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Dispersion of orbital excitations in 2D quantum antiferromagnets

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Abstract. We map the problem of the orbital excitation (orbiton) in a 2D antiferromagnetic and ferroorbital ground state onto a problem of a hole in 2D antiferromagnet. The orbiton turns out to be coupled to magnons and can only be mobile on a strongly renormalized scale by dressing with magnetic excitations. We show that this leads to a dispersion relation reflecting the two-site unit cell of the antiferromagnetic background, in contrast to the predictions based on a mean-field approximation and linear orbital-wave theory.

1. Introduction

Calculating collective excitations in nonfrustrated but interacting spin systems may be considered as one of the few extremely successful stories in solving the strongly correlated electron systems. Independently on whether the approach which is used to calculate such excitations stems from the linear spin wave theory (for ordered states) or the Bethe Ansatz solutions (for quantum disordered states in 1D), a remarkable qualitative and quite often also quantitative agreement with a number of experimental results is usually achieved, see e.g. [1].

On the other hand, collective excitations in interacting *orbital* systems have attracted much less attention of the community, primarily due to experimental problems in detecting the collective orbital excitations (orbitons) [2]. *A priori*, excitations in the orbital degree of freedom of Mott insulators should behave in a similar manner as those of the spin sector: in both cases the large Coulomb repulsion in the Mott insulators ‘freezes’ the charge degrees of freedom and largely reduces the effective low energy Hilbert space so that instead of electrons it is given by spin or orbital (pseudospin) degrees of freedom. In place of the ‘spin-wave theory’ for magnetic excitations, one would then use ‘orbital-wave theory’ [3].

It has recently been shown [4], however, that this orbital-wave picture does not hold in many realistic systems. Here, we prove that in a generic 2D Kugel-Khomskii (KK) spin-orbital model [5] with the antiferromagnetic (AF) and ferroorbital (FO) ground state the linear orbital wave theory breaks down and one needs to explicitly take care of the coupling between spins and orbitals. Furthermore, we show that for realistic parameters of the KK Hamiltonian, the dispersion of the coherent excitation changes qualitatively and reflects the two-site unit cell of the antiferromagnetic background, in contrast to expectations based on linear orbital-wave theory.

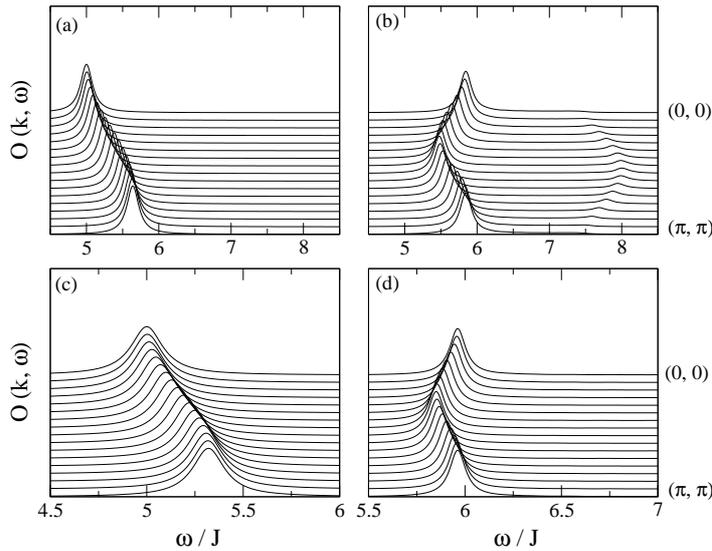


Figure 1. Spectral function for the orbital excitation $O(\mathbf{k}, \omega)$ [Eq. (2)] calculated in the linear orbital wave picture [(a) and (c)] and using the exact mapping onto the effective t - J model [(b) and (d)]. Upper (lower) panels for equivalent (inequivalent) values of the hoppings between the two orbitals, see text. Note the different scales on upper and lower panels and that the incoherent spectrum in panel (d) is extremely small and not visible at this scale. Parameters: $E_z = 5J$ and broadening $\eta = 0.05J$.

