAN FIELD SOLUTION OF THE GENERALIZED COMPASS MODEL

Here we will present a MF solution of the GCM assuming a typical order. As the GCM includes OCM as a special case for $\theta = \pi/2$, this solution will be used later on for both the GCM and its simple version, the OCM. As usually in a MF approach, we start from decoupling interaction term, i.e., the interaction term of Eq. (4) is rewritten as,

$$n_{i,\alpha} n_{i,\beta} = \frac{1}{2} (n_{i,\alpha} + n_{i,\beta}) - \frac{1}{2} \left[ \left( \cos \frac{\varphi}{2} c_{i,\alpha}^\dagger c_{i,\beta} + c_{i,\beta}^\dagger c_{i,\alpha} \right) + \sin \frac{\varphi}{2} (n_{i,\alpha} - n_{i,\beta}) \right]$$  \hspace{1cm} (19)

where $\varphi$ is an arbitrary angle. In any case we are interested AF type of ordering so the lattice must be divided into two sublattices. This introduces fermion operators with two flavors defined as follows,

$$\forall i \in A : \quad c_{i,\mu}^\dagger = c_{A,\mu}^\dagger, \quad c_{i,\alpha + \beta}^\dagger = c_{B,\mu}^\dagger.$$  \hspace{1cm} (20)

Now we introduce mean field $h$ which interpolates between $\sigma^x$ or $\sigma^z$ magnetization depending on $\varphi$, \hspace{1cm} (21)

$$h = \left\langle \cos \frac{\varphi}{2} (B_{i,\alpha}^\dagger B_{i,\beta} + B_{i,\beta}^\dagger B_{i,\alpha}) + \sin \frac{\varphi}{2} (n_{i,\alpha} - n_{i,\beta}) \right\rangle.$$  \hspace{1cm} (21)

Using the above equation we are ready to write the $t$-$U$ Hamiltonian of Eq. (4) in a MF form in the $k$-space,

$$\mathcal{H}_{t-U}^{MF} = 2t \sum_{k,\alpha,\beta} \sum_{\mu,\nu} \gamma^{\mu\nu}_{k} c_{k,\alpha}^\dagger c_{k,\beta}^\dagger + H.c.$$  \hspace{1cm} (22)

so all the $b$-bonds remain unchanged. This brings us to the conclusion that $\mathcal{H}_i^0$ is covariant under the action of the $\tilde{Q}_i$; the exact form of the Hamiltonian changes, but the change is such that the properties of the new Hamiltonian are the same as before — only the orbitals along one line are renamed which is not relevant for the physics. Also the the pseudospin part $\mathcal{H}_i^0$ derived out of such a Hamiltonian is the same as before.

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$$H_{t-U}^{MF} = 2t \sum_{k,\alpha,\beta} \sum_{\mu,\nu} \gamma^{\mu\nu}_{k} c_{k,\alpha}^\dagger c_{k,\beta}^\dagger + H.c.$$  \hspace{1cm} (22)

where

$$\gamma^{\mu\nu}_{k} \equiv A_{\mu,\nu} \cos k_{\alpha} + B_{\mu,\nu} \cos k_{\beta}.$$  \hspace{1cm} (23)

The last step is Bogoliubov transformation. We introduce new fermion operators $f_{k,\mu}^S$ for $S = A, B$ and $\mu = \alpha, \beta$ being linear combination of the old ones,

$$f_{k,\mu}^S = \mathcal{L} \left( A_{k,\alpha}^S \right) \left( B_{k,\beta}^S \right).$$  \hspace{1cm} (24)

The eigenmodes can be determined by the equation,

$$[H_{t-U}^{MF}, f_{k,\mu}^S] = E_{k,\mu} f_{k,\mu}^S.$$  \hspace{1cm} (25)
Thus the transformation matrix \( B \) reads,

\[
B = \frac{U}{2} \left[ \begin{array}{c}
-h \sin \frac{\varphi}{2} & -h \cos \frac{\varphi}{2} & \frac{4t_\uparrow}{U} \gamma_\uparrow & \frac{4t_\downarrow}{U} \gamma_\downarrow \\
-h \cos \frac{\varphi}{2} & h \sin \frac{\varphi}{2} & \frac{4t_\uparrow}{U} \gamma_\downarrow & \frac{4t_\downarrow}{U} \gamma_\uparrow \\
\frac{4t_\uparrow}{U} \gamma_\uparrow & \frac{4t_\downarrow}{U} \gamma_\downarrow & h \cos \frac{\varphi}{2} & h \sin \frac{\varphi}{2} \\
\frac{4t_\uparrow}{U} \gamma_\downarrow & \frac{4t_\downarrow}{U} \gamma_\uparrow & h \sin \frac{\varphi}{2} & h \cos \frac{\varphi}{2}
\end{array} \right] + \frac{U}{2}.
\]

