Spin correlations in the Heisenberg chain

Let's look at the (staggered) spin correlation function

$$C(r) = \langle \mathbf{S}_i \cdot \mathbf{S}_{i+r} \rangle (-1)^r$$

versus the distance r and at r=N/2 versus system size N

Theory (bosonization, conformal field theory) predicts (for large r, N)

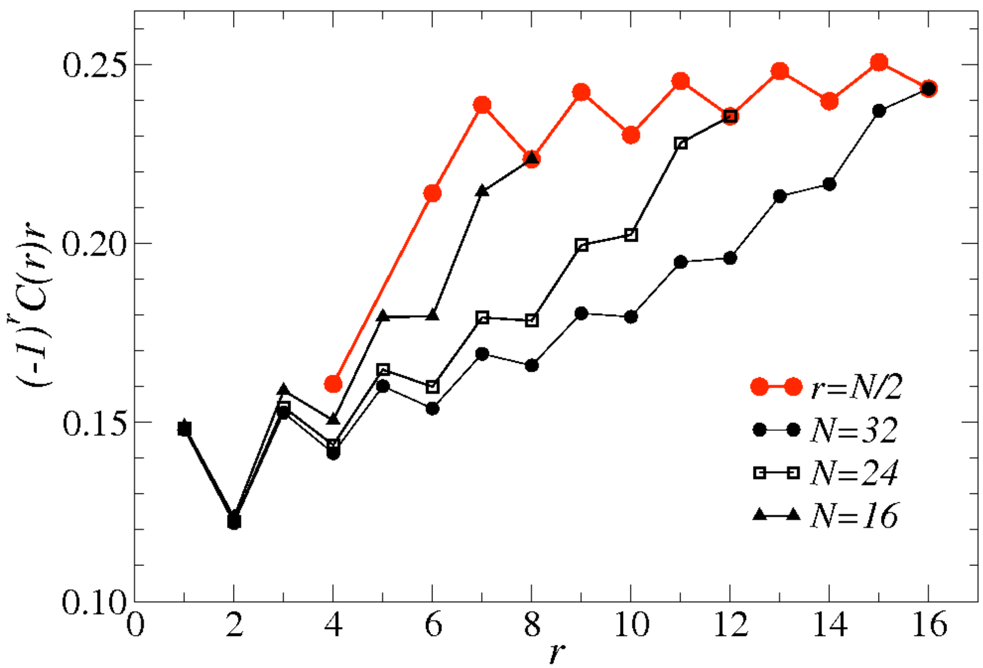
$$C(r) \propto \frac{\ln^{1/2}(r/r_0)}{r}$$

Plausible based on N up to 32

- other methods for larger N

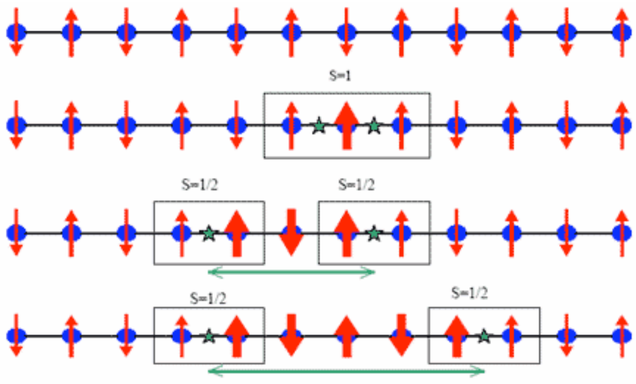
Power-law correlations are a sign of a "critical" state; at the boundary between

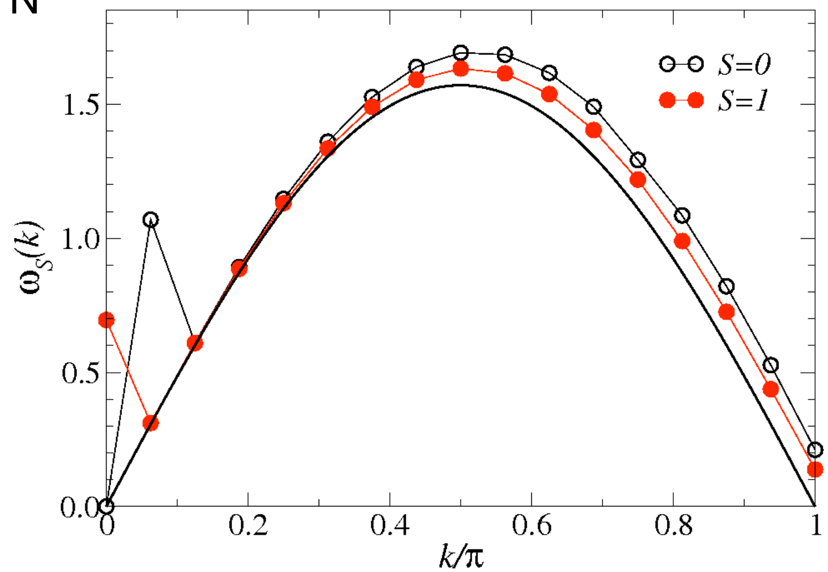
- ordered (antiferromagnetic)
- disordered (spin liquid)



