

# The dynamics of a doped hole in a cuprate is not controlled by spin fluctuations

Hadi Ebrahimnejad<sup>1</sup>, George A. Sawatzky<sup>1,2</sup> and Mona Berciu<sup>1,2\*</sup>

**Understanding what controls the dynamics of the quasiparticle that results when a hole is doped into an antiferromagnetically ordered CuO<sub>2</sub> layer is the first necessary step in the quest for a theory of the high-temperature superconductivity in cuprates. Here we show that the long-held belief that the quantum spin fluctuations of the antiferromagnetic background play a key role in determining this dynamics is wrong. Indeed, we demonstrate that the correct, experimentally observed quasiparticle dispersion is generically obtained for a three-band model describing the hole moving on the oxygen sublattice and coupled to a Néel lattice of spins without spin fluctuations. We argue that results from one-band model studies actually support this conclusion, and that this significant conceptual change in our understanding of this phenomenology opens the way to studying few-hole dynamics, to accurately gauge the strength of the ‘magnetic glue’ and its contribution to superconductivity.**

Twenty-seven years after the discovery of high-temperature superconductivity<sup>1</sup>, consensus on its theoretical explanation is still absent. To a good extent, this is due to the difficulty of studying strongly correlated systems near half-filling, needed to understand the behaviour of one or a few holes doped into a CuO<sub>2</sub> layer. To simplify this task it is customary to replace three-band models<sup>2</sup> describing the doping holes as entering the O *2p* orbitals of these charge-transfer insulators<sup>3</sup> with much simpler one-band Hubbard or *tJ* models<sup>4,5</sup>.

The simplification from three-band to one-band models is based on the idea that the quasiparticle resulting when one hole is doped in the system has predominantly Zhang–Rice singlet (ZRS) character<sup>6,7</sup>. Agreement between the quasiparticle dispersion for a generalized *tJ* model (with longer-range hopping) and that measured by angle-resolved photoemission spectroscopy (ARPES) in parent compounds<sup>8–13</sup> is taken as evidence that one-band models are valid. Whether this is a good approximation in all of the Brillouin zone and also for finite doping, or whether it is valid only near the ( $\pi/2$ ,  $\pi/2$ ) minimum, is still debated<sup>14</sup>. In one-band models, moreover, spin and charge fluctuations arise from the same particle–hole excitations, making it difficult to envisage a separation between the quasiparticles and the pairing glue. Such a separation, however, is assumed in most theories describing spin-fluctuation-mediated pairing<sup>4</sup>. Even more problematic are recent arguments that such a strong attractive interaction mediated by spin fluctuations is actually ignored by one-band models<sup>15</sup>. In other words, even if these one-band models capture the quasiparticle dispersion accurately, they may still fail to properly describe their effective interactions.

To fully answer these questions, one needs to be able to compare predictions of the three-band and one-band models not just in the single-hole sector, where a single quasiparticle forms and its dispersion can be calculated, but also in the two-hole sector, where the effective interactions between quasiparticles can be studied. Carrying out two-hole calculations by exact numerical means is still too difficult a task: quantum Monte Carlo algorithms suffer from sign problems, and at present exact diagonalization can be carried out only on rather small clusters, where the finite-size

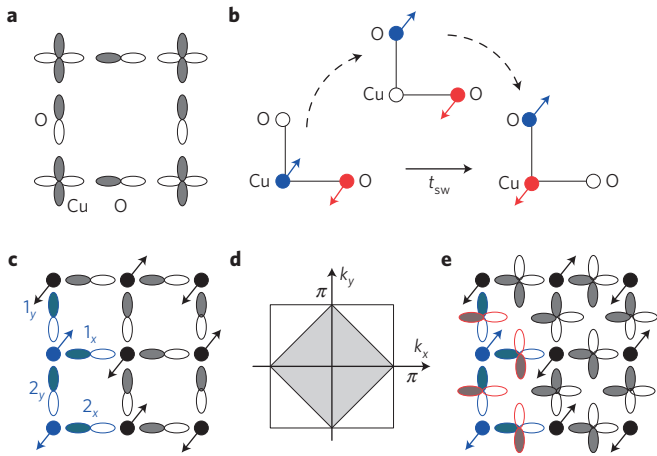
effects are still considerable and render the interpretation of the results difficult<sup>16</sup>.

