The $J_1 - J_2$ model on the square lattice: Exact Diagonalization and Coupled Cluster Method

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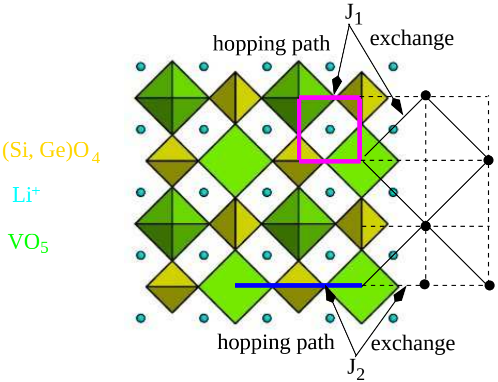
Motivation

Various materials are well described by the $J_1 - J_2$ model (e.g. Li_2VOSiO_4 and Li_2VOGeO_4)

- canonical model to investigate quantum phase transitions driven by frustration
- benchmark for approximativ techniques
- non-magnetic quantum phase (quantum paramagnet)
- nature of quantum phase under discussion
- nature of quantum phase transitions under discussion (deconfined quantum criticality ?)

Motivation

Li_2VOSiO_4 and Li_2VOGeO_4 formed by layers of V^{4+} ($s = \frac{1}{2}$)



The quantum Heisenberg-AFM in 2d

- $T > 0$: Mermin/Wagner '66

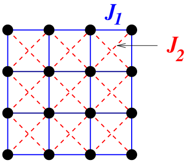
  no magnetic long-range order

- $T = 0$ **square lattice:**
  - LRO exists for $S \geq 1$ (Neves and Perez 1986)

    (till now) no proof for LRO for $S = 1/2$ but: LRO by a lot of papers (1987-1992) well-established
  - $s = 1/2$: magnet. moment $m_{qu} \approx 0.6 m_{clas}$
  - generally: Néel like order favoured in 2d quantum AFM
  - **competing** interactions, e.g. frustration, may destroy magntic order in the GS

    $\rightarrow$ order-disorder quantum phase transitions

The Model

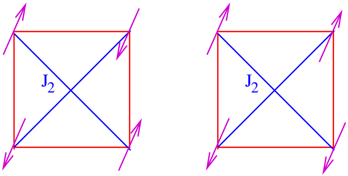


- Hamiltonian

$$H = J_1 \sum_{\langle i,j \rangle} \vec{S}_i \vec{S}_j + J_2 \sum_{\langle\langle i,j \rangle\rangle} \vec{S}_i \vec{S}_j$$

- here focus on: $J_1 = +1$ (AFM), frustrating $J_2 \geq 0$ (AFM)

Frustration in the J1 – J2 model



The $J_1 - J_2$ model has been studied by many authors (about 200 papers) – but still unresolved questions exist

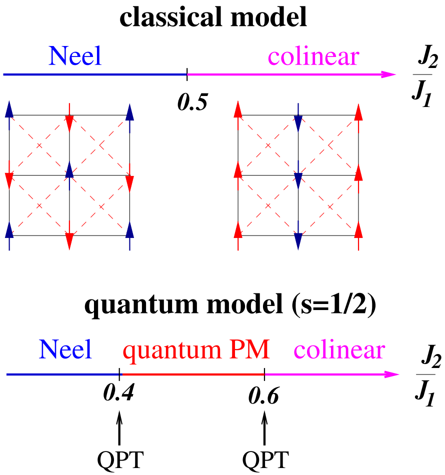
see,e.g:

Chandra and Doucot, Phys. Rev. B **38**, 9335 (1988); H.J. Schulz, T.A.L. Ziman, and D. Poilblanc J. Phys. I **6**, 675 (1996) (Lanczos till N=36); R.F. Bishop, D.J.J. Farnell, and J.B. Parkinson, Phys. Rev. B **58**, 6394 (1998) (CCM); L. Capriotti, F. Becca, A. Parola, and S. Sorella, Phys. Rev. Lett. **87**, 097201 (2001); $\cdots$; J. Sirker, Z. Weihong, O. P. Sushkov, and J. Oitmaa, Phys. Rev. B **73**, 184420 (2006); R. Darradi, O. Derzhko, R. Zinke, J. Schulenburg, S. E. Krüger, and J. Richter, Phys. Rev. B **78**, 214415 (2008); L. Isaev, G. Ortiz, and J. Dukelsky, Phys. Rev. B **79**, 024409 (2009); $\cdots$

papers also by:
R. Bishop; J. Dukelsky; D. Farnell; A. Honecker; A. Läuchli; J. Schulenburg; S. Sorella

Ground state phases – General scenario

frustration drives zero-temperature phase transitions:



The Methods

- Lanczos exact diagonalization (ED) of finite lattices up to $N = 40$ sites (size of matrix 10^{10}) using *spinpack* code
  $\rightarrow$ see talk J. Schulenburg
  see also talks A. Honecker, A. Läuchli
- Coupled Cluster Method (CCM)
  - exponential ansatz for GS

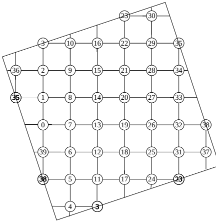
$$|\Psi\rangle = e^S|\Phi\rangle \quad , \quad |\Phi\rangle = |\downarrow\downarrow\downarrow\downarrow\downarrow\ldots\rangle \quad S = \sum_{i_1 i_2 \cdots i_l} [i_1 i_2 \cdots i_l] s^+_{i_1} s^+_{i_2} \cdots s^+_{i_l}$$

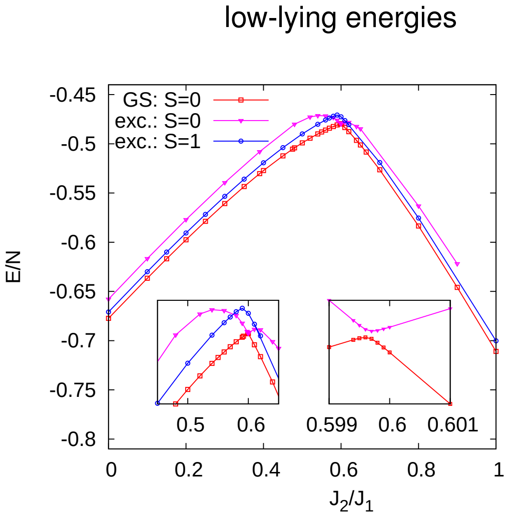
  - we use LSUB*n* approximation
    take in to account all possible many-body cluster configurations $I = i_1 i_2 \cdots i_l$ in all different localised regions of n contiguous sites on the lattice
  - square lattice up to LSUB10: 45825 terms using *CCCM* code

