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

Luis O. Manuel

Instituto de Física Rosario
Rosario, Argentina

Collaborators:

Adolfo E. Trumper (Rosario)
Ignacio J. Hamad (Rosario)
Adrian E. Feiguin (UCSB, Santa Barbara)

CORPES'07 - April 17.2007

Outline

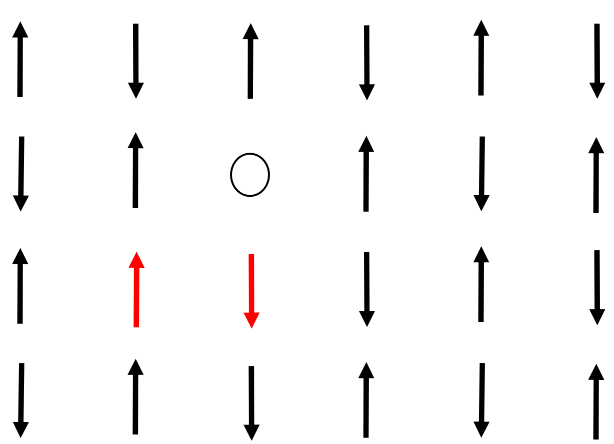
- Introduction: Hole dynamics in antiferromagnets
- Hole motion in different magnetic backgrounds

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

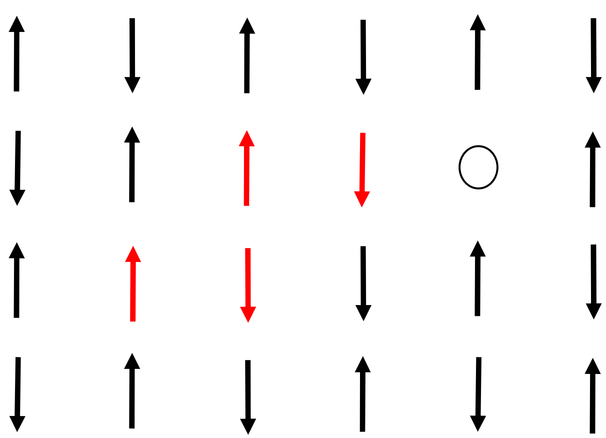


“wrong” spin

The hole can move only by disturbing the antiferromagnetic background

If J >> t then τ_{exch}~ 1/J << τ_{hopp}~1/t

→the hole can propagate “easily”



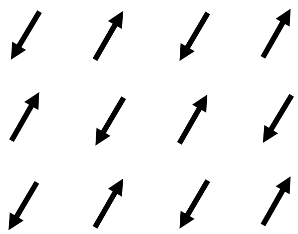
Hole + surrounding cloud of spin flips = quasiparticle or spin polaron

If J << t then τ_{exch} >> τ_{hopp}

→ the hole will leave behind a string of “wrong” spins, increasing its effective mass

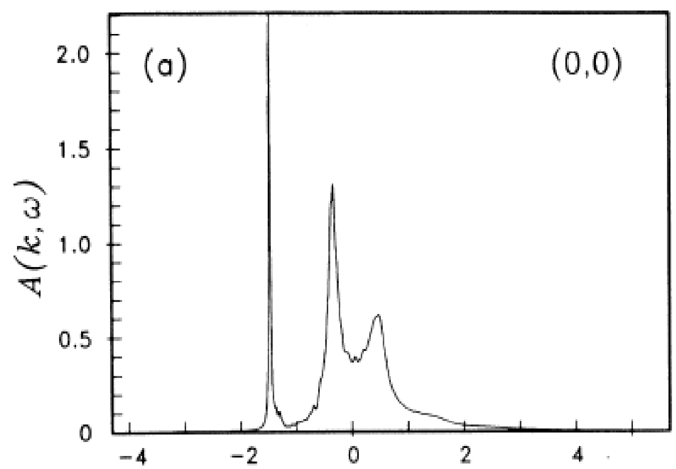
Hole motion and magnetic order: non-frustrated lattices

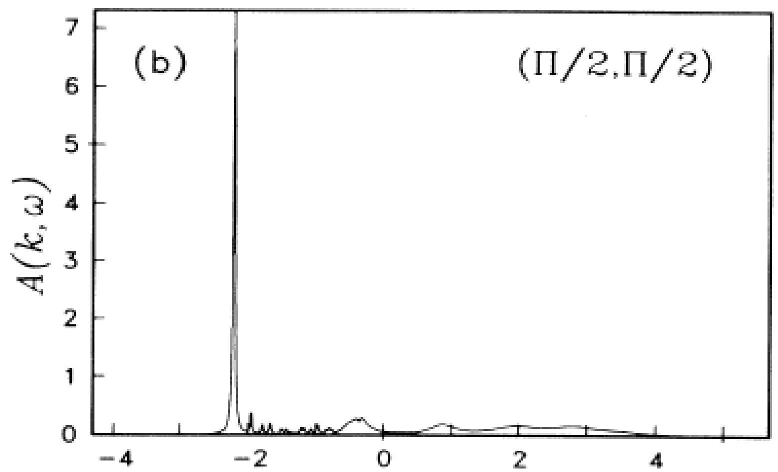
The hole motion will strongly depend on the magnetic correlations of the underlying magnetic order



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

Martinez and Horsch PRB 44, 317 (1991) ; Dagotto RMP 66, 763 (1994); Brunner *et al* PRB 62, 15480 (2000)

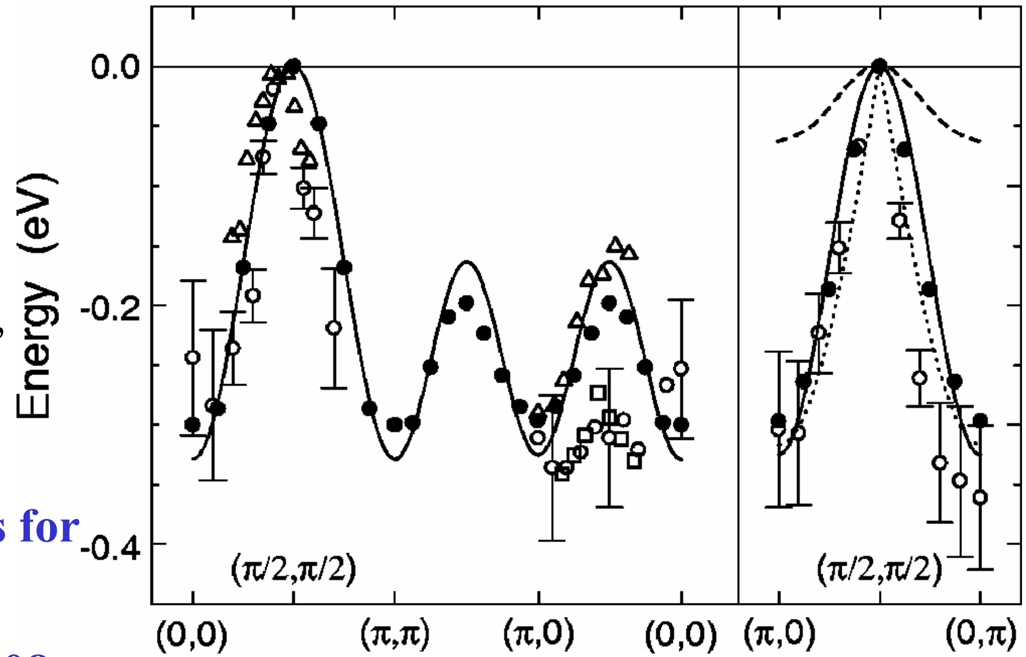




Experimental

Electronic dispersions for $Sr_2CuO_2Cl_2$ and $Ca_2CuO_2Cl_2$ measured by ARPES seem to confirm this picture

