

Altermagnetic Polarons: The Fate of Altermagnetic Band Splittings at Strong Coupling

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While a spin-dependent band splitting is one of the characteristic features of altermagnets, the conventional band picture itself breaks down in the many altermagnets that are correlated Mott materials. We employ two numerical many-body methods, the self-consistent Born approximation and a variational cluster approach, to explore this strongly correlated regime and investigate hole motion in Mott altermagnets. Our results reveal that spin-dependent spectral-weight transfer is the dominant signature of Mott altermagnetism. This pronounced spin-momentum locking of the quasiparticle spectral weight arises from the formation of altermagnetic polarons, whose dynamics are governed by the interplay between free hole motion and the coupling of the hole to magnon excitations in the altermagnet. We demonstrate this effect by calculating angle-resolved photoemission spectroscopy spectra for three canonical altermagnetic systems: the checkerboard J – J' model, a variant describing the transition-metal-ion sites of the inverse Lieb lattice, and the Kugel-Khomskii spin-orbital altermagnet based on cubic vanadates RVO_3 ($\text{R} = \text{La}, \text{Pr}, \text{Nd}, \text{Y}$).

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It was recently discovered that, depending on their symmetries, collinear antiferromagnets may break spin degeneracy in momentum space, even in the absence of spin-orbit coupling, giving rise to a set of magnetic materials referred to as altermagnets (AMs) [1–6]. At a single-particle level, valid for systems with weak electron-electron interactions, this gives rise to electronic bands with anisotropic, spin-split isoenergy surfaces. The anisotropic bands in turn lead to a series of unusual electric, magneto-electric and optical properties [7–11]. Indeed, such spin-split bands corresponding to (very) weak correlations without band renormalization have been observed in angle-resolved photoemission spectroscopy (ARPES) experiments—for instance in metallic CrSb or semiconducting MnTe [12–18].

However, a large set of AMs are actually strongly correlated Mott insulators, with band gaps determined by the Hubbard electron-electron interaction [6]. This comprises, e.g., a series of transition metal fluoride AMs with rutile structure [6], vanadates [19], recently discovered

layered AM $\text{La}_2\text{O}_3\text{Mn}_2\text{Se}_2$ [20,21], and, potentially, transition metal oxychalcogenides [22,23]. It is well-known that in canonical correlated antiferromagnets the band picture fails as many-body effects strongly renormalize quasiparticle dispersions all the way down to the magnetic energy scale, and at the same time vehemently reorganize spectral weights (SWs) [24,25]. This raises the question as to the fate of altermagnets and their dynamical properties in the strongly correlated and Mott insulating regime.

In strong-coupling correlated antiferromagnets the large difference with the bare single-particle electronic dispersions is due to the disruptions in the antiferromagnetic (AF) background that are caused by a moving charge carrier. Its motion dynamically creates and annihilates excitations of the AF background, usually magnons, and the interplay of hole and magnons strongly modifies hole propagation. While a quasiparticle (QP)—the spin polaron—often survives, it contains only part of the SW and has a dispersion of the order of the magnetic exchange J rather than of the bare hopping t [26]. The missing weight is lost into an incoherent continuum [27,28] that is usually separated from the polaronic QP band and distributed over a width $\propto t$. The description of charge carriers in terms of spin polarons in antiferromagnets is widely used [29–31] to interpret ARPES measurements on cuprates [32,33] and has been extended to describe orbital excitations in iridates [34] and cuprates [35], as well as been investigated in ultracold-atom quantum simulators [36–38].

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Certain theoretical aspects of AMs beyond the weak-coupling regime have been considered, in particular the existence of lower and upper Hubbard bands in addition to altermagnetic band splitting [39], the persistence of altermagnetic signatures into a frustrated and/or fluctuating regime [40,41], and nontrivial temperature effects [42,43]. However, the impact of altermagnetic symmetries on the properties of strongly interacting quasiparticles and spin polarons, which are directly related to the spectral function measured in ARPES, have not been considered so far.