$\rightarrow$ see also talks R. Bishop, D. Farnell

Results

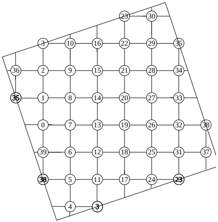
Results ED N=40

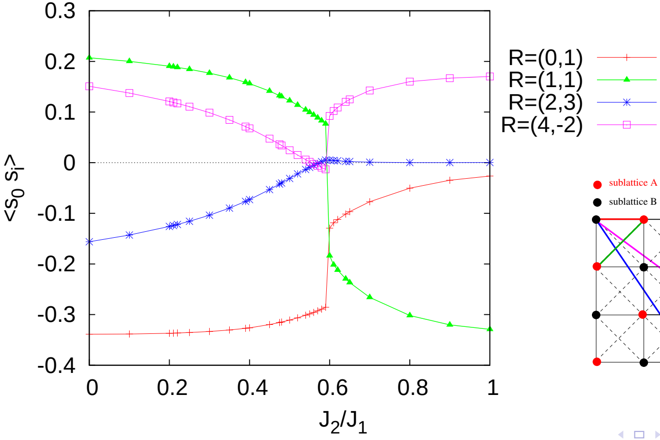


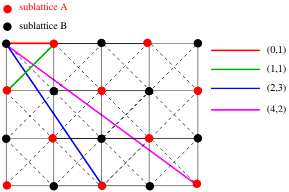


Results ED N=40

spin-spin correlation $\langle \mathbf{S}_i \mathbf{S}_j \rangle$

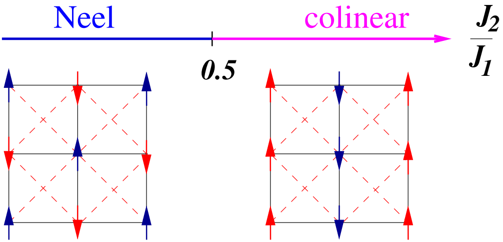






Order parameter for ED

remember: frustration drives zero-temperature phase transitions

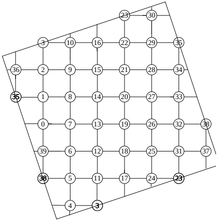


corresponding order parameters: structure factor

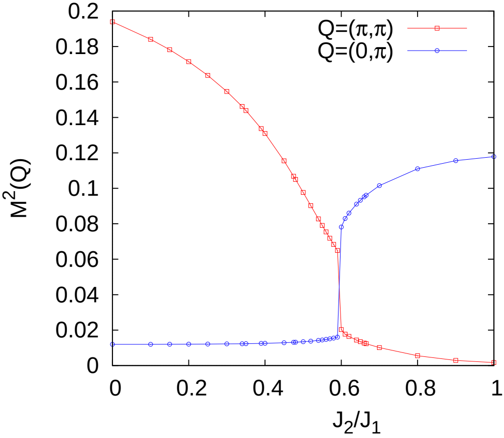
$$M_N^2(\mathbf{Q}) = \frac{1}{N(N+2)} \sum_{i,j} \langle \mathbf{s}_i \cdot \mathbf{s}_j \rangle e^{i\mathbf{Q}(\mathbf{R}_i - \mathbf{R}_j}$$

$\mathbf{Q} = (\pi, \pi)$ – Néel , $\mathbf{Q} = (0, \pi)$ or $\mathbf{Q} = (\pi, 0)$ – colinear

Results ED N=40



square of order parameter



Exact Diagonalization – Finite-size extrapolation

seminal papers: Neuberger and Ziman PRB 1989; Hasenfratz and Niedermayer, Z.Phys.B 1993; Schulz, Ziman, and Poilblanc, J.Phys.I 1996

formulas:

order parameter I: $$M_N^2(\pi,\pi) = \frac{1}{4} m_1^2 \left(1 + \frac{0.62075c}{\rho\sqrt{N}} + \cdots\right)$$

c - spin-wave velocity ; ρ - spin stiffness

order parameter II: $$M_N^2(\pi,0) = \frac{1}{8} m_2^2 + \frac{\text{const.}}{\sqrt{N}} + \cdots .$$

GS energy: $$\frac{E_{GS}(N)}{N} = e_0 - 1.4372 \frac{c}{N^{3/2}} + \cdots .$$

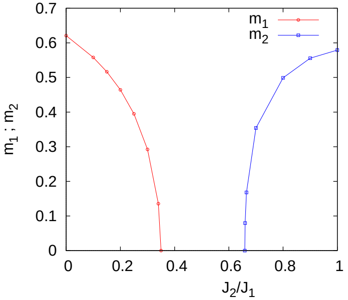
spin gap: $$\Delta_T(N) = \Delta_T + \frac{A}{N} + \cdots$$

susceptibility: $$\chi(N) = \chi + \frac{B}{N} + \cdots \quad ; \quad \chi(N) = N\Delta_T(N)$$

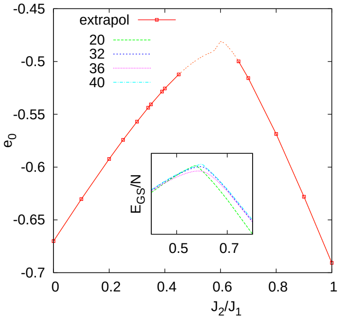
$\rightarrow$ we get m_1, m_2, e_0, ρ, Δ, χ