Excitations of the Heisenberg chain

- the ground state is a singlet (S=0) for even N
- the first excited state is a triplet (S=1)
- can be understood as pair of “spinons”

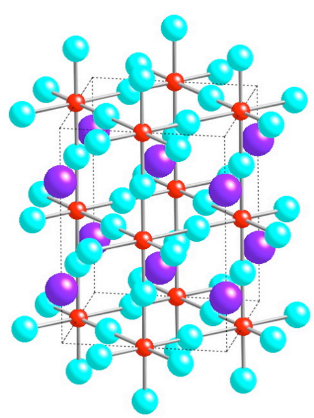


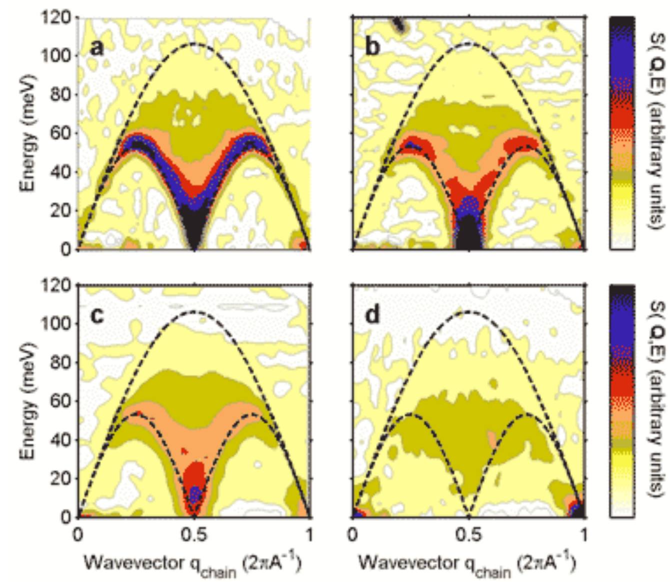


Neutron scattering experiments

- quasi-one-dimensional $KCuF_3$

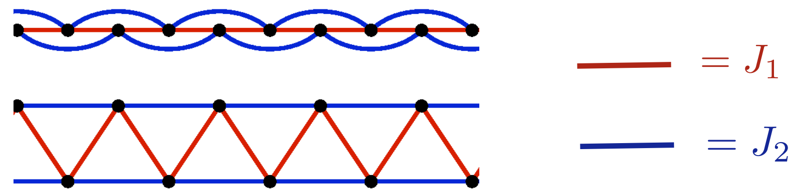
B. Lake et al., Nature Materials 4 329-334 (2005)





Heisenberg chain with frustrated interactions

$$H = \sum_{i=1}^{N} \left[J_1 \mathbf{S}_i \cdot \mathbf{S}_{i+1} + J_2 \mathbf{S}_i \cdot \mathbf{S}_{i+2} \right]$$

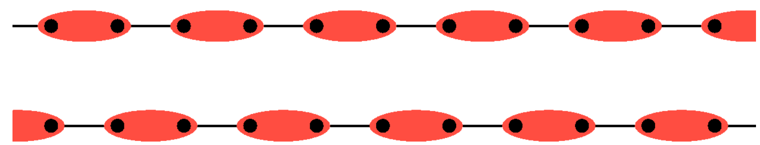


For the special point $J_2/J_1=0.5$, this model has an exact solution

Singlet-product states

$$|\Psi_A\rangle = |(1,2)(3,4)(5,6)\cdots\rangle$$

$$|\Psi_B\rangle = |(1,N)(3,2)(5,4)\cdots\rangle$$



It is not hard to show that these are eigenstates of H (we will do later)

$$(a,b) = (\uparrow_a \downarrow_b - \downarrow_a \uparrow_b)/\sqrt{2}$$

The system has this kind of order (with fluctuations, no exact solution) for all $J_2/J_1>0.2411$..... This is a **quantum phase transition** between