Wells et al, PRL 74, 964, (1995); Ronning et al, Science 282, 2067 (1998)



ARPES data and SCBA results for the t-t’-t’’-J model

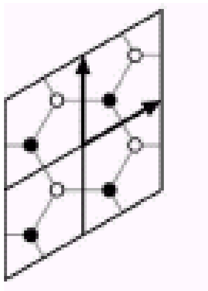
(t=0.35 eV, t’=-0.12 eV, t”=0.08 eV, and J=0.14 eV)

$$\text{min}: \quad E(0,0) \sim E(\pi,0)$$

$$\text{max}: \quad E(\frac{\pi}{2},\frac{\pi}{2})$$

$$E(\frac{\pi}{2},\frac{\pi}{2}) - E(0,0) \sim 2[E(\frac{\pi}{2},0) - E(0,0)]$$

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



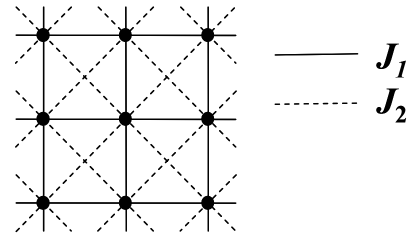
Another non-frustrated lattice: honeycomb lattice

A. Luscher et al, PRB 73, 155118 (2006)

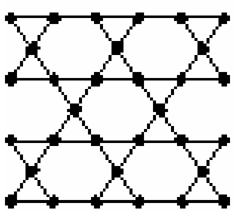
SCBA, series expansions, and exact diagonalization results show well defined quasiparticle peaks at the bottom of the spectrum throughout the whole Brillouin zone

Frustrated lattices: weakly frustrated J_1-J_2 model

Y. Shibata, T. Tohyama, and S. Maekawa, PRB 59, 1840 (1999)



J_2 weakens the AF spin background. The frustration supresses the QP weight and makes the spectrum broad for small momentum



A highly frustrated lattice: kagomé lattice

A. Lauchli and D. Poilblanc, PRL 92, 236404 (2004)

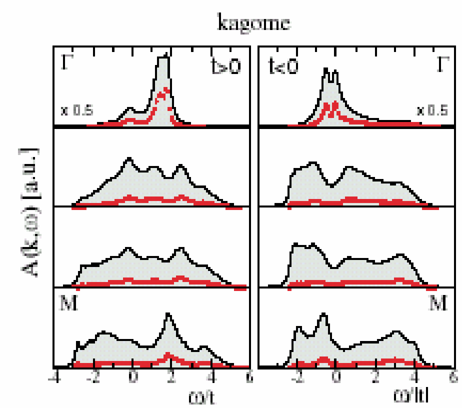


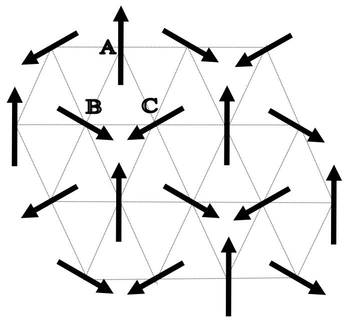
FIG. 5 (color online). Single hole spectral functions (black lines) along the line $\Gamma \leftrightarrow M$ computed on a 27 site kagome cluster for $t = +1$ (left panel) and for $t = -1$ (right panel). In both cases $J/|t| = 0.4$. The red circles denote pole locations and their residues. Note that no quasiparticle peaks are visible for all momenta.

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

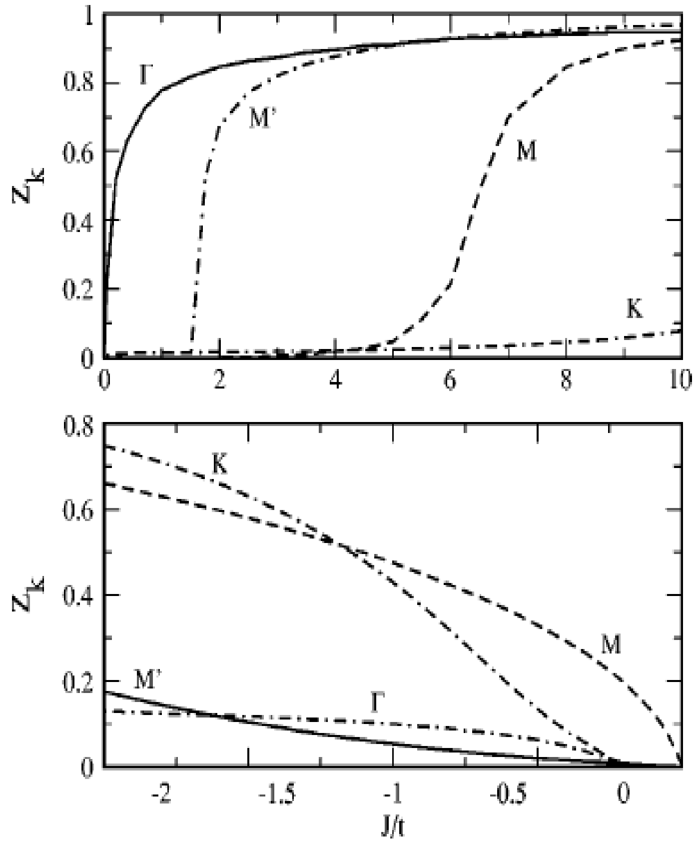
A. Trumper, C. Gazza, and L.O.M., PRB 69, 184407 (2004)

The ground state is a "simple" semiclassical 120° Néel order

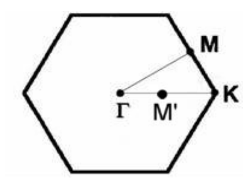


t > 0

t < 0



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 → spinless fermion
spin fluctuations → Holstein-Primakov bosons

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

$$S_i^x \sim \frac{1}{2}(a_i^\dagger + a_i) \qquad S_i^y \sim \frac{i}{2}(a_i^\dagger - a_i) \qquad S_i^z = \frac{1}{2} - a_i^\dagger a_i$$

Effective Hamiltonian

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

Free hopping (due to the ferromagnetic component)

Free magnon energy

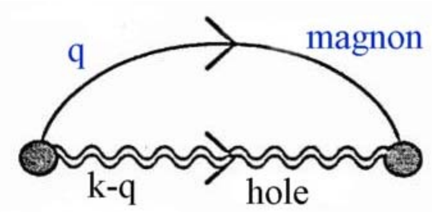
hole-magnon interaction

Self-consistent Born approximation (SCBA)

