Spin-charge separation in doped 2D frustrated quantum magnets

Didier Poilblanc

Laboratoire de Physique Théorique, UMR5152-CNRS, Toulouse, France

Outline

1. Disordered state in frustrated magnets
2. Lanczos methods & ARPES
3. Spin-charge separation in single hole dynamics ?
4. New results for the J_1-J_2-J_3 model

(Exotic superconductivity in VBS host)

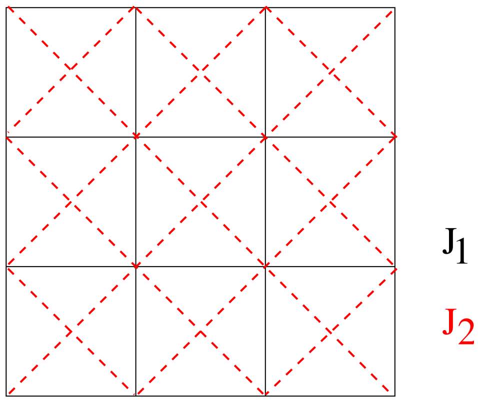
Collaborations and references

- Single hole dynamics
  A. Läuchli & DP, PRL **92**, 236404 (2004)
- On the J_1-J_2-J_3 model: ongoing work with
  A. Läuchli, M. Mambrini & F. Mila
- Other work: doped Shastry-Sutherland lattice
  P W. Leung, PRB **69**, 180403 (2004)
- Pairing in VBS host
  DP, PRL **93**, 197204 (2004)

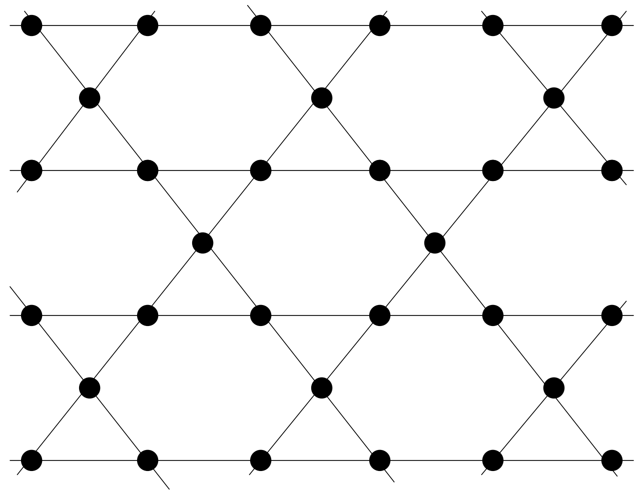
2D Frustrated magnets

Lattices with AF frustrating interactions

Melzi et al., PRB **85**, 1318 (2000)



frustrated square lattice (S=1/2): Li_2VOSiO_4



Kagome lattice like $SrCr_{9-x}Ga_{3+x}O_{19}$ (S=3/2)

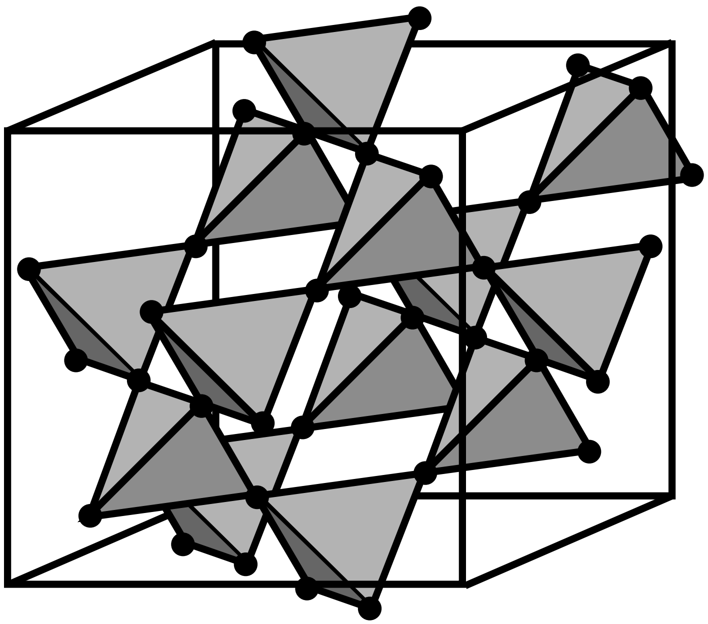
Ramirez et al., PRL **64** ('90)

Broholm et al., PRL **65** ('90)

Uemura et al., PRL **73** ('94)

3D Frustrated magnets

pyrochlores and spinels



Transition metal oxides

- $ZnCr_2O_4$ spinel
- $A_2Ti_2O_7$ titanates

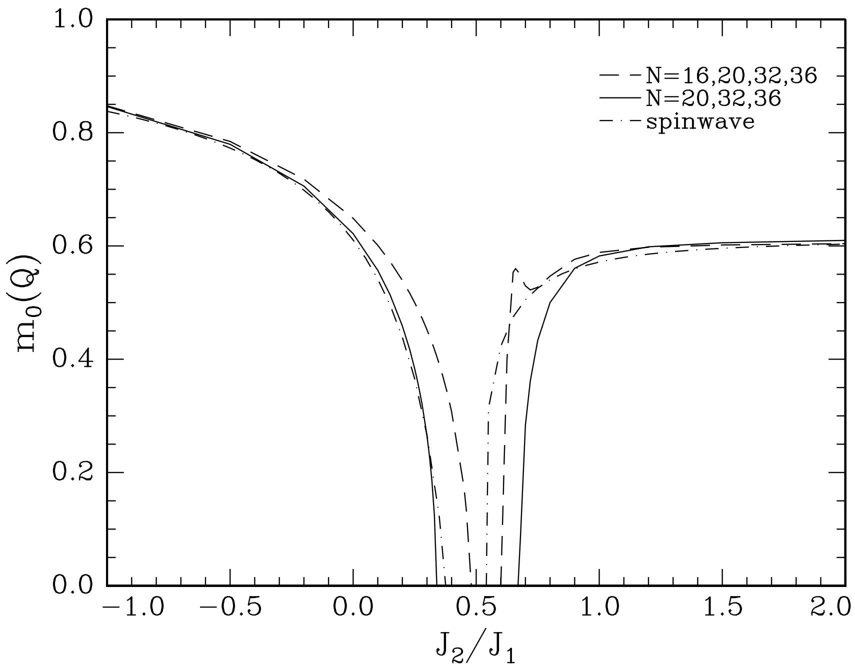
Ramirez et al., PRL 89, 067202 (2002)

-no ordering at low temperatures

-spin gap formation

Exotic disordered groundstates

Low-spin (S=1/2) $\Rightarrow$ strong quantum fluctuations



nature of disordered phases ?