- a critical state
- a valence-bond-solid (VBS) state

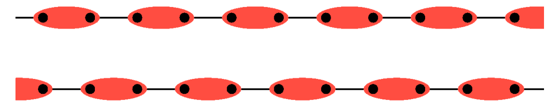
The symmetry is not broken for finite N

- the ground state is a superposition of the two ordered states

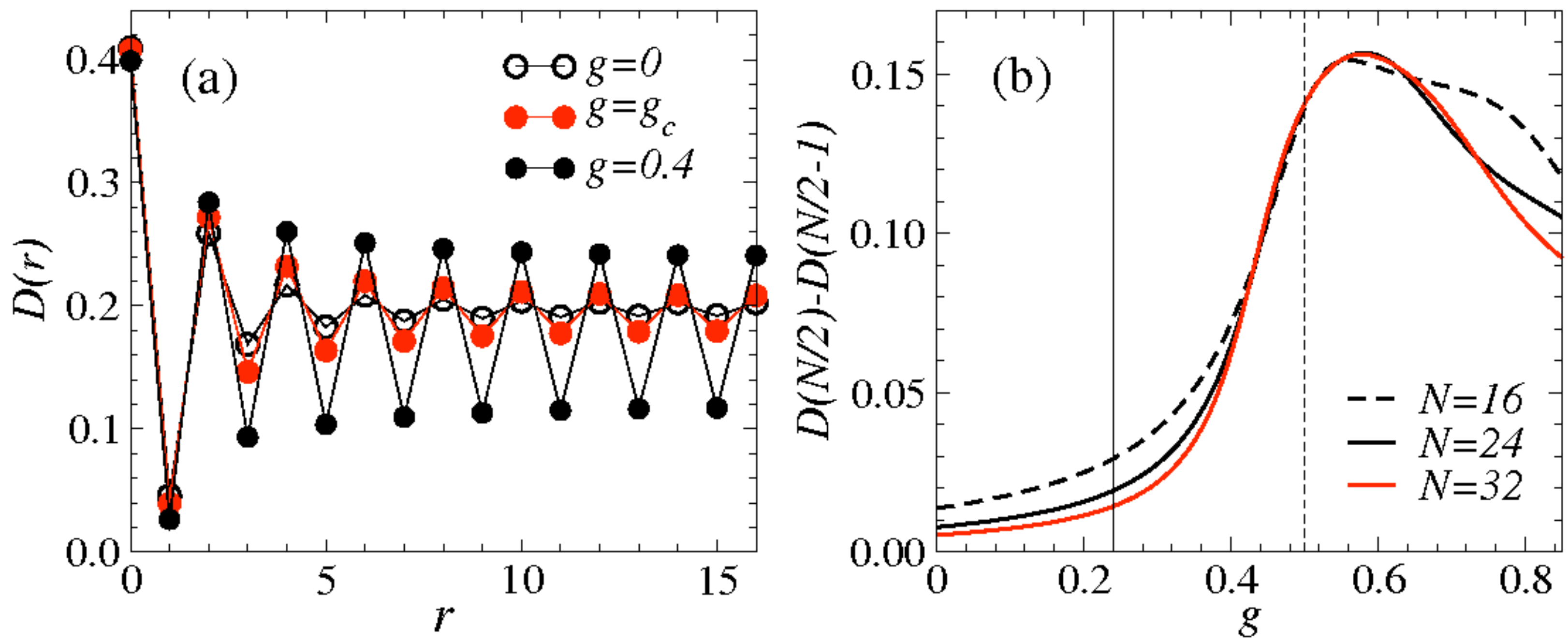
$$|\Psi_0\rangle \sim |\Psi_A\rangle + |\Psi_B\rangle, \qquad |\Psi_1\rangle \sim |\Psi_A\rangle - |\Psi_B\rangle$$

The VBS state can be detected in finite systems using “dimer” correlations

$$D(r) = \langle B_i B_{i+r} \rangle = \langle (\mathbf{S}_i \cdot \mathbf{S}_{i+1})(\mathbf{S}_{i+r} \cdot \mathbf{S}_{i+1+r}) \rangle$$



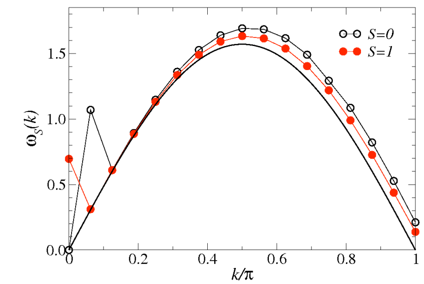
Results from Lanczos diagonaization; different coupling ratios ***$g=J_2/J_1$***



It is not easy to detect the transition this way

- “infinite-order” transition; exponential (slow) growth of the VBS order
- much larger systems are needed for observing a sharp transition
- other properties can be used to accurately determine the critical point g_c
  -level crossings [K. Okamoto and K. Nomura, Phys. Lett. A 169, 443 (1992)]