We calculate the hole **spectral function**

$$A_{\mathbf{k}}(\omega) = -\frac{1}{\pi} Im G^h_{\mathbf{k}}(\omega)$$

$$G^h_{\mathbf{k}}(\omega) = \langle AF | h_{\mathbf{k}} \frac{1}{(\omega + i\eta^+ - H)} h^\dagger_{\mathbf{k}} | AF \rangle$$



solving the self-consistent equation for the self-energy

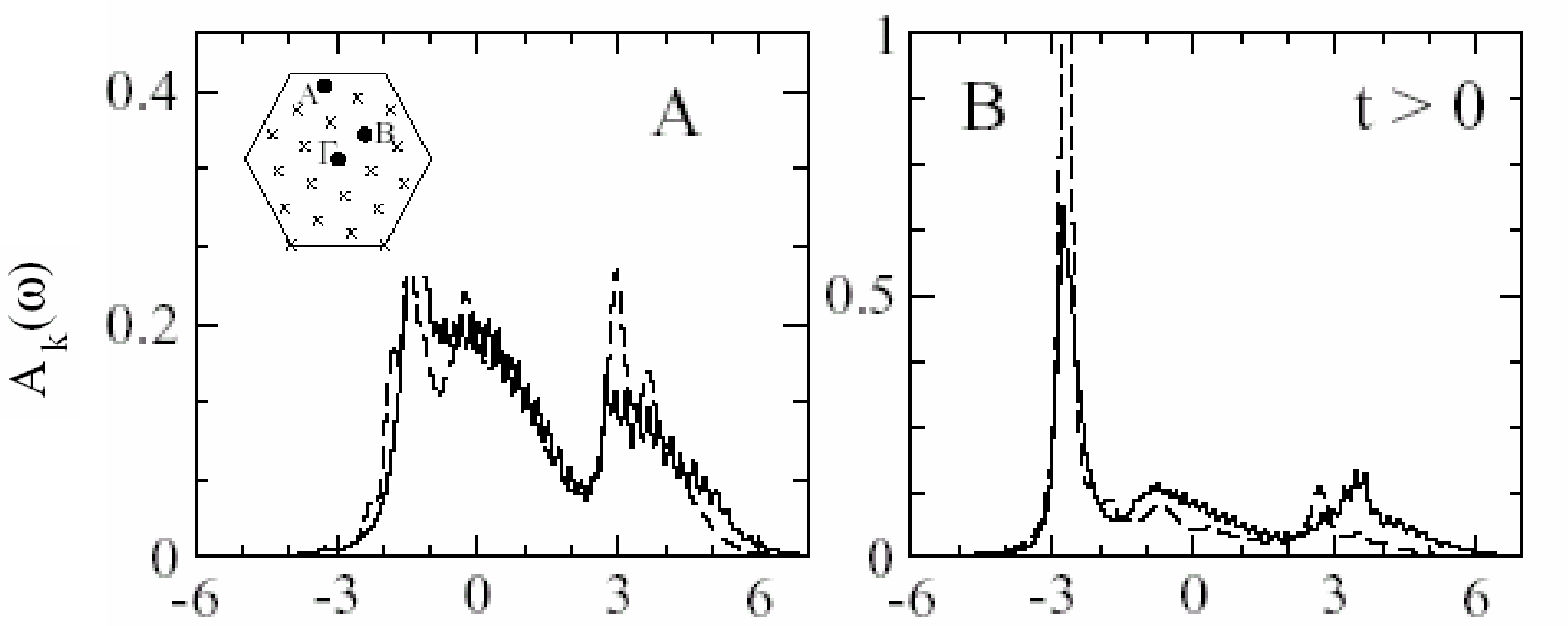
$$\Sigma_{\mathbf{k}}(\omega) = \frac{3t^2}{N_s} \sum_{\mathbf{q}} \frac{| M_{\mathbf{kq}} |^2}{\omega - \omega_{\mathbf{q}} - \epsilon_{\mathbf{k-q}} - \Sigma_{\mathbf{k-q}}(\omega - \omega_{\mathbf{q}})}$$

Quasiparticle weight
(How much of the hole survives)

$$z_{\mathbf{k}} = \left(1 - \frac{\partial \Sigma_{\mathbf{k}}(\omega)}{\partial \omega}\right)^{-1} \Big|_{\ E_{\mathbf{k}} = \Sigma_{\mathbf{k}}(E_{\mathbf{k}})}$$

Comparison SCBA vs exact results

N = 21 sites



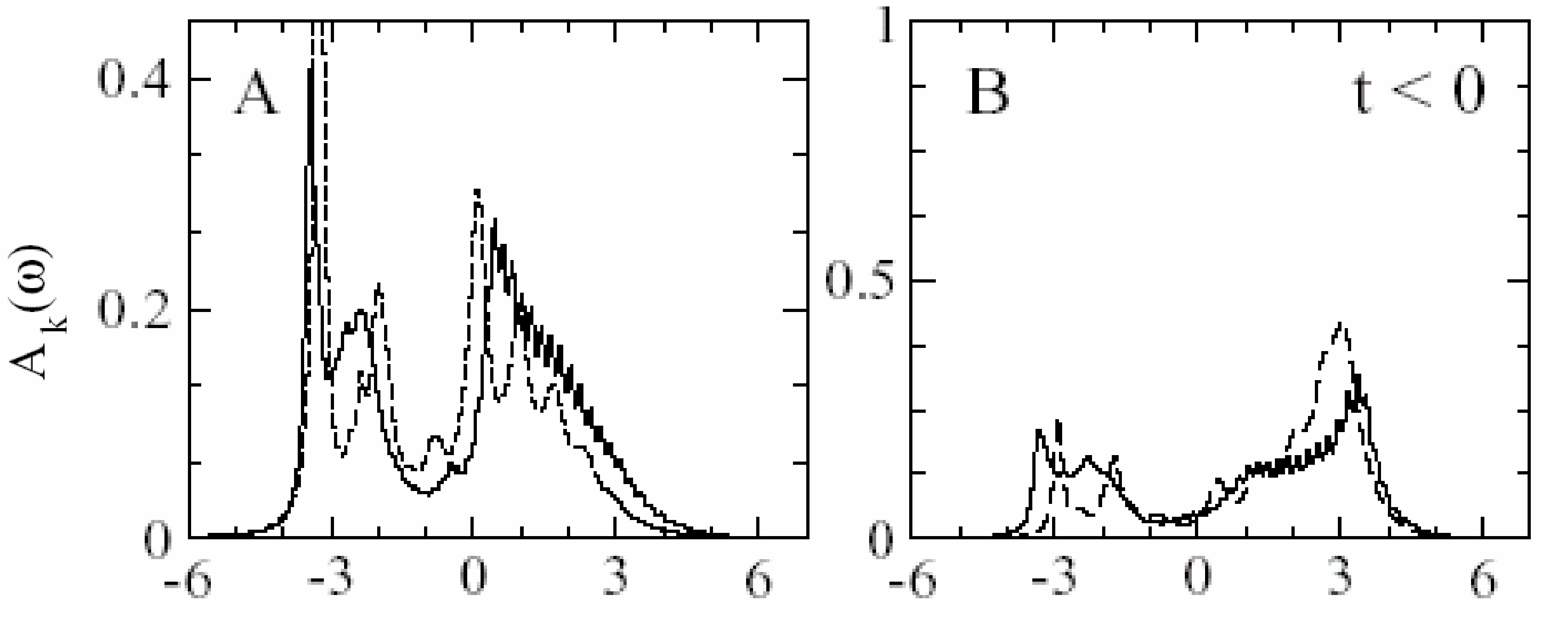
- **Positive t**
- **J /t=0.4 → strong coupling regime**

