Hole dynamics in frustrated antiferromagnets: Coexistence of many-body and free-like excitations

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Hole spectral functions: spin polaron quasiparticle excitation at low energy and broad resonances at higher energies.

Conclusions

Outline

- Introduction: Hole dynamics in antiferromagnets
- Hole motion in different magnetic backgrounds
  - Frustration effects: weakening of AF correlations, competing correlations, and a new mechanism for hole motion
- t-J models solved with the self-consistent Born approximation (SCBA)
- Hole spectral functions: spin polaron quasiparticle excitation at low energy and broad resonances at higher energies.
- Conclusions
A single hole dynamics in an antiferromagnet

**t-J model**

\[
H = - \sum_{ij\sigma} t_{ij} \hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} + \sum_{\langle ij \rangle} J_{ij} \vec{S}_i \cdot \vec{S}_j
\]

The hole can move only by disturbing the antiferromagnetic background.

- **If** \(J >> t\) then \(\tau_{\text{exch}} \approx 1/J << \tau_{\text{hopp}} \approx 1/t\)
  
  \(\rightarrow\) the hole can propagate "easily"

- **If** \(J << t\) then \(\tau_{\text{exch}} >> \tau_{\text{hopp}}\)
  
  \(\rightarrow\) the hole will leave behind a string of "wrong" spins, increasing its effective mass

"wrong" spin

Hole + surrounding cloud of spin flips = quasiparticle or spin polaron
Hole motion and magnetic order: non-frustrated lattices

The hole motion will strongly depend on the magnetic correlations of the underlying magnetic order.

In the square lattice antiferromagnet the spin polaron is always well defined, for all momenta and $J > 0$

Experimental

Electronic dispersions for Sr$_2$CuO$_2$Cl$_2$ and Ca$_2$CuO$_2$Cl$_2$ measured by ARPES seem to confirm this picture


But the width of the peaks is too large to correspond to physical lifetimes of QP! Polaronic effects? (Ronning, Rosch, Gunnarsson, etc)

ARPES data and SCBA results for the t-t’-t”-J model
(t=0.35 eV, t’=-0.12 eV, t”=0.08 eV, and J=0.14 eV)

\[ E(0,0) \sim E(\pi,0) \]
\[ E(\pi/2,\pi/2) - E(0,0) \sim 2|E(\pi/2,0) - E(0,0)| \]
Another non-frustrated lattice: honeycomb lattice
A. Luscher et al, PRB 73, 155118 (2006)

SCBA, series expansions, and exact diagonalization results show well defined quasiparticle peaks at the bottom of the spectrum throughout the whole Brillouin zone

Frustrated lattices: weakly frustrated J$_1$-J$_2$ model

J$_2$ weakens the AF spin background. The frustration suppresses the QP weight and makes the spectrum broad for small momentum

A highly frustrated lattice: kagomé lattice

Lanczos exact diagonalization results show no QP peaks for J/t=0.4 and all momenta, for both signs of t
Hole dynamics in the triangular lattice

The ground state is a “simple” semiclassical 120° Néel order

SCBA results show no QP only for $t > 0$, and for momenta away from the magnetic Goldstone modes
Model and method

We use the $t$-$J$ model in local spin quantization axis, assuming a semiclassical magnetic order

Representations: hole $\rightarrow$ spinless fermion
spin fluctuations $\rightarrow$ Holstein-Primakov bosons

$$\hat{c}_{i\uparrow} = h_{i}^{\dagger} \quad \hat{c}_{i\downarrow} = h_{i}S_{i}^{-}$$

$$S_{i}^{x} \sim \frac{1}{2}(a_{i}^{\dagger} + a_{i}) \quad S_{i}^{y} \sim \frac{i}{2}(a_{i}^{\dagger} - a_{i}) \quad S_{i}^{z} = \frac{1}{2} - a_{i}^{\dagger}a_{i}$$

Effective Hamiltonian

$$H = \sum_{k} \epsilon_{k} h_{k}^{\dagger}h_{k} + \sum_{q} \omega_{q} \alpha_{q}^{\dagger}\alpha_{q} - t\sqrt{\frac{3}{N_{s}}} \sum_{k,q} \left[ M_{kq} h_{k}^{\dagger}h_{k-q}\alpha_{q} + h.c. \right]$$

Free hopping (due to the ferromagnetic component)
Free magnon energy
hole-magnon interaction
Self-consistent Born approximation (SCBA)

We calculate the hole spectral function

\[ A_k(\omega) = -\frac{1}{\pi} \text{Im} G_k^h(\omega) \]

\[ G_k^h(\omega) = \langle AF | h_k \frac{1}{\omega + i\eta^+-H} h_k^\dagger | AF \rangle \]

solving the self-consistent equation for the self-energy

\[ \Sigma_k(\omega) = \frac{3t^2}{N_s} \sum_q \frac{|M_{kq}|^2}{\omega - \omega_q - \epsilon_{k-q} - \Sigma_{k-q}(\omega - \omega_q)} \]

Quasiparticle weight
(How much of the hole survives)

\[ z_k = \left( 1 - \frac{\partial \Sigma_k(\omega)}{\partial \omega} \right)^{-1} \quad | \quad E_k = \Sigma_k(E_k) \]
Comparison SCBA vs exact results

N = 21 sites

Positive $t$

$J/t=0.4 \rightarrow$ strong coupling regime

Lanczos

SCBA
SCBA vs exact results

N = 21 sites

A

\[ A_k(\omega) \]

0.4

0.2

-6

-3

0

3

6

B

\[ t < 0 \]

\[ J / |t| = 0.4 \]

Negative t

Lanczos

SCBA
Hole spectral functions: negative $t$

- **Quasiparticle** (spin polaron)
- **t-resonance**: free hopping
- **Strings**
- **Incoherent background**

$J/|t|=0.4$
Hole spectral functions: positive $t$

No quasiparticle!

