Quasiparticle vanishing driven by geometrical frustration

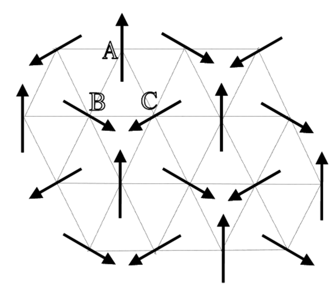
Luis Manuel and Adolfo Trumper

Instituto de Física Rosario and Universidad Nacional de Rosario, Argentina

We have studied the dynamics of a single hole injected in a triangular antiferromagnet. Using a hole-magnon effective Hamiltonian we have computed the hole spectral function and the quasiparticle wave function within the self-consistent Born approximation. We have found remarkable differences, under sign reversal of the transfer integral *t*, regarding the multi-magnon processes and the own existence of the quasiparticle excitations. Such differences are due to the subtle interplay between magnon-assisted and free hopping mechanisms. We conclude that the conventional quasiparticle picture can be broken by geometrical magnetic frustration without invoking spin liquid phases.

How does the magnetic frustration affect the dynamics of a single hole in an antiferromagnet?

Let's look what happens when a hole is doped in an antiferromagnet on a triangular lattice with a semiclassical 120° Néel ordered ground state



Model and Method

We use the *t-J* model in local spin quantization axis

$$H = -\sum_{ij\sigma} t_{ij} \hat{c}^{\dagger}_{i\sigma} \hat{c}_{j\sigma} + \sum_{<ij>} J_{ij} \mathbf{S}_i . \mathbf{S_j}$$

Representations: hole → spinless fermion

spin fluctuations → Holstein-Primakov bosons

$$\hat{c}_{i\uparrow} = h^{\dagger}_i \qquad \hat{c}^{\dagger}_{i\downarrow} = h_i S^{-}_i$$

$$S^x_i \sim \frac{1}{2}(a^{\dagger}_i + a_i) \qquad S^y_i \sim \frac{i}{2}(a^{\dagger}_i - a_i) \qquad S^z_i = \frac{1}{2} - a^{\dagger}_i a_i$$

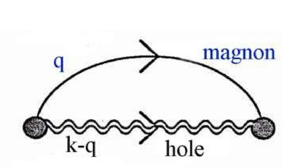
Effective Hamiltonian

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

free hopping (due to non-collinearity) — free magnon energy — hole-magnon interaction (quasiparticle origin in non-frustrated antiferromagnets)

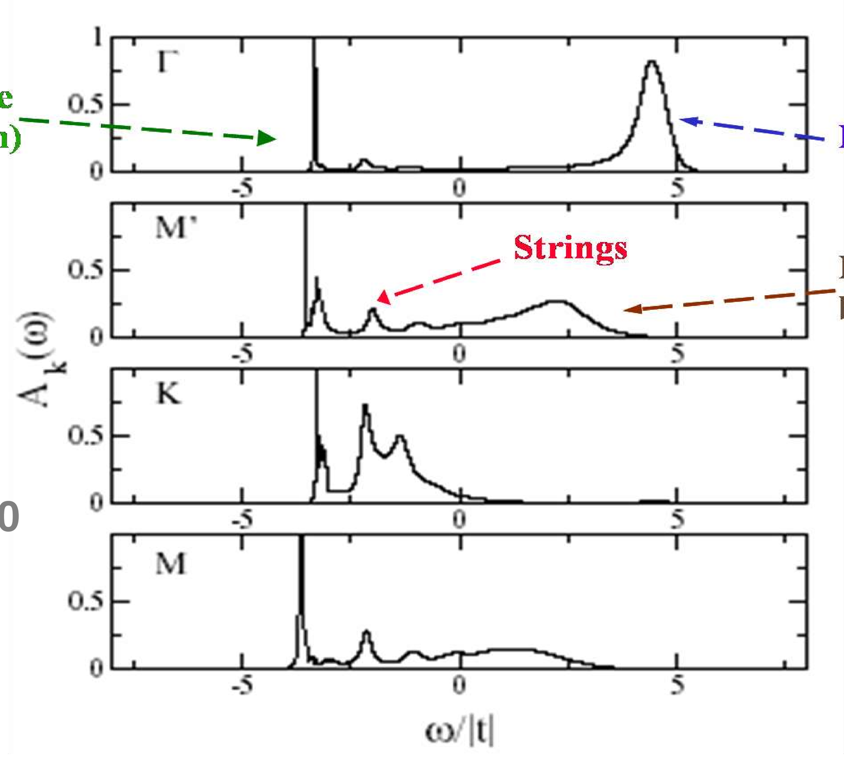
Due to non-collinearity there are two mechanisms for hole motion and they interfere. **Will the quasiparticle survive?**