____________ Lanczos

_ _ _ _ _ _ _ SCBA

SCBA vs exact results

N = 21 sites

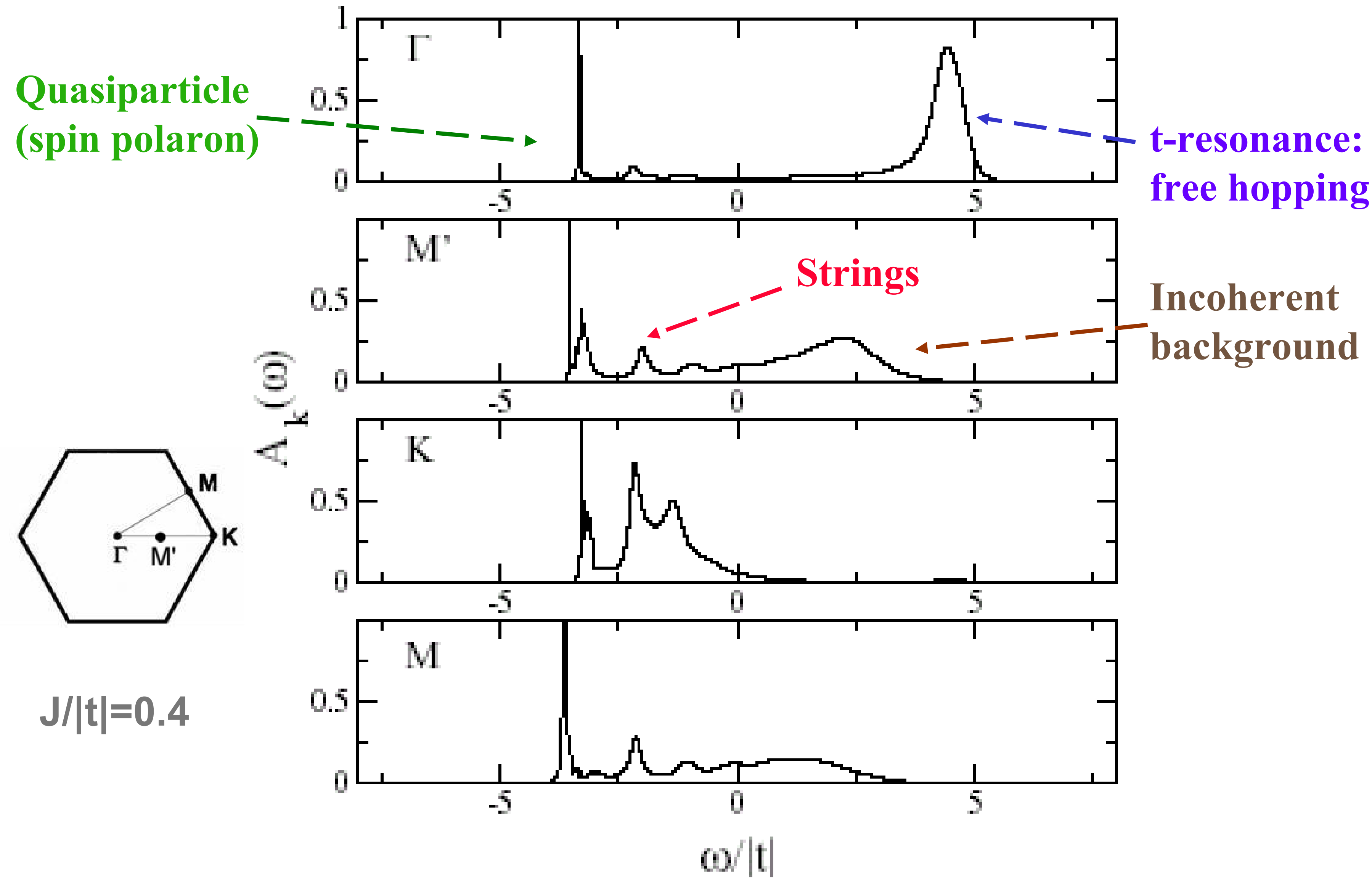


- **Negative t**
- **J /|t|=0.4**

Lanczos (solid line)

SCBA (dashed line)

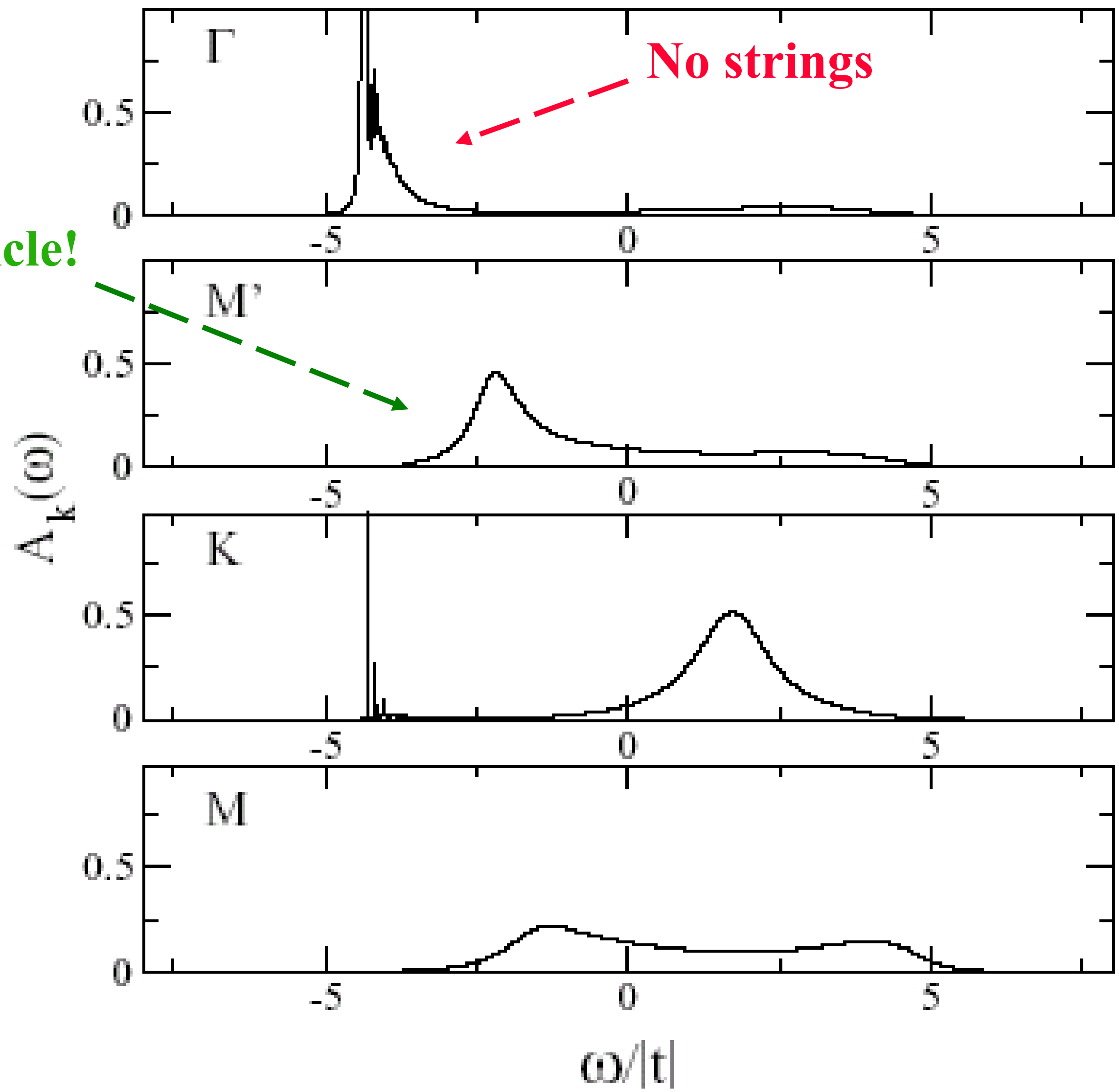
Hole spectral functions: negative *t*



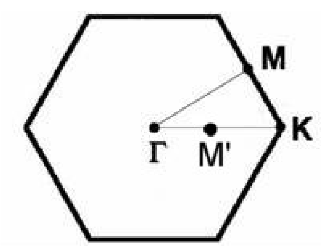
Hole spectral functions: positive *t*

No strings

No quasiparticle!



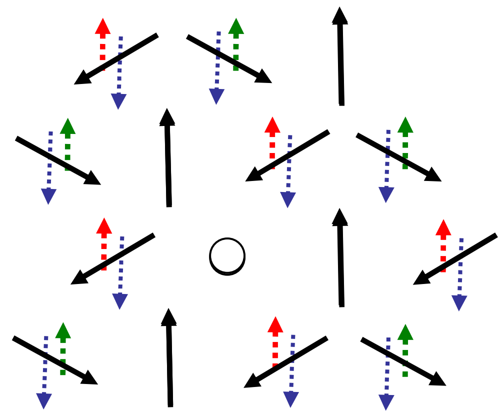
Sign reversal of *t* is not trivial!



