Quasiparticle vanishing driven by geometrical frustration

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Outline

- Introduction: Hole dynamics in antiferromagnets

  How does the frustration affect the hole dynamics?

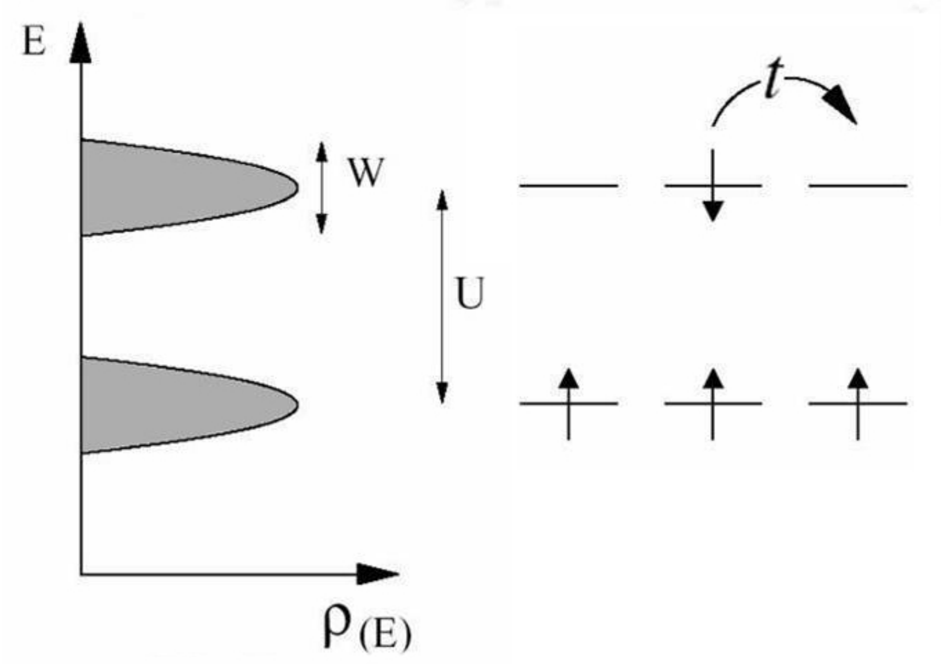
- Model and methods
- Hole spectral functions: quasiparticle and string excitations
- Quasiparticle wave function
- Conclusions

Mott insulators

Strong electronic correlation **W < U**

⬇

Mott insulating state



metal-transition oxides →
d orbitals **W ~U ~ 2 eV**

Hubbard model

$$H = \sum_{ij\sigma} t_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

Low energy physics of a Mott insulator

The low energy physics is dominated by spin fluctuations

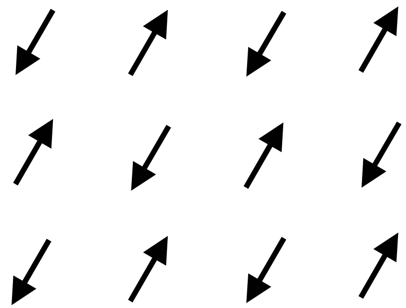
↓

Heisenberg model (localized spins)

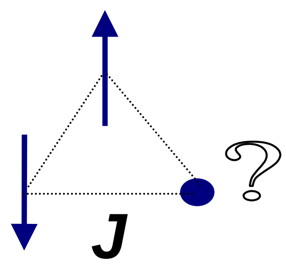
$$H = \sum_{<ij>} J_{ij} \mathbf{S_i}.\mathbf{S_j}$$

$$J_{ij} = \frac{4t_{ij}^2}{U}$$

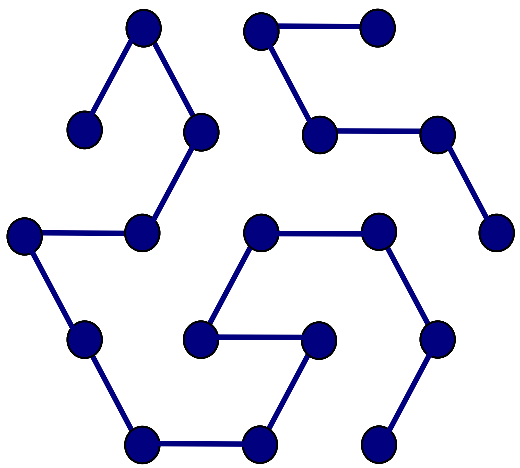
Square lattice → Nèel order is the ground state, e.g. La_2CuO_4



Triangular lattice → geometrical frustration might prevent magnetic long range order



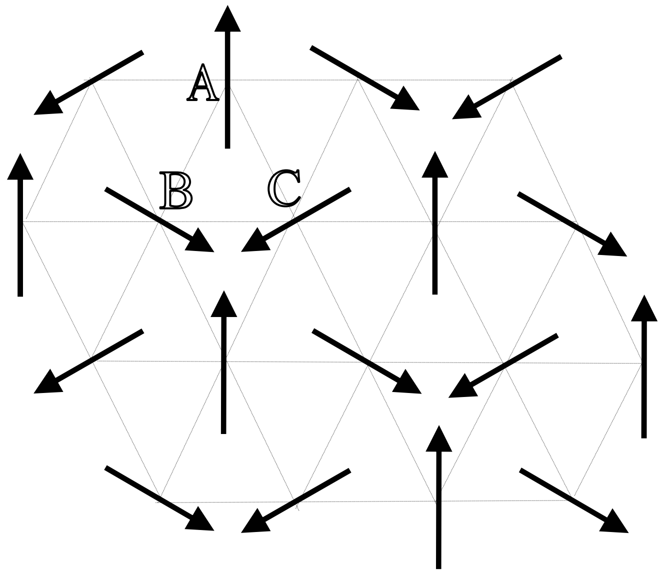
Ground state of a triangular antiferromagnet



In 1973 P. W. Anderson proposed a
Resonant Valence Bond State (RVB)

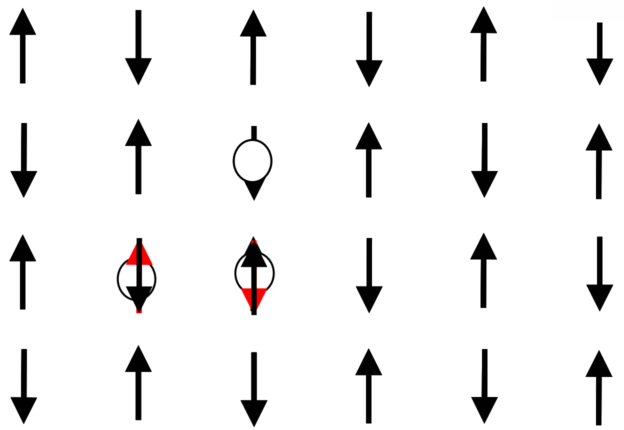
 $= \frac{1}{2}\left[\left|\uparrow\downarrow\right\rangle - \left|\downarrow\uparrow\right\rangle\right]$

…but the ground state is a “simple” semiclassical **120° Néel order**
(Bernu at al, PRL ’92,
Trumper et al, PRL ’99)



A single hole dynamics in an antiferromagnet

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

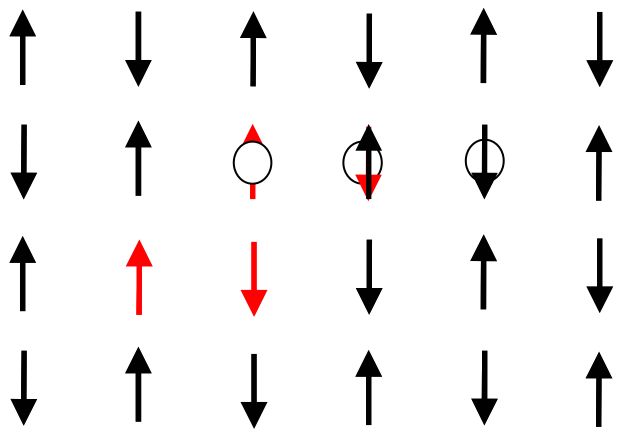


"wrong" spin

The hole can move only by disturbing the antiferromagnetic background

If J >> t then $\tau_{exch} \sim 1/J << \tau_{hopp} \sim 1/t$

→the hole can propagate "easily"