After diagonalization of \( B \) we get four eigenenergies two of which are smaller than the others — we denote them as \( \{ E_{E,1}^c, E_{E,2}^c \} \). After filling the system with one fermion per site we obtain the ground state energy per site, \( \mathcal{E}_0 \), as an integral over the reduced Brillouin zone, i.e.,

\[
\mathcal{E}_0 = \frac{1}{8\pi^2} \int_{-\pi}^{\pi} dk_\uparrow dk_\downarrow \left\{ E_{E,1}^c + E_{E,2}^c \right\},
\]

with \( k_\uparrow = (k_x + k_y)/2 \) and \( k_\downarrow = (k_x - k_y)/2 \). The self-consistency equation of the form,

\[
\frac{2}{U} \frac{d}{dh} \mathcal{E}_0 = h,
\]

can be solved numerically by performing the numerical integration in \( \mathcal{E}_0 \).

Following the results for the generalized compass model presented in Ref. 39 we impose two different orderings depending on the angle \( \theta \), entering hopping matrices \( \{ A, B \} \) as shown by Eqs. (7), (8). The first order occurs below the critical angle \( \theta_{\text{MERA}} \approx 84.8^\circ \) (according to the MERA results of Ref. 39) and this is AF order in the \( \sigma^\uparrow \) components of the pseudospins (AFx), thus we take MF h with \( \varphi = \pi \) to simulate this phase. Above \( \theta_c \) the order changes into AF order that tracks one of the effective pseudospins \( \tilde{\sigma}(\theta) \) or \( \tilde{\sigma}(-\theta) \) (AFy) of Eq. (3), so we set \( \varphi = \theta \) in the definition of \( h \). In Fig. 1 we show the energies \( \mathcal{E}_0 \) for these two phases as functions of \( \theta \) at \( U = 20t \). We can see that their behavior is qualitatively correct, i.e., for \( \theta = 0 \) the two phases are the same, so the energies are equal. When \( \theta \) increases, the AFx becomes favorable until \( \theta = \theta_{\text{MERA}} \) and in our case \( \theta_{\text{MERA}} \approx 68^\circ \). Above \( \theta_c \) the AFy phase is favorable.

V. SPECTRAL FUNCTIONS OF THE ORBITAL COMPASS MODEL AT DIFFERENT \( U \)

In order to address the strong-coupling limit at large \( U \), where the \( t-U \) models come close to the OCM and GCM models, we use the VCA. It builds on cluster-perturbation theory, where the self-energy is calculated exactly (using exact diagonalization) for a small cluster and used to evaluate the one-particle Green’s function of a much larger system. This is complemented by optimization, where the grand potential is minimized with respect to a proposed order parameter. However, the method is only applicable to order parameters that are quadratic in fermion operators, e.g. magnetic, orbital or superconducting order. The order parameter for a nematic phase, in contrast, is proportional to \( \langle \sigma_x^\uparrow \sigma_x^\downarrow - \sigma_y^\uparrow \sigma_y^\downarrow \rangle \), and the VCA can consequently not be used to self-consistently detect this order in the GCM. Nevertheless, cluster-perturbation theory has been shown to be useful in obtaining spectral function for a nematic ground state imposed on models for iron-based superconductors.

Here, where the microscopic character of the nematic state is slightly different, we use a different approach. We make use of the facts that: (i) the nematic state is (in the thermodynamic limit) given by mutually decoupled AF chains, and (ii) the \( t-U \) Hamiltonian for the hole does not depend on the mutual orientation of the chains, see Sec. III. To treat the nematic state, we thus set the order parameter to select one configuration out of the ground state manifold, e.g. the AF one. The grand potential can be optimized just as in the AF state and the spectral density can be obtained, which is identical to that of all other ground states. This approach neglects tunneling from one nematic state to any other, but as the time scale of the related flip of a whole chain is much longer than the time scale of hole motion, especially in large systems, this is not expected to affect the hole’s motion.