Here, we consider the correlated charge propagation in Mott-insulating altermagnets, i.e., the spin polaron in an altermagnet instead of an antiferromagnet. Both the bare dispersion, which one would observe without correlations, and the magnon spectrum [44,45], which strongly modifies the effective dispersion of a spin polaron, have momentum-dependent band splittings in altermagnets that are not present in antiferromagnets. Focusing on a $t - J$ model on the checkerboard lattice, we find that momentum and spin of the polaron are similarly strongly linked. However, in contrast to weakly interacting altermagnets, this is not necessarily reflected in a band splitting, but rather in the particle lifetime: one spin projection is pushed into the incoherent spectrum, losing its quasiparticle character, so that the surviving quasiparticle shows spin-momentum locking.

We also look at hole motion in a Mott-insulating Kugel-Khomskii-type model for vanadates of the form RVO_3 ($R = \text{La, Pr, Nd, Y}$) that combine orbital and magnetic order [46–48]. Orbital order is driven by a combination of lattice and superexchange effects, with $LaVO_3$ being most clearly dominated by superexchange [48]. Looking at a single two-dimensional plane, spin and orbital alternate together in an antiferromagnetic and antiferro-orbital pattern as sketched in Fig. 1(b), suggesting an AM state [49]. In fact, band-structure calculations have found YVO_3 to be an altermagnet [19], and we will show that holes are then expected to move as altermagnetic polarons.

Spectral function of the checkerboard altermagnetic polaron—Our considerations start from a $t - J$ model on the checkerboard lattice [see Fig. 1(a)], defined by

$$H = -t \sum_{\langle i,j \rangle, \sigma} c_{i,\sigma}^\dagger c_{j,\sigma} - t' \sum_{\langle\langle i,j \rangle\rangle \parallel (1,1) \atop i,j \in A, \sigma} c_{i,\sigma}^\dagger c_{j,\sigma} - t' \sum_{\langle\langle i,j \rangle\rangle \parallel (1,-1) \atop i,j \in B, \sigma} c_{i,\sigma}^\dagger c_{j,\sigma} \quad (1)$$

$$+ J \sum_{\langle i,j \rangle} \mathbf{S}_i \mathbf{S}_j + J' \sum_{\langle\langle i,j \rangle\rangle \parallel (1,1) \atop i,j \in A} \mathbf{S}_i \mathbf{S}_j + J' \sum_{\langle\langle i,j \rangle\rangle \parallel (1,-1) \atop i,j \in B} \mathbf{S}_i \mathbf{S}_j, \quad (2)$$

where $c_{i,\sigma}^\dagger$ ($c_{i,\sigma}$) creates (annihilates) an electron with spin $\sigma = \uparrow, \downarrow$ on site i . $\mathbf{S}_i$ denotes the corresponding vector of spin operators $S_i^\alpha = \frac{1}{2} \sum_{s,s'} c_{i,s}^\dagger \sigma_{s,s'}^\alpha c_{i,s'}$ with Pauli matrices σ^α . Nearest-neighbor (NN) bonds $\langle i, j \rangle$ connect the two