Determining the transition point using level crossings



Lowest excitation for the g=0 Heisenberg chain is a triplet

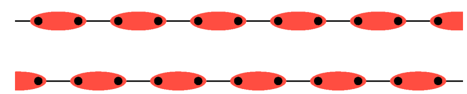
- this can be expected for all $g<g_c$

The VBS state is 2-fold degenerate for infinite N

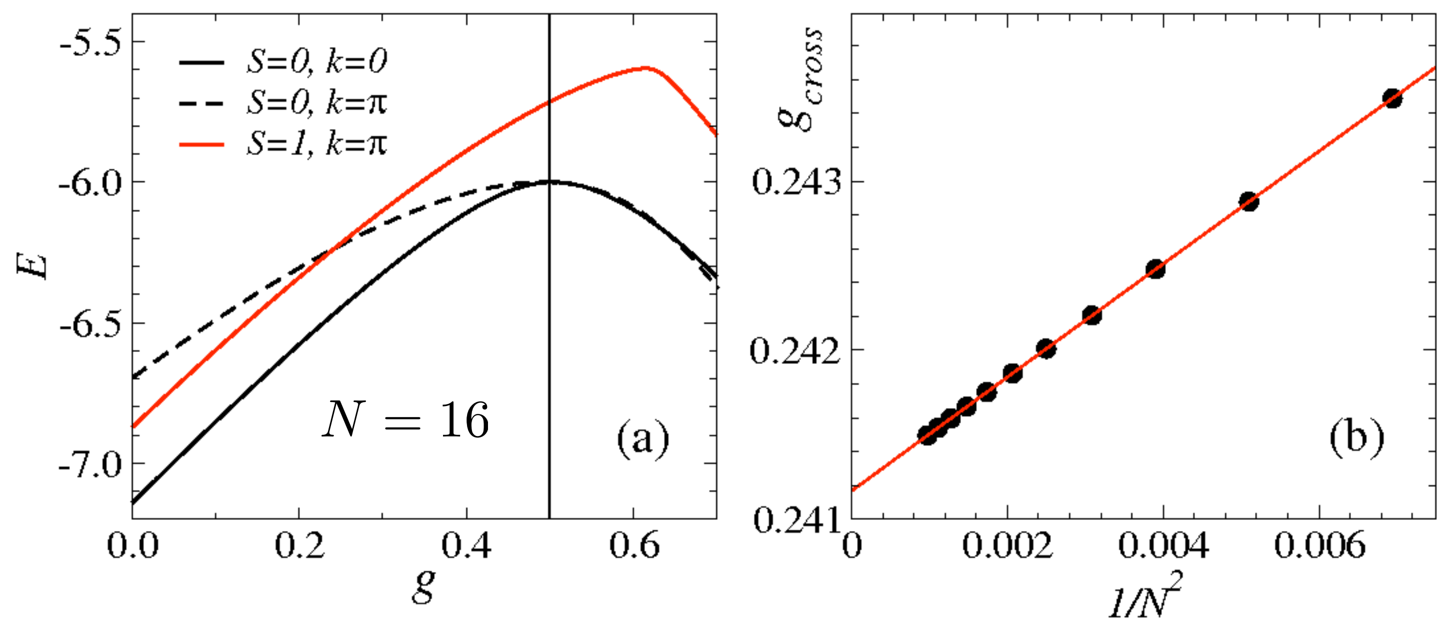
- and for any N at g=1/2
- these two states are singlets
- gap between them closes exponentially as $N\to\infty$
- the lowest excitation is the second singlet

$$|\Psi_0\rangle \sim |\Psi_A\rangle + |\Psi_B\rangle$$

$$|\Psi_1\rangle \sim |\Psi_A\rangle - |\Psi_B\rangle$$



The two lowest excited state should cross at g_c



Extrapolating point for different N up to 32 gives g_c=0.2411674(2)

Heisenberg chains with long-range interactions

The spin-rotational symmetry cannot be spontaneously broken
in 1D Heisenberg systems with short-range interactions
- with long-range interactions magnetic (e.g., Neel) order can form

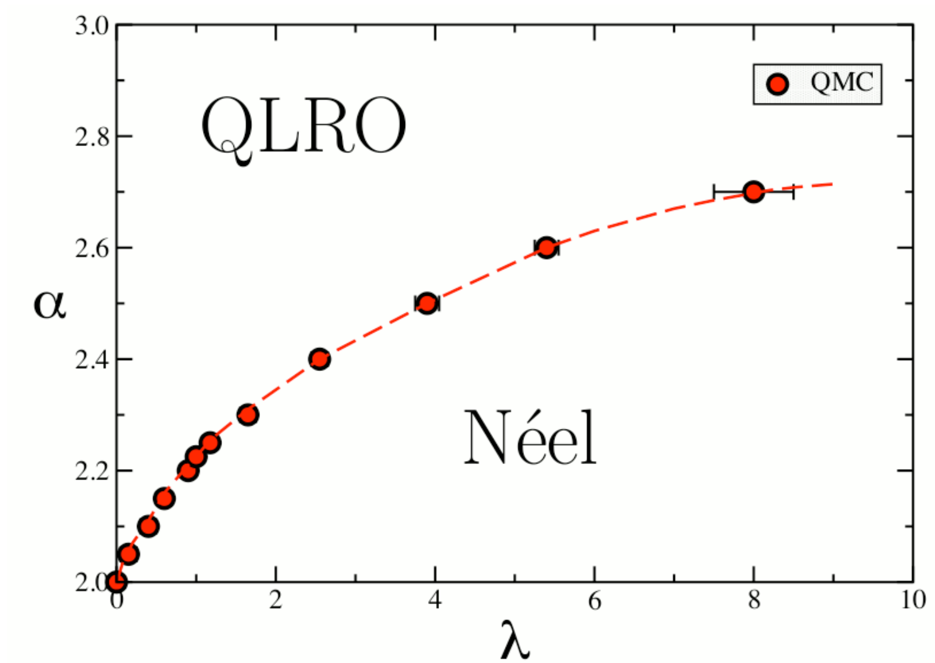
Consider power-law decaying unfrustrated antiferromagnetic interactions
[N. Laflorencie, I. Affleck, and M. Berciu, JSTAT (2006)]

$$H = \sum_{r=1}^{N/2} (-1)^{r-1} J_r \sum_{i=1} \mathbf{S}_i \cdot \mathbf{S}_{i+r} \qquad J_1 = \lambda, \quad J_{r>1} = \frac{1}{r^\alpha}$$