We present here the VCA results obtained for a directly solved cluster of \( 3 \times 4 \) sites, with superlattice translation vectors, being \( \vec{x} = (3,1) \) and \( \vec{y} = (0,4) \), so that the AF order within the cluster implies that the whole lattice is AF. We also used other cluster geometries and sizes, e.g. \( \sqrt{10} \times \sqrt{10} \), for comparison and found consistent results, suggesting that the features that we observe in spectral functions are not cluster-dependent.

In Fig. 2, we present the VCA spectral functions in the limit of small \( U \) together with the MF bands. Figure 2(a) shows the spectral function for \( U = 1t \) along a standard path in the Brillouin zone. In this weak-interaction limit, the VCA spectral function exhibits two coherent bands coinciding with the bands obtained in the MF approach. This confirms the correctness of the numerical treatment.
The dispersion of the bands shows the high mobility of the hole especially around the point \( \vec{k} = (\pi/2, \pi/2) \), and it is clearly visible that one band is more dispersive than the other. For \( U = 2t \), see Fig. 2(b), the system has already gone through a metal-insulator transition in the MF approach and two subbands have formed that turn out to correspond to the upper and lower Hubbard bands. In the VCA, the system is indeed close to the transition, so that some spectral weight is transferred to the new (shadow) bands, but this weight is very small so that the bands are not yet visible in the plot. The coherent part of the VCA spectral function still coincides with the MF bands, but some incoherent features can already be recognized. Further increase in \( U \) up to \( U = 4t \) is enough to drive the cluster through the metal-insulator transition and to split the hole and electron parts of the spectral function in the VCA — in Fig. 2(c) we show the hole spectral function for \( U = 4t \), i.e., the lower Hubbard band. Except for some momentum-space regions around \( \vec{k} = (0,0) \), interactions now induce more incoherence. Nevertheless, coherent bands can be clearly observed, see e.g., the sharp features in the lowest and highest energy part of the spectral function around \( \vec{k} = (\pi,\pi) \). Qualitatively the VCA and MF bands look quite similar on the path between \( \vec{k} = (\pi,\pi) \) and \( \vec{k} = (\pi,0) \). This is not the case for the section between \( \vec{k} = (\pi,0) \) and \( \vec{k} = (0,0) \), where the sharp feature around \( \vec{k} = (\pi/2,\pi/2) \) has opposite convexity than the MF band. Finally, around \( \vec{k} = (\pi,0) \) the VCA spectral function does not exhibit any coherent features, but has only incoherent spectral weight.

Figure 3 shows the spectral functions in the limit of large \( U \). For \( U = 8t \), see Fig. 3(a), we can see that the spectral weight is distributed more equally among the states around \( \vec{k} = (0,0) \) and \( \vec{k} = (\pi,\pi) \) than for smaller values of \( U \). The bottom band is seen as a coherent feature roughly agreeing with the MF prediction, but much less dispersive. The upper band cannot be identified easily with any MF band, even though although the features around \( \vec{k} = (\pi/2,\pi/2) \) resemble the MF bands. Especially in the large-\( U \) limit, see Fig. 3(b) for \( U = 20t \), the weight imbalance between \( \vec{k} = (0,0) \) and \( \vec{k} = (\pi,\pi) \) is no longer visible and the bands are flatter than for lower \( U \), both in qualitative agreement with the MF results. Also
the shapes of the bands in VCA agree to some extent with the MF bands, especially around \( \vec{k} = (\pi/2, \pi/2) \). Strong coupling differences to the MF bands are on one hand the incoherent weight and on the other the separation of bottom and top bands. Even the MF bands do not really cross, but they remain very close to each other at \( \vec{k} = (\pi/2, \pi/2) \). In the VCA, the are much further separated, which means there is a strong effective interaction at this value of \( \vec{k} \) that cannot be captured by a simple MF approach.

Maybe the most obvious new feature seen at large \( U \) is, however, a rather coherent band in the middle of the spectrum. It has strongest intensity around \( \vec{k} = (\pi, \pi) \) and can be best seen in Fig. 4(b) for \( U = 20t \), where it is the sharpest feature of the spectral function. The extra band is absent from the MF approach and in the VCA, it seems to strongly repel the two bands at the top and bottom of the spectrum, thus making them flatter and the overall spectrum much wider than in the MF approach.