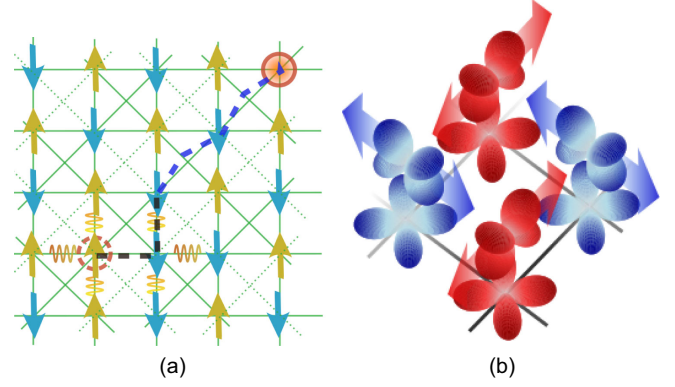


FIG. 1. (a) Cartoon for hole propagation in the (generalized) checkerboard model: The hole has moved from its original position (dashed empty circle) to the current one (filled circle) via two NN hoppings (black dashed horizontal and vertical line) and two NNN hopping processes (blue dashed diagonal lines). The NN processes have disturbed the AF background and thus created magnons, the NNN hopping left it intact. Adding (different) couplings along the dotted lines as well describes the transition-metal sublattice of the inverse Lieb lattice [50]. (b) Cartoon for the spin-orbital model based on $LaVO_3$. The xy orbital is half filled and superexchange leads to AF order, indicated by red and blue color. Additionally, the xz/yz orbitals share one electron, which can only hop along one direction (indicated by the fat arrows) and whose spin is aligned to the xy spin on the same site. Superexchange processes due to xz/yz hopping induce Ising spin coupling.

sublattices A and B . Bonds $\langle\langle i, j \rangle\rangle$ connect sites from the same sublattice and are active only along direction $(1,1)$ for the A sublattice and $(1, -1)$ for B ; see the solid lines in Fig. 1(a). NN hopping t is used as the unit of energy.

We employ the self-consistent Born approximation (SCBA) [26] by largely following Refs. [51–53]. Throughout this Letter, we remain in the regime of dominant NN exchange, so stabilizing Néel magnetic order [54]. The spin part (2) of the Hamiltonian becomes

$$\tilde{H}_J = \omega_{\alpha, \mathbf{k}} \alpha_{\mathbf{k}}^\dagger \alpha_{\mathbf{k}} + \omega_{\beta, \mathbf{k}} \beta_{\mathbf{k}}^\dagger \beta_{\mathbf{k}}, \quad (3)$$

where $\alpha_{\mathbf{k}}^\dagger$ ($\alpha_{\mathbf{k}}$) and $\beta_{\mathbf{k}}^\dagger$ ($\beta_{\mathbf{k}}$) create (annihilate) magnons of the two branches, which are expected to survive magnon-magnon interactions [55]. For details as well as the treatment of the kinetic energy (1), see [56].

The primary advantage of SCBA is that it very accurately captures the unavoidable coupling between the hole and the collective excitations from the ordered state—the magnons. NN hole hopping between sublattices always creates or annihilates magnons and thus couples hole motion and magnons, see Fig. 1(a). Only the subdominant next-nearest-neighbor (NNN) hole hopping within a sublattice does not disturb the AM background; see Fig. 1(a). The SCBA captures both of these processes in the self-consistent equations for the self-energy,

