The fate of the spin polaron in the 1D antiferromagnet: supplementary materials

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THE t–J MODEL FOR QUASI-1D CUPRATES: TUNEABLE STAGGERED MAGNETIC FIELD VS. TUNEABLE MAGNON-MAGNON INTERACTION

In order to construct the t–J model for quasi-1D cuprates, we make the following assumptions:

First, to get qualitative insight into the hole motion, we note that hopping between the chains can be neglected [1] and that the longer-range hopping is very small for quasi-1D cuprates [2]. Besides, the recently postulated strong coupling to phonons in 1D cuprates [3], not included here, would only further disrupt the (mentioned below and in the main text of the paper) fine balance between the magnon-magnon interactions and the magnon on-site energy.

Second, the remaining Heisenberg exchange interaction between the chains can be represented as the staggered magnetic field (which, due can be obtained from the spin exchange between the chains [4], hence is called $J_\perp$ below and in the main text of the paper):

$$H_{J_\perp} = \frac{J_\perp}{2} \sum_{\langle i,j \rangle} \left[(-1)^i S_i^z + (-1)^j S_j^z \right]. \tag{1}$$

The above term follows by assuming the onset of the long-range magnetic order at low temperatures, the magnetic interactions between the chains can be treated on a mean-field level—which, irrespectively of the sign of the interchain coupling, yields a staggered magnetic field acting on the antiferromagnetic chain in which the hole moves [4–6]. We note that, also at higher temperatures, i.e. when there is no long-range order and the staggered field cannot be used to simulate the coupling between the chains, the (mentioned in the main text of the paper) fine balance between the magnon-magnon interactions and their onsite energies will *also* be disrupted due to the change of magnon on-site energies by the exchange interaction between the chains. Thus, all of the presented results, obtained below will qualitatively model the quasi-1D cuprates also at temperatures higher than the Neel temperature. (We do not present such calculations, since they require exact diagonalisation of a full 2D problem, which heavily suffers from finite size effects and is beyond the scope of this work.) Following [4] one can estimate the value of $J_\perp$ in various quasi-1D cuprates: e.g. for $KCuF_3$ we obtain $J_\perp \approx 0.06J$ [hence the assumed in Fig. 4(d) of the main text value $J_\perp = 0.1J$, being the upper bound of that estimate].

Now let us investigate how the additional staggered field looks like in the polaronic description already used in the main text. In order to do this we firstly show in detail the polaronic descritpion of the 1D t–J model [i.e. how to go from Eq. (1) to Eq. (2) of the main text]. To this end, we start with a rotation of spins in one of the system's sublattices. This results in

$$H_{\rm rot} = -t \sum_{\langle i,j \rangle} \left(\tilde{c}^\dagger_{i\sigma} \tilde{c}_{j\bar{\sigma}} + H.c \right) + J \sum_{\langle i,j \rangle} \left[\frac{1}{2} \left(S_i^+ S_j^+ + S_i^- S_j^- \right) - S_i^z S_j^z - \frac{1}{4} \tilde{n}_i \tilde{n}_j \right]. \tag{2}$$

This allows for the introduction of holes and magnons according to the following transformations

$$\begin{aligned} \tilde{c}^\dagger_{i\uparrow} &= h_i, \qquad & \tilde{c}_{i\uparrow} &= h_i^\dagger (1 - a_i^\dagger a_i), \\ \tilde{c}^\dagger_{i\downarrow} &= h_i a_i^\dagger, \qquad & \tilde{c}_{i\downarrow} &= h_i^\dagger a_i, \end{aligned} \tag{3}$$

$$\begin{aligned} S_i^+ &= h_i h_i^\dagger (1 - a_i^\dagger a_i) a_i, \qquad & S_i^z &= \left(\frac{1}{2} - a_i^\dagger a_i \right) h_i h_i^\dagger, \\ S_i^- &= a_i^\dagger (1 - a_i^\dagger a_i) h_i h_i^\dagger, \qquad & \tilde{n}_i &= 1 - h_i^\dagger h_i = h_i h_i^\dagger, \end{aligned} \tag{4}$$

where $a_i^\dagger$ are bosonic creation operation at site i denoting magnons and $h_i^\dagger$ are fermionic creation operators at site i denoting holons. Here magnons can be understood as deviations from the state that has all the spins pointing up after the applied sublattice rotation. In the end, the 1D t–J model (up to a shift by a constant energy) reads:

$$\mathcal{H} = \mathcal{H}_t + \mathcal{H}_J, \tag{5}$$

where,

$$\mathcal{H}_t = t \sum_{\langle i,j \rangle} \left\{ h_i^\dagger h_j \left[a_i + a_j^\dagger (1 - a_i^\dagger a_i) \right] + h_j^\dagger h_i \left[a_j + a_i^\dagger (1 - a_j^\dagger a_j) \right] \right\}, \tag{6}$$

$J_\perp/J$	Δ	λ
0.01	0.01	$\frac{100}{101}$
0.1	0.1	$\frac{10}{11}$
0.5	0.5	$\frac{2}{3}$

TABLE I. Table presenting the relation between the value of the staggered field $J_\perp$ in the quasi-1D t–J model and the t–J model with rescaled magnon-magnon interaction λ and the XXZ anisotropy Δ.

$$\begin{aligned}\mathcal{H}_J = &\frac{J}{2}\sum_{\langle i,j\rangle} h_i h_i^\dagger \left[(1-a_i^\dagger a_i)(1-a_j^\dagger a_j)a_i a_j + a_i^\dagger a_j^\dagger (1-a_i^\dagger a_i)(1-a_j^\dagger a_j)\right] h_j h_j^\dagger \\ &+ \frac{J}{2}\sum_{\langle i,j\rangle} h_i h_i^\dagger \left(a_i^\dagger a_i + a_j^\dagger a_j - 2a_i^\dagger a_i a_j^\dagger a_j - 1\right) h_j h_j^\dagger.\end{aligned} \tag{7}$$