We show that a simple variational approximation for a three-band model on an infinite lattice captures all main known aspects of the quasiparticle behaviour not just qualitatively, but also quantitatively. This approximation can also be systematically improved by increasing the variational space; this provides an estimate for the relevance of the excluded states. Most importantly, this method can be straightforwardly generalized to calculate few-hole propagators<sup>15,17</sup>.

Here we present the one-hole solution, which already reveals several major surprises. First, we find that the spin fluctuations of the antiferromagnetic (AFM) background play a negligible role in determining the quasiparticle dispersion, because the hole moves on a different sublattice. In contrast, in one-band models it is widely believed that the dynamics of a ZRS is controlled by these fluctuations, because not only does the ZRS move in the magnetic sublattice but it is also a coherent mix of spin and charge degrees of freedom. We argue that this view is wrong, and that the necessary inclusion of longer-range hopping in one-band models has precisely the effect of minimizing the role of the spin fluctuations. Second, the quasiparticle's dispersion in our model has the characteristic shape measured experimentally for any reasonable choice of parameters, unlike in one-band models where addition of longer-range hoppings is necessary to obtain the correct dispersion, as mentioned above. Third, our method allows us to study five-band models to understand the importance of the in-plane O *2p* orbitals that do not hybridize directly with Cu  $3d_{x^2-y^2}$ . As expected, we find that the quasiparticle dispersion is little affected; however, the ARPES spectral weight is significantly changed and now exhibits a strong suppression outside the magnetic Brillouin zone (MBZ) in agreement with ARPES findings<sup>8,11</sup>. This suggests that even three-band models do not fully capture all of the quasiparticle properties<sup>18</sup>.

The model we study can be thought of as the *tJ* analogue of the three-band Emery model<sup>2</sup>: double occupancy on the Cu sites is forbidden because of the large on-site Hubbard repulsion, so there is a spin-1/2 at each Cu site and the doping hole enters the O *2p* ligand

<sup>1</sup>Department of Physics and Astronomy, University of British Columbia, Vancouver, British Columbia V6T 1Z1, Canada. <sup>2</sup>Quantum Matter Institute, University of British Columbia, Vancouver, British Columbia V6T 1Z4, Canada. \*e-mail: [berciu@phas.ubc.ca](mailto:berciu@phas.ubc.ca)



orbitals (see Fig. 1a). The resulting Hamiltonian is<sup>14,19,20</sup>:

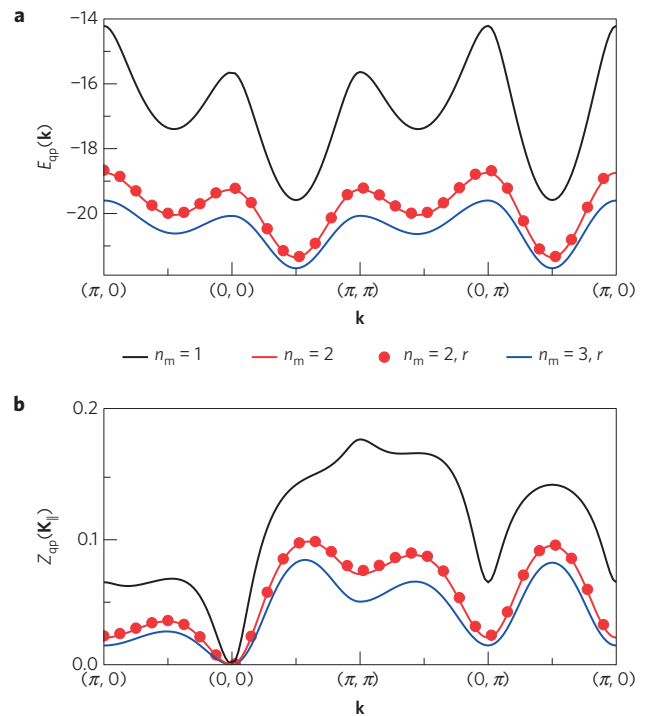
$$\mathcal{H} = T_{pp} + T_{\text{swap}} + H_{J_{pd}} + H_{J_{dd}}$$