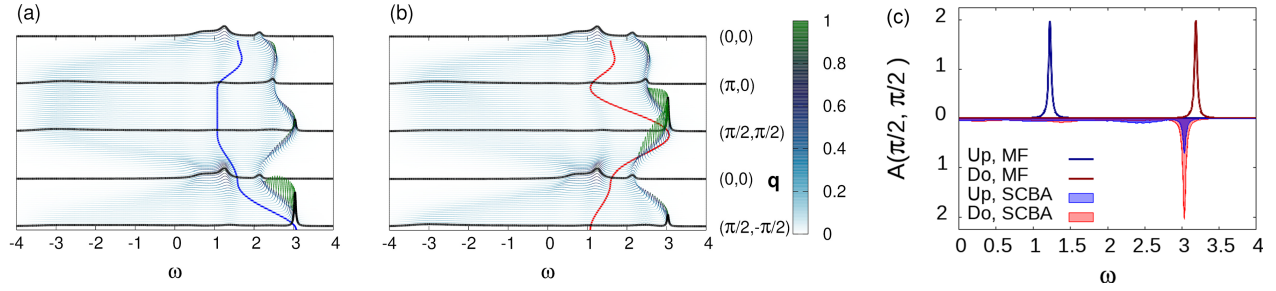


FIG. 2. One-particle spectral density obtained with SCBA for the checkerboard model with $J = 0.4t$, NNN $J' = 0.15t$ and $t' = -0.5t$, and (a) spin-up, (b) spin-down. Momenta are here given in terms of a one-site unit cell; peaks were broadened with a Lorentzian of width $0.02t$ for plotting. For comparison to the usual square-lattice antiferromagnet, momenta $\mathbf{q}$ here correspond to a one-site unit cell. They can be obtained from momenta $\mathbf{k}$ of the two-site unit cell as $q_{x/y} = (k_a \pm k_b)/2$. The lines in the floor correspond to the mean-field (MF) bands for a Hubbard model with $t = 1$, $t' = -0.5t$, and $U = 10t$. Panel (c) shows the spectral density for spin up (blue) and down (red) at momentum $\mathbf{q} = (\pi/2, \pi/2)$ and compares the MF approximation (plotted upward) to the SCBA (plotted downward).

$$\Sigma^\alpha(\mathbf{k}, \omega) = \frac{z^2 t^2}{N_u} \sum_{\mathbf{k}'} M_{\mathbf{k}, \mathbf{k}'}^2 G^{\bar{\alpha}}(\mathbf{k} - \mathbf{k}', \omega - \omega_{\bar{\alpha}, \mathbf{k}'}), \quad (4)$$

for sublattice $\alpha = A, B$. As NN hopping changes the sublattice, the Green's function $G^{\bar{\alpha}}$ entering the sum is the one of the opposite sublattice $\bar{\alpha} = B, A$ and the energy difference $\omega_{\bar{\alpha}, \mathbf{k}'}$ is the energy of the emitted and reabsorbed $\alpha(\beta)$ magnon for $\Sigma^B(\Sigma^A)$. The vertex $M_{\mathbf{k}, \mathbf{k}'}$ is given in Supplemental Material [56], $z = 4$ is the coordination number, and N_u the number of unit cells. The Green's function is obtained from the self-energy via the Dyson equation,

$$[G^\alpha(\mathbf{k}, \omega)]^{-1} = \omega - \epsilon^\alpha(\mathbf{k}) - \Sigma^\alpha(\mathbf{k}, \omega) + i\delta, \quad (5)$$

with the free dispersion $\epsilon^\alpha(\mathbf{k}) = 2t' \cos k_\alpha$ coming from NNN hopping. Higher-order processes are here effectively included, as long as they do not contain crossing magnon lines. For square-lattice AF states, the lowest crossing terms vanish, and the impact of the noncrossing approximation has been found to be negligible [57]. Finally, we again include quantum fluctuations when going from the sublattice-dependent Green's function G^α to the spin-dependent $G^{\sigma=\uparrow, \downarrow}$ [56].

Figure 2 shows the resulting one-particle spectrum for $J' = 0.15t$ and $t' = -0.5t$ and compares it to mean-field (MF) bands. In both approaches—and especially around momenta $[(\pi/2), \pm(\pi/2)]$ —spectra clearly depend on spin both in MF and SCBA, while they would coincide in a standard AF due to symmetry. However, as shown in detail in (c), the spin dependence manifests itself very differently: while MF theory predicts a second peak of opposite spin and at significantly different energy, this peak is largely lost within the incoherent part of the spectrum in the SCBA. Instead, we find at strong coupling a single coherent QP with spin-dependent spectral weight rather than spin-split bands.

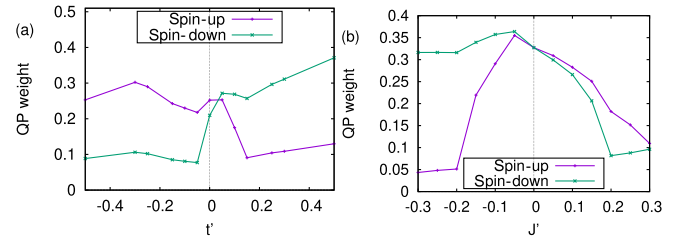


FIG. 3. QP weights [56] at momentum $[(\pi/2), (\pi/2)]$ for (a) $J' = 0.15t$ and variable t' and (b) $t' = 0$ and variable J' .