2. Model and results

The Hamiltonian of the generic 2D KK model that we want to study describes a two-orbital system with orbital-conserving hopping and reads

$$H = J \sum_{\langle i,j \rangle} \left(\mathbf{S}_i \cdot \mathbf{S}_j + \frac{1}{4} \right) \left(\mathbf{T}_i \cdot \mathbf{T}_j + \frac{1}{4} \right) + E_z \sum_i T_i^z, \quad (1)$$

where \mathbf{S} (\mathbf{T}) are the spin (pseudospin) operators which fulfill the $SU(2)$ algebra and J is the superexchange constant which describes the interaction of $S = 1/2$ spins and $T = 1/2$ (orbital) pseudospins. Besides, E_z is the crystal field which is implicitly assumed to be so large that in the ground state $|\phi\rangle$ of H only one type of orbital is occupied (the FO order of orbitals) and consequently there is long-range AF order in temperature $T = 0$.

The purpose of this study is to calculate the orbital excitations from the ground state $|\phi\rangle$ of Hamiltonian (1), as defined by the spectral function $O(\mathbf{k}, \omega)$:

$$O(\mathbf{k}, \omega) = \frac{1}{\pi} \lim_{\eta \rightarrow 0} \Im \left\langle \phi \left| T_{\mathbf{k}}^- \frac{1}{\omega + E_\phi - H - i\eta} T_{\mathbf{k}}^+ \right| \phi \right\rangle, \quad (2)$$

where E_ϕ is the ground state energy and $T_{\mathbf{k}}^+$ is the momentum-dependent orbital raising operator.

In the ‘standard’ orbital-wave approach [6, 7], this spectral function can be easily calculated (see, e.g., Ref. [4]) by mean-field decoupling of spins and orbitals and by: (i) introducing the Holstein-Primakoff bosons for orbital pseudospins (cf. Ref. [8]) and (ii) neglecting interactions between bosons. We then obtain:

$$O(\mathbf{k}, \omega) = \delta \left[\omega - E_z + \frac{1}{2} z J_{\text{OW}} (1 - \gamma_{\mathbf{k}}) \right], \quad (3)$$

with $z = 4$ is the coordination number in 2D and $\gamma_{\mathbf{k}} = (\cos k_x + \cos k_y)/2$ is the lattice structure factor in 2D. Here $J_{\text{OW}} = 2J \langle \phi | \mathbf{S}_i \cdot \mathbf{S}_j + \frac{1}{4} | \tilde{\phi} \rangle \simeq -0.16J$ where $|\tilde{\phi}\rangle$ is the 2D AF, i.e. spin-only part of ground state $|\phi\rangle$. The spectrum consists of a single quasiparticle peak with a relatively large dispersion, cf. Fig. 1(a) for the spectrum along the high symmetry direction $(0, 0) \rightarrow (\pi, \pi)$ in the Brillouin zone.

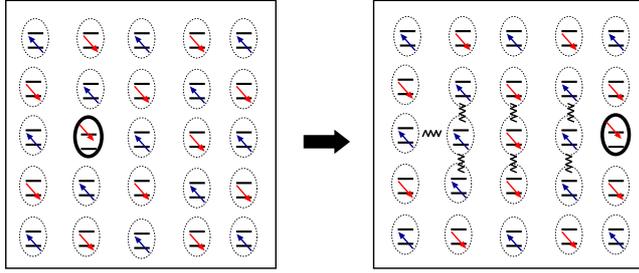


Figure 2. Artist's view of the defects (springs) in the spin background (up and down arrows) created by the moving orbiton (bold oval). Only if these defects are healed by quantum fluctuations the orbiton can move coherently – otherwise, the orbiton is trapped in a string-like potential, see text.

However, it was shown in detail in Ref. [4] that the above mean-field decoupling of spins and orbitals does not lead to a reliable description of orbital dynamics in a coupled spin-orbital system. Therefore, following Ref. [4] and using *inter alia* the Jordan-Wigner transformation [9] for spin and orbital degrees of freedom,¹ we map the above problem of a single orbiton in the AF and FO ground state Eq. (2) onto a a problem of a single hole in the AF ground state

$$O(\mathbf{k}, \omega) = \frac{1}{\pi} \lim_{\eta \rightarrow 0} \Im \left\langle \tilde{\phi} \left| p_{\mathbf{k}\uparrow}^\dagger \frac{1}{\omega + E_{\tilde{\phi}} - \tilde{H} - E_z - i\eta} p_{\mathbf{k}\uparrow} \right| \tilde{\phi} \right\rangle, \quad (4)$$

described by an effective t - J Hamiltonian

$$\tilde{H} = -t \sum_{\langle i,j \rangle, \sigma} (p_{i\sigma}^\dagger p_{j\sigma} + h.c.) + J \sum_{\langle i,j \rangle} \left(\mathbf{S}_i \cdot \mathbf{S}_j + \frac{1}{4} n_i n_j \right). \quad (5)$$

Here the electron operators $p_{i\sigma}$ ($p_{i\sigma}^\dagger$) act in the restricted Hilbert space without double occupancies and create (annihilate) holes in the 2D AF ground state $|\tilde{\phi}\rangle$. Besides, $n_i = \sum_{\sigma} n_{i\sigma}$ and the effective hopping parameter t describing the motion of orbital excitation is given by $t \equiv J/2$.