$T_{pp}$  describes first- and second-nearest-neighbour hopping of the hole;  $T_{\text{swap}}$  describes effective hopping of the hole mediated by the Cu spin, whereby first the Cu hole hops onto a neighbouring O followed then by the original hole filling the Cu orbital (see Fig. 1b). Note that this leads to a swap of the spins of the hole and the Cu;  $H_{J_{pd}}$  describes the AFM exchange between the spins of the hole and of its two neighbouring Cu; and  $H_{J_{dd}}$  describes the nearest-neighbour AFM superexchange between Cu spins except on the bond occupied by the hole. If  $J_{dd} = 1$  is the energy unit, then  $t_{pp} = 4.13$ ,  $t'_{pp} = 2.40$ ,  $t_{sw} = 2.98$  and  $J_{pd} = 2.83$ , respectively. We set the lattice constant  $a = 1$ . See ref. 14 for further details on the Hamiltonian, and on its exact diagonalization solution for a hole on a  $32\text{ Cu} + 64\text{ O}$  cluster.

To study this Hamiltonian on an infinite lattice, we make the key simplification of reducing  $H_{J_{dd}}$  to an Ising form, instead of its full Heisenberg form. As a result, the undoped ground state  $|\text{AFM}\rangle$  is a simple Néel state without any spin fluctuations. This approach will be justified a posteriori on the basis of the results it leads to.

We define Green's functions and generate their exact equations of motion as described in the Methods. We note that each time a new magnon is created in a configuration, its energy is increased by (about)  $2J_{dd}$  because up to four Cu–Cu bonds become ferromagnetic. Many-magnon states are thus energetically expensive and unlikely to be significant components of the lowest-energy eigenstates. We therefore define a variational approximation by choosing an integer  $n_m$  and setting all propagators with more than  $n_m$  magnons to zero. This leads to a manageable (although still infinite) sparse system of equations that can be solved efficiently.

As exact diagonalization results show a distortion of the AFM background only rather close to the hole (Fig. 3 of ref. 14) it is reasonable to expect that small  $n_m$  may already give a good approximation. To check this, we calculate the results for  $n_m \leq 3$ . For  $n_m = 2$  we do both the full variational calculation that allows the magnons to be at any distance from one another, and the restricted calculation where only configurations with the two magnons on adjacent sites are kept (the hole can be located anywhere). In the



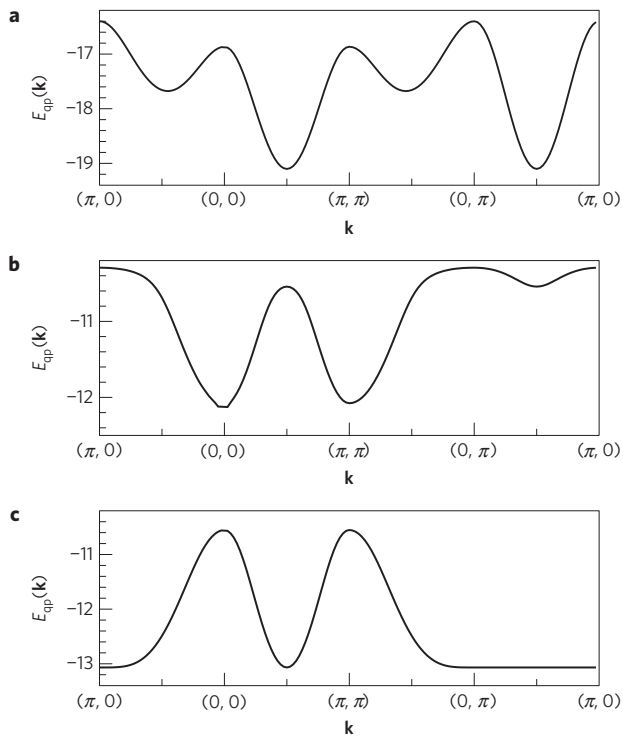
**Figure 2 | Results for the three-band model.** **a**, Quasiparticle energy (in units of  $J_{dd}$ ) along various cuts in the Brillouin zone. The results are for the three-band model using  $n_m = 1$  (black line),  $n_m = 2$  (red line), restricted  $n_m = 2$  (red circles) and restricted  $n_m = 3$  (blue line) approximations. **b**, The corresponding ARPES quasiparticle spectral weights.