Very close to the AF limit, i.e., for small $|t'| \ll t$, a second QP with the opposite dominant spin is seen at very slightly different energy; see Supplemental Material [56]. However, as soon as larger $|t'|$ increases this energy splitting, the second QP reaches the continuum states, broadens, and thus loses its QP character. The associated QP weight then drops sharply [see Fig. 3(a)], and total QP weight becomes spin-polarized. J' has a weaker effect on the bands than t' , so that two QPs of opposite spin can be found up to quite substantial values of $|J'| \lesssim 0.2t = 2J/3$; see Fig. 3(b). However, their energy difference remains small throughout [56].

The transition-metal ions of the inverse Lieb lattice (ILL), which hosts a number of altermagnets [23,50], form a generalization of the checkerboard lattice, where additional couplings t'_b and J'_b are introduced along the dotted diagonals of Fig. 1(a). In the Mott insulator $\text{La}_2\text{O}_3\text{Mn}_2\text{Se}_2$, for instance, the two exchange couplings $J'_b \approx J'$ between NNN Mn ions happen to be rather similar, but band structure clearly indicates quite different NNN hoppings $t'_b \neq t'$ [20,21]. Hoppings $t'_b \ll t' \approx (t/2)$ for the Mn xy orbital, given in Fig. 4(a), show a single QP with spectral-weight transfer, as above in Fig. 2. As a second case, we look at the Mn $3z^2 - r^2$ orbital, which has small NN hopping t , so that $t' \approx t$ and $t'_b \approx 3t$. Sublattice-conserving hoppings thus dominate: the hole decouples from the spin

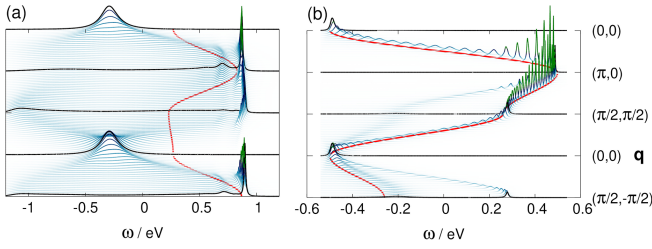


FIG. 4. One-particle spectral density obtained with SCBA for spin-down on the generalized checkerboard (representing transition-metal ions on the ILL) with $J = 10$ meV, $J' = 2.5$ meV $\approx J'_b = 3$ meV, and $|S| = \frac{5}{2}$. In (a), NN hopping $t = 300$ meV, $t' = 150$ meV $= (t/2)$, and $t'_b = 10$ meV describe an xy orbital. (b) is for the $3z^2 - r^2$ orbital with $t = t' = 60$ meV and $t'_b = 180$ meV $= 3t$ [21]. Lines on the floor correspond to the large- U limit of MF, where the hole only hops on the spin-down sublattice.

background and the two spin-split bands survive to a significant extent; see Fig. 4(b). Note, however, that t_{2g} and e_g bands are expected to hybridize and overlap in $\text{La}_2\text{O}_3\text{Mn}_2\text{Se}_2$, so that measured spectra would show a mixed character.

We have complemented the SCBA study with the variational cluster approximation (VCA) [58–61] applied to the checkerboard Hubbard model. The J and J' terms of (2) are here replaced by an on-site Hubbard repulsion $U \sum_i n_{i,\uparrow} n_{i,\downarrow}$. We choose $U = 10t$, which gives an effective NN superexchange $J = (4t^2/U) = 0.4t$ as before, and puts us solidly in the Mott insulating regime at half filling. Further setting $t' = \pm 0.2t$ and $\pm 0.5t$, we then verified [56], that the magnetically ordered state has a QP with momentum-dependent spin polarization analogous to the SCBA spectra discussed in Fig. 2 above.