To better understand the results in the strong coupling regime we have projected the spectral function on \( \alpha \) and \( \beta \) orbitals for \( U = 20t \). This is shown in Fig. 4(a) and 4(b). Comparing Fig. 4(a) with the initial, nonprojected, result of Fig. 3(b) we can see that almost only the central band is visible in the \( \alpha \) channel and is very sharp. The \( \beta \)-projection in Fig. 4(b) conversely only shows the top and bottom bands. The central band absent from MF spectra can now be identified as due to three-site hopping of \( \alpha \) orbitals along the AF chains. Noting this and assuming classical AF order in the OCM ground state, we can easily derive an approximate form of the three-site hopping band from the general three-site hopping Hamiltonian of Eq. (A3) by putting \( \bar{n}_{i,\alpha} = 0 \) and \( \bar{n}_{i,\beta} = 1 \) for \( i \in A \) and thus \( \bar{n}_{i,\alpha} = 1 \) and \( \bar{n}_{i,\beta} = 0 \) for \( i \in B \) in the central site of the hopping term. This leads to the kinetic Hamiltonian of the form,

\[
H^{\alpha}_{t^2} = -\frac{2t^2}{U} \sum_{\vec{k} \in A} \epsilon^{B \dagger}_{\vec{k},\alpha} \epsilon^{B}_{\vec{k},\alpha} \left\{ \cos (2k_\alpha) + \frac{1}{4} \cos (2k_\beta) + \cos (k_\alpha + k_\beta) + \cos (k_\alpha - k_\beta) \right\}.
\]

This dispersion relation is shown in Fig. 5(a) and indeed reproduces well the band obtained by the VCA.

Alternative plots of the projected spectral functions of Figs. 4 are presented in Figs. 5. Here the 3D fence plots are used instead of the map plots. As before, the three-site hopping band is well visible in Fig. 5(a) as a ridge of tall, coherent peaks and the other features can be seen in Fig. 5(b). Most of them are incoherent.

VI. SPECTRAL FUNCTIONS OF THE GENERALIZED COMPASS MODEL

In this Section we present spectral functions of the GCM obtained via the VCA for a few selected values
of angle $\theta$. We have used the same procedure as for the original OCM: the $t$-$U$ Hamiltonian $H$ for the GCM was implemented into a VCA input file and the optimization of the grand potential $\Omega$ was done with respect to the order parameter. Following the results from Ref. 39 and Sec. IV, we assumed two possible orders, AF$\alpha$ and AF$x$ one, and we compared the optimal values of $\Omega$ for each of them to decide which configuration is more favorable for a selected value of $\theta$. We have verified that the VCA results for lower values of $U \lesssim 8t$ show a preference for the AF$x$ direction for all values of $\theta$. For $\theta \to \pi/2$, this is in contrast to the expectations (and to the VCA results) for the strong coupling limit, where the model goes over into the OCM and prefers AF$\alpha$ order for $\theta > \theta_c^{VCA} \approx 88^\circ$.

We note here that the ground state manifold of the classical OCM model has in fact an accidental degeneracy that makes AF$x$ and AF$\alpha$ (as well as orientation along any other direction) equivalent and which is only lifted by quantum and thermal fluctuations. In the case of the itinerant model, orbital fluctuations in the weak-coupling regime have been noted to differ from strong coupling, which has been attributed to a different degree of band hybridization. The importance of $U$-dependent hybridization and the close energies of various orientations are probably the reason for the basis-sensitivity of the VCA results. As we are here interested in hole dynamics of the OCM and GCM, we focus on larger values of $U$, where all results are consistent.

We are here going to analyze how the spectral density of the 2D Ising magnet with AF$x$ order evolves when going from the pure Ising model towards the transition to nematic order, i.e., for increasing $\theta$. In Figs. 3(a) and 3(b) we show the VCA spectral functions of GCM at three different angles $\theta < \theta_c$ for $U = 20t$. As for OCM, the results were tested for finite-size effects by changing cluster geometry and size; results presented here are for a $3 \times 4$ cluster. Figure 3(a) shows the hole spectral function for $\theta = 0$, where the GCM reduces to the classical AF Ising model. The overall spectrum has approximately ladder character, as expected, because the hole is confined in a string potential and quantum fluctuations which might relieve the confinement are absent. The only mechanism allowing for weak dispersion is three-site hopping, which acts on the scale of $t^2/U$. The two MF bands cannot of course reflect the ladder spectrum, i.e., both energies and total width of the spectrum are wrong, but they do reflect the low hole mobility.