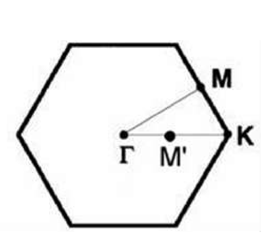
To answer this question we calculate the hole spectral functions, using the self-consistent Born approximation for the self-energy.



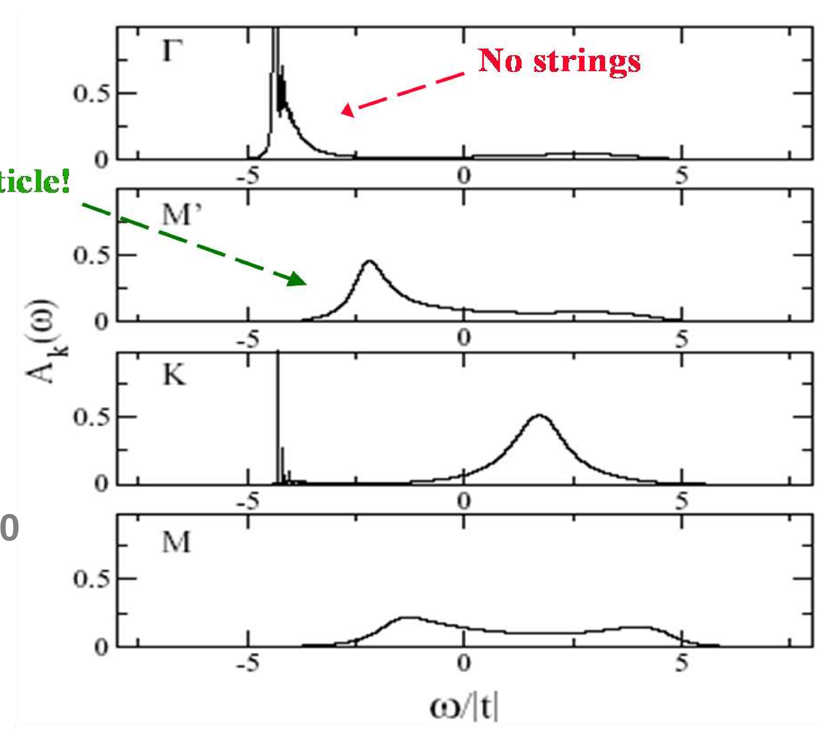
Hole spectral functions

For positive *t*, and in the strong coupling regime, we find that the low energy quasiparticle excitations vanish outside the neighborhood of the magnetic Goldstone modes; while for negative *t* the quasiparticle excitations are always well defined. This strong momentum and *t* sign dependence is related to the underlying magnetic structure and the particle-hole asymmetry of the model.