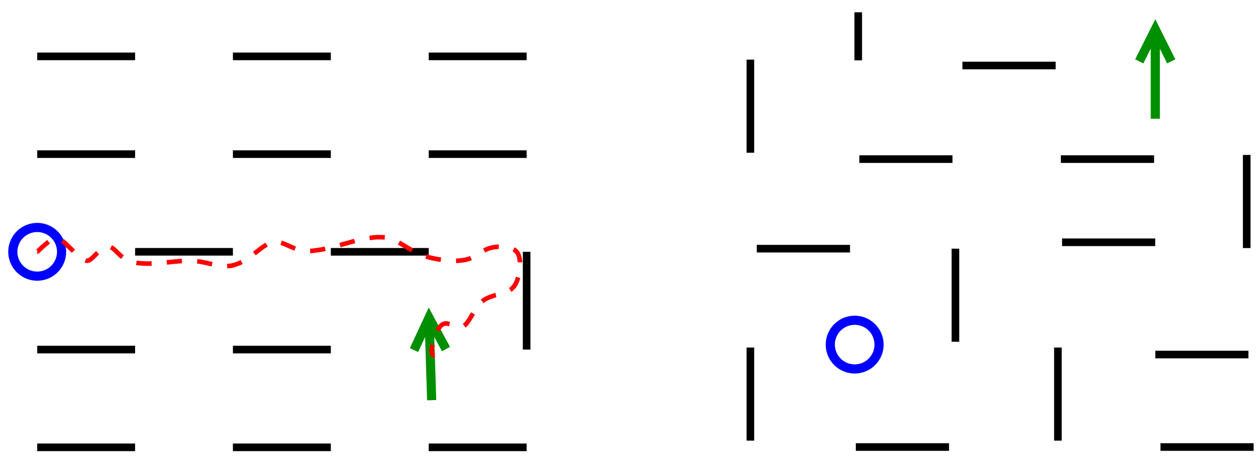
$\rightarrow$ many studies (and controversies !)

Misguich & Lhuillier, "*Frustrated spin systems*", Ed. H.T. Diep, World-Scientific (2003)

Schulz, Ziman & DP, "*Magnetic systems with competing interactions*", p120, Ed. H.T. Diep, W.-S.(1994)

Confinement vs deconfinement

Idea: use doping (or ARPES) to probe nature of the ground state



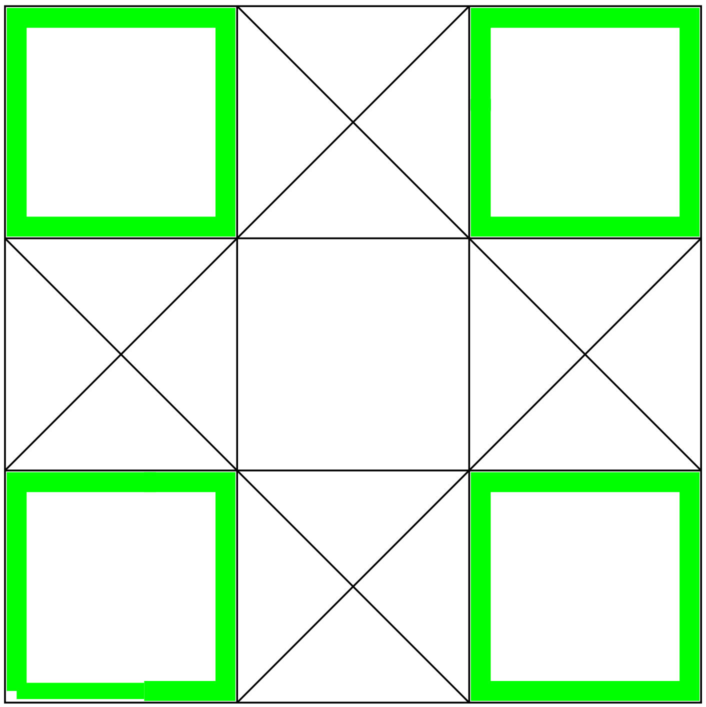
(a)

(b)

"string potential"

"deconfined" spinon

Checkerboard lattice: a Valence Bond Solid



2D array of corner-sharing tetrahedra: ”2D pyrochlore”

VBS phase (plaquette)

Fouet et al., PRB (2003)

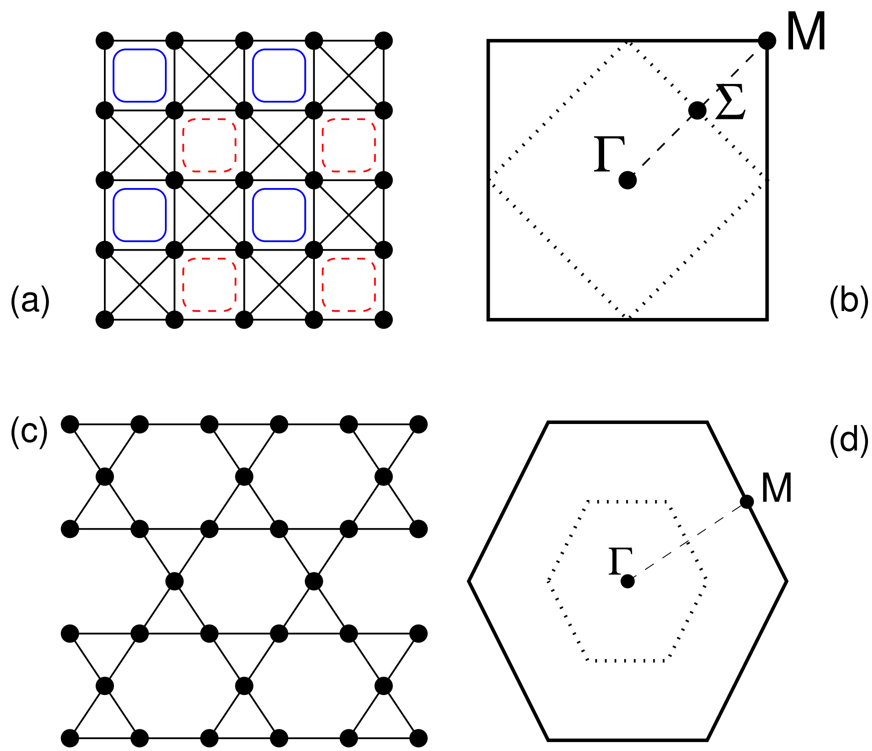
- Finite spin gap $\sim 0.6J$
- Translation symmetry breaking

1. $E_{\text{singlet}}(\mathbf{Q}=(\pi,\pi)) - E_0 \to 0$ when $N \to \infty$
2. $\langle \text{Plaq}_l \text{Plaq}_{l'} \rangle \to \text{finite}$ when $|l' - l| \to \infty$

Kagome: paradigm of a "spin liquid" (?)

- Magnetically disordered
  Leung & Elser PRB **47**, 5459 (1993)
- Small spin gap $\sim 0.05J$
  Lechemninant et al., PRB **56**, 2521 (1997)
- No symmetry breaking (neither SU(2) nor lattice symmetries)
- Large number of low energy singlets
  Waldtmann et al., EPJB **2**, 501 (1998)
  Mila et al., PRL **81**, 2356 (1998)

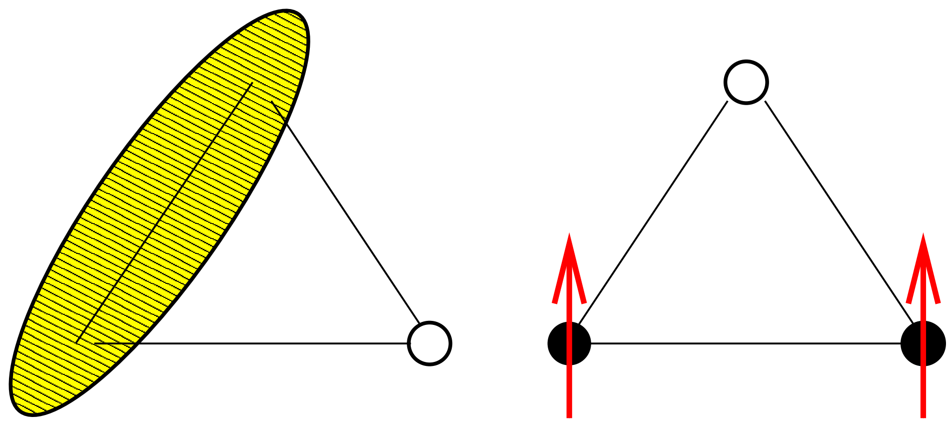
framework



$$H = -t \sum_{\langle i,j \rangle, \sigma} \mathcal{P} \left(c^{\dagger}_{i,\sigma} c_{j,\sigma} + \text{h.c.} \right) \mathcal{P} + J \sum_{\langle i,j \rangle} S_i \cdot S_j - \frac{1}{4} n_i n_j$$