Now let us investigate the staggered magnetic field term given by Eq. (1) above. Performing the same set of transformations we obtain (up to a constant energy shift),

$$\mathcal{H}_{J_\perp} = \frac{J_\perp}{2}\sum_{\langle i,j\rangle}\left(a_i^\dagger a_i h_i h_i^\dagger + a_j^\dagger a_j h_j h_j^\dagger\right) \approx \frac{J_\perp}{2}\sum_{\langle i,j\rangle} h_i h_i^\dagger \left(a_i^\dagger a_i + a_j^\dagger a_j\right) h_j h_j^\dagger. \tag{8}$$

The omitted terms on the right hand side of the approximation modify the magnetic field only around the hole and they are $\propto J_\perp \left(a_i^\dagger a_i h_j h_j^\dagger + a_j^\dagger a_j h_i h_i^\dagger\right)$. In the end, we obtain for the spin part of the Hamiltonian [$\mathcal{H}_t$ is not affected, i.e. given by Eq. (6) above]

$$\begin{aligned}\mathcal{H}_{J+J_\perp} \equiv\; &\mathcal{H}_J + \mathcal{H}_{J_\perp} \\ \approx\; &\frac{J}{2}\sum_{\langle i,j\rangle} h_i h_i^\dagger \left[(1-a_i^\dagger a_i)(1-a_j^\dagger a_j)a_i a_j + a_i^\dagger a_j^\dagger (1-a_i^\dagger a_i)(1-a_j^\dagger a_j)\right] h_j h_j^\dagger \\ &+ \frac{J}{2}\sum_{\langle i,j\rangle} h_i h_i^\dagger \left[\left(1+\frac{J_\perp}{J}\right)\left(a_i^\dagger a_i + a_j^\dagger a_j\right) - 2a_i^\dagger a_i a_j^\dagger a_j - 1\right] h_j h_j^\dagger.\end{aligned} \tag{9}$$

Let us introduce the XXZ anisotropy

$$\Delta = \frac{J_\perp}{J} \tag{10}$$

and the rescaled magnon-magnon interaction parameter

$$\lambda = \frac{1}{1+\Delta}. \tag{11}$$

Then, in the single hole limit, we can write

$$\begin{aligned}\mathcal{H}_{J+J_\perp} \approx\; &\frac{J}{2}\sum_{\langle i,j\rangle} h_i h_i^\dagger \left[(1-a_i^\dagger a_i)(1-a_j^\dagger a_j)a_i a_j + a_i^\dagger a_j^\dagger (1-a_i^\dagger a_i)(1-a_j^\dagger a_j)\right] h_j h_j^\dagger \\ &+ (1+\Delta)\frac{J}{2}\sum_{\langle i,j\rangle} h_i h_i^\dagger \left(a_i^\dagger a_i + a_j^\dagger a_j - 2\lambda a_i^\dagger a_i a_j^\dagger a_j\right) h_j h_j^\dagger.\end{aligned} \tag{12}$$

Thus, once $J_\perp \neq 0$ the final model is the t–J model with the XXZ anisotropy Δ *and* rescaled magnon-magnon interaction λ. In TABLE I. we present the values of λ, Δ calculated for the corresponding values of $J_\perp$ used in calculations for Fig. 4(b) and 4(d) in the main text.

SU(2) SYMMETRY BREAKING IN THE t–J MODEL WITH TUNEABLE MAGNON-MAGNON INTERACTIONS

We start by re-expressing the magnon-magnon interaction term in the 'standard' (i.e. spin) language,

$$a_i^\dagger a_i a_j^\dagger a_j = -S_i^z S_j^z + \frac{1}{4}\tilde{n}_i\tilde{n}_j - \frac{1}{2}\left(\xi_i^{\mathcal{A}} S_i^z \ + \xi_j^{\mathcal{A}} S_j^z\right)\tilde{n}_i\tilde{n}_j, \tag{13}$$

where $\xi_i^{\mathcal{A}}$ equals -1 for $i \in \mathcal{A}$ and 1 otherwise, with $\mathcal{A}, \mathcal{B}$ denoting the two sublattices of the bipartite lattice. Thus, Hamiltonian (2) of the main text (i.e. the t–J model with tuneable magnon-magnon interactions) reads,

$$H = -t\sum_{\langle i,j\rangle}\left(\tilde{c}_{i\sigma}^\dagger \tilde{c}_{j\sigma} + \text{H.c.}\right) + J\sum_{\langle i,j\rangle}\left\{S_i S_j - \frac{1}{4}\tilde{n}_i\tilde{n}_j + (\lambda-1)\left[S_i^z S_j^z - \frac{1}{4}\tilde{n}_i\tilde{n}_j + \frac{1}{2}\left(\xi_i^{\mathcal{A}} S_i^z \ + \xi_j^{\mathcal{A}} S_j^z\right)\tilde{n}_i\tilde{n}_j\right]\right\}. \tag{14}$$

In the above Hamiltonian (14), the term

$$\frac{1}{2}\left(\xi_i^{\mathcal{A}} S_i^z \ + \xi_j^{\mathcal{A}} S_j^z\right)\tilde{n}_i\tilde{n}_j \tag{15}$$

can be understood as a staggered field acting on all spins although it is halved for the neighbors of the hole. This term contributes to the Hamiltonian once $\lambda \neq 1$ and explicitly breaks the SU(2) symmetry.

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