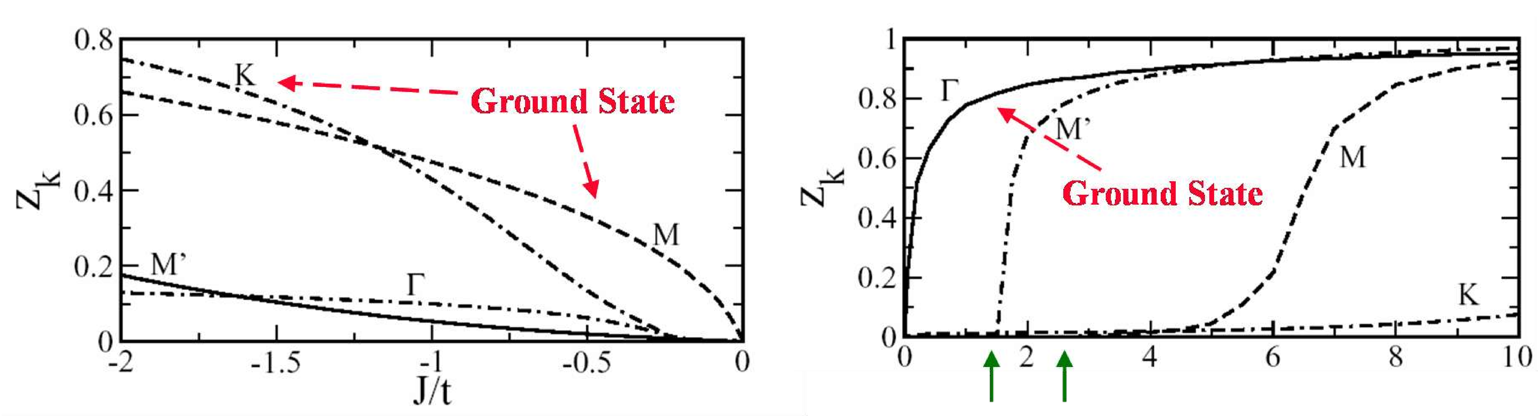


J/|t|=0.4



Sign reversal of *t* is not trivial!

Quasiparticle weight

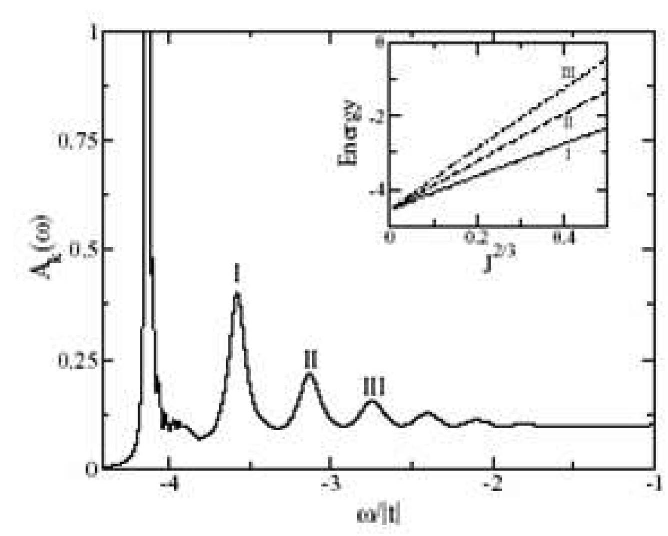


String excitations

For negative *t* we find resonances of magnetic origin identified with string excitations of a hole confined by an effective linear potential of order *J*

$E_{string} \sim (J/t)^{2/3}$

Like a particle bounded by a linear potential



Quasiparticle energy scaling with *J/t*

$E_{qp} \sim (J/t)^{0.65}$ for negative *t* → local environment around the hole enhances its antiferromagnetic character.

$E_{qp} \sim (J/t)^{0.55}$ for positive *t* → the ferromagnetic character is favored.

Quasiparticle wavefunction

$$|\Psi_{\mathbf{k}}\rangle = a^{(0)}_{\mathbf{k}} h^{\dagger}_{\mathbf{k}} |AF\rangle + \frac{1}{\sqrt{N}} \sum_{\mathbf{q}_1} a^{(1)}_{\mathbf{k},\mathbf{q}_1} h^{\dagger}_{\mathbf{k}-\mathbf{q}_1} \alpha^{\dagger}_{\mathbf{q}_1} |AF\rangle + \frac{1}{N} \sum_{\mathbf{q}_1,\mathbf{q}_2} a^{(2)}_{\mathbf{k},\mathbf{q}_1,\mathbf{q}_2} h^{\dagger}_{\mathbf{k}-\mathbf{q}_1-\mathbf{q}_2} \alpha^{\dagger}_{\mathbf{q}_2} \alpha^{\dagger}_{\mathbf{q}_1} |AF\rangle + \cdots$$