Results ED: finite size extrapolation

order parameter

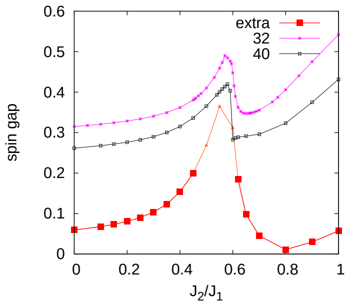


GS energy

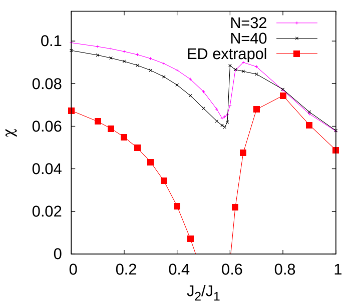


Results ED: finite size extrapolation

spin gap Δ_T

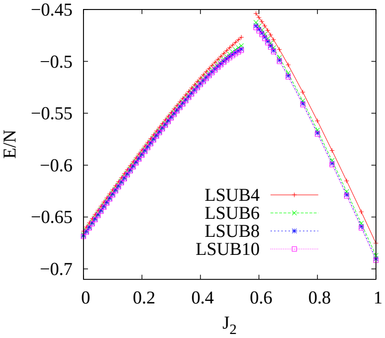


uniform susceptibility χ

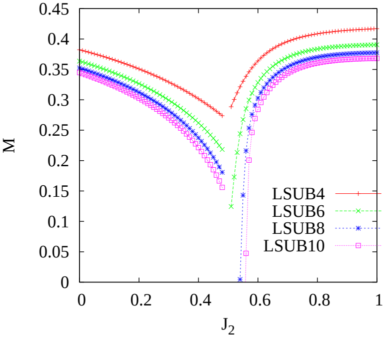


Results CCM – LSUBn approximation

GS energy



sublattice magnetization



CCM - Extrapolation of the LSUBn results

- polynomial scaling based on previous experience (no exact scaling laws)
- GS energy

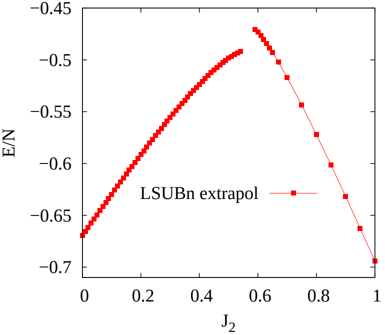
$$E(n) = E_\infty + a_1(1/n)^2 + a_2(1/n)^4$$

- order parameter (sublattice magnetization)

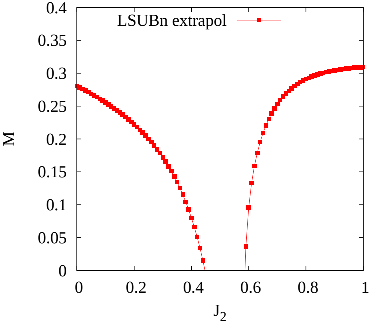
$$M(n) = M_\infty + b_1(1/n)^{0.5} + b_2(1/n)^{1.5}$$