Phase transition between
- crititrical state
- Neel-ordered state

The critical (or "quasi-long-range ordered") phase has the normal Heisenberg chain critical fluctuations/correlations

Transition curve $\alpha_c(\lambda)$
- varying critical exponents



Combining long-range interactions and frustration [AWS, PRL 2010]

Un-frustrated power-law decaying J_r, frustrating J_2

$$H = \sum_{r=1}^{N/2} (-1)^{r-1} J_r \sum_{i=1}^{N} \mathbf{S}_i \cdot \mathbf{S}_{i+r}$$

$$J_r \propto \frac{1}{r^\alpha} \quad (J_r > 0), \quad \text{except for :} \quad J_2 = -g \ (< 0)$$

$$J_1 + \sum_{r=3}^{N/2} J_r = 1$$ (convenient normalization of un-frustrated terms)

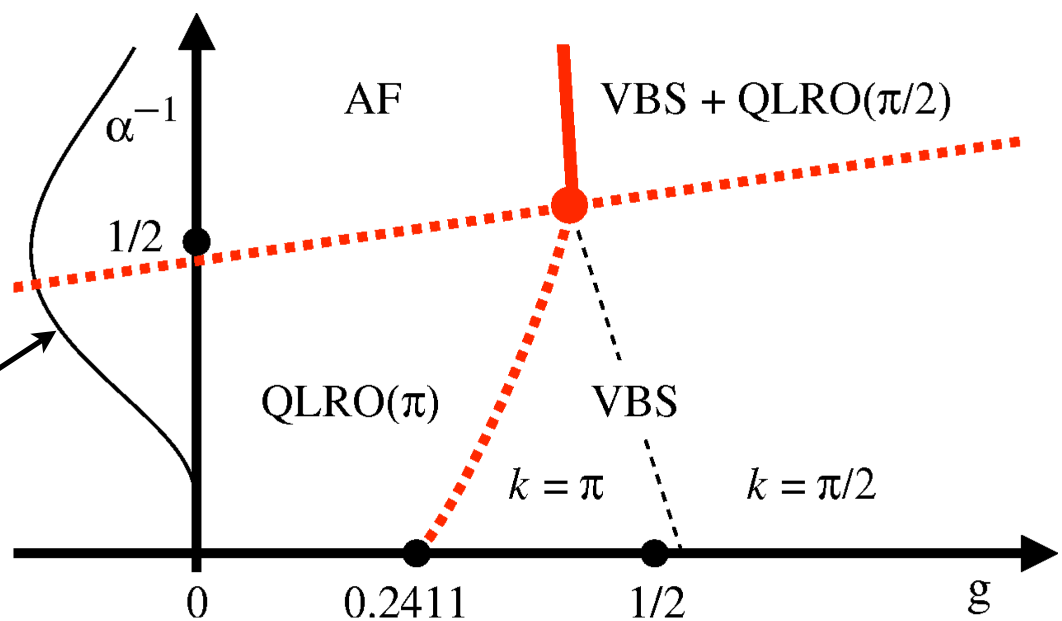
For $\alpha \to \infty$ the system reduces to the J_1-J_2 chain with $g=J_2/J_1$

Technically challenging

- QMC sign problem
- long-range interactions
  - DMRG difficulties
- What can Lanczos tell?