Frustrated hole motion

$J \to 0$ limit



singlet triplet

$$t < 0 \qquad E = -|t| \qquad E = -2|t|$$

$$t > 0 \qquad E = -2t \qquad E = -t$$

Single particle Green-function

"time-ordered" Green's function $\rightarrow$ "electron" ($\omega < 0$) and "hole" ($\omega > 0$) parts

$$
\begin{aligned}
G(\mathbf{q},\omega) &= \langle N_e | c^{\dagger}_{-\mathbf{q},\sigma} \frac{1}{\omega - i\epsilon + H - E_{N_e-1}} c_{\mathbf{q},\sigma} | N_e \rangle \\
&+ \langle N_e | c_{\mathbf{q},\sigma} \frac{1}{\omega + i\epsilon - H + E_{N_e+1}} c^{\dagger}_{-\mathbf{q},\sigma} | N_e \rangle
\end{aligned}
$$

- half-filling: $N_e = N$, system size
- "hole" and "electron" parts related: $t \Leftrightarrow -t$
- Spectral fct $\mathrm{Im}\, G(\mathbf{q},\omega) \rightarrow$ IPES & ARPES

Dynamics within Lanczos ED

- Continued-fraction: $z = \omega + i\epsilon$, $A = c_{\mathbf{q},\sigma}$ or $A = c^{\dagger}_{-\mathbf{q},\sigma}$

$$G(z) = \cfrac{\langle \Psi_0 | A A^{\dagger} | \Psi_0 \rangle}{z + E_0 - \tilde{e}_1 - \cfrac{\tilde{b}_2^2}{z + E_0 - \tilde{e}_2 - \cfrac{\tilde{b}_3^2}{z + E_0 - \tilde{e}_3 - \ldots}}}$$

- Physical meaning:

$$I(\omega) = \sum_m |\langle \Psi_m | A^{\dagger} | \Psi_0 \rangle|^2 \delta(\omega - E_m + E_0)$$

1. poles and weights $\rightarrow$ dynamics of $A^{\dagger}$
2. symmetry of $A^{\dagger}$ $\rightarrow$ well defined quantum numbers & selection rules
3. ! calculation of eigen-states/vectors not required !

Static hole (checkerboard)

- Switch off t first $\Rightarrow$ already some insight !

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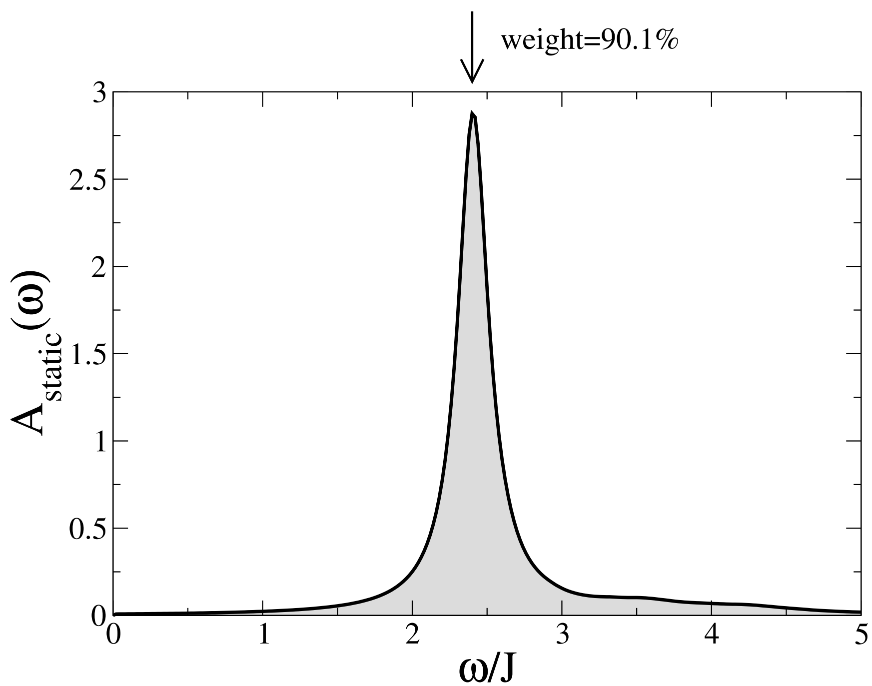

Overlap

$$Z = |\langle \Phi_{1h} | c_{i,\uparrow} | \Phi_{0h} \rangle|^2$$

finite

on checkerboard lattice

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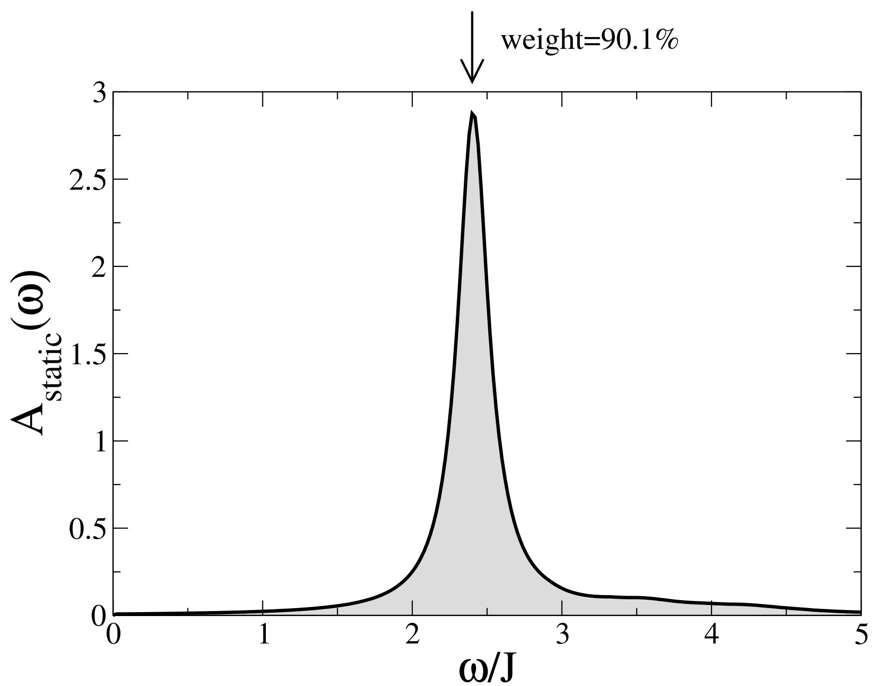

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Similarity with 1D spin-Peierls g.s.