Sign reversal of $t$ is not trivial!

No strings
Triangular lattice

Descomposing the spins in an up-down basis

Two mechanisms for hole motion

Magnon-assisted hopping (hole-magnon interaction)

spin-polaron origin in non-frustrated antiferromagnets

Free hopping: no absorption or emission of magnons (due to the ferromagnetic component of the magnetic order)
These two mechanisms for hole motion will interference

To study this interference we can go from the pure AF state (only magnon-assisted propagation) to the pure ferromagnetic state (only free hopping propagation) by canting the AF order

We solve the $t$-$J$ model with a Zeeman term that couples only with spin, to stabilize the canted phase, using the SCBA

$$H = H_t + H_J = -t \sum_{\langle i,j \rangle} (\hat{c}^\dagger_{i,\sigma} \hat{c}_{j,\sigma} + h.c.) +$$

$$+ J \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j + B \sum_i S^z_i$$

Hole spectral functions: $k = (\pi/2, \pi/2)$

- Quasiparticle (spin polaron): always magnon assisted
- Propagation along ferromagnetic clusters induced by spin fluctuations
- Free hopping (classical ferro. component): $t$-resonance

As the angle increases the QP weight decreases

$J/t = 0.1$

$A_k(\omega)$
Hole spectral functions: $k=(0.8\pi,0.8\pi)$

$\theta=0^\circ$  

$\theta=30^\circ$  

$\theta=60^\circ$  

$J/t=0.1$
Quasiparticle weight vs. canting angle \( J/t=0.4 \)

\[
\begin{align*}
\theta & \quad \text{(deg.)} \\
0 & \quad 0.2 \quad 0.4 \quad 0.6 \quad 0.8 \quad 1 \\
Z_k & \\
\end{align*}
\]

Inside the magnetic BZ the QP weight goes to zero at 60°.

Outside the MBZ the QP weight goes to zero only for \( \theta=90° \).

\((\pi,\pi)\) is a unique case: constructive interference.

\((\pi/2,\pi/2)\) and \((0,0)\) are the same case.

MBZ
Contributions of the magnetic bands to the hole spectral function

\[
J/t=0.4, \ \theta=40°
\]

- 'Ferromagnetic' magnons only.
- Complete spectral function
- AF magnons only

AF: For all \( k \) and \( q \sim 0 \), \( M_{k,q} \sim \sqrt{q} \)

F: For all \( k \) and \( q \sim \pi \), \( M_{k,q} \sim \text{const} + |q - \pi| \)

The coupling with ferromagnetic magnons is more coherent: more spectral weight.
J/t dependence of QP excitations.

As $J/t$ increases, there is a crossover from

**Strong coupling: $J/t < 1$**  \rightarrow \text{QP: many-body state: hole coupled with magnons}

**Weak coupling: $J/t > 1$**  \rightarrow \text{One hole + one magnon}

\[
|\Psi_k\rangle = a_k^{(0)} h_k^\dagger |AF\rangle + \frac{1}{\sqrt{N}} \sum_{q_1} a_k^{(1)} h_{k-q_1}^\dagger \alpha_{q_1}^\dagger |AF\rangle + \frac{1}{N} \sum_{q_1,q_2} a_k^{(2)} h_{k-q_1-q_2}^\dagger \alpha_{q_2}^\dagger \alpha_{q_1}^\dagger |AF\rangle + \cdots
\]

\begin{align*}
\uparrow & \quad \text{bare hole} \quad \uparrow \quad \text{one magnon} \quad \uparrow \quad \text{multi-magnon}
\end{align*}

In weak coupling (Rayleigh-Schrodinger)

\[
a_{kq}^{(1\sigma)} = M_{k,q}^\sigma / (\epsilon_k - \epsilon_{k-q} - \omega_{q}^\sigma)
\]

\begin{align*}
\uparrow & \quad \text{Free hole, weakly renormalized by one magnon excitation}
\end{align*}

\[z_k \rightarrow 1 \quad \text{and} \quad E_k \rightarrow \epsilon_k\]
Bare hole and t-resonance

The t-resonance is always the bare hole weakly perturbed by a magnon

QP, t-resonance and bare hole are the same
J1-J2 Heisenberg model: Collinear phases

Experimental realization: \( \text{Li}_2\text{VOSiO}_4 \)
(see Trumper’s poster next week)

What happens when antiferromagnetic and ferromagnetic chains coexist?
Néel phase ($J_2 < 0.5J_1$)
Frustration $\rightarrow$ weakened QP spectral weight

Collinear phase ($J_2 > 0.5J_1$)
Frustration $\rightarrow$ weakened QP spectral weight and prominent t-resonance

Lanczos results confirm the SCBA picture
Conclusions

Competing frustrated interactions can induce ferromagnetic correlations, resulting in two mechanisms for hole motion:

A magnon assisted propagation, due to AF fluctuations of the background.
A free-like hoping mechanism due to the ferromagnetic component of the magnetic order.

As a consequence of the competition between both mechanisms, the QP spectral weight vanishes in some cases (triangular lattice for $t>0$, canted phase for $\theta \geq 60^\circ$, etc.)

In the strong coupling regime, $t>J$, the hole propagates preferably at two well separated energies
At low energies as a coherent spin polaron.
At higher energies as a free hole weakly renormalized by magnons.

For $t<J$ there is a crossover of the QP excitation from a many body state to a quasi-free hole.