For $\theta = \pi/4$, see Fig. 3(b), the bands become significantly more dispersive, especially the ones on the top, while the ones on the bottom are less dispersive. The shape of the topmost band is qualitatively well reproduced by the MF and this band is the sharpest feature seen in the spectral function at $\theta = \pi/4$. As in the case of the original OCM at high $U$ (Fig. 3), the bands predicted by MF repel each other in the VCA and new features emerge at the intermediate energies, with rather incoherent weight. Similarly to the generic OCM case, bands are most dispersive along the direction $(0, 0) \to (\pi, \pi)$.

The increased dispersion, especially of the rather coherent topmost band, is here not primarily driven by quantum fluctuations, because the ground state is still Ising ordered, as it is fond for $\theta = 0$, see above. However, interorbital hopping is now active, see Eqs. (7) and (8), which allows the hole to evade the string potential and to propagate, similar to the case of a hole in $e_g$ orbital order.

Finally, in Fig. 3(c), we show the spectral function infinitesimally close to the transition angle $\theta_c$, thus $\theta = 88^\circ - \epsilon$. As in the MF results the bands are more dispersive and the agreement between both approximations is better. Comparing to $\theta = \pi/4$, spectral weight is distributed more equally on the energy scale and it shows imbalance between $k = (\pi, \pi)$ and $k = (0, 0)$, similar to the OCM at $U = 8t$, see Fig. 3(a). Despite a rela-
tively large value of $\theta$ the overall ladder modulation of the spectrum, characteristic for the Ising model at $\theta = 0$, is still well visible. This is a consequence of small quantum fluctuations in the ground state of the undoped GCM, as shown in Ref. [39]. Therefore we should attribute all the difference in hole’s behavior induced by growing $\theta$ rather to its $\theta$-dependent hopping term than to the change of its background. Note that the inter-orbital hopping of the hole may induce quantum fluctuations as well, but they should be distinguished from fluctuations inherent in the undoped ground state. On the other hand, for values of $\theta$ higher than $\theta_c^{\text{VCA}}$ the system is already in the AFa phase and its spectral function is very similar to the one already discussed in case of the OCM.

VII. SUMMARY AND CONCLUSIONS

We have derived an itinerant $t$-$U$ model for the generic as well as for generalized compass models by choosing proper hopping amplitudes of the respective spinless two-band Hubbard models. The itinerant models studied here reproduce the form of the generalized (and generic orbital) compass model in the limit of large interaction $U$, when electrons localize and orbital degrees of freedom are coupled by the superexchange processes. The $t$-$U$ models were then solved in the mean field approximation by splitting the interaction term and assuming antiferromagnetic order of checkerboard type (either AFa or AFx type). The mean field approach predicted correctly the transition between AFa and AFx order in the generalized compass model, however, the critical angle $\theta_c^{\text{MF}} \approx 68^\circ$ (at strong coupling, $U = 20t$) is found to be far from the quasi-exact result of Ref. [39] $\theta_c^{\text{MERA}} \approx 84.8^\circ$. On the other hand, the variational cluster approach gives a value of the critical angle $\theta_c^{\text{VCA}} \approx 88^\circ$ much closer to $\theta_c^{\text{MERA}}$, however in both cases, i.e. in mean field and in the variational cluster approach, the result is potentially $U$-dependent, in agreement with earlier studies on the weak-coupling limit. As the variational cluster approach cannot directly detect nematic order by construction, we used here as a proxy the preferred spin direction, which is known to be different in the antiferromagnetic Ising and the nematic phases. However, at smaller $U \lesssim 8t$, where the space of plausible candidate phases is not known, the variational cluster approach results were inconclusive for large $\theta$. Bands at large $U$, where results are consistent, were interpreted with the help of mean field results.

We have obtained the spectral functions for the orbital compass model at different couplings $U$, as well as for the generalized compass model at strong coupling and different values of $\theta$. We compared these variational cluster-approximation results with the mean field bands, where agreement at weak coupling, up to $U = 2t$, is as expected good. (Only the metal-insulator transition occurred for smaller $U$ in case of the mean field.) For higher values of $U$, where the interacting spectra in the variational cluster approach become less coherent, agreement becomes worse. However, the bands obtained in mean field typically still reproduce some features of the most coherent bands seen at the top and the bottom of the spectra given by the variational cluster approach.