bare hole — one magnon — multi-magnon

We solve the Schrodinger equation for the spin polaron in the self-consistente Born approximation

$$H|\Psi_{\mathbf{k}}\rangle = E_{\mathbf{k}} |\Psi_{\mathbf{k}}\rangle$$

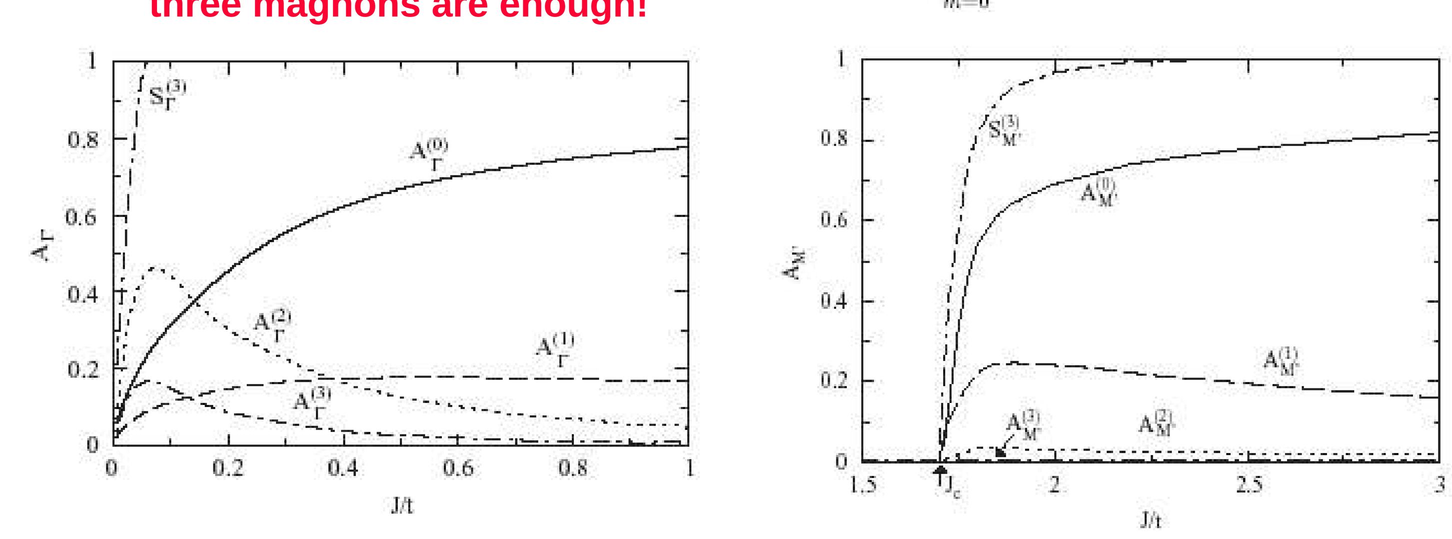
Normalization condition $\langle \Psi_{\mathbf{k}} | \Psi_{\mathbf{k}} \rangle = \sum_n A^{(n)}_{\mathbf{k}} = 1$

weight of the *n*-magnon contribution

For positive *t* there is a strong momentum dependence of the multi-magnon contributions

three magnons are enough!

$$S^{(n)}_{\mathbf{k}} = \sum_{m=0}^{n} A^{(m)}_{\mathbf{k}}$$



magnon proliferation

Conclusions

- The magnetic frustration induces qualitative changes in the hole dynamics:
  - t < 0 → well defined quasiparticle and string excitations
  - t > 0 → no quasiparticle, no strings, magnon proliferation
- We give firm evidence that non-conventional excitations can be found in *non-collinear* spin-crystal phases like the one present in the triangular antiferromagnet. There is no need of spin liquid phases!
- Experiments? There is a plenty of strongly correlated materials with a triangular topology: organic salts (BEDT-TTF)X, cobaltates, silicon surfaces, etc. Our findings could be of relevance for these compounds.

References:

A. E. Trumper, C. J. Gazza, and L. O. Manuel, Phys. Rev. B 69, 184407 (2004).

A. E. Trumper, C. J. Gazza, and L. O. Manuel, Physica B 354, 252 (2004).