Spin-charge separation in doped 2D frustrated quantum magnets

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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

- On the $J_1$-$J_2$-$J_3$ model: ongoing work with
  A. Läuchli, M. Mambrini & F. Mila

- Other work: doped Shastry-Sutherland lattice

- 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$_2$VOSiO$_4$

Kagome lattice like SrCr$_{9-x}$Ga$_3^+$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
  - $\text{ZnCr}_2\text{O}_4$ spinel
  - $\text{A}_2\text{Ti}_2\text{O}_7$ 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 !)

Confinement vs deconfinement

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

(a) “string potential”

(b) “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. $E_{\text{singlet}}(Q = (\pi, \pi)) - E_0 \to 0$ 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 $\sim 0.05 J$
  Lecheminant 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

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

\[ J \to 0 \text{ limit} \]

\begin{align*}
\text{singlet} & : t < 0 & \quad E = -|t| \\
\text{triplet} & : t > 0 & \quad E = -2|t|
\end{align*}

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\end{align*}
Single particle Green-function

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

$$G(q, \omega) = \langle N_e | c_{-q, \sigma}^\dagger \frac{1}{\omega - i\epsilon + H - E_{N_e-1}} c_{q, \sigma} | N_e \rangle$$

$$+ \langle N_e | c_{q, \sigma} \frac{1}{\omega + i\epsilon - H + E_{N_e+1}} c_{-q, \sigma}^\dagger | N_e \rangle$$

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

- Continued-fraction: \( z = \omega + i \epsilon, \ A = c_{q,\sigma} \) or \( A = c_{-q,\sigma}^\dagger \)

\[
G(z) = \frac{\langle \Psi_0 | AA^\dagger | \Psi_0 \rangle}{z + E_0 - \tilde{e}_1 - \frac{\tilde{b}_2^2}{z + E_0 - \tilde{e}_2 - \frac{\tilde{b}_3^2}{z + E_0 - \tilde{e}_3 - \ldots}}}
\]

- 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 !
- Switch off $t$ first $\implies$ already some insight!
Static hole (checkerboard)

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

Overlap finite on checkerboard lattice

$$Z = \left| \langle \Phi_{1h} | c_{i,\uparrow} | \Phi_{0h} \rangle \right|^2$$
Static hole (checkerboard)

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

\[
Z = |\langle \Phi_{1h} | c_{i,\uparrow} | \Phi_{0h} \rangle|^2
\]
finite
on checkerboard lattice

Similarity with 1D spin-Peierls g.s.
\[
\Rightarrow \text{confining potential between "holon" and "spinon"}
\]
Static hole (Kagome)

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

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

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

Incoherent spectrum
Weights distributed on many poles even at low energies
Hole dynamics in the VB Solid

Checkerboard

\[ A(k, \omega) \text{ [a.u.]} \]

\[ \omega/t \]

\[ t > 0 \]

\[ t < 0 \]

\[ \Gamma \]

\[ \Sigma \]

\[ M \]

\[ 0.2\% \]

\[ 6.7\% \]

\[ 7.1\% \]

\[ 13.5\% \]

\[ 1.3\% \]

\[ 2.9\% \]

\[ 0.04\% / 2\% \]

\[ 4.2\% \]

\[ \omega/|t| \]
Single hole doped in a spin liquid

A(k,0) [a.u.]

kagome

\[ A(k,0) \ [\text{a.u.}] \]

\[ \omega/t \]

\[ \Gamma \ x 0.5 \]

\[ t>0 \]

\[ t<0 \]

\[ \omega/|t| \]

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spin & charge repel!

(a) Dimer correlations

(b) Hole-spin correlations

Hole-spin correlations in "Holon" wavefct

(c) t>0

(d) t<0

Hole-spin correlations in neighboring triangle (like static case: see e.g. Dommange et al, PRB)
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
  - single hole almost localized
  - singlet corr. robust & no Nagaoka F

![Graphs showing hole localisation in the VBS host](image-url)
$J_1 - J_2 - J_3$ square lattice Heisenberg

- Classical phase diagram (Moreo et al., PRB 90)
  - collinear vs spiral

- Quantum case
  - VBS vs spin liquid
$J_1 - J_2 - J_3$ square lattice Heisenberg

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

Columnar dimer: Leung & Lam, PPB 96

Spin liquid: Capriotti, Scalapino & White, PRL 2004

$$Z_{\text{imp}} = \left| \langle \Phi_{1h} | \Phi_{1h}^{\text{bare}} \rangle \right|^2 \text{ with } | \Phi_{1h}^{\text{bare}} \rangle = c_i, \uparrow | \Phi_{0h} \rangle \ (t = 0)$$
Spin distribution

\[ \langle S^z_i \rangle \] at distance \( r = r_i - r_O \) from defect on a \( \sqrt{32} \times \sqrt{32} = 32 \)-site square cluster

- \( \langle S^z_i \rangle_{\text{bare}} \) → spin-spin correlation in host
- \( \langle S^z_i \rangle_{\text{gs}} \) → location of “spinon”

Typically, \( \xi_{\text{conf}} > \xi_{\text{AF}} \)

\( \xi_{\text{conf}} \) finite when \( N \rightarrow \infty \)
Discussion & Conclusions

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

- Spinel oxide LiTi$_2$O$_4$
  Sun et al., PRB 70, 054519 (2004)

- 5d transition-metal pyrochlores as Cd$_2$Re$_2$O$_7$
or KOs$_2$O$_6$
  Hanawa et al., PRL 87, 187001 (2001)
  Hiroi et al., JPSJ 73, 1651 (2004)

- CoO triangular layer based compound

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:

\[
\begin{pmatrix}
 z' - \tilde{e}_1 & -\tilde{b}_2 & \ldots & 0 \\
 -\tilde{b}_2 & \ddots & \ddots & \vdots \\
 \vdots & \ddots & \ddots & -\tilde{b}_M \\
 0 & \ldots & -\tilde{b}_M & z' - \tilde{e}_M
\end{pmatrix}
\]

(1)
Non-magnetic dopant in spin-Peierls chain

Experiment
Doping in CuGeO$_3$: Cu$^{2+}$ → 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 $4 \times 4$ & $\sqrt{32} \times \sqrt{32}$-site clusters

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

Feynman-Hellmann:
- magnetic energy: $E_B^{\text{mag}} = J \frac{dE_B}{dJ}$
- kinetic energy: $E_B^{\text{kin}} = E_B - E_B^{\text{mag}} < 0$ ⇒ gain !!

s-wave and d-wave symmetries favored

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Hole-hole correlations

- No hole-hole repulsion for $t > 0$
- Pair size $\sim 3$ lattice spacings
Correlated pair hopping

- Analogy with fully frustrated TB model: interaction-induced delocalized 2-particle BS
  Vidal & Douçot, PRB 65, 045102 (2002)