$n_m = 3$  case we perform only the restricted calculation where the magnons are in a connected cluster. The corresponding dispersions of the low-energy quasiparticle are shown in Fig. 2a along several cuts in the full Brillouin zone (FBZ).

The most striking observation is that the dispersions have a shape like that measured experimentally, with deep isotropic minima at  $(\pi/2, \pi/2)$ . This shows that even the very simple  $n_m = 1$  solution already captures important aspects of the correct quasiparticle dynamics.

As expected for bigger variational spaces, the dispersions for larger  $n_m$  lie at lower energies. The bandwidths for  $n_m = 2, 3$  are about half of that for  $n_m = 1$ , owing to standard polaronic physics. Consider  $n_m = 2$ : it is energetically favourable for the hole to be near the second emitted magnon, as they have antiparallel spins, but configurations with the hole near the first magnon are not favourable because of their parallel spins. If the first magnon is bound in the cloud it must be adjacent to the second magnon, to limit the number of broken AFM bonds. Alternatively, this magnon can dissociate from the cloud resulting in excited states starting from  $E_{1,gs} + 2J_{dd}$ ; that is, the ground-state energy of the  $n_m = 1$  quasiparticle plus the  $2J_{dd}$  cost for a magnon located far from it. For our parameters, this continuum starts at  $\approx -17.58J_{dd}$  so the  $n_m = 2$  quasiparticle band must become narrower to fit below it. The comparison between the full and the restricted  $n_m = 2$  cases confirms that the connected magnon clusters (which cost less exchange energy) account for the overwhelming contribution to the low-energy quasiparticle, as expected.

The  $n_m = 3, r$  results show an additional narrowing of the bandwidth from  $2.6J_{dd}$  for  $n_m = 2$ , to  $2.05J_{dd}$ . This solution is thus very close to the  $2J_{dd}$  bandwidth of the fully converged case. This is not surprising because the quasiparticle cannot possibly bind too many magnons in its cloud, given that each magnon is at a different location and that the hole can interact with at most one favourable magnon (with antiparallel spin) in any configuration.

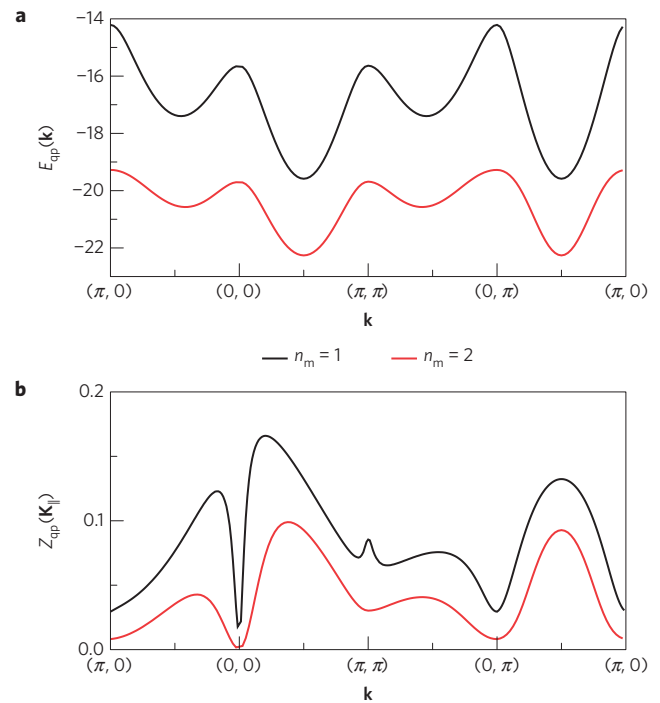


**Figure 3 | Role of various parameters. a–c.** Quasiparticle dispersion for the three-band model and  $n_m = 2$ , when we set  $J_{pd} = 0$  (**a**), or  $t_{sw} = 0$  (**b**) or  $t_{pp} = 0$  (**c**). In each case, the other parameters are kept at their stated values.

We conclude that the  $n_m = 3, r$  solution is already quantitatively accurate, and indeed its dispersion is in excellent agreement with the exact diagonalization dispersion of ref. 14.