The most striking feature of the orbital compass model, with respect to the corresponding itinerant model, is its nematic order, where chains with antiferromagnetic order stagger along one direction, say $a$, and are mutually decoupled along the other, $b$. The main topic of this paper is hole motion in such a phase. We have shown in Sec. III that the same symmetries that decouple orbital order between chains also render the kinetic Hamiltonian for the hole independent of their relative orientation. As a consequence of the symmetry considerations, we can thus conclude that doping with a hole does not lift the degeneracy of the nematic ground state manifold. On a technical side, this permits us to calculate one-particle spectra in one of the ground states, e.g., the AF one, instead of having to average over many of them. This was confirmed by choosing different spin configurations from the ground state manifold and getting the same result in the variational cluster approach. The disorder of the nematic ground state manifold does thus not affect hole motion and the variational cluster-approach spectra reveal rather coherent bands that also disperse along the $b$ direction, see Fig. 3 in Sec. V. This is in contrast to a spin-orbital model for narrow-band manganites, where a nematic phase emerges spontaneously without the Hamiltonian having similar symmetries, and where spectra differ for different states. For of a hole inserted into the $\alpha$ orbital, which can hop along the AF ordered $a$ direction, comparison to mean field reveals that three-site terms are crucial for the hole propagation, see Sec. V. This reflects the Ising-character of order along the $a$ axis, where there is moreover no inter-orbital hopping.

In our study of the generalized compass model with two dimensional magnetic Ising order, we focused on the impact of interorbital hopping terms, parametrized by $\theta$, see Sec. IV. At $\theta = 0$, interorbital hopping is absent and superexchange of the model is equivalent to the classical Ising model. The consequence for the hole’s motion is clearly visible in the spectral function — the bands are sharp but very flat. This is coherent with Ref. [49], saying that for classical Ising model the hopping of the hole is possible only via three-site terms. For $\theta > 0$, where the strong-coupling limit no longer reduces to the Ising model, dispersion is strongly increased, even though the magnetic order is still 2D and Ising-like. Finite $\theta$ allows on one hand more quantum fluctuations into the ground state which enables hole propagation via spin-flips healing the defects produced by the hole, as in the Heisenberg model. On the other hand, inter-orbital hopping allows the hole to move even in an Ising-ordered background without quantum fluctuations, because it can hop without creating defects in the first place. This latter effect dominates in the generalized compass model, where order remains almost perfectly Ising-like.

The final conclusion on the mobility of a single hole in
the above models is that the hole can move coherently
in the generic orbital compass model and its generalized
version. In the Ising limit (at $\theta = 0$ in the generalized
compass model) as well as for the $a$ orbital along the
antiferromagnetic chains in a direction of the orbital compass
model, the dominant process is three-site hopping.
Apart from this process, mobility in this latter case can
be associated with the form of the hopping matrix $B_{0}$
in the direction of the $x$-bonds containing hopping be-
tween any pair of orbitals. This inter-orbital hopping
allows the hole to avoid creating defects in the AF order
by choosing the lowest-energy hopping for each bond in
the $b$ direction. However, this is de facto more subtle
for it would suggest coherent hopping to be only along
the $b$ direction, while it is 2D in the variational cluster-
approach spectra. In the generalized compass model, the
analogous role is played by the $\bar{\theta}$ terms, see
Eq. (3). This qualitatively explains, using essentially the
same argument as for the generic orbital case, why the
hole is confined in the generalized compass model when
$\theta = 0$, and becomes mobile when $\theta$ grows.

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Appendix A: General three-site hopping

The three-site hopping can be derived in the same way
as the superexchange. The only difference is that the
fermions after creating a virtual excitation with double
occupancy do not come back to their initial positions
but move further on. In the Hamiltonians written below
the excitation was created at site $i$ and the fermion can
either move straight ahead either in the $a$ or $b$ directions,
or can turn left or right after deexcitation. The general
three-site hopping for the Hamiltonian $H_{t-U}$ of Eq. (1)
reads,

$$H_{t-U}^{ab} = -\frac{t^{2}}{U} \sum_{i} \sum_{\mu,\nu,\alpha,\beta} \left\{ \hat{c}_{i+a,\mu}^{\dagger} (A_{\mu\nu} A_{\nu\bar{\nu}} \hat{n}_{i,\bar{\nu}} + B_{\bar{\nu}} A_{\nu\nu} \hat{n}_{i,\nu}) \hat{c}_{i-a,\nu}^{\dagger} + \hat{c}_{i+a,\mu}^{\dagger} \left[ A_{\mu\nu} A_{\nu\nu} \left( \hat{c}_{i,\nu}^{\dagger} \hat{\bar{\nu}} + \hat{c}_{i,\bar{\nu}} \hat{\nu} \right) \right] \hat{c}_{i-a,\nu}^{\dagger} \right\} \tag{A1}$$