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

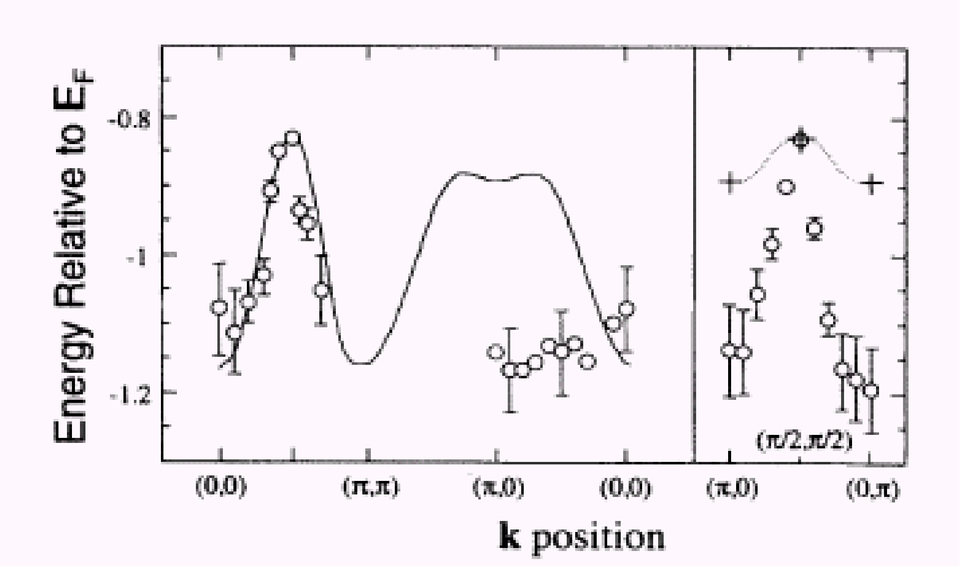
If J << t then $\tau_{exch} >> \tau_{hopp}$

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

In the square lattice antiferromagnet the spin polaron is always well defined (Martinez & Horsch PRB '91, Dagotto RMP '94).

ARPES seems to confirm this picture, e.g. $Sr_2CuO_2Cl_2$

(Wells et al, PRL '95)



How does the frustration affect the hole dynamics?

Let's look what happens when a hole is doped in an antiferromagnet on a triangular lattice

Model and method

We use the *t-J* model in local spin quantization axis, assuming a 120° Néel 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 non-collinearity)

Free magnon energy

hole-magnon interaction

Model and method (contd.)

$$\epsilon_{\mathbf{k}} = -3t\gamma_{\mathbf{k}} \qquad \gamma_{\mathbf{k}} = \tfrac{1}{3}\Sigma_{\mathbf{e}}\cos(\mathbf{k}\cdot\mathbf{e})$$

half of the tight-binding energy dispersion in the triangular lattice

$$\omega_{\mathbf{q}} = \frac{3}{2}J\sqrt{(1-\gamma_{\mathbf{q}})(1+2\gamma_{\mathbf{q}})}$$

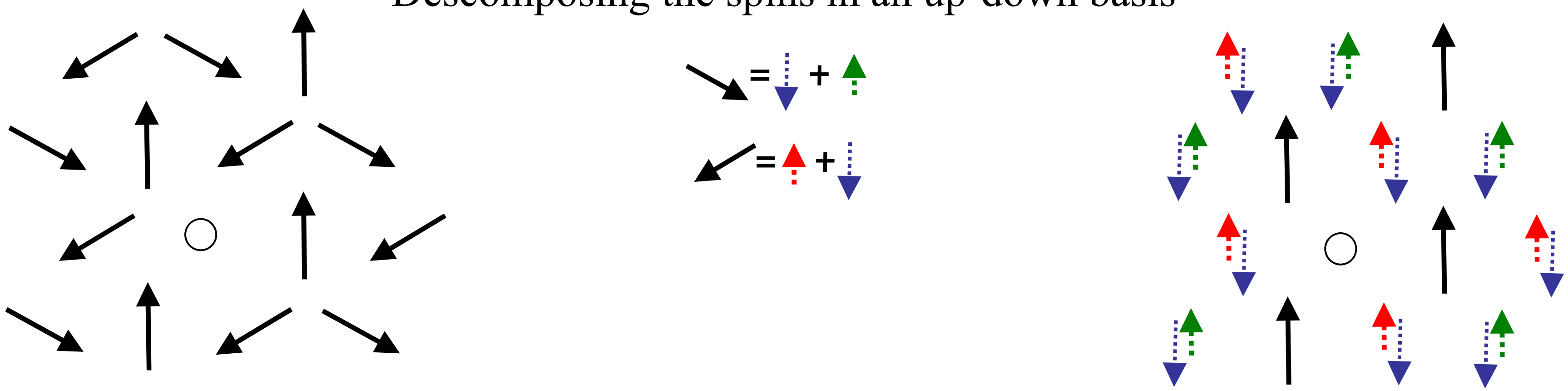
spin wave dispersion

$$M_{\mathbf{kq}} = i(\beta_{\mathbf{k}}v_{-\mathbf{q}} - \beta_{\mathbf{k\text{-}q}}u_{\mathbf{q}}) \qquad \beta_{\mathbf{k}} = \Sigma_{\mathbf{e}}\sin(\mathbf{k}\cdot\mathbf{e})$$

hole-magnon vertex interaction

u and v are the usual Bogoliubov coefficients

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

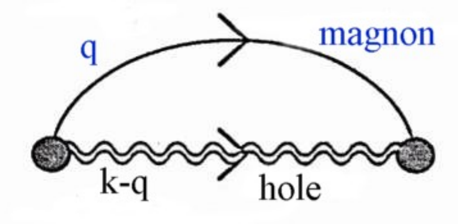
Free hopping: no absorption or emission of magnons (due to the non-collinearity)