This quantitative agreement between the variational and exact diagonalization results shows that quantum spin fluctuations of the AFM background (fully included in exact diagonalization but frozen in our variational approach) have little or no effect on the quasiparticle’s dynamics. This is because in three-band models the hole can move freely on the O sublattice, so it can easily absorb magnons created previously and then emit others at new locations to move the cloud, resulting in fast quasiparticle dynamics. Spin fluctuations of the background, which act on a slower timescale ( $J_{dd}$  is the smallest energy), are then not essential for this dynamics. Indeed, we have attempted to gauge the effect of spin fluctuations for  $n_m = 2$  by adding in the equations of motion terms that directly link two-magnon and zero-magnon propagators, mimicking spin fluctuations that either produce or remove a pair of nearest-neighbour magnons close to the hole. Such terms lead to very minor quantitative changes, as will be reported elsewhere.

This conclusion may seem surprising because for one-band models it is believed that spin fluctuations are essential in determining the quasiparticle dispersion: as a ZRS moves it creates a string of wrongly oriented spins (magnons) whose energy increases linearly with its length, and which ‘ties’ it near the starting position. In the absence of spin fluctuations, the quasiparticle acquires a finite mass only by executing Trugman loops<sup>21</sup>, which are many-step (and thus very slow) processes that lead to a very heavy quasiparticle<sup>22</sup>. Spin fluctuations act faster to remove pairs of nearest-neighbour magnons from the string and thus release the ZRS. These arguments, however, depend essentially on the assumption that only nearest-neighbour hopping of the ZRS is possible, despite the knowledge that the resulting dispersion is wrong, being nearly flat along  $(0, \pi) - (\pi, 0)$ . To obtain agreement with experiments, second- and third-nearest-neighbour hopping must be added<sup>8,10</sup>. These allow



**Figure 4 | Results for the five-band model. a,b.** Quasiparticle energy (**a**) and ARPES quasiparticle spectral weight (**b**) for variational solutions with one and two magnons.

the ZRS to move freely on its magnetic sublattice and get away from the string of defects that nearest-neighbour hopping creates, similar to what happens in three-band models. The longer-range hopping thus changes the phenomenology qualitatively and in its presence, we find that spin fluctuations are no longer essential for the quasiparticle dynamics in one-band models either, unlike when only nearest-neighbour hopping is allowed.

A natural follow-up question is whether careful tuning of the parameters is needed to achieve this dispersion, or whether this shape is generic. The answer is the latter. Specifically,  $\mathcal{H}_{J_{pd}}$  has almost no effect on the shape of  $E_{qp}(\mathbf{k})$ : even setting  $J_{pd} = 0$  leaves it virtually unchanged, only shifting the overall value as exchange energy is lost (see Fig. 3a). Setting either  $t_{sw} = 0$  or  $t_{pp} = 0$  leads to very different dispersions (Fig. 3b,c); however, if  $t_{pp}$  and  $t_{sw}$  are comparable, the correct shape appears. In fact, a deep minimum at  $(\pi/2, \pi/2)$  is then achieved even for  $n_m = 0$  (not shown). This confirms the speculation in ref. 14 that  $E_{qp}(\mathbf{k})$  arises through constructive interference between  $T_{pp}$  and  $T_{sw}$ , and shows that both terms are needed to properly describe the quasiparticle dynamics. Note that many studies of three-band models ignore  $T_{pp}$  or treat it as a perturbation<sup>23–25</sup> (for further discussion, see the supplementary material of ref. 14).

Having established that the shape of  $E_{qp}(\mathbf{k})$  is robust, we now analyse the quasiparticle ARPES weight, calculated as described in the Methods. In Fig. 2b we plot  $Z_{qp}(\mathbf{K}_{\parallel})$  along various cuts in the FBZ. The first observation is that unlike  $E_{qp}(\mathbf{k})$ ,  $Z_{qp}(\mathbf{K}_{\parallel})$  does not have MBZ periodicity: the evolution along  $(0, 0) - (\pi, \pi)$  is not symmetric about  $(\pi/2, \pi/2)$ . This is expected: all of the propagators must, and indeed do, exhibit MBZ periodicity; however, the ARPES spectral weight does not because the interference between contributions from like orbitals switches from constructive (inside the MBZ) to destructive (in the remaining part of the FBZ).