for the hopping along $a$ axis and analogous expression
holds for the $b$ axis. In case of turn at site $i$ the relevant
expression is,

$$H_{t-U}^{ab} = -\frac{t^{2}}{U} \sum_{i} \sum_{\mu,\nu,\alpha,\beta} \left\{ \hat{c}_{i+a,\mu}^{\dagger} (B_{\nu\mu} A_{\nu\nu} \hat{n}_{i,\nu} + B_{\bar{\nu}} A_{\nu\nu} \hat{n}_{i,\nu}) \hat{c}_{i-a,\nu}^{\dagger} + \hat{c}_{i+a,\mu}^{\dagger} \left[ B_{\nu\mu} A_{\nu\nu} \left( \hat{c}_{i,\nu}^{\dagger} \hat{\bar{\nu}} + \hat{c}_{i,\bar{\nu}} \hat{\nu} \right) \right] \hat{c}_{i-a,\nu}^{\dagger} \right\} + H.c., \tag{A2}$$

where $\alpha(\beta) = \beta(\alpha)$.

Now we can derive the three-site hopping Hamiltonians
for the cases of OCM and GCM using hopping matrices of Eqs. (6), (7) and (8). For OCM we get,

$$H_{t-U}^{0} = -\frac{t^{2}}{2} \sum_{i} \sum_{\mu,\nu=\alpha,\beta} \left\{ \hat{c}_{i+a,\mu}^{\dagger} \left( \hat{n}_{i,\nu} - \frac{\sin \theta}{2} \hat{\sigma}_{\nu}^{\zeta} - \cos \frac{\theta}{2} \hat{\sigma}_{\nu}^{\zeta} \right) A_{\mu\nu}^{\theta} \hat{c}_{i-a,\nu}^{\dagger} + \hat{c}_{i+a,\mu}^{\dagger} \left[ A_{\mu\nu}^{\theta} \left( \hat{c}_{i,\nu}^{\dagger} \hat{\bar{\nu}} + \hat{c}_{i,\bar{\nu}} \hat{\nu} \right) \right] \hat{c}_{i-a,\nu}^{\dagger} \right\} + H.c., \tag{A3}$$

with $\hat{n}_{i,\beta} = n_{i,\beta} (1 - n_{i,\alpha})$, and for the GCM,

$$H_{t-U}^{0} = -\frac{\sqrt{2} t^{2}}{2} \sum_{i} \sum_{\mu,\nu=\alpha,\beta} \left\{ \hat{c}_{i+a,\mu}^{\dagger} \left( \hat{n}_{i,\nu} - \frac{\sin \theta}{2} \hat{\sigma}_{\nu}^{\zeta} - \cos \frac{\theta}{2} \hat{\sigma}_{\nu}^{\zeta} \right) A_{\mu\nu}^{\theta} \hat{c}_{i-a,\nu}^{\dagger} + \hat{c}_{i+a,\mu}^{\dagger} \left[ A_{\mu\nu}^{\theta} \left( \hat{c}_{i,\nu}^{\dagger} \hat{\bar{\nu}} + \hat{c}_{i,\bar{\nu}} \hat{\nu} \right) \right] \hat{c}_{i-a,\nu}^{\dagger} \right\} + H.c., \tag{A4}$$

with $\hat{n}_{i} = \hat{n}_{i,\alpha} + \hat{n}_{i,\beta}$ and new hopping matrix $C_{\theta}$ similar to previous ones,

$$C_{\theta} = \frac{\sqrt{2}}{2} \left( \frac{1 + \sin \frac{\theta}{2}}{\cos \frac{\theta}{2}} - \frac{\cos \frac{\theta}{2}}{\sin \frac{\theta}{2}} - 1 \right). \tag{A5}$$