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

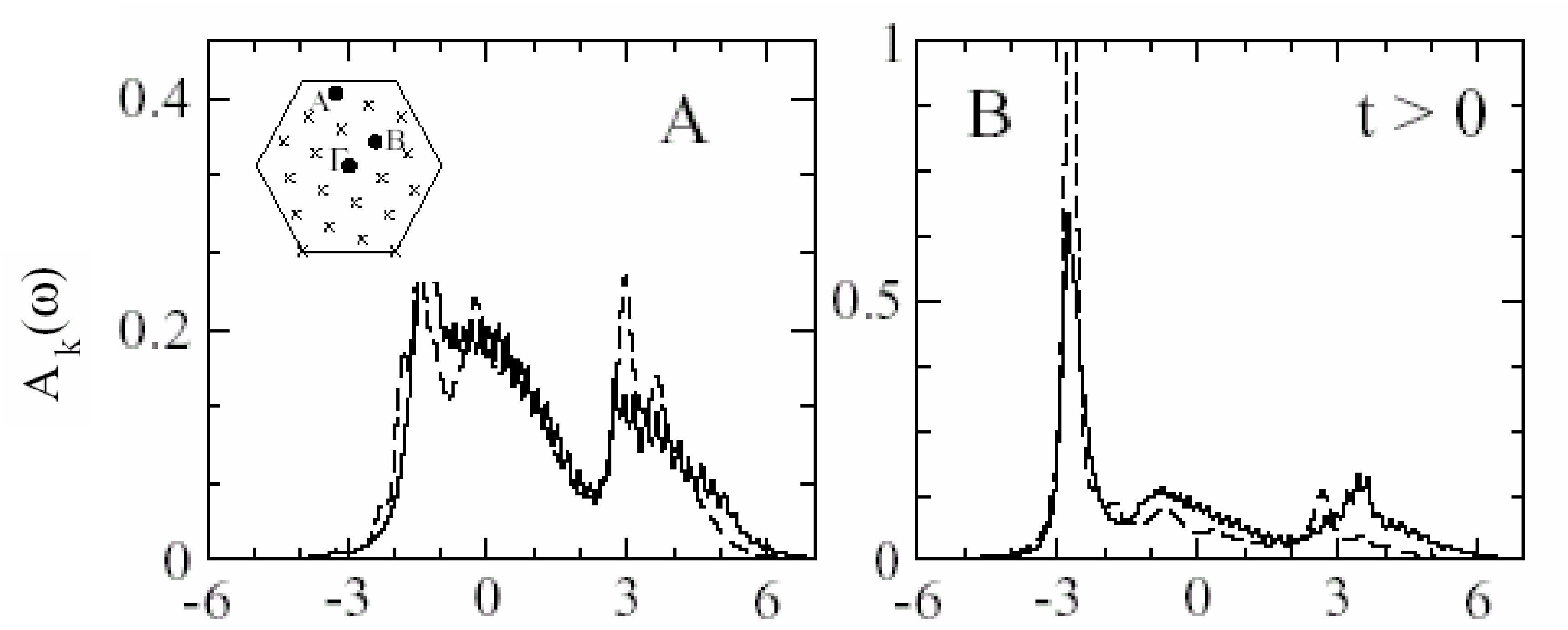
$$\Sigma_{\mathbf{k}}(\omega) = \frac{3t^2}{N_s} \sum_{\mathbf{q}} \frac{| M_{\mathbf{kq}} |^2}{\omega - \omega_{\mathbf{q}} - \epsilon_{\mathbf{k-q}} - \Sigma_{\mathbf{k-q}}(\omega - \omega_{\mathbf{q}})}$$

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



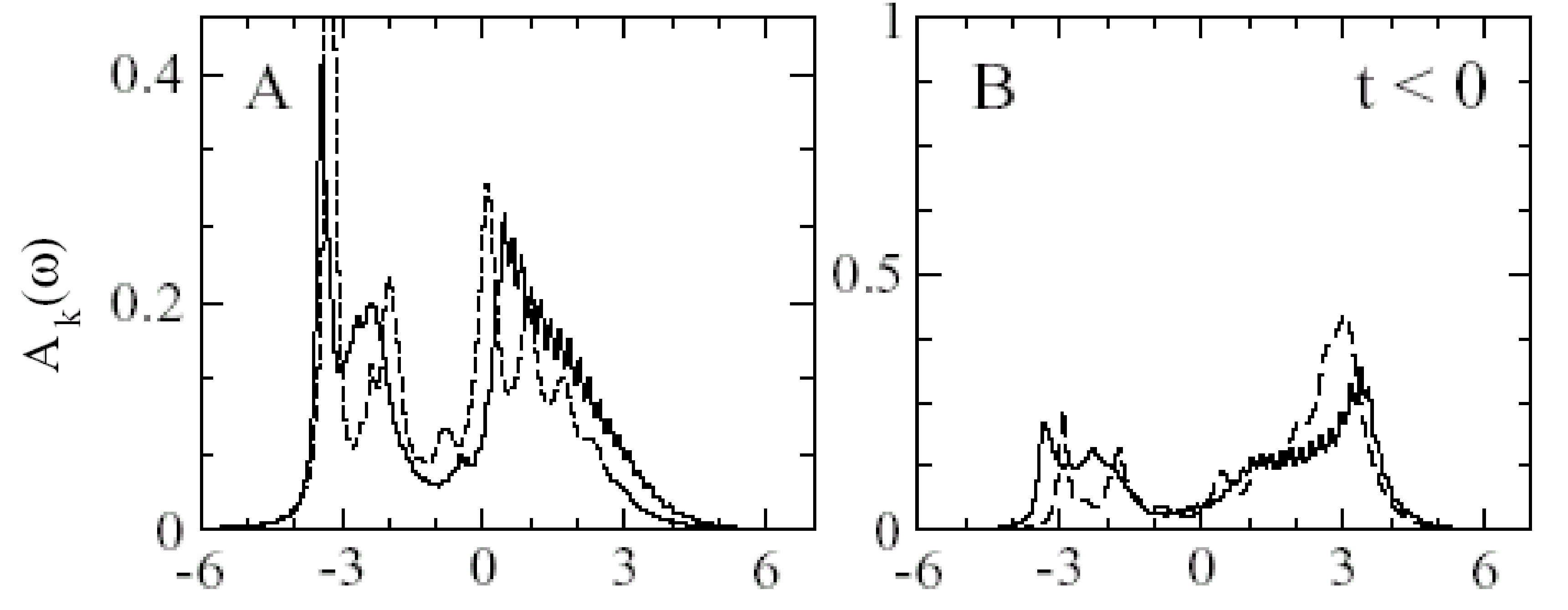
- **Positive t**
- **J /t=0.4 → strong coupling regime**