$\Rightarrow$ confining potential between "holon" and "spinon"

Static hole (Kagome)

- Static correlations: Dommange et al., PRB 68, 224416 (2003)
- Dynamic correlations: $Z = |\langle \Phi_{1h} | c_{i,\uparrow} | \Phi_{0h} \rangle|^2 \simeq 0$

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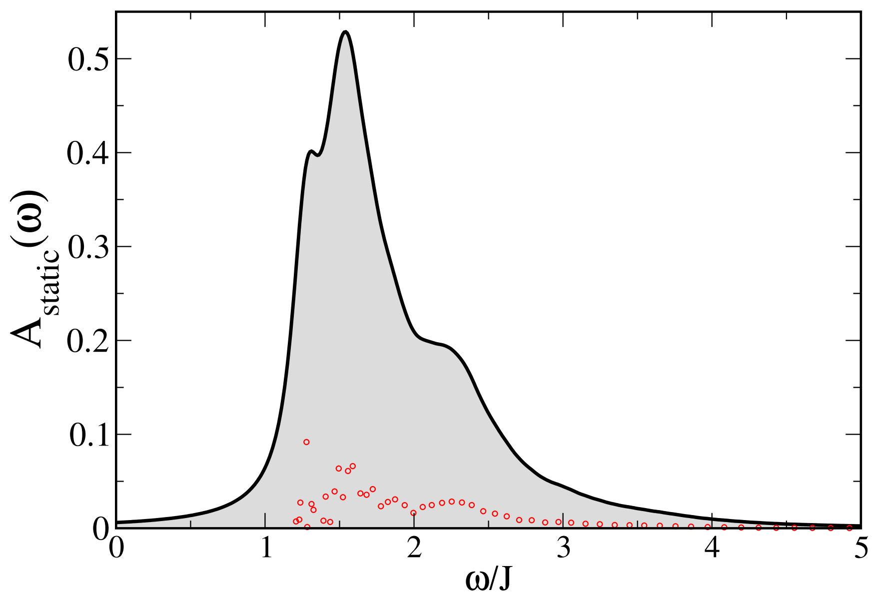

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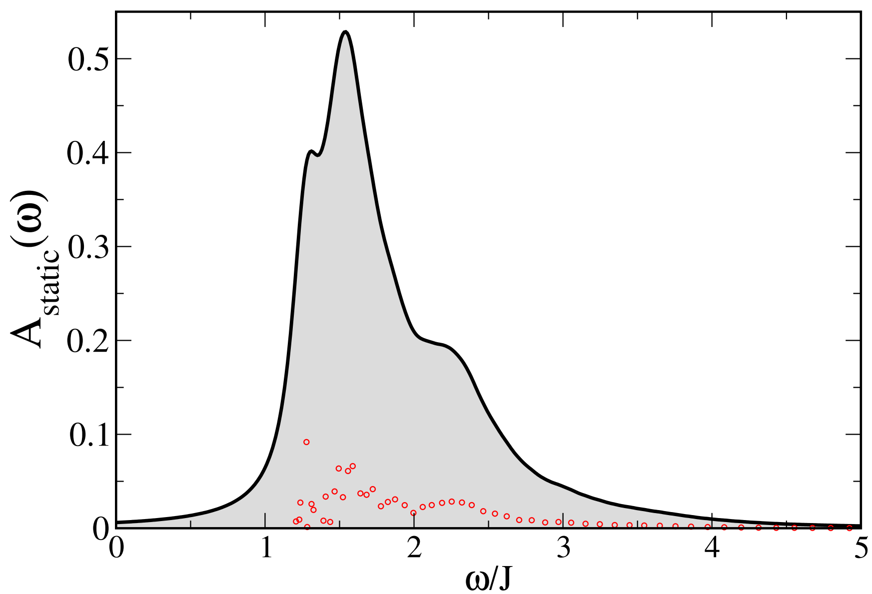
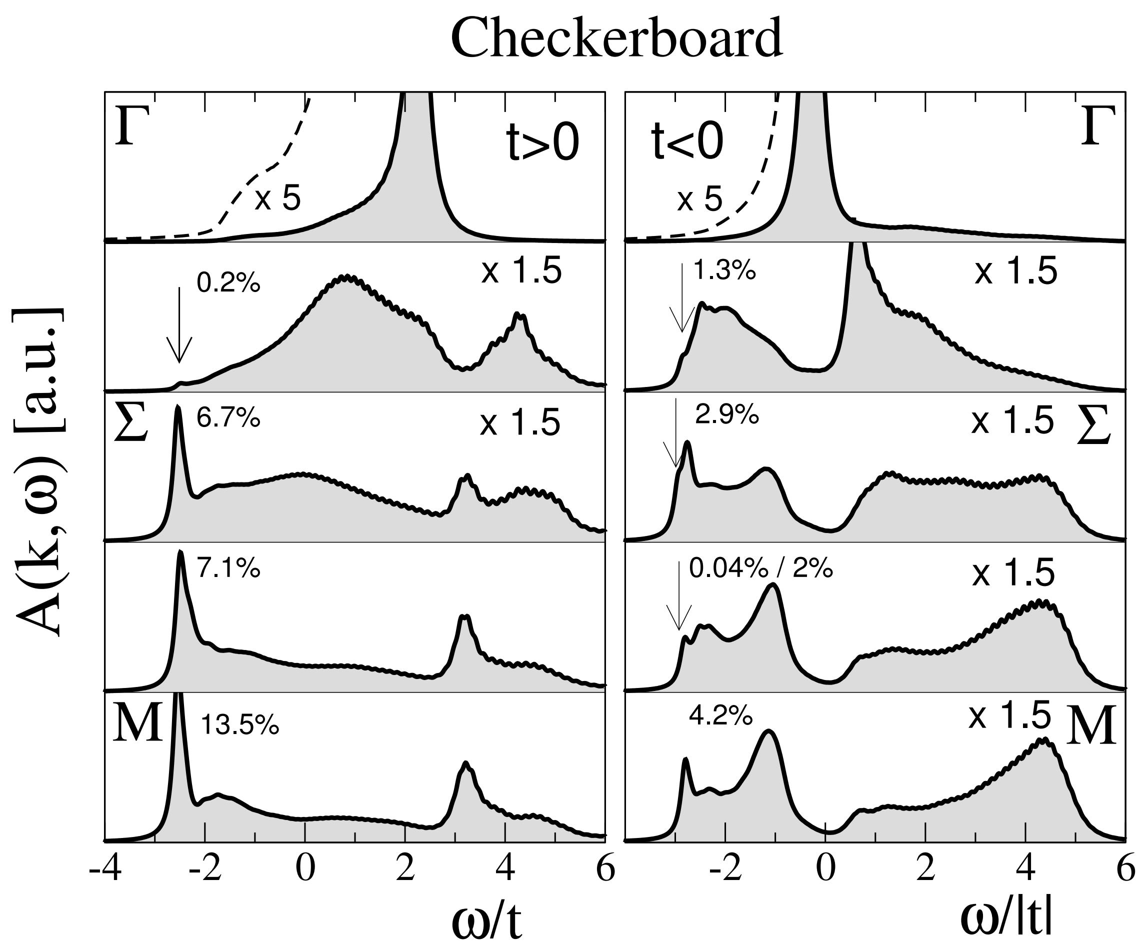