It is worth pointing out that a similar approach (Néel order plus a few magnons) for one-band models does not lead to any asymmetry. This is because even though there are two sublattice Bloch states with the ZRS located on either magnetic sublattice, there is no

interference between them as they belong to sectors with different total spin  $S_z$ . Additional Hubbard and spin-fluctuation corrections must be included to obtain an asymmetric spectral weight (see, for example, ref. 26).

The second observation is that  $Z_{\text{qp}}(\mathbf{K}_{\parallel})$  disagrees along the  $(0, 0) - (\pi, \pi)$  cut with the experimental measurements that find large weight near  $(\pi/2, \pi/2)$  that decreases fast on both sides<sup>8,11</sup>. (Note that exact diagonalization predicts  $Z_{\text{qp}}(\pi, \pi) = 0$  because its quasiparticle has spin  $3/2$  in that region. Such an object cannot be fully described with a Néel background that breaks invariance to spin rotations.) As the situation improves with increasing  $n_m$ , it is possible that going to higher  $n_m$  may fix this problem. However, such an explanation is rather unsatisfactory because it suggests a sensitive dependence of the ARPES weight on the precise structure of the magnon cloud, unlike the robust insensitivity of the dispersion.

To check for an alternative explanation, we add the second set of in-plane O  $2p$  orbitals to our model, resulting in the new unit cell sketched in Fig. 1e. These orbitals are usually ignored because they do not hybridize directly with the Cu  $3d_{x^2-y^2}$  orbitals. However, they do hybridize heavily with the ligand  $2p$  orbitals occupied by the hole, so their role should be evaluated more carefully and this can be done easily with our method.

For the Hamiltonian, this requires us to expand  $T_{\text{pp}}$  accordingly. This is achieved without introducing new parameters because nearest-neighbour hopping between two new orbitals also has magnitude  $t_{\text{pp}}$ , and between new and old orbitals  $\tilde{t}_{\text{pp}}/t_{\text{pp}} = (t_{\text{pp},\sigma} - t_{\text{pp},\pi})/(t_{\text{pp},\sigma} + t_{\text{pp},\pi}) = 0.6$  because  $t_{\text{pp},\pi} = t_{\text{pp},\sigma}/4$ . We can also add next-nearest-neighbour hopping  $t'_{\text{pp}}$  for the new orbitals. As  $t_{\text{pp},\sigma}$  scales with distance as  $1/d^4$ , it follows that  $\tilde{t}'_{\text{pp}} = t'_{\text{pp},\sigma}/4 = 0.2t_{\text{pp}}$  (ref. 27). This is smaller than  $t'_{\text{pp}} \approx 0.6t_{\text{pp}}$  for the old orbitals for which next-nearest-neighbour hopping is boosted through hybridization with the  $4s$  orbital of the bridging Cu. In any event, we find very little sensitivity to the precise values we use for  $\tilde{t}'_{\text{pp}}$ .

We study the five-band model with the same variational approximations, suitably generalized. Figure 4 shows the quasiparticle dispersion and ARPES spectral weight for the  $n_m = 1, 2$  solutions. For  $E_{\text{qp}}(\mathbf{k})$ , the results are very similar to those shown in Fig. 2a, but the bands are slightly wider, as expected because of the increased bare kinetic energy. We have checked that the dependence on  $J_{\text{pd}}$ ,  $t_{\text{sw}}$  and  $t_{\text{pp}}$  is essentially unchanged. Indeed, the expectation that this other set of orbitals has little effect on the quasiparticle dispersion is correct.

However, their addition has a significant effect on the evolution of  $Z_{\text{qp}}(\mathbf{K}_{\parallel})$  on the  $(0, 0) - (\pi, \pi)$  cut. The asymmetry is maintained but the results now show a decrease of the ARPES spectral weight on both sides of the MBZ boundary, in agreement with experimental data<sup>8,11</sup>.