Altermagnetic polaron spectral function in LaVO_3 —To establish a platform where the altermagnetic polaron can be experimentally identified and investigated, we propose layers or surfaces of LaVO_3 . Bulk LaVO_3 has a G -type orbital and a C -type spin order, which yields an AM state for single planes. We apply the VCA to a two-dimensional three-orbital t_{2g} model with kinetic energy,

$$H_{t_{2g}} = -t \sum_{\langle i,j \rangle, \sigma} c_{i,xy,\sigma}^\dagger c_{j,xy,\sigma} + \Delta \sum_{i,\sigma} n_{j,xy,\sigma} \quad (6)$$

$$-t \sum_{\langle i,j \rangle \| a, \sigma} c_{i,xz,\sigma}^\dagger c_{j,xz,\sigma} - t \sum_{\langle i,j \rangle \| b, \sigma} c_{i,yz,\sigma}^\dagger c_{j,yz,\sigma}, \quad (7)$$

on the square lattice, where $c_{i,\alpha,\sigma}^\dagger$ refers to an electron with spin σ in orbital α on site i . The dominant energy scale is here on-site interaction U together with Hund’s-rule coupling [56], so that a filling of two electrons corresponds to a Mott insulator with large spin one. Crystal field splitting $\Delta < 0$ ensures that one electron is found in the xy orbital, and this half-filled xy orbital strongly promotes AF

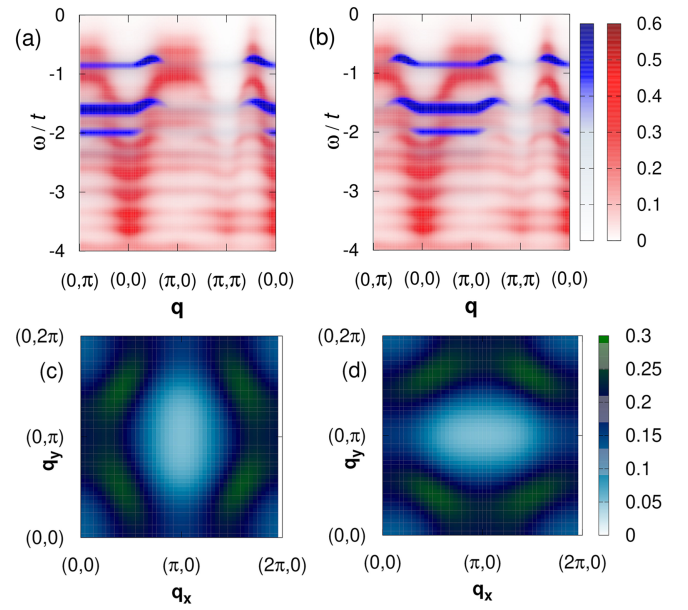


FIG. 5. Occupied states obtained with VCA for the three-orbital t_{2g} model with $t = 1$, $U = 14t$, $J_H = 2t$, $\Delta = -0.5t$ in the AF and AO state illustrated in Fig. 1(b). (a) gives the energy- and momentum-dependent spectrum for spin-up and (b) for spin-down. Weight in red comes from the xy orbital, while the combined xz and yz weight is shown in blue. (c) and (d) show the weight of up and down states, respectively, integrated over the energy range $-1.2t < \omega < -0.5t$, all orbitals.

magnetic order. The second electron can be in either the xz or the yz state and the VCA here finds the AF and AO order of Fig. 1(b) to be favorable.

The orbital order has a strong Ising-like—rather than Heisenberg-like—character, and the AF and AO state transfers this to the spin degree of freedom as well [53]. The VCA spectra for the AF and AO state are shown in Fig. 5 and show the QP peaks with spin-dependent dispersion, as expected from earlier work [53]. Hole motion is almost completely driven by three-site hopping of the hole [52,62] that acts along the $x(y)$ axis for a hole inserted into the $xz(yz)$ orbital. As spin and orbitals are locked together by the AO and AF order, a hole inserted into a particular orbital also has a definite spin polarization. The spin-dependent dispersion is then repeated in a few replica bands with increasing excitation energy (“ladder spectrum”), which are due to the polaronic motion in an Ising-like AO and AF state.