(g,α^{-1}) phase diagram

- Laflorencie et al. model
- other phases from Lanczos



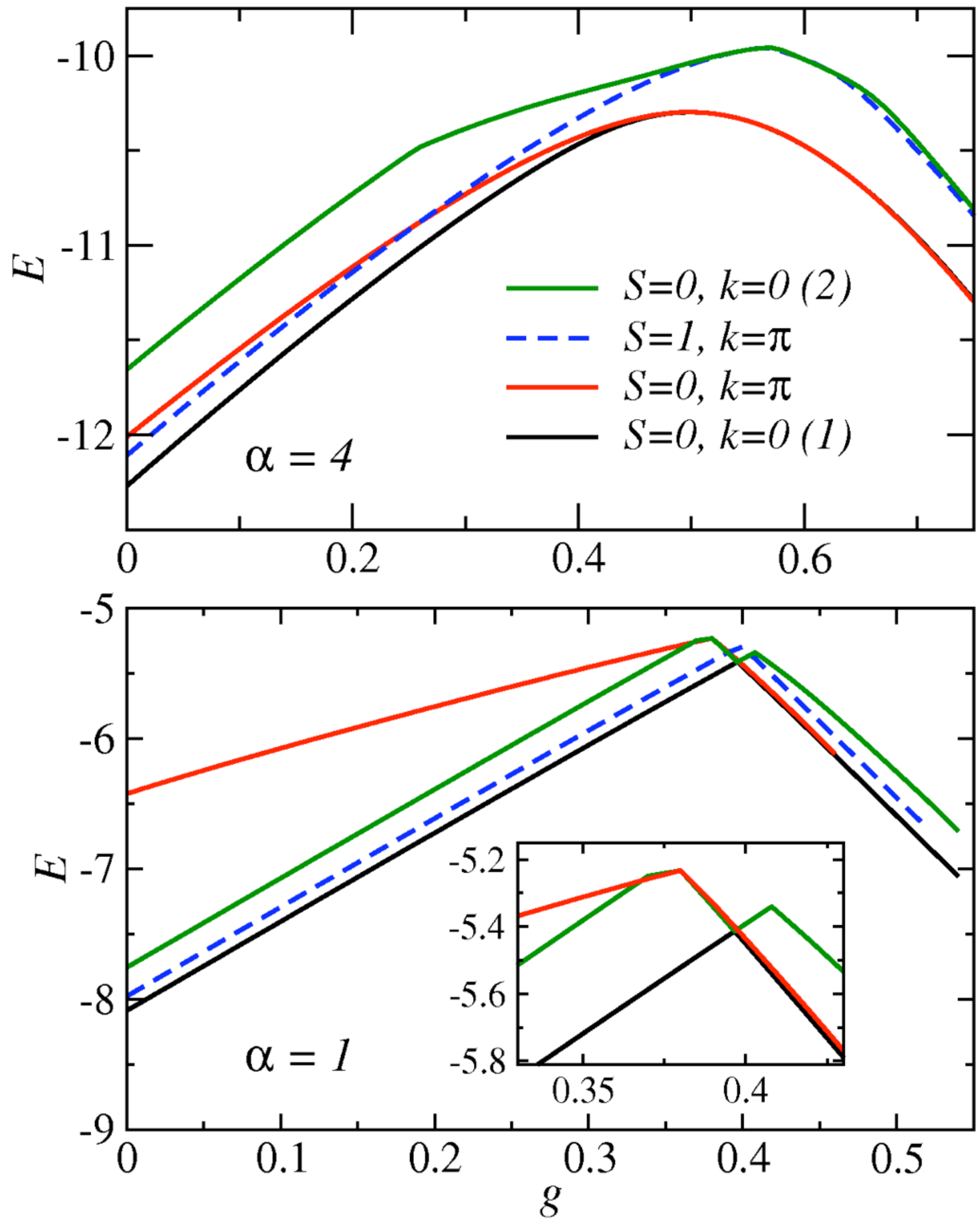
Lanczos results for ground state and excitation **energies**

Similar to the J_1-J_2 chain for large α (>2)

- singlet-triplet crossing
- rounded E_0 maximum

Different curve shapes for small α (<2)

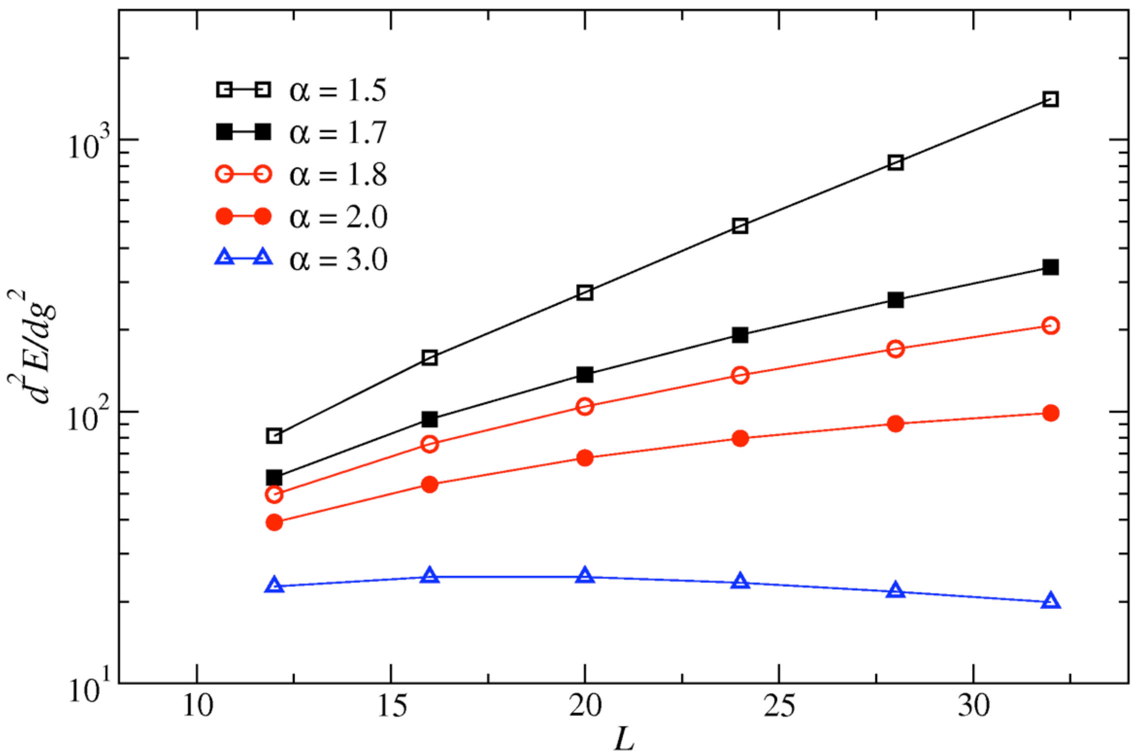
- sharp breaks
- avoided level crossings
- indicative of 1st order phase transition