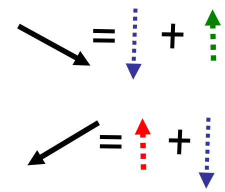
J/t=0.4

Triangular lattice

Triangular lattice: semiclasical 120° order



Descomposing the spins in an up-down basis



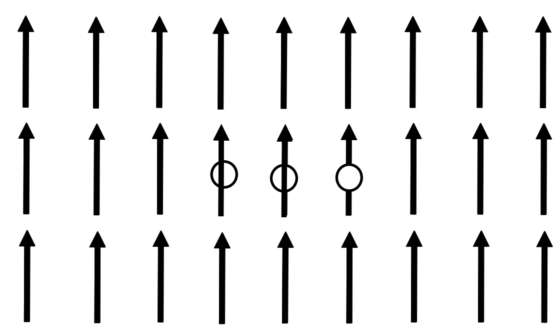
Two mechanisms for hole motion

Magnon-assisted hopping (hole-magnon interaction)

↓

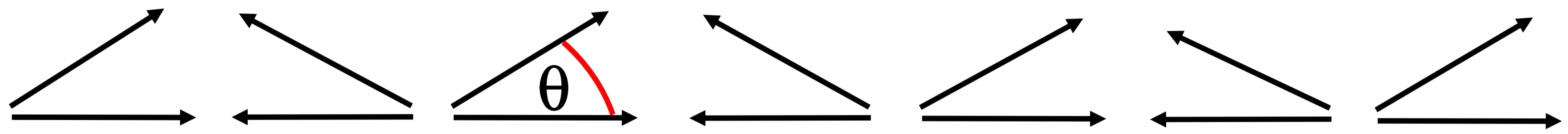
spin-polaron origin in non-frustrated antiferromagnets

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

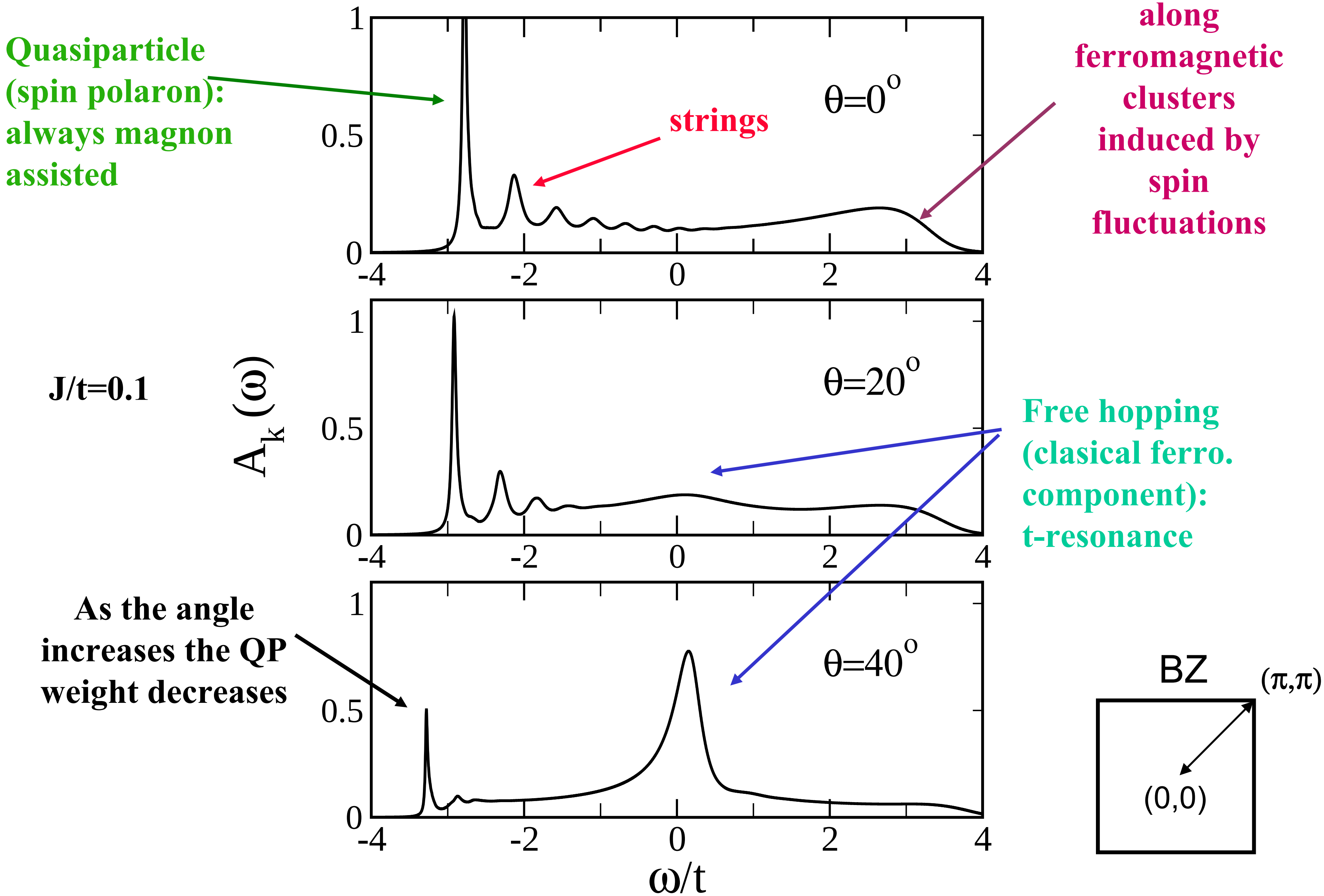


We solve the *t-J* model with a Zeeman term that couples only with spin, to stabilize the canted phase, using the SCBA