In addition to spin-dependent dispersion, however, we also find substantial spin-dependent SW transfer—see spectra at the special AM momenta as well as the integrated SW in Figs. 5(c) and 5(d). Spectra around momenta $\mathbf{q} = (\pi, 0)$ and $(0, \pi)$ are strongly spin-polarized, especially within the combined xz/yz sector. (In the xy orbital, both spins can hop in both directions, which somewhat dilutes polarization.) SW is here not transferred into higher-energy incoherent features; all peaks of the ladder spectrum in

contrast have a similar weight distribution. Instead, the interplay between polaronic and free holon motion moves some weight of opposite spin into the upper Hubbard band.

Conclusions and outlook—We have here extended the discussion of altermagnetic symmetries to the strong-coupling case of a spin polaron formed by holes in altermagnetic Mott insulators. Spin-split QP peaks of both spin species, as would be expected at weak coupling, may be preserved when coupling to spin fluctuations is suppressed. This can happen in the case of an Ising spin background, as discussed here for a t_{2g} model that could be realized in surfaces or layers of orbitally ordered LaVO_3 . Nevertheless, weights of the two QPs are even here found to be quite different, resulting in a modification of the weak-coupling picture and in effective spin-momentum locking of the QP sector. Similarly, when a hole in the $3z^2 - r^2$ orbital of the ILL Mott altermagnet $\text{La}_2\text{O}_3\text{Mn}_2\text{Se}_2$ [20,21] moves mostly on one largely spin-polarized sublattice, two spin-split QPs are expected. If the hole instead couples more strongly to spin fluctuations, as in the checkerboard model or the xy orbital of $\text{La}_2\text{O}_3\text{Mn}_2\text{Se}_2$, the two spin-polarized QPs are replaced by a single QP peak with clear spin-momentum locking, while the spectral weight of opposite spin is incoherent and broad.

The effect of altermagnetic band splitting on superconductivity has already become an extensive area of research. For instance, the band splitting can give Cooper pairs a finite momentum even without a magnetic field [63,64]. One may think of a superconducting diode effect [65], and the Lieb lattice formed by Cu and O ions in cuprate superconductors can form an AM [66]. In this context our findings raise the question of what happens when stronger correlations not only shift the band energies but also render bands of one spin species incoherent. Indeed, QP coherence has recently been found to have a significant impact on superconducting instabilities [67,68].

This point immediately relates to a long-standing debate in the field of high-temperature superconductors on pairing mediated by correlations [69]. The spin polaron suppresses spin order in the vicinity of the mobile charge, which self-consistently traps the charge [70]. This so-called spin bag does not carry a spin in antiferromagnets, but from our results it is clear that in altermagnets it does and it will be interesting to establish how this affects the pairing mediated by a shared bag. Very recently, numerical studies of the square-lattice Hubbard model have addressed the relative importance of pairing mechanisms due to spin fluctuations vs others based more directly on short-range interactions [71–73]. The difference between AM and AF when it comes to polaron spin and spin-momentum locking suggest that numerical investigations of superconductivity in strongly correlated altermagnets, beyond MF [23,74,75], may here contribute further insights, as might experimental realizations based on strongly correlated building blocks [76].

Note added—We recently became aware of work by L. Lanzini *et al.* discussing related issues [77]. Two more preprints on lifetime and spectral-weight aspects of Mott altermagnets have appeared since [78,79].

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Data availability—The data that support the findings of this article are not publicly available upon publication because it is not technically feasible and/or the cost of preparing, depositing, and hosting the data would be prohibitive within the terms of this research project. The data are available from the authors upon reasonable request.

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