Results CCM - extrapolated LSUBn

GS energy

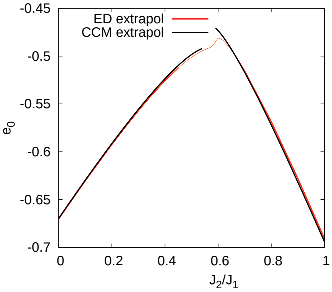


sublattice magnetization

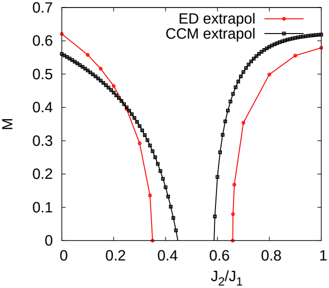


Comparison CCM - ED

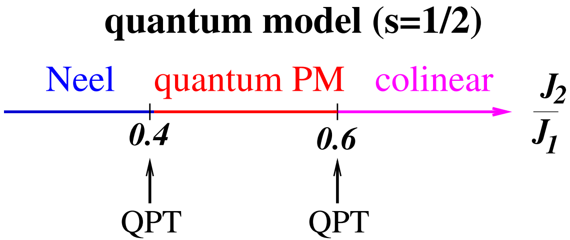
GS energy



order parameter



Ground-state phase diagram

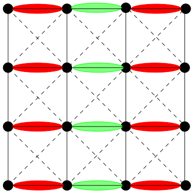


- The existence of the quantum paramagnetic phase can be confirmed by CCM and ED
- What about the nature of the quantum phase ?
- What about the quantum phase transitions?

Nature of the quantum phase around $J_2 = 0.5J_2$

Valence bond crystal?

valence-bond pattern



calculate generalized susceptibility (CCM, ED)

- add approriate perturbation to H_{J1J2}:

  $H = H_{J1J2} + \delta \sum_{i,j} (-1)^i \mathbf{s}_{i,j} \mathbf{s}_{i+1,j}$

- generalized susceptibility is defined as

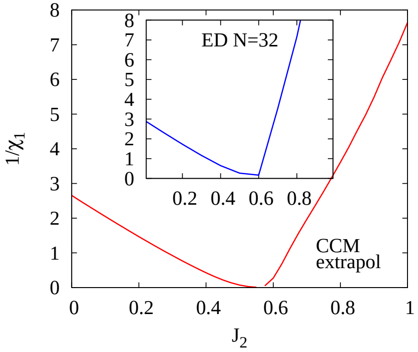
  $$\chi = - \left. \frac{\partial^2 e(\delta)}{\partial \delta^2} \right|_{\delta=0}$$

- extrapolation of LSUBn data

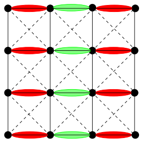
  $\chi(n) = \chi_\infty + c_1(1/n) + c_2(1/n)^2$

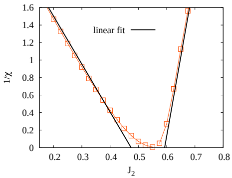
Results: Nature of the quantum phase

inverse susceptibility



perturbation





ED and CCM support existence of valence-bond GS around $J_2 = 0.5J_1$

Nature of the transition at $J_2 \sim 0.4J_1$

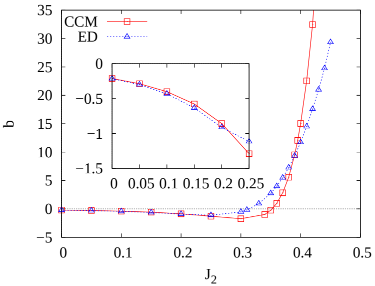
effective field theory yields

$$e(\delta) - e(\delta = 0) = -\frac{1}{2A}\delta^2 + \frac{u_\phi}{4A^4}\delta^4 + \frac{Ar_\phi - 3u_\phi^2}{6A^7}\delta^6 + \mathcal{O}(\delta^8).$$

1st order: $\frac{u_\phi}{4A^4} < 0$ 2nd order: $\frac{u_\phi}{4A^4} > 0$

numerical data fit to: $$e(\delta) - e(0) = \frac{a}{2}\delta^2 + \frac{b}{4}\delta^4 + \frac{c}{6}\delta^6$$

coefficient b in front of δ^4



$b > 0$ near the transition point at $J_2 \sim 0.4J_1$

note: Sirker et al. (PRB 2005) found $b < 0$ by series expansion

Some conclusions

- CCM and ED are appropriate methods to study quantum phase transitions in 2D
- **no problems with frustration**
- ED: restricted to 1d and 2d
- CCM: 3d also possible