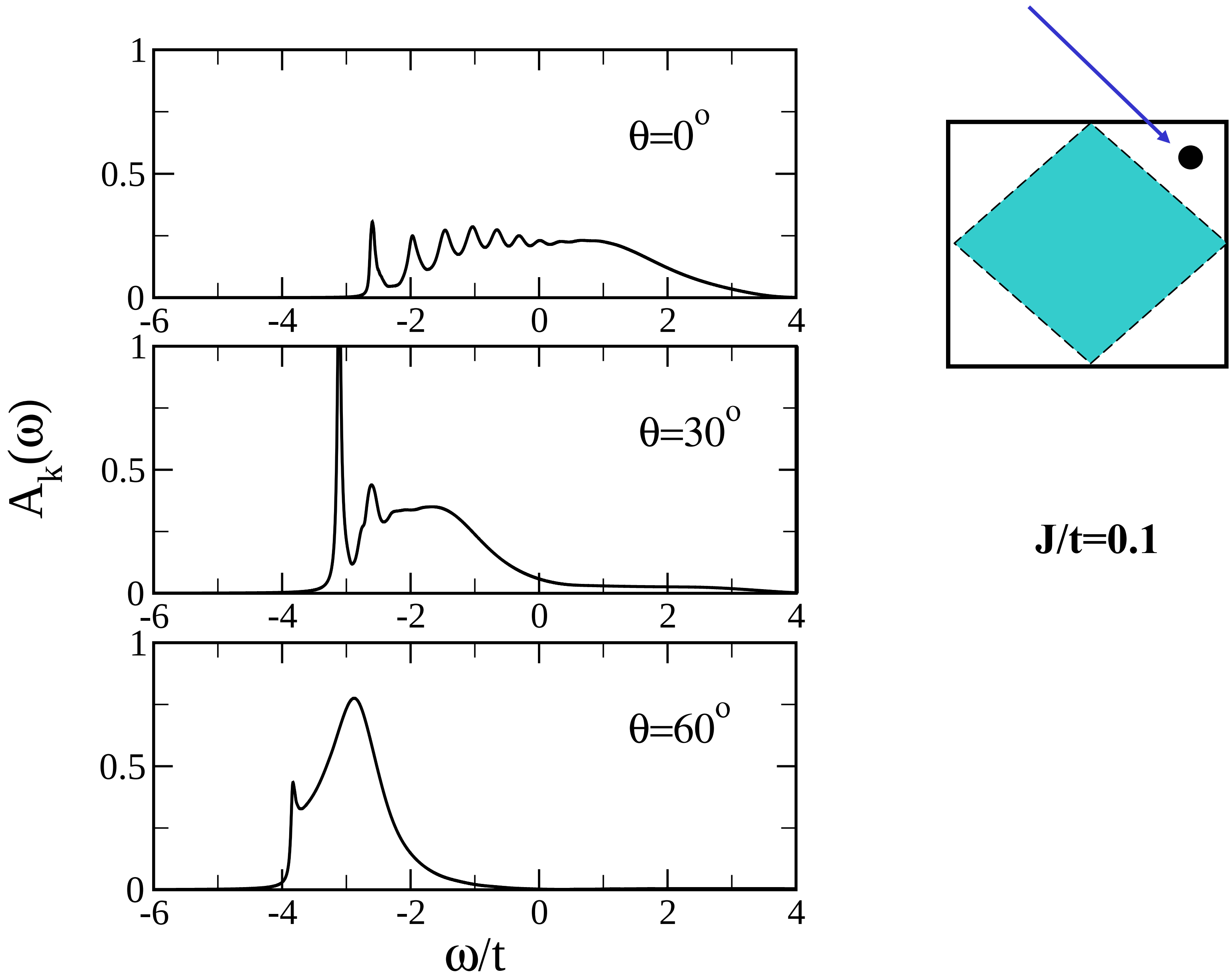
$$H = H_t + H_J = -t \sum_{\langle i,j \rangle} (\hat{c}^{\dagger}_{i,\sigma} \hat{c}_{j,\sigma} + h.c.) + \\ + J \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j + B \sum_i S_i^z$$

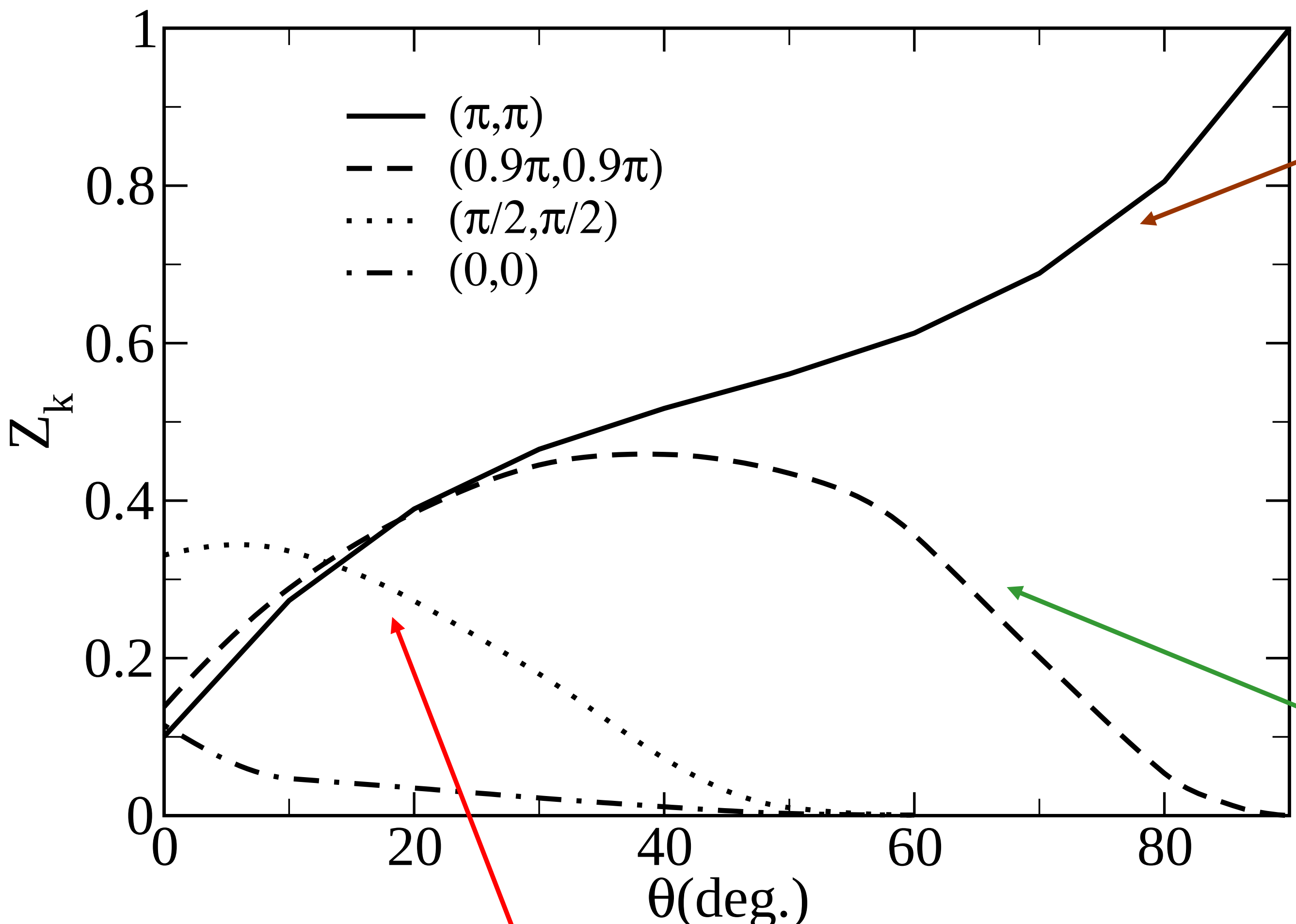
I. Hamad, L.O.M., *et al*, PRB 74, 094417 (2006)

Hole spectral functions:k=(π/2,π/2)

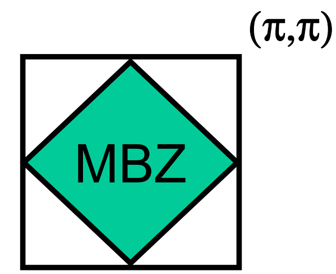


Hole spectral functions: k=(0.8π,0.8π)