The fact that the weight is significantly changed even though the dispersion is not much affected should not be a surprise. As ARPES measures interference between like  $2p$  orbitals, the quasiparticle weight can be significantly affected even by rather small redistributions of the wavefunction among orbitals, unlike the energy. These results suggest that a full understanding of the evolution of the spectral weight at low dopings, still missing at present, may require inclusion into theoretical models of these additional orbitals. This will only increase the need for accurate approximations such as the one we propose here, because exact numerical approaches become even more challenging to implement in larger Hilbert spaces.

To summarize, we used a simple variational approach to study a quasiparticle in three- and five-band models of an infinite  $\text{CuO}_2$  layer, while also being able to gauge accuracy by increasing the variational space. Our results compare well with available results from exact diagonalization of small clusters. As the variational approach ignores the effect of spin fluctuations in the AFM layer,

the good agreement for the dispersion strongly supports the idea that these spin fluctuations do not play the important role in the quasiparticle dynamics attributed to them on the basis of results for one-band models with only nearest-neighbour hopping.

This is a very important finding because properly describing the background spin fluctuations is very difficult and a major barrier to studying the two-hole sector to understand the effective interactions between quasiparticles, which is the second piece of knowledge (besides the quasiparticle dispersion) needed to propose accurate simple(r) effective models. Our method allows us to distinguish the magnons emitted and absorbed by holes, which are treated exactly, from those due to background fluctuations, which are ignored. As the method also generalizes to treat few-hole states, we are now able to investigate the role of magnon exchange in mediating strong attractions between holes, and to verify whether this attraction is indeed absent from the one-band effective models used at present, as speculated in ref. 15. This work is now in progress.

## Methods

For the three-band model, the unit cell of the Néel AFM has two Cu spins and thus four distinct O sites; this and the corresponding MBZ are shown in Fig. 1c,d. Thus, there are four inequivalent hole Bloch states  $p_{\mathbf{k}\alpha,\sigma}^{\dagger} = 1/\sqrt{N} \sum_{i \in A_{\alpha}} e^{i\mathbf{k}\cdot\mathbf{R}_{i,\alpha}} p_{i,\alpha,\sigma}^{\dagger}$ , where  $N \rightarrow \infty$  is the number of unit cells,  $\alpha \in \{1_x, 1_y, 2_x, 2_y\}$  labels the type of O orbital,  $A_{\alpha}$  is the sublattice of all O of type  $\alpha$ ,  $\mathbf{R}_{i,\alpha}$  is the location of the  $\alpha$  O of unit cell  $i$ ,  $\mathbf{k}$  is a quasimomentum inside the MBZ and  $p_{i,\alpha,\sigma}^{\dagger}$  creates a spin- $\sigma$  hole at  $O_{i,\alpha}$ . In the following we set  $\sigma = \uparrow$  (the  $\sigma = \downarrow$  case is treated similarly and gives identical results) and define the single-hole propagators  $G_{\beta\alpha}(\mathbf{k}, \omega) = \langle \text{AFM} | p_{\mathbf{k}\beta,\uparrow} \hat{G}(\omega) p_{\mathbf{k}\alpha,\uparrow}^{\dagger} | \text{AFM} \rangle$ , where  $\hat{G}(\omega) = [\omega + i\eta - \mathcal{H}]^{-1}$ ,  $\hbar = 1$  and  $\eta > 0$  is a small broadening. The energy  $\omega$  is measured from the undoped ground state; that is, we set  $\mathcal{H}_{\text{dd}} | \text{AFM} \rangle = 0$ . The one-hole spectrum  $E_n(\mathbf{k})$  is given by the poles of these propagators, and from the residues one can find the overlaps  $\langle n, \mathbf{k}, \uparrow | p_{\mathbf{k}\alpha,\uparrow}^{\dagger} | \text{AFM} \rangle$ , where  $\mathcal{H} | n, \mathbf{k}, \uparrow \rangle = E_n(\mathbf{k}) | n, \mathbf{k}, \uparrow \rangle$  are the one-hole eigenstates for band  $n$ .