The spectrum Eq. (4) was calculated using the self-consistent Born approximation on 32×32 sites (which gives results in very good agreement with the exact diagonalization studies, cf. Ref. [10]) and consists of a large quasiparticle peak and a very small incoherent spectrum, cf. Fig. 1(b). The bandwidth W of the coherent orbiton peak, as obtained from Fig. 1(b) or from perturbative calculations cf. Ref. [10], is $W \simeq 2t^2/J \simeq J/2$ (for $t = J/2$) and thus somewhat smaller than the mean-field one for which $W \simeq 0.64J$. In more striking contrast to the mean-field results, the dispersion has a minimum at $(\pi/2, \pi/2)$ instead of $(0, 0)$, as a result of the coupling between orbitons and the AF ‘background’.

In many realistic cases, the spin-orbital model (1) has to be modified to account for the different hoppings for electrons in the two active orbitals. We have verified that the effective hopping t is then no longer $t = J/2$ but instead $t = 2t_1 t_2 / U$ where t_1 and t_2 denote the bare hopping of an electron in orbital 1 and 2 and U is the on-site Hubbard repulsion. Furthermore, quite often the hopping of the occupied orbital (defined below as orbital 1) is larger, as the gain in hybridization energy contributes to its energy gain with respect to the empty orbital, i.e., $t_1 > t_2$. For example for copper oxides with an occupied $x^2 - y^2$ orbital and empty t_{2g} orbital, $t_2 \approx t_1/2$ and thus $t = J/4$ since $J = 4t_1^2/U$. In the orbital-wave picture, the dispersion width is then likewise reduced by a factor of two to $W = 0.32J$, but the effect is stronger in the interacting t - J model, where we find $W \simeq 0.125J$, cf. Fig. 1(c)-(d).

¹ See also supplementary material in Ref. [4] which discusses the validity of this mapping in the 2D case.

3. Discussion

Let us now try to understand the physical origin of these large differences between the orbiton motion obtained in the mean-field approximation and in a far more exact way (i.e. via mapping onto the effective t - J model), cf. Fig. 2. As in the mean-field case the orbiton moves freely and does not excite any spin excitations, the whole effect of the spin background is taken into account by renormalizing the superexchange constant J into its reduced value J_{OW} . This stays in contrast with the result obtained from the mapping onto the t - J model: now the orbiton is effectively a ‘hole’ in the AF spin background which, when moving, flips the spins of the 2D AF, cf. Fig. 2. In fact, the further the orbiton moves the more spin flips (defects in 2D AF) it excites which leads to the so-called string-like potential acting on the orbiton, cf. Fig. 2. The orbiton can then move coherently only due to the presence of quantum spin fluctuations in the ground state which ‘heal’ these defects, ‘attach’ to the orbiton and jointly move as an orbiton quasiparticle on a renormalized scale (cf. Ref. [11, 10] with the hole in 2D AF moving effectively as a spin polaron). We also note that this result is entirely different from that in the 1D case [4], where the orbital flip excitation fractionalizes into free ‘spinon’ and ‘orbiton’ quasiparticles, similar to decay of a doped hole into spinon and holon.

4. Conclusions

In summary, we showed that a single orbital excitation in the 2D AF and FO ground state moves similarly to a hole in the 2D AF state. Therefore, it can only be mobile by coupling to the spin fluctuations which leads to a minimum in the orbiton dispersion for the $(\pi/2, \pi/2)$ point in the Brillouin zone and to the very strong renormalization of the orbiton bandwidth. In particular, in the realistic case which can correspond to the dd excitations in copper oxides, the orbiton bandwidth is of the order of $\sim 0.1J$ which explains why typically such dd excitations in the AF ground state are nearly dispersionless and can be well modelled using quantum chemistry calculations on small clusters [12].

Acknowledgments

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