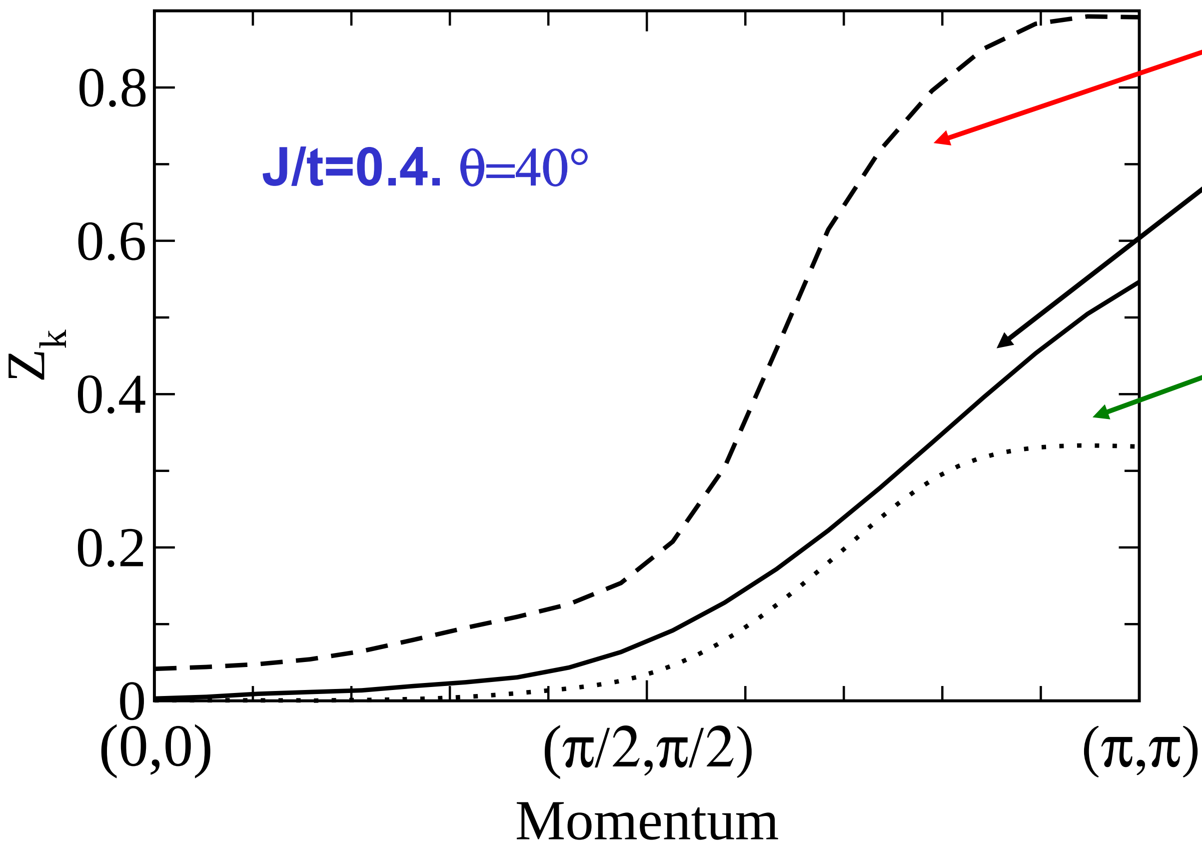
(π,π) is a unique case: constructive interference



Outside the MBZ the QP weight goes to zero only for θ=90°

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

Contributions of the magnetic bands to the hole spectral function



'Ferromagnetic' magnons only.

$\mathbf{q} \sim \pi$

Complete spectral function

AF magnons only

$\mathbf{q} \sim 0,$

AF: For all $\mathbf{k}$ and $\mathbf{q} \sim 0$, $M_{\mathbf{k},\mathbf{q}} \sim \sqrt{q}$

F: For all $\mathbf{k}$ and $\mathbf{q} \sim \pi$, $M_{\mathbf{k},\mathbf{q}} \sim \mathrm{const} + |\mathbf{q} - \pi|$

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 → QP: many-body state: hole coupled with magnons

Weak coupling: J/t>1 → One hole + one magnon

$$|\Psi_{\rm k}\rangle = a^{(0)}_{\rm k} h^\dagger_{\rm k}|AF\rangle + \frac{1}{\sqrt{N}}\sum_{\rm q_1} a^{(1)}_{\rm k,q_1} h^\dagger_{\rm k-q_1}\alpha^\dagger_{\rm q_1}|AF\rangle + \frac{1}{N}\sum_{\rm q_1,q_2} a^{(2)}_{\rm k,q_1,q_2} h^\dagger_{\rm k-q_1-q_2}\alpha^\dagger_{\rm q_2}\alpha^\dagger_{\rm q_1}|AF\rangle + \cdots$$

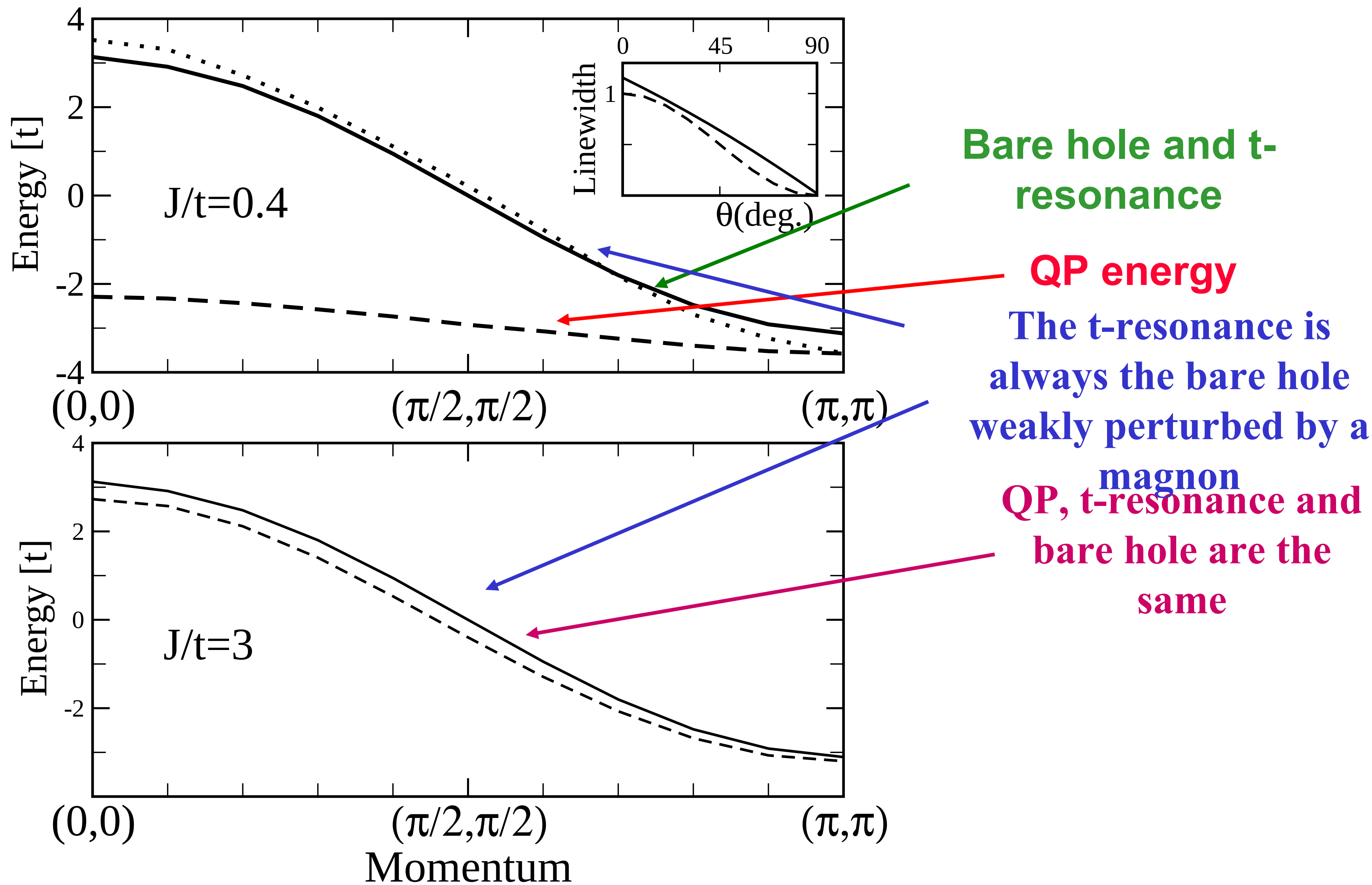
↑ bare hole ↑ one magnon ↑ multi-magnon

$$z_{\mathbf{k}} \rightarrow 1 \text{ and } E_{\mathbf{k}} \rightarrow \epsilon_{\mathbf{k}}$$