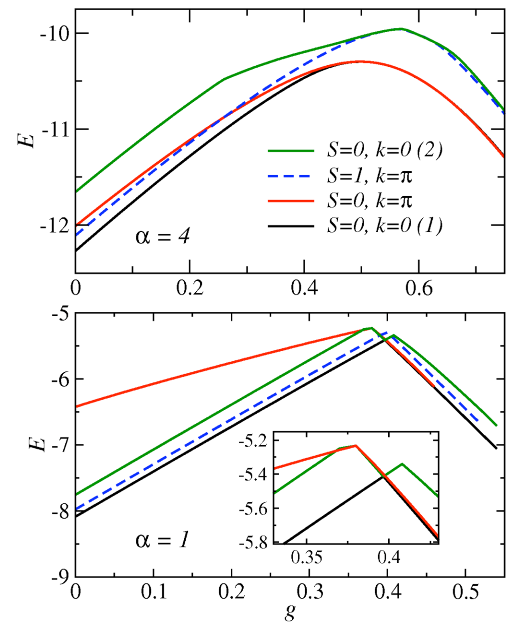


Analysis of the ground state energy curve $E_0(g)$

Characterize the sharpness of the maximum
by the second derivative versus chain length

$$\frac{d^2E_0(g)}{dg^2} \quad \text{(at the peak value } g_{\text{peak}}\text{)}$$

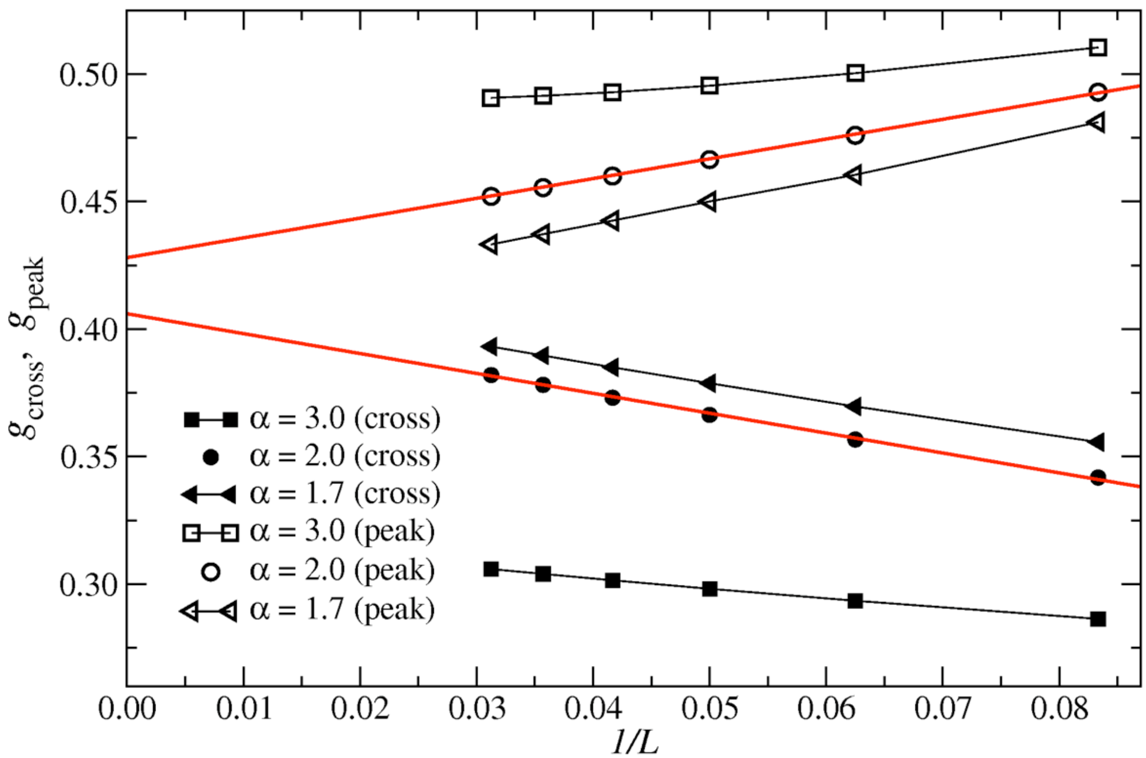




Exponentially divergent peak curvature for α<2

- First-order transition due to avoided level crossing

How do the singlet-triplet crossing point g_{cross} and g_{peak} move with L?



For α>1.8

- singlet-triplet crossing at frustrated coupling $g_{cross} < g_{peak}$
- indicative of same QLRO-VBS$_2$ transition as in standard J_1-J_2 chain

For α<1.8

- the two special points coincide when L→∞
- what is the nature of the transition
- Neel state expected for small g
- Is it a Neel-VBS transition?