———————— **Lanczos**

_ _ _ _ _ _ _ _ **SCBA**

SCBA vs exact results

N = 21 sites

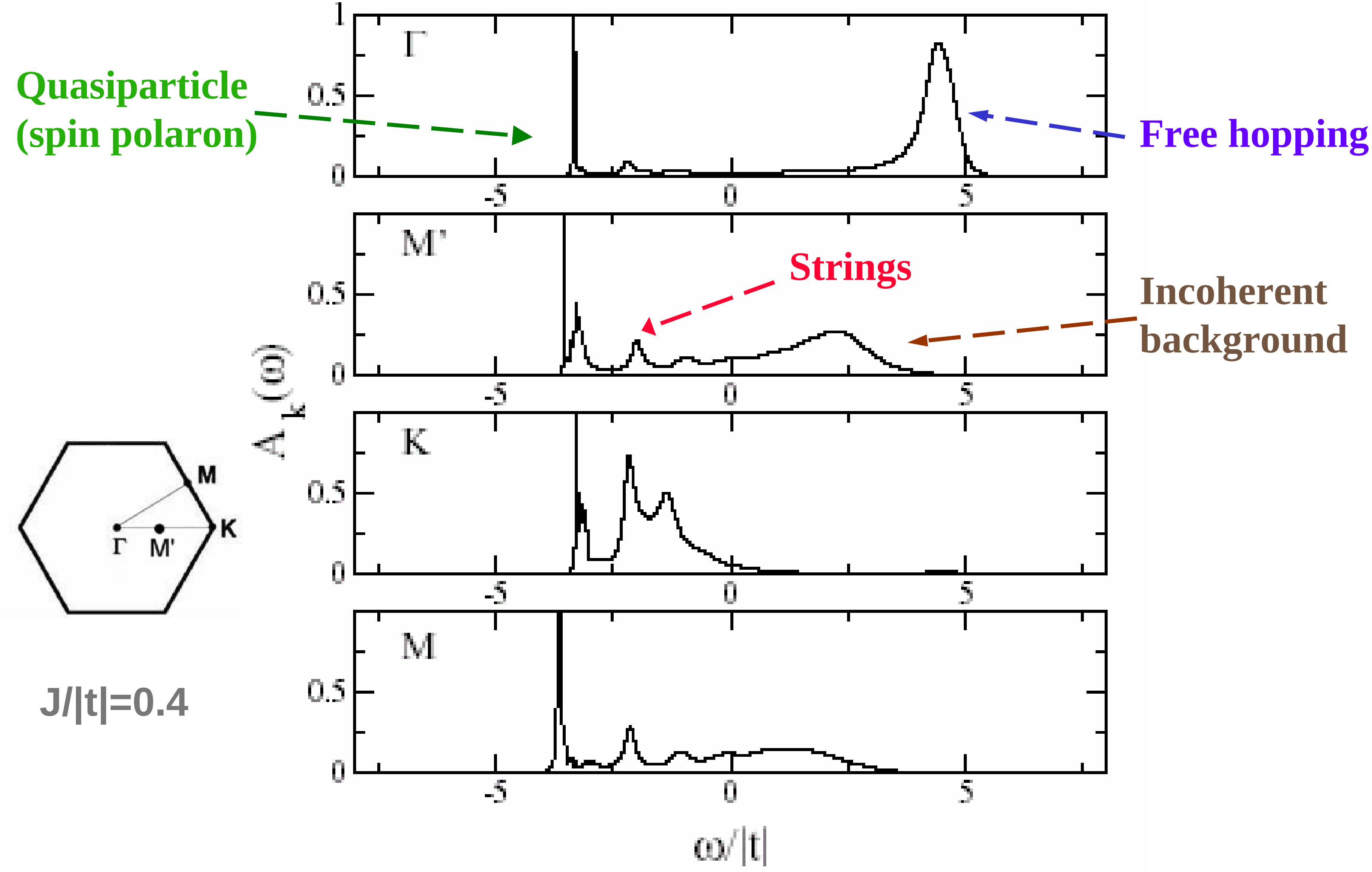


- **Negative t**
- **J /|t|=0.4**

___________ **Lanczos**

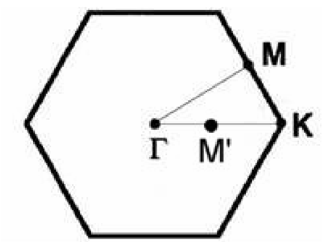
_ _ _ _ _ _ _ **SCBA**

Hole spectral functions: negative *t*

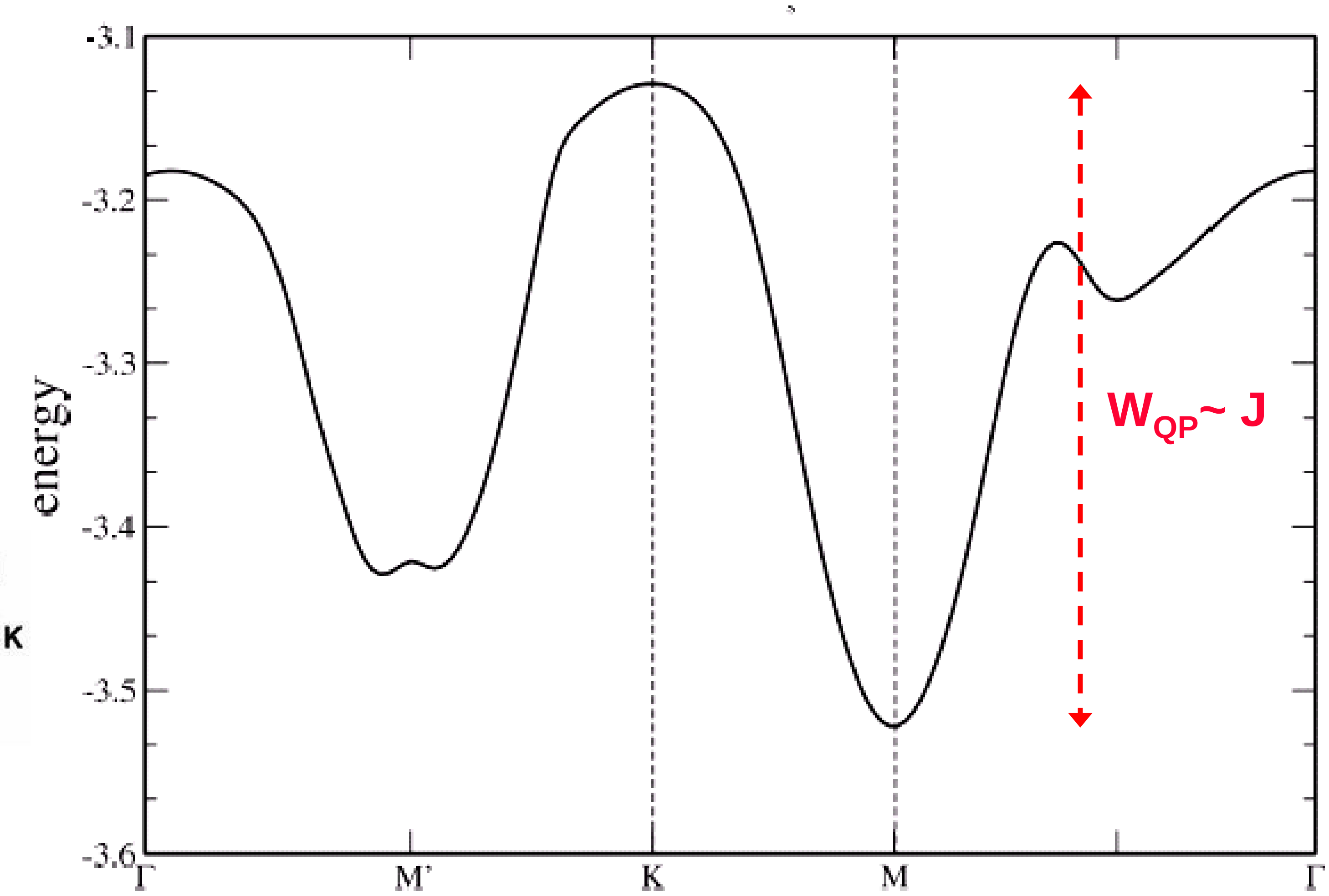


J/|t|=0.4

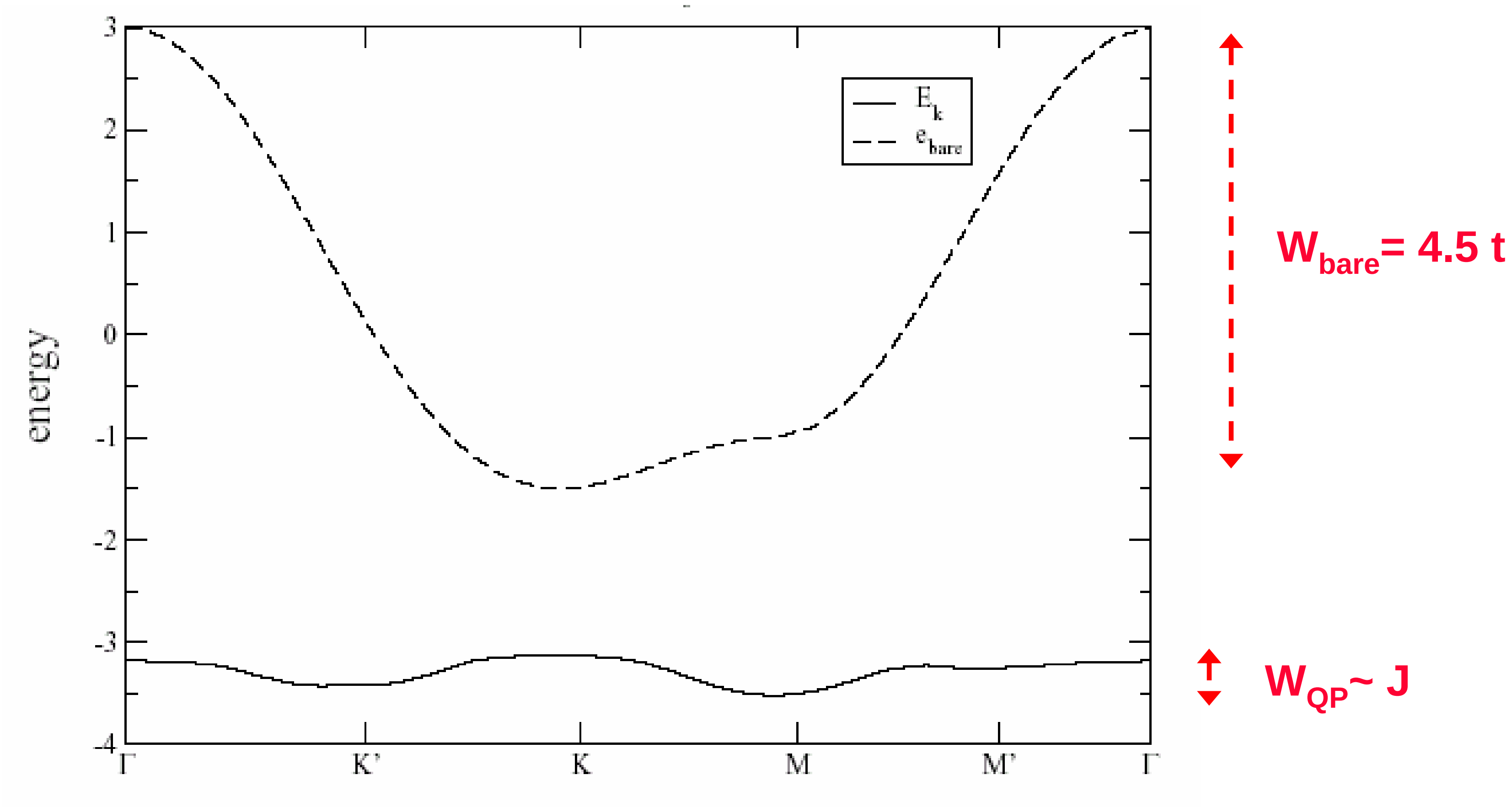
Quasiparticle energy dispersion: negative *t*