In weak coupling (Rayleigh-Schrodinger)

$$a^{(1\sigma)}_{\mathbf{kq}} = M^{\sigma}_{\mathbf{k},\mathbf{q}}/(\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k}-\mathbf{q}} - \omega^{\sigma}_{\mathbf{q}})$$

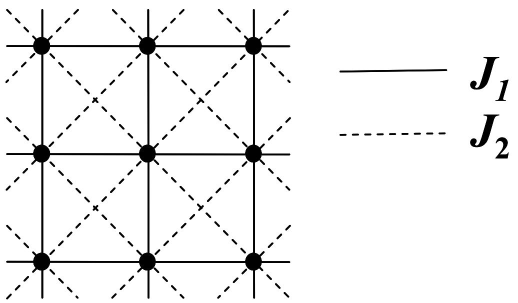
↑ Free hole, weakly renormalized by one magnon excitation

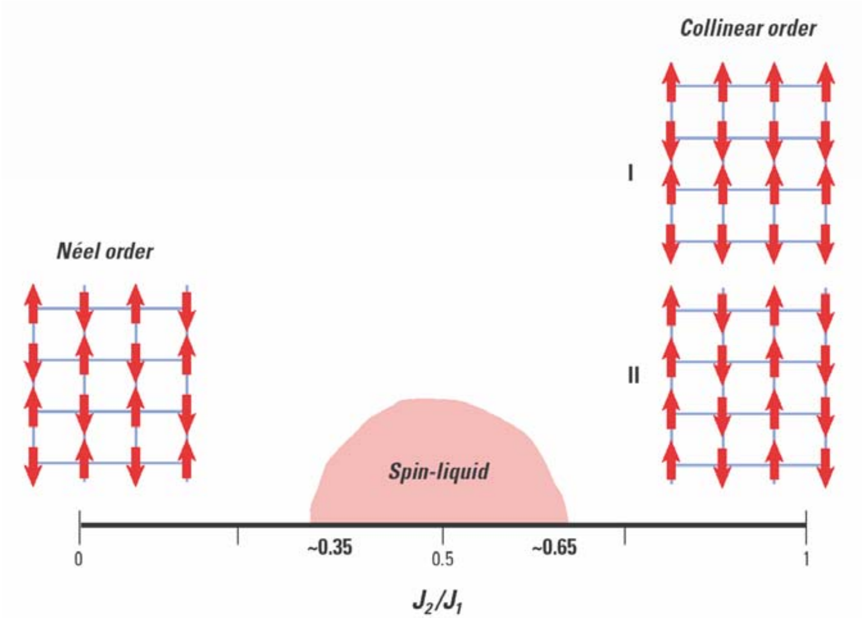


4
2
0
-2
-4
Energy [t]
J/t=0.4
0
45
90
Linewidth
1
θ(deg.)
(0,0)
(π/2,π/2)
(π,π)
4
2
0
-2
Energy [t]
J/t=3
(0,0)
(π/2,π/2)
(π,π)
Momentum
Bare hole and t-resonance
QP energy
The t-resonance is always the bare hole weakly perturbed by a magnon
QP, t-resonance and bare hole are the same

J1-J2 Heisenberg model: Collinear phases

I. Hamad, A. Trumper, L.O.M., Physica B (2007)



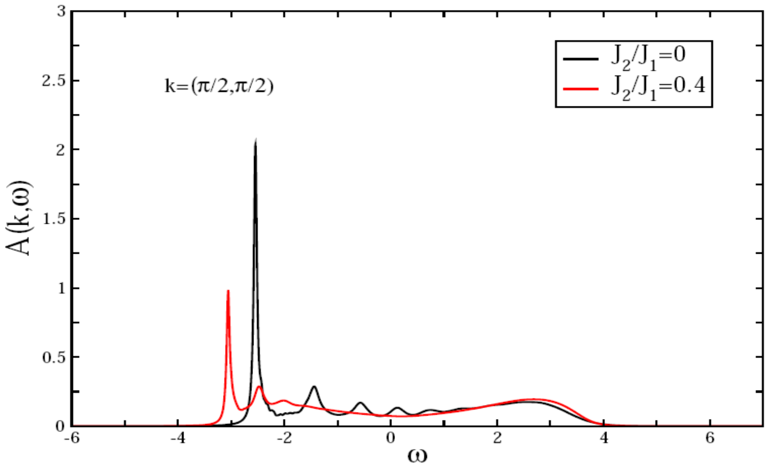


Experimental realization: **Li_2VOSiO_4**

(see Trumper's poster next week)

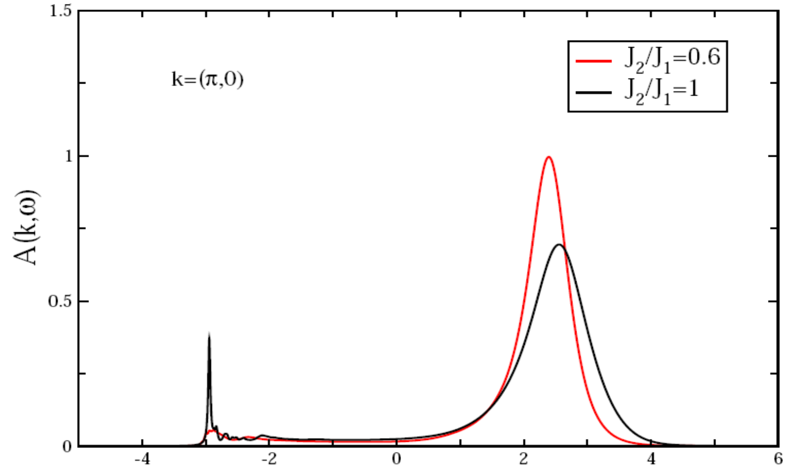
What happens when antiferromagnetic and ferromagnetic chains coexist?

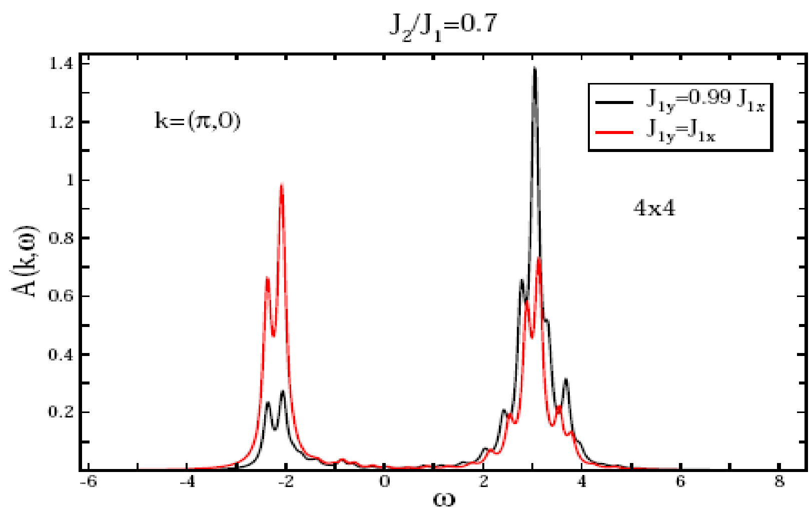
Néel phase ($J_2 < 0.5J_1$)
Frustration → weakened QP spectral weight



J_1=0.4t

Collinear phase ($J_2 > 0.5J_1$)
Frustration → 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 $\theta\geq 60°$, 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.**