The equations of motion are generated using the identity  $\hat{G}(\omega)(\omega + i\eta - \mathcal{H}) = 1$  to find  $(\omega + i\eta)G_{\beta\alpha}(\mathbf{k}, \omega) = \delta_{\alpha,\beta} + \langle \text{AFM} | p_{\mathbf{k}\beta,\uparrow} \hat{G}(\omega) \mathcal{H} p_{\mathbf{k}\alpha,\uparrow}^{\dagger} | \text{AFM} \rangle$ . The Hamiltonian has: terms that do not change either the hole location or its spin ( $\mathcal{H}_{\text{dd}}$  and the diagonal part of  $\mathcal{H}_{\text{pd}}$ ) and lead to a simple energy shift; terms that change the hole location but not its spin ( $T_{\text{pp}}$  and terms in  $T_{\text{swap}}$  that move the hole past the Cu with the same spin orientation) and link  $G_{\beta\alpha}$  to other  $G_{\beta\alpha'}$ ; and terms that flip the hole's spin, while also flipping a neighbouring Cu spin (terms in  $T_{\text{swap}}$  that move the hole past the Cu with antiparallel spin, and the off-diagonal part of  $\mathcal{H}_{\text{pd}}$ ). These last terms define generalized propagators that we call one-magnon propagators because they are projected on states that have a magnon (flipped Cu spin) beside the hole. Equations of motion for the one-magnon propagators are obtained similarly, and link them to other one-magnon propagators with a different hole-magnon distance, to two-magnon propagators, because the hole can flip a second Cu spin, and—if the hole and magnon are on neighbouring sites—back to various  $G_{\beta\alpha}$ . The equations for two-magnon propagators link them to other two- and three-, and possibly also to one-magnon propagators, and so on and so forth. Although the full set of exact equations of motion can be thus generated, they are impossible to solve exactly. As described in the main text, we use a variational principle to simplify this system by removing all propagators with more than  $n_m$  magnons. The resulting system remains infinite but can be solved efficiently as described, for instance, in ref. 17.

If  $\mathbf{K} = (\mathbf{K}_{\parallel}, K_z)$  is the photoelectron's momentum and  $\omega$  is the transferred energy, and assuming an unpolarized beam, the ARPES intensity<sup>28</sup> is then obtained as  $A(\mathbf{K}, \omega) \sim \sum_{\mathbf{k}, \mathbf{G}} \delta_{\mathbf{K}_{\parallel} + \mathbf{k}, \mathbf{G}} \sum_{\alpha, \beta} e^{i\mathbf{G}\cdot\mathbf{R}_{\alpha\beta}} \eta_{\alpha\beta} A_{\alpha\beta}(\mathbf{k}, \omega)$ . We checked that this gives the correct unfolding if we decouple the hole from the spins, because then the dispersion in the FBZ can be calculated analytically. Here  $\mathbf{G}$  are the reciprocal lattice vectors of the MBZ and  $\mathbf{k}$  are momenta in the first MBZ. The first sum shows that ARPES detects quasiparticles of quasimomentum  $\mathbf{k}$  equal to the photohole's in-plane momentum  $-\mathbf{K}_{\parallel}$ , modulo  $\mathbf{G}$ .  $\mathbf{R}_{\alpha\beta} = \mathbf{R}_{i,\alpha} - \mathbf{R}_{i,\beta}$  is the distance between the O sites  $\alpha, \beta$  and  $A_{\alpha\beta}(\mathbf{k}, \omega) = -1/\pi \text{Im} G_{\alpha\beta}(\mathbf{k}, \omega)$  are the spectral weights of the sublattice propagators. Finally,  $\eta_{\alpha\beta} = 1$  if the orbitals  $\alpha$  and  $\beta$  are both either  $2p_x$  or  $2p_y$ , and zero otherwise. The quasiparticle ARPES spectral weight,  $Z_{\text{qp}}(\mathbf{K}_{\parallel})$ , is the weight at the energy  $\omega = E_{\text{qp}}(\mathbf{k})$  of the quasiparticle; that is,  $A(\mathbf{K}, \omega \rightarrow E_{\text{qp}}(\mathbf{k})) \rightarrow Z_{\text{qp}}(\mathbf{K}_{\parallel}) \delta(\omega - E_{\text{qp}}(\mathbf{k}))$ .

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### Author contributions

H.E. and M.B. performed the numerical calculations. All authors contributed to the data analysis and the writing of the manuscript.

### Additional information

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### Competing financial interests

The authors declare no competing financial interests.