J/|t|=0.4



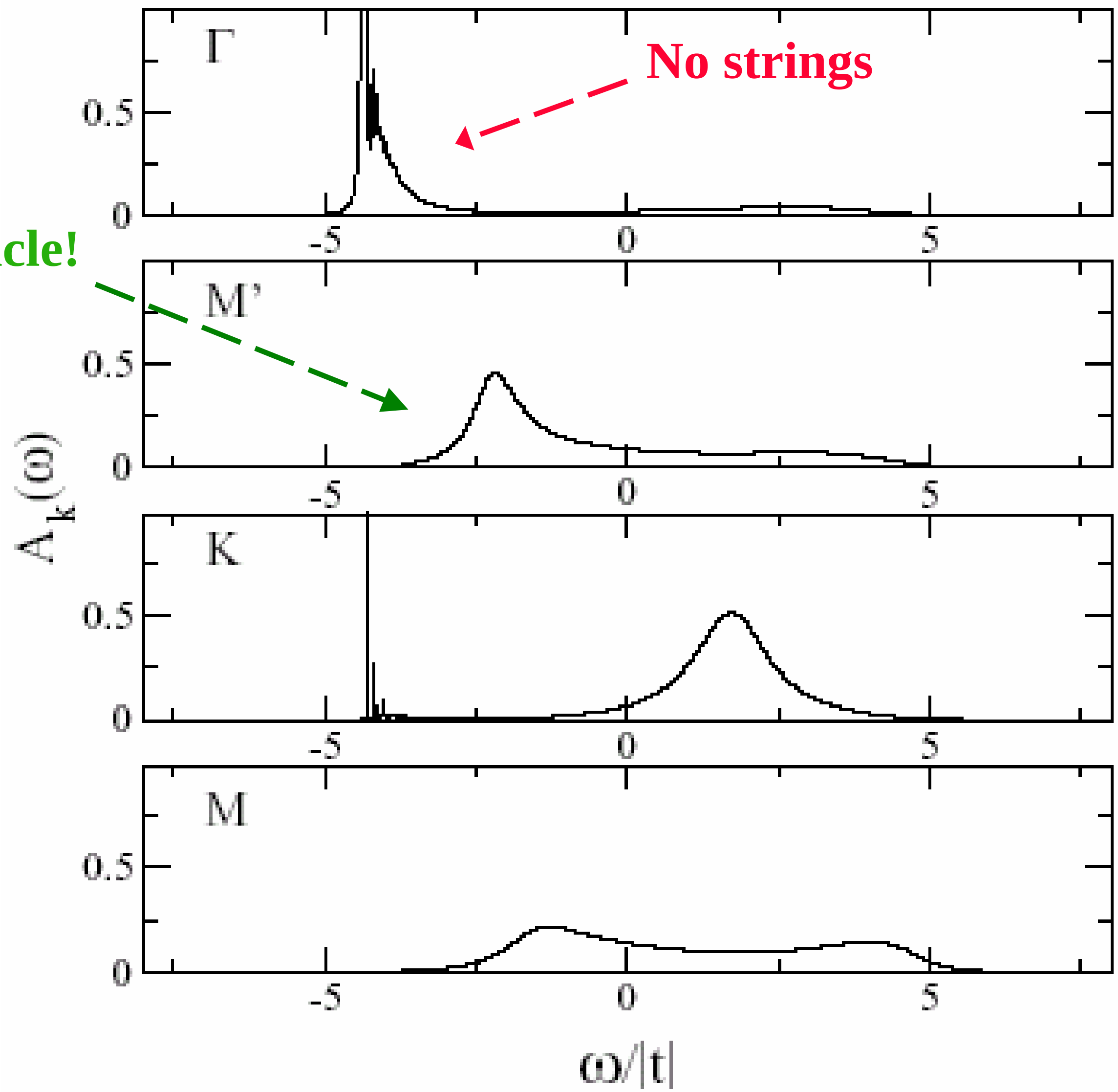
Quasiparticle energy dispersion

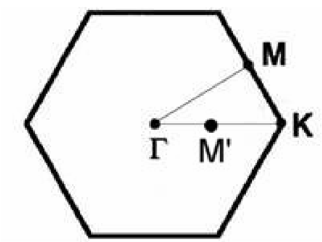


Hole spectral functions: positive *t*

No strings

No quasiparticle!