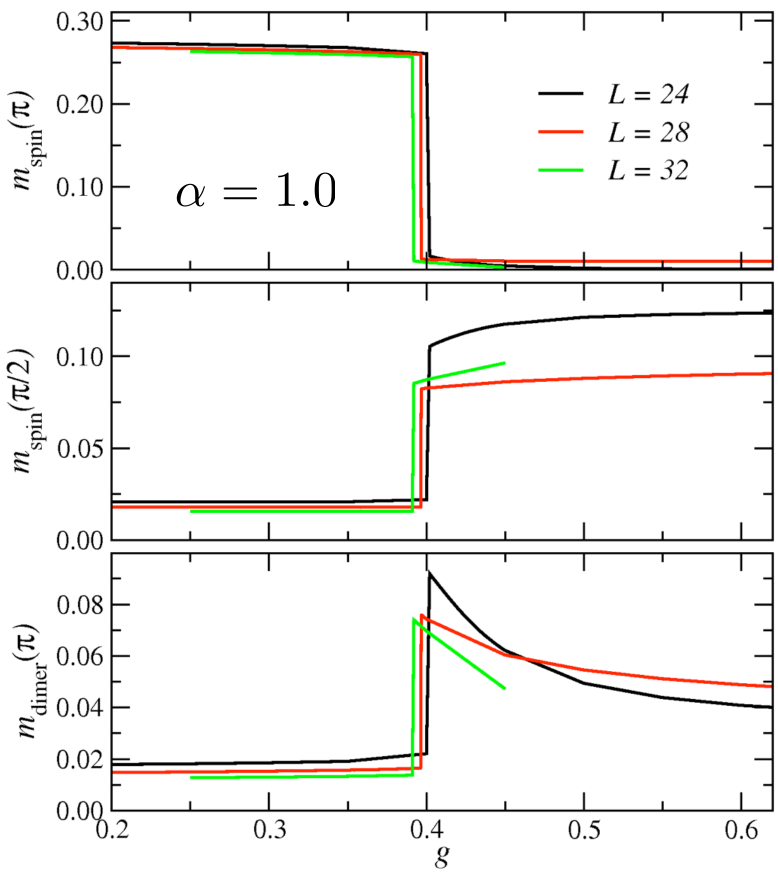
Spin correlations C(r)

- staggered (Neel) for g<gc
- period 4 for g>gc (critical?)

Dimer correlations D(r)

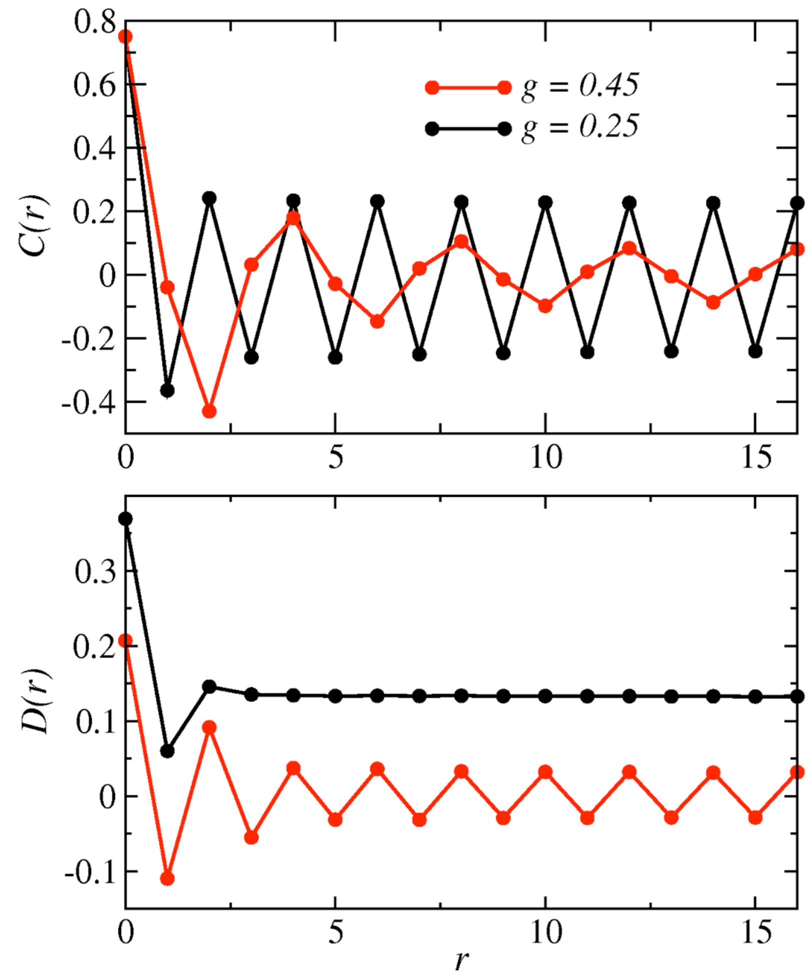
- short-ranged for g<gc
- period-2 VBS for g>gc

1st order transition



$$C(r) = \langle \mathbf{S}_i \cdot \mathbf{S}_{i+r} \rangle$$

$$D(r) = \langle (\mathbf{S}_i \cdot \mathbf{S}_{i+1})(\mathbf{S}_{i+r} \cdot \mathbf{S}_{i+1+r}) \rangle$$



$$m(q) = \frac{1}{N} \sum_{r=0}^{N-1} \mathrm{e}^{-iqr} C(r) \quad [\text{or } D(r)]$$