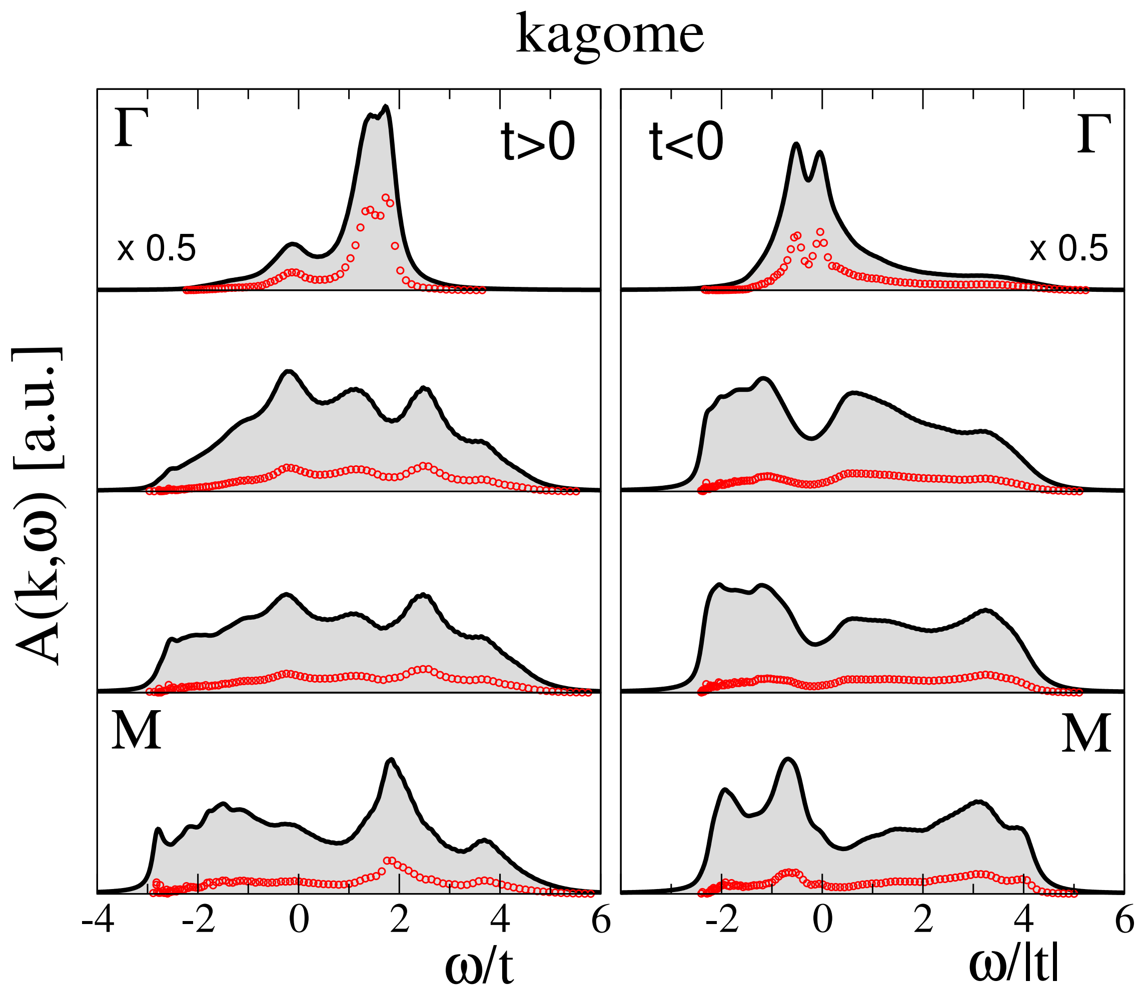
Incoherent spectrum

Weights distributed on many poles even at low energies

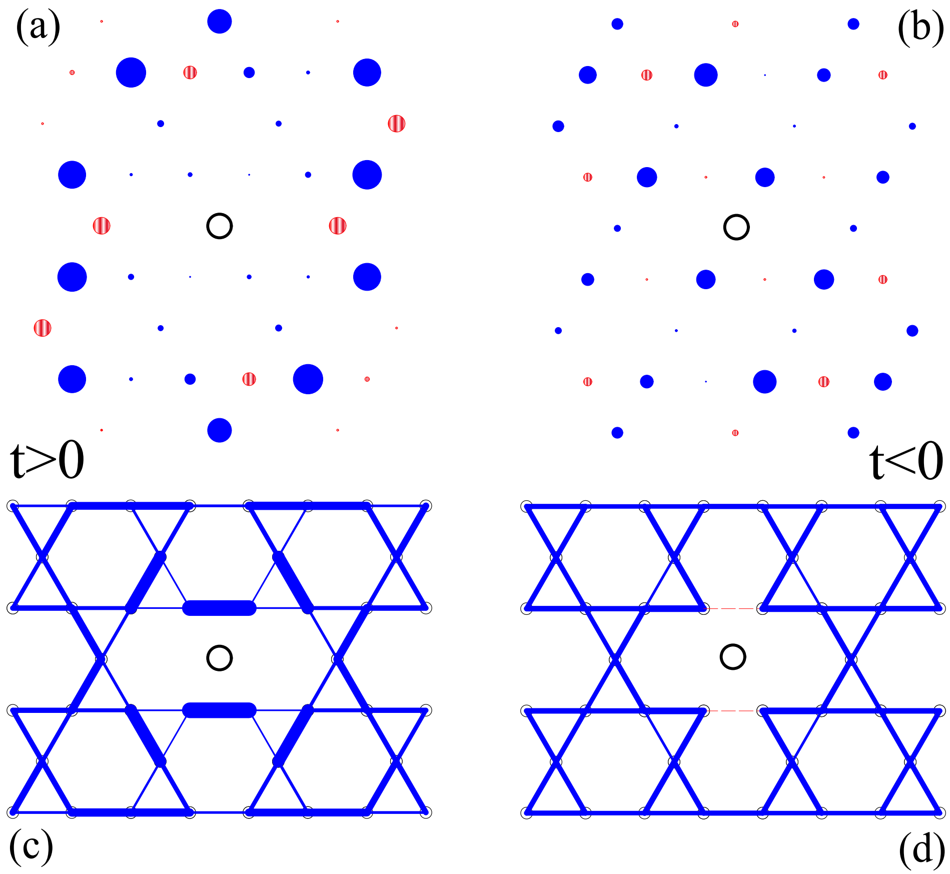
Hole dynamics in the VB Solid



Single hole doped in a spin liquid



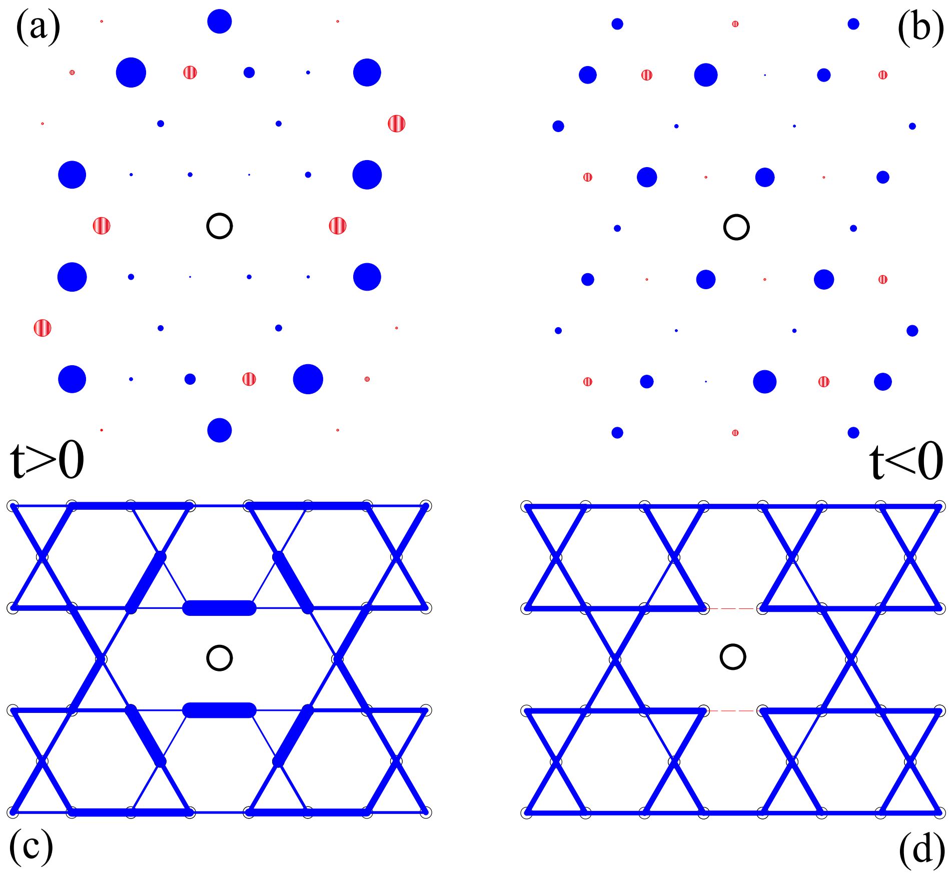
spin & charge repel !



⇐ Hole-spin correlations

Dimer correlations in "Holon" wavefct

spin & charge repel !

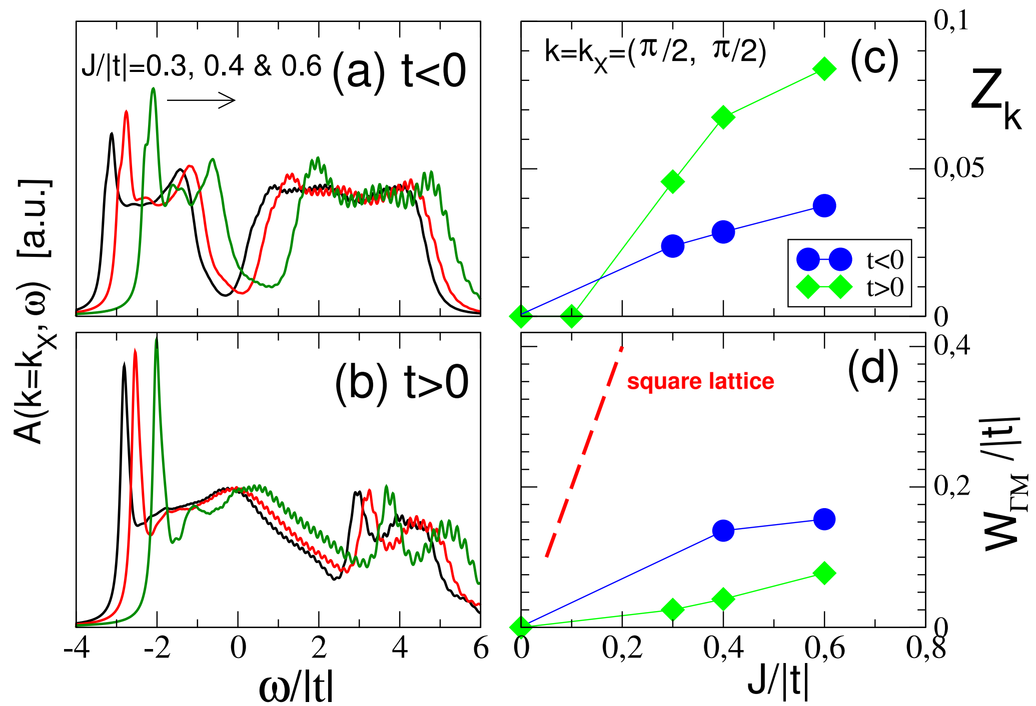


⇐ Hole-spin correlations