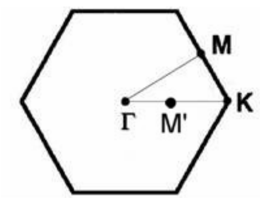


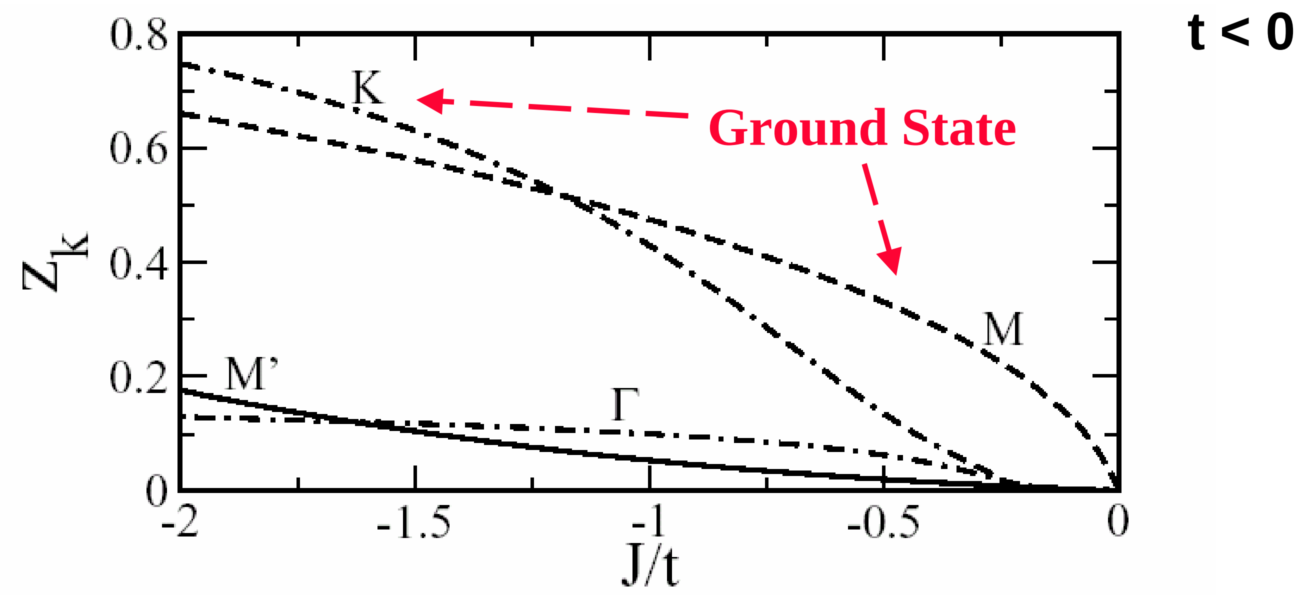


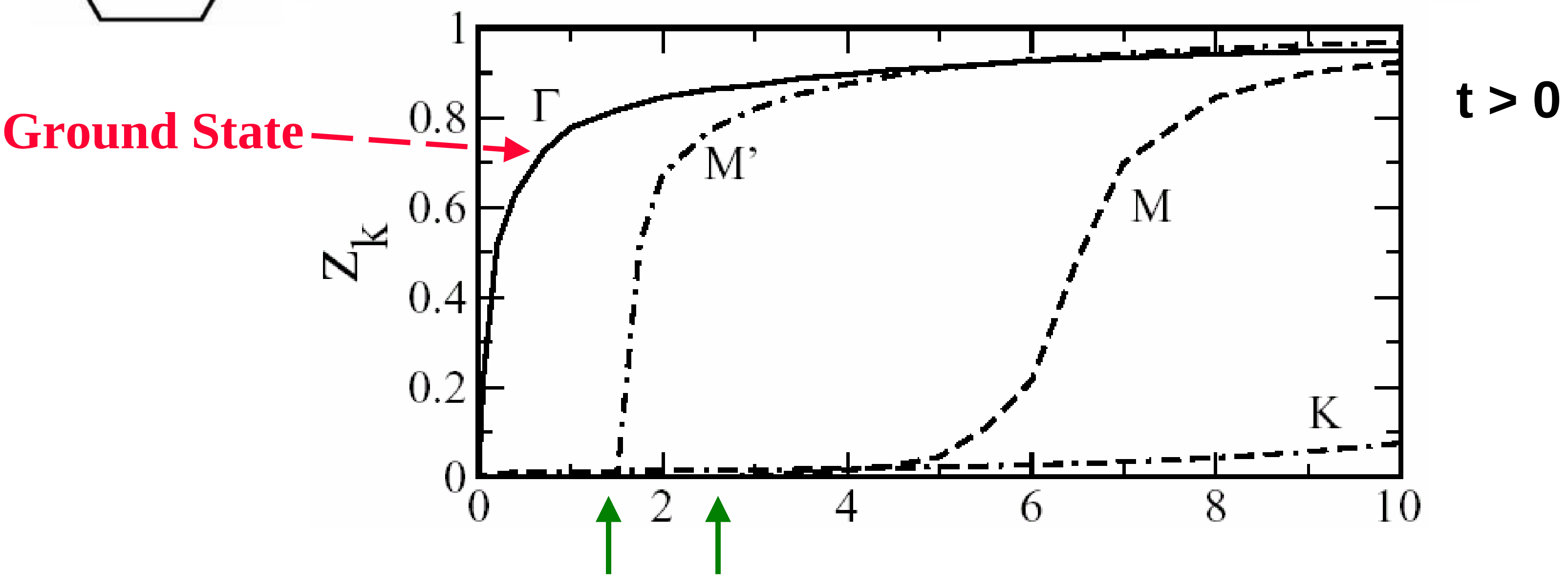
J/t=0.4

Sign reversal of *t* is not trivial!

Quasiparticle weight vs J/t

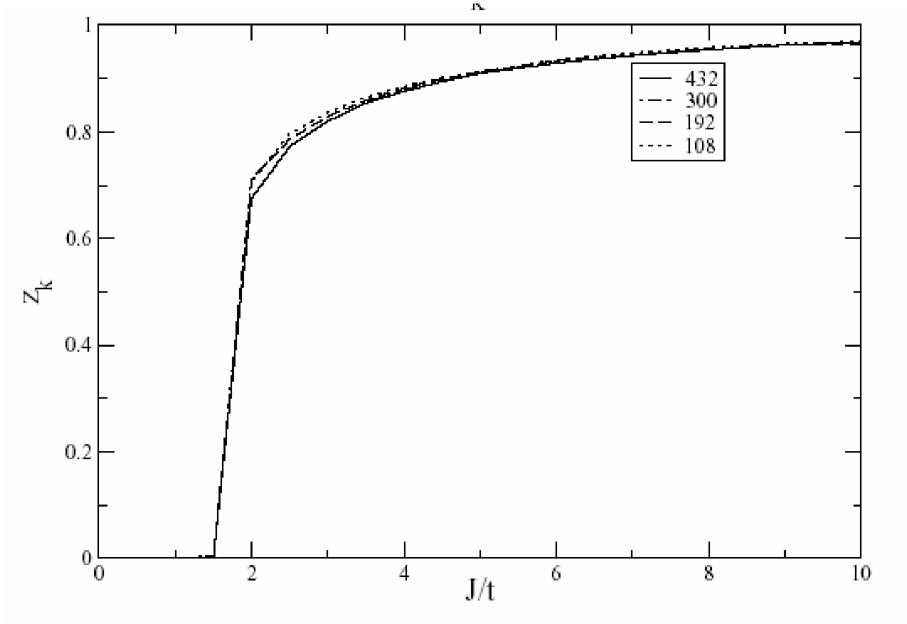




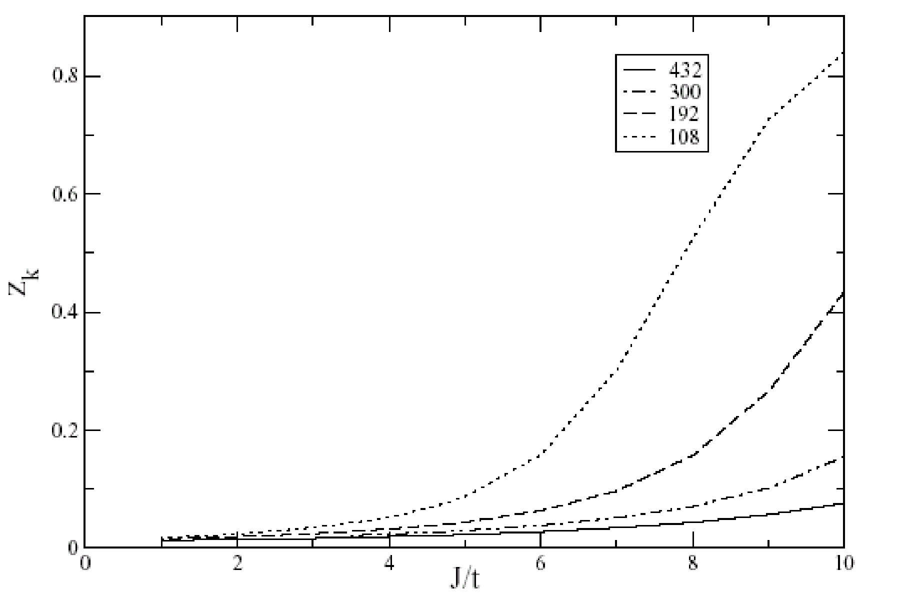


Quasiparticle weight: finite size effects

M’