Appendix B: Change of basis for the $t-U$ model

We start with the $t-U$ Hamiltonian for the compass
model of Eq. (1),

$$H_{t-U}^{0} = t \sum_{i} \left\{ \hat{c}_{i,\alpha}^{\dagger} \hat{c}_{i+a,\alpha}^{\dagger} + \frac{1}{2} \sum_{\mu,\nu=\alpha,\beta} \hat{c}_{i,\mu}^{\dagger} \hat{c}_{i+\mu,\nu}^{\dagger} \right\} + H.c., \tag{B1}$$

and we will transform it into the $t-U$ Hamiltonian of the
GCM Eq. (2) at $\theta = \pi/2$. The key transformation is rotation by $\pi/4$ in the fermionic space,

$$\begin{pmatrix} c_{i,\alpha} \\ c_{i,\beta} \end{pmatrix} = \begin{pmatrix} \cos \frac{\pi}{4} & \sin \frac{\pi}{4} \\ -\sin \frac{\pi}{4} & \cos \frac{\pi}{4} \end{pmatrix} \begin{pmatrix} b_{i,\alpha} \\ b_{i,\beta} \end{pmatrix}. \tag{B2}$$
Following this one can express the hopping part in a new basis of fermions $b_{\mu,i}^\dagger$ as,

$$
\mathcal{H}_t^0 = \frac{t}{\sqrt{2}} \sum_i \sum_{\gamma=a,b} \left\{ \frac{\sqrt{2}+1}{2} b_{i,\alpha}^\dagger b_{i+\gamma,\alpha} + \frac{\sqrt{2}-1}{2} b_{i,\beta}^\dagger b_{i+\gamma,\beta} \right\}
$$

$$
\mp \frac{1}{2} b_{i,\alpha}^\dagger b_{i+\gamma,\beta} \mp \frac{1}{2} b_{i,\beta}^\dagger b_{i+\gamma,\alpha} \right\}.
$$

(B3)

Surprisingly, the interaction part keeps its simple form after the substitution, i.e.,

$$
\mathcal{H}_U^0 = U \sum_i \left( b_{i,\alpha}^\dagger b_{i,\alpha} \right) \left( b_{i,\beta}^\dagger b_{i,\beta} \right).
$$

(B4)

Comparing Eqs. (B3) and (B4) with Eqs. (4), (7) and (8) we see that the rotated $t-U$ compass model is equivalent to the generalized $t-U$ compass model at $\theta = \pi/2$ if we only renormalize the hopping amplitude $t$ by $1/\sqrt{2}$ in the compass model.

### Appendix C: The $Y$ antisymmetry

The quantum compass model is known to anticommute with an operator being a product of $\sigma_i^y$ on a chosen sub-lattice, i.e.,

$$
Y = \prod_{i \in A} \sigma_i^y.
$$

(C1)

Anticommutation means that,

$$
Y \mathcal{H}_0^I Y = -\mathcal{H}_0^I.
$$

(C2)

In the presence of a hole however, the $Y$ operator has to be modified because $\sigma_i^y = 0$ for a site with zero or double occupancy. To cure this problem one can substitute $\sigma_i^y$ as follows

$$
\sigma_i^y \rightarrow (1-n_i)^2 + \sigma_i^y,
$$

(C3)

with $n_i = n_{i,\alpha} + n_{i,\beta}$. Now at zero/double occupied site, $\sigma_i^y = 1$ and for other sites $\sigma_i^y$ remains unchanged. The form of $Y$ for a single hole is,

$$
Y_{1h} = \prod_{i \in A} \sigma_i^y + \sum_{p \in A} (1-n_p)^2 \prod_{A \ni p \neq p} \sigma_i^y.
$$

(C4)

Surprisingly, this does not change the anticommutation relation for the pseudospin Hamiltonian, i.e.,

$$
Y_{1h} \mathcal{H}_0^I Y_{1h} = -\mathcal{H}_0^I,
$$

(C5)

but the change in the kinetic part is less trivial,

$$
Y_{1h} \mathcal{H}_t^0 Y_{1h} = \frac{t}{2} \sum_{i \in A} \left( \tilde{c}_{i,\alpha}^\dagger - \tilde{c}_{i,\beta}^\dagger \right) \sum_{\mu=\alpha,\beta} \left( \tilde{c}_{i+b,\mu} + \tilde{c}_{i-b,\mu} \right)
$$

$$
- t \sum_{i \in A} \tilde{c}_{i,\beta}^\dagger \left( \tilde{c}_{i+a,\alpha} + \tilde{c}_{i-a,\alpha} \right) + \text{H.c.}
$$

(C6)

These two results, Eqs. (C5) and (C6) show that on one hand the pseudospin interactions can be changed freely from AF to FM, but on the other hand the kinetic part changes in such a way that the physics of the moving hole remains unchanged. For instance, along $a$ the hopping transforms from pseudospin-conserving to pseudospin-flipping so the hole motion can frustrate the FM exchange in the $a$ direction.