Dimer correlations in "Holon" wavefct

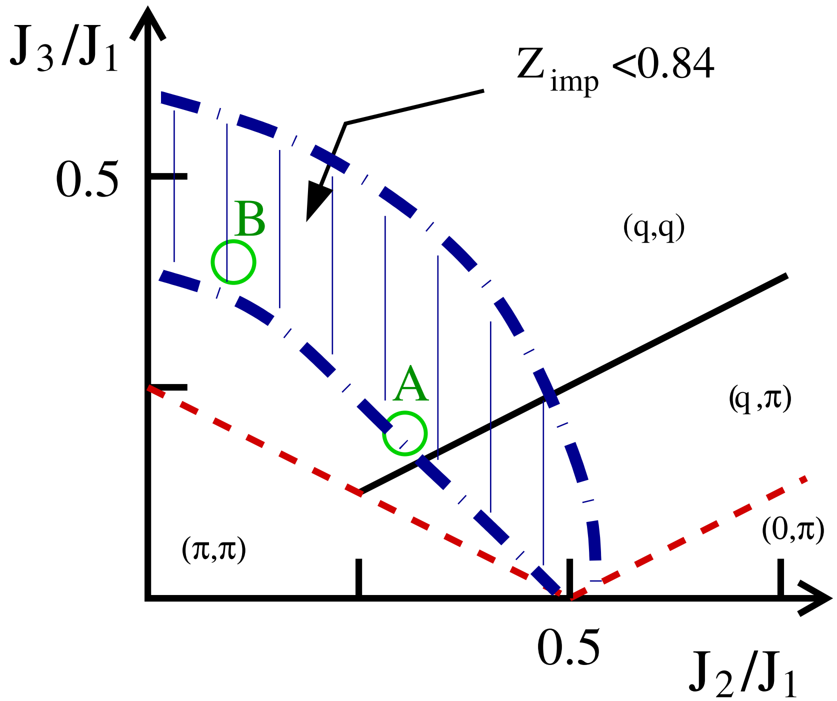
Spin & charge separation: holon benefits from large dimer correlations in neighboring triangle (like static case: see e.g. Dommange et al, PRB)

Hole localisation in the VBS host



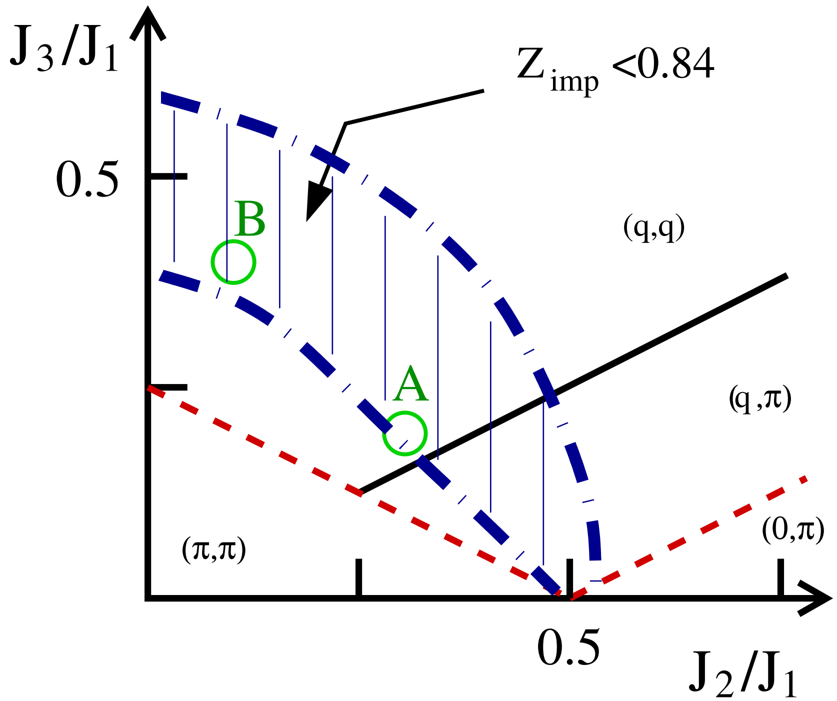
- Electron-hole asymmetry
- For $t > 0$: destructive interference effects
  $\rightarrow$ single hole almost localized
  $\rightarrow$ singlet corr. robust & no Nagaoka F