K

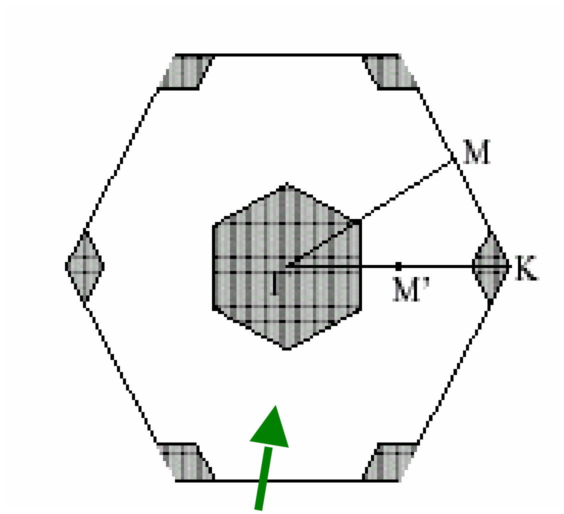


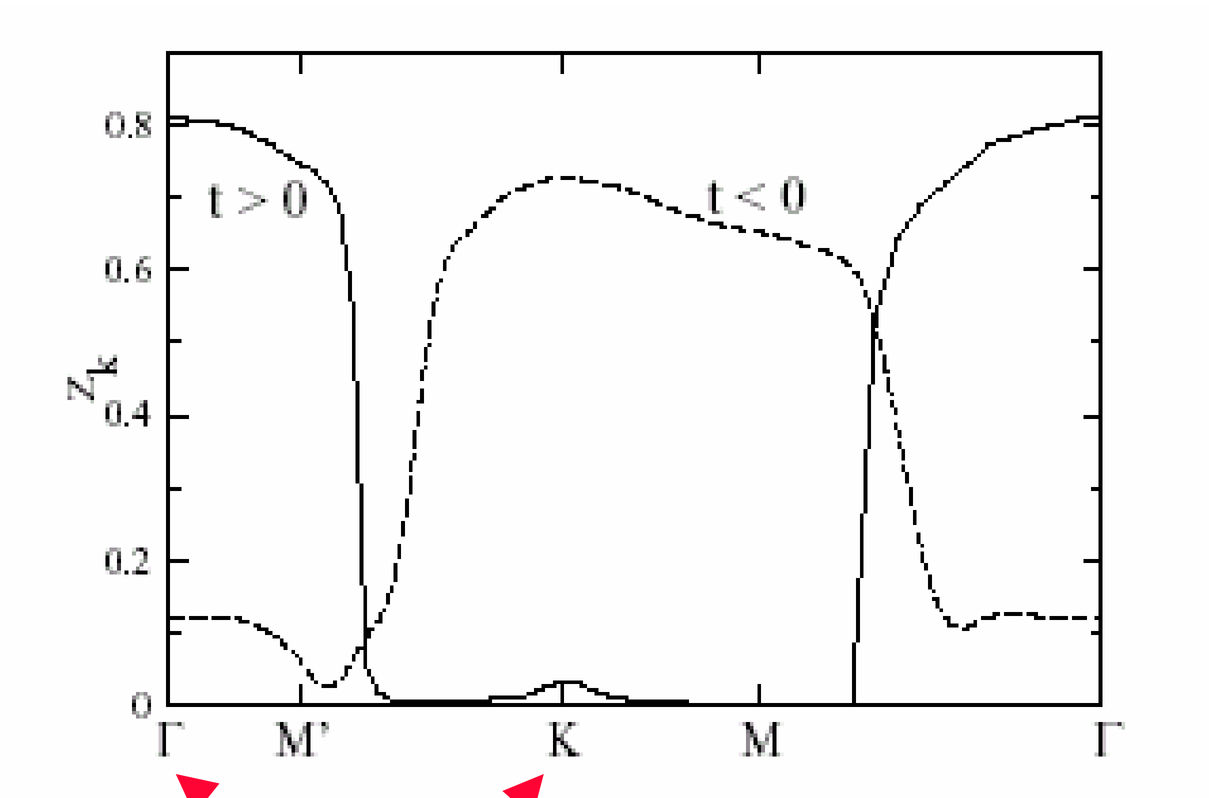
For positive t and in the weak coupling regime there are very strong finite size effects for momenta around the magnetic wave vector K

Momentum dependence of the quasiparticle weight

J/|t| = 2.0

J/t = 0.4

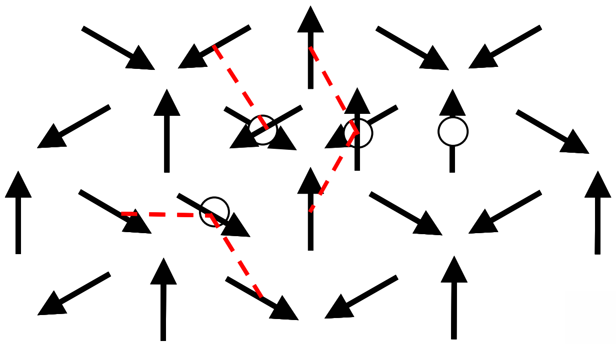




no quasiparticle

Goldstone modes

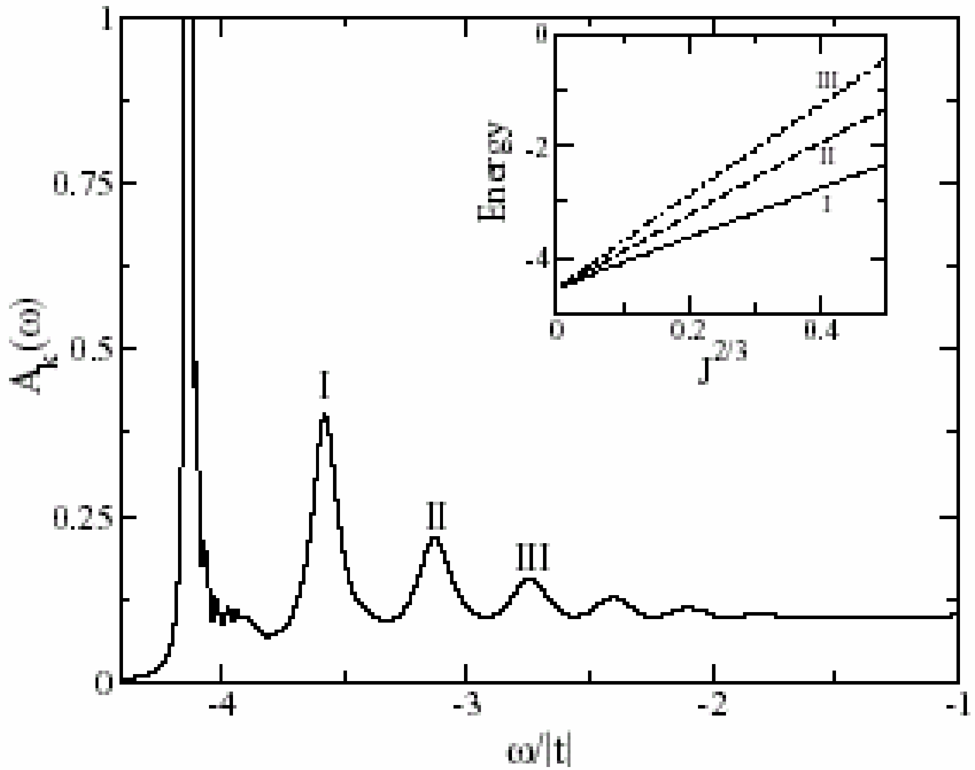
Strings excitations: Only for negative *t* !



For J < |t| there will be a lot of "wrong" strings, leading to long lived resonances

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

Like a particle bounded by a linear potential



Quasiparticle energy scaling with J/t

For an antiferromagnetic spin polaron $E_{qp} \sim (J/t)^{2/3}$

For a ferromagnetic spin polaron ("ferron") $E_{qp} \sim (J/t)^{1/2}$

In the thermodynamic limit we have found

- **$t < 0$ → $E_{qp} \sim (J/t)^{0.64}$ → enhanced local AF environment around the hole**
- **$t > 0$ → $E_{qp} \sim (J/t)^{0.54}$ → enhanced ferromagnetic environment**

…while for small cluster sizes (N < 21) we have found the opposite behaviour, as in Koretsune & Ogata, PRL'02.

Quasiparticle wavefunction

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

↑ bare hole ↑ one magnon ↑ multi-magnon

We solve the Schrodinger equation for the spin polaron in the retraceable paths approximation **[Ramsak & Horsch PRB'93, Reiter PRB'94]**

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

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

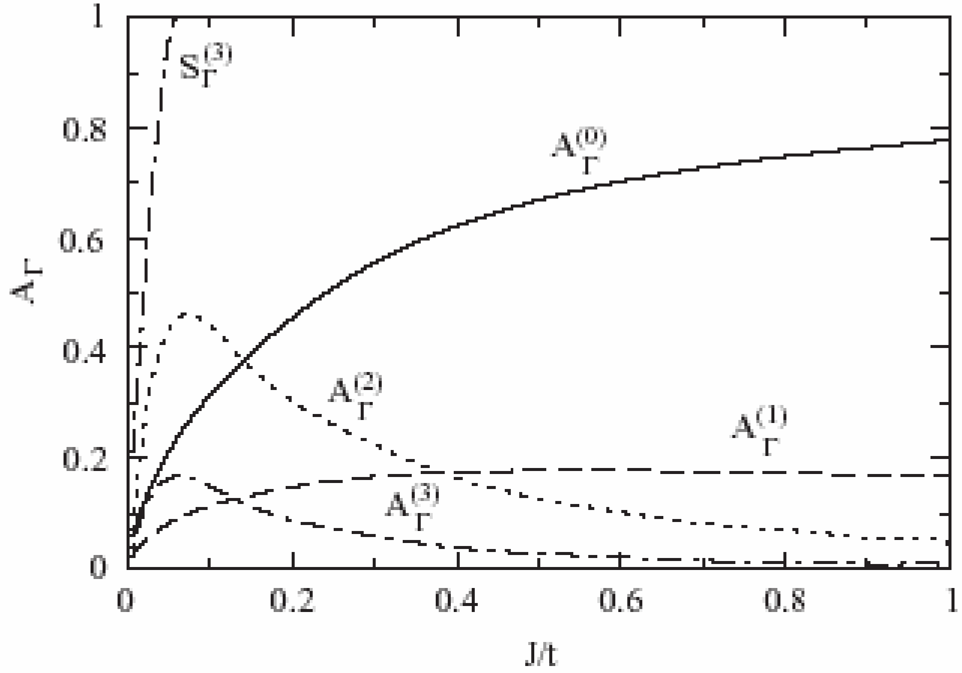
↑ **weight of the *n*-magnon contribution**

In particular → $A_{\mathbf{k}}^{(0)} = \langle\Psi_{\mathbf{k}}|h_{\mathbf{k}}^{\dagger}|AF\rangle \equiv z_{\mathbf{k}}$

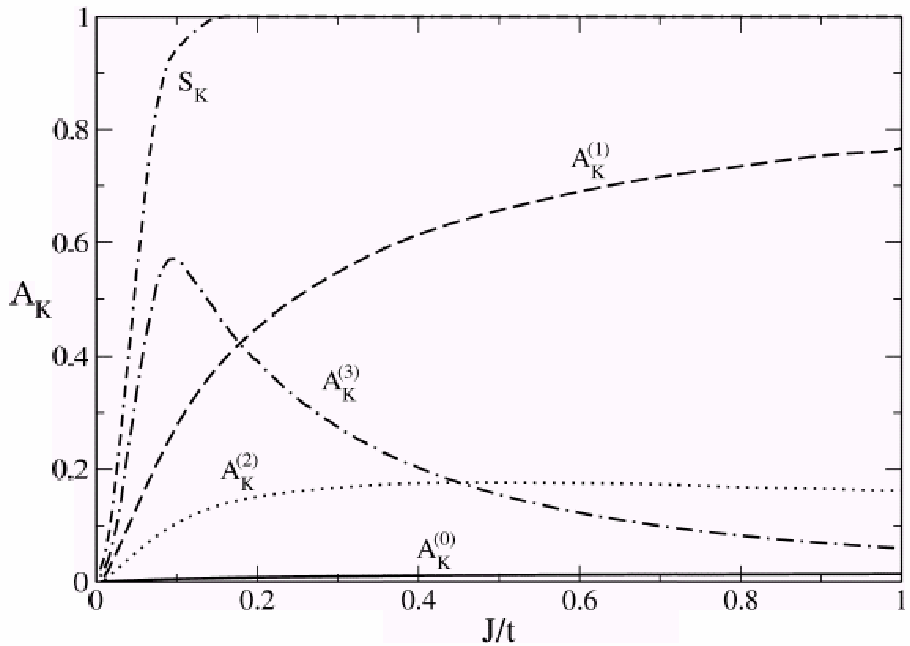
How many magnons?

Positive *t*

Three magnons are enough!

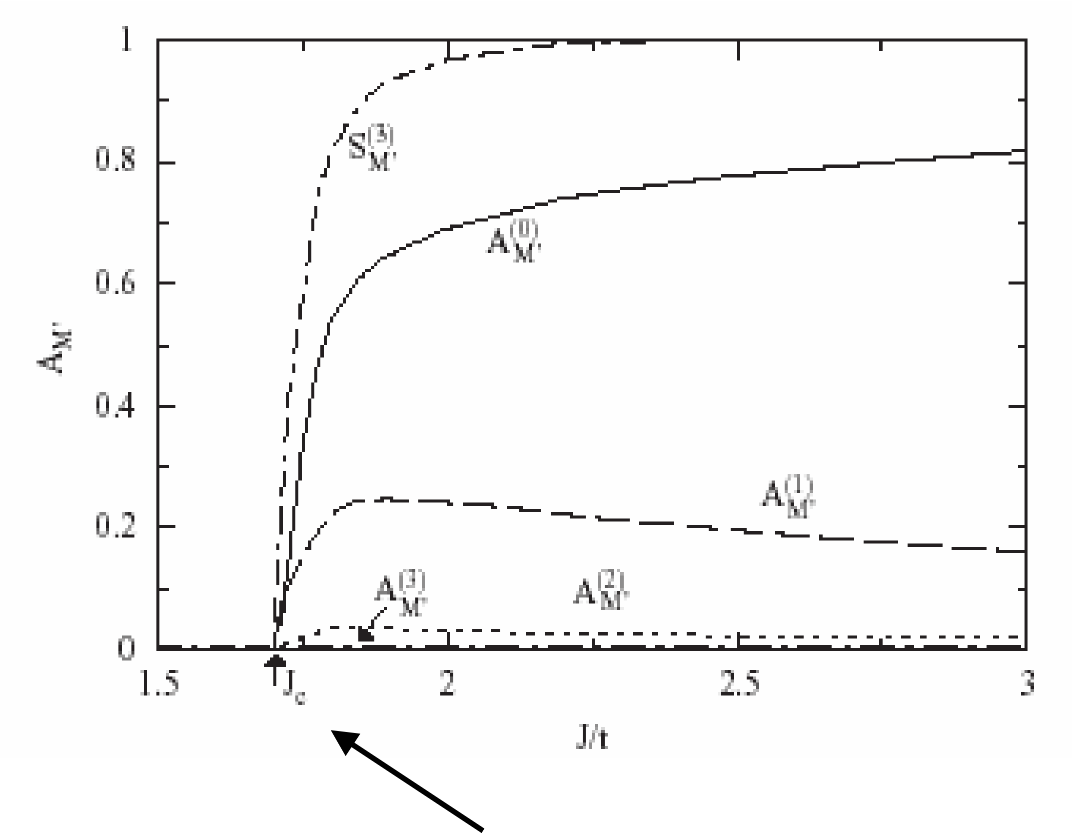


One magnon even for J >> t



$$S_{\mathbf{k}}^{(n)} = \sum_{m=0}^{n} A_{\mathbf{k}}^{(m)}$$

How many magnons?



Magnon proliferation even for a relative large J/t!

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 triangular topology: organic salts (BEDT-TTF)-X, cobaltates, silicon surfaces, etc, etc. Our findings could be of revelance for these compounds.**