J_1-J_2-J_3 square lattice Heisenberg



- Classical phase diagram (Moreo et al., PRB 90)
  $\rightarrow$ collinear vs spiral
- Quantum case
  $\rightarrow$ VBS vs spin liquid

J_1-J_2-J_3 square lattice Heisenberg



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- Quantum case
  $\longrightarrow$ VBS vs spin liquid

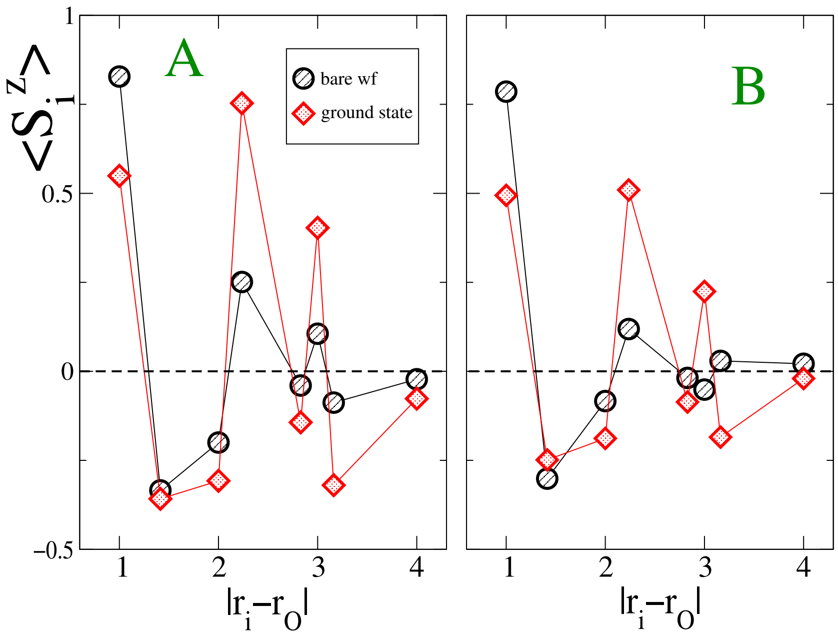
columnar dimer: Leung & Lam, PPB 96

spin liquid: Capriotti, Scalapino & White, PRL 2004

$\Longrightarrow Z_{\rm imp} = |\langle \Phi_{1h} | \Phi_{1h}^{\rm bare} \rangle|^2$ with $|\Phi_{1h}^{\rm bare}\rangle = c_{i,\uparrow} |\Phi_{0h}\rangle$ $(t=0)$

Spin distribution

$\langle S_i^z \rangle$ at distance $\mathbf{r} = \mathbf{r_i} - \mathbf{r_O}$ from defect on a $\sqrt{32} \times \sqrt{32}$ = 32-site square cluster



- $\langle S_i^z \rangle_{\rm bare} \rightarrow$ spin-spin correlation in host
- $\langle S_i^z \rangle_{\rm gs} \rightarrow$ location of "spinon"

Typically, $\xi_{\rm conf} > \xi_{\rm AF}$

$\xi_{\rm conf}$ finite when $N \rightarrow \infty$?

Discussion & Conclusions

- Spin-charge separation in a spin-liquid
  $\longrightarrow$ Generic ? Finite density of holes ?
- Spinon-holon bound-state in translational symmetry breaking VBS
- Frustration of hopping $\longrightarrow$ electron-hole asymmetry
- Progress on frustrated square lattice AF
  $\longrightarrow$ help from dimer basis (Mambrini et al.)
- Pairing mechanism based on kinetic energy (another time!)

Metallic frustrated systems ?

- spinel oxide $LiTi_2O_4$
  Sun et al., PRB **70**, 054519 (2004)
- 5d transition-metal pyrochlores as $Cd_2Re_20_7$ or KOs_2O_6
  Hanawa et al., PRL **87**, 187001 (2001)
  Hiroi et al., JPSJ **73**, 1651 (2004)
- CoO triangular layer based compound
  Takada et al., Nature **422**, 53 (2003)

All superconducting with T_c up to 13.7 K !

Dynamics within Lanczos ED

- $A^\dagger$ is applied to GS:

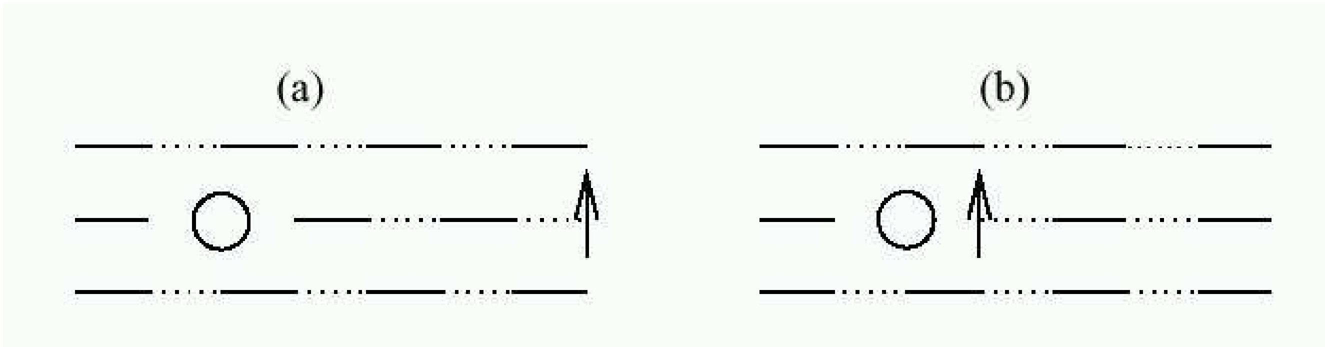
$$|\tilde{\Phi}_1\rangle = \frac{1}{(\langle\Psi_0|AA^\dagger|\Psi_0\rangle)^{1/2}} A^\dagger|\Psi_0\rangle$$

$$\Rightarrow \quad \tilde{C}(z) = \langle\Psi_0|AA^\dagger|\Psi_0\rangle\langle\tilde{\Phi}_1|(z' - H)^{-1}|\tilde{\Phi}_1\rangle$$

- Lanczos procedure:

$$z' - H = \begin{matrix} z' - \tilde{e}_1 & -\tilde{b}_2 & \dots & 0 \\ -\tilde{b}_2 & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & -\tilde{b}_M \\ 0 & \dots & -\tilde{b}_M & z' - \tilde{e}_M \end{matrix} \qquad (1)$$

Non-magnetic dopant in spin-Peierls chain



Experiment

Doping in $CuGeO_3$: $Cu^{2+} \longrightarrow Zn^{2+}$ or Mg^{2+}

Hase et al., PRL **71**, 4059 (1993)

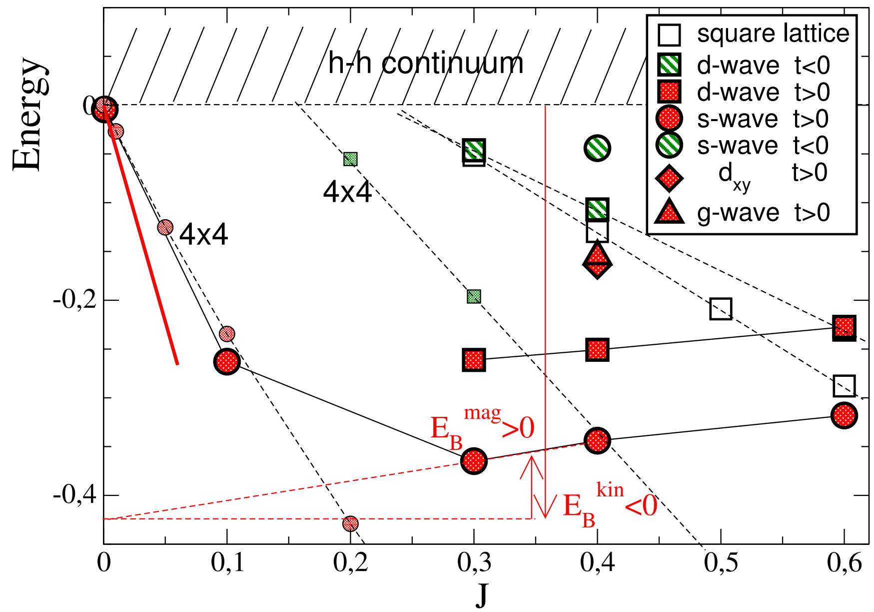
Theory (numerics)

Augier et al., PRB **60**, 1075 (1999)

Pairing energy

Binding on 4×4 & $\sqrt{32} \times \sqrt{32}$-site clusters

$$\Delta_{\text{binding}} = E_{2holes} + E_{Heis} - 2E_{1hole}$$



Feynman-Hellmann:

magnetic energy:

$$E_B^{\text{mag}} = J \frac{dE_B}{dJ}$$

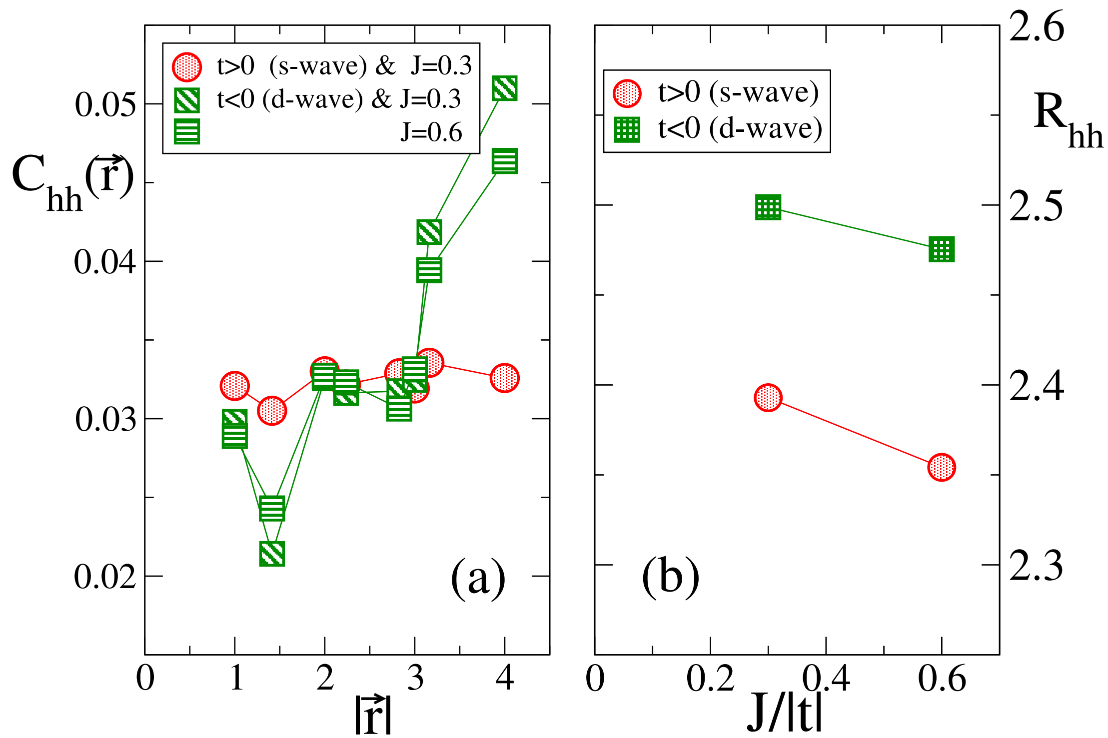
kinetic energy:

$$E_B^{\text{kin}} = E_B - E_B^{\text{mag}} < 0$$

$\Rightarrow$ gain !!

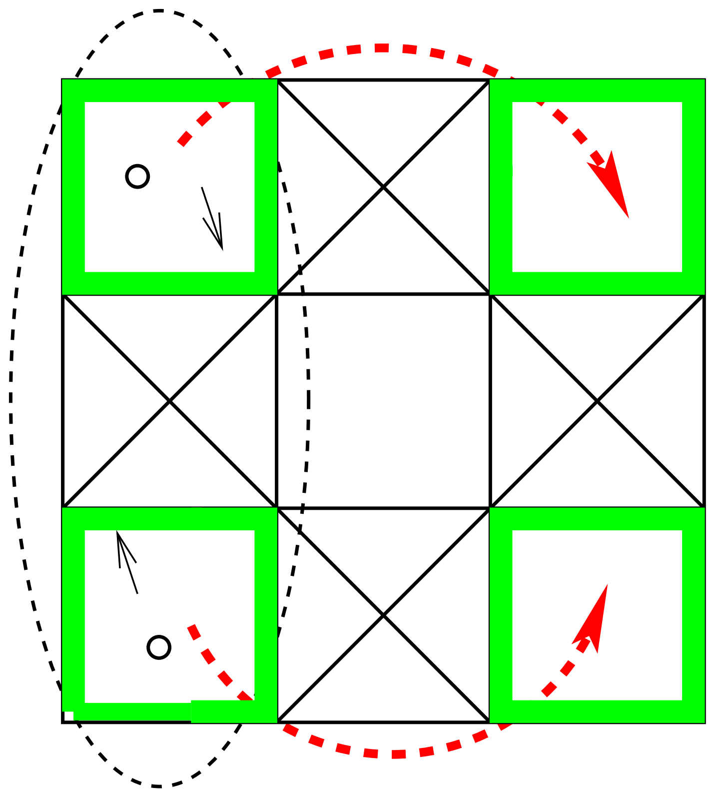
s-wave and d-wave symmetries favored

Hole-hole correlations



- No hole-hole repulsion for $t > 0$
- Pair size ~ 3 lattice spacings

Correlated pair hopping



- Analogy with fully frustrated TB model: interaction-induced delocalized 2-particle BS

Vidal & Douçot, PRB **65**, 045102 (2002)