Mahabaleshwar Condensed Matter School, December 5-12, 2009

Computational methods for quantum spin systems

Quantum spin systems discussed from a computational perspective

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Lecture contents

Models

- S=1/2 Heisenberg models
- beyond nearest-neighbor interactions (1D)
- also including multi-spin (4,6,...) interactions (2D)

Methods

- finite-lattice methods
- exact diagonalization (use of symmetries)
- Stochastic series expansion (finite-T quantum Monte Carlo)
- Valence-bond projector (ground state quantum Monte Carlo)

Physics

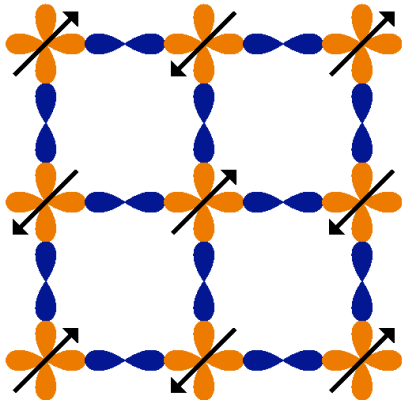
- various types of ordered and disordered ground states
  - Neel (antiferromagnetic); AF
  - Quantum disordered (chain and ladder systems)
  - Valence-bond solid; VBS
- quantum phase transitions
  - frustration driven transitions in 1D
  - 2D Neel - VBS transition (candidates for deconfined quantum criticality)

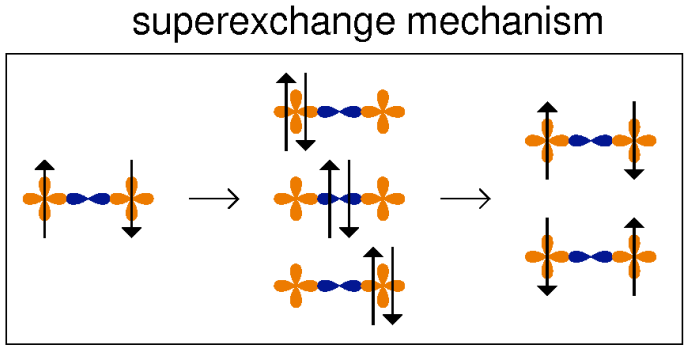
Level and choise of topics

- from basics to on-going research (including some unpublished results)

Introduction to Heisenberg models

Localized spins → spin-only model, Heisenberg (super)exchange interaction

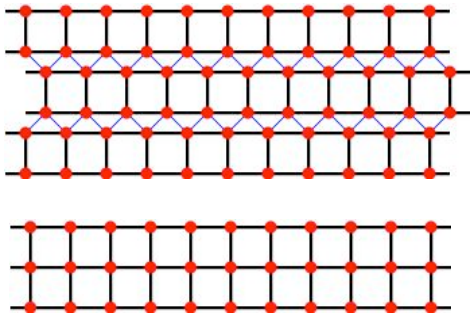


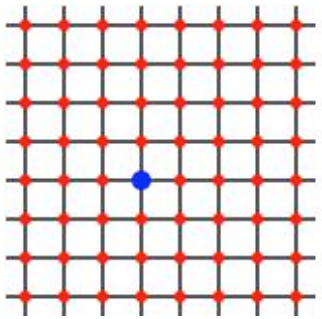


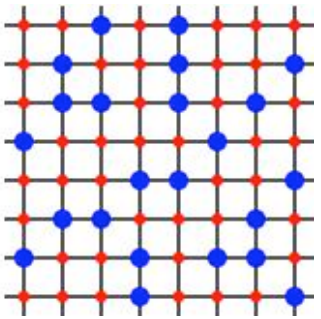
$$H = J \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j$$

Many quasi-1D and quasi-2D **antiferromagnetic** materials (cuprates, organics,...)

- chains, ladders, 2D planes, impurities, frustrated interactions, ...



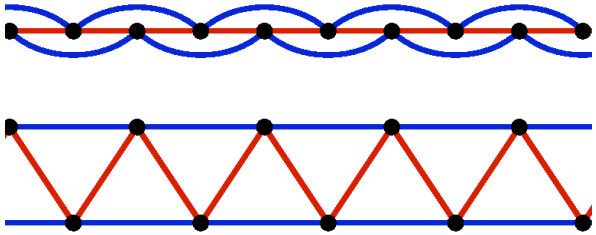




The physics of the Heisenberg model depends strongly on the geometry

- different types of ground states and excitations
- quantum phase transitions between different ground states

1D S=1/2 Heisenberg chain with frustrated interactions



$= J_1$

$= J_2$

Two types of ground states, depending on the ratio **$g=J_2/J_1$**

- **Antiferromagnetic "quasi order" (critical state) for g<0.25**
  - exact solution - Bethe Ansatz - for $J_2=0$
  - bosonization approach gives additional information
  - spin-spin correlations decay as 1/r

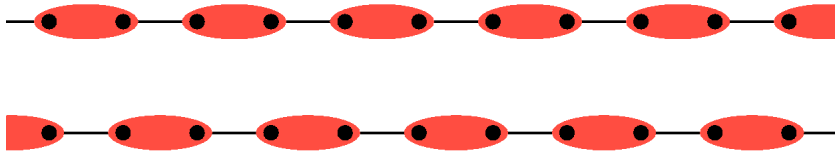
$$\langle \vec{S}_i \cdot \vec{S}_j \rangle \sim \frac{(-1)^{r_{ij}}}{r_{ij}}$$

  - gapless spin excitations

- **Valence-bond solid (VBS) order for g>0.25; doubly-degenerate state**
  - gap to spin excitations; exponentially decaying spin correlations

$$\langle \vec{S}_i \cdot \vec{S}_j \rangle \sim \exp(-r_{ij}/\xi)(-1)^{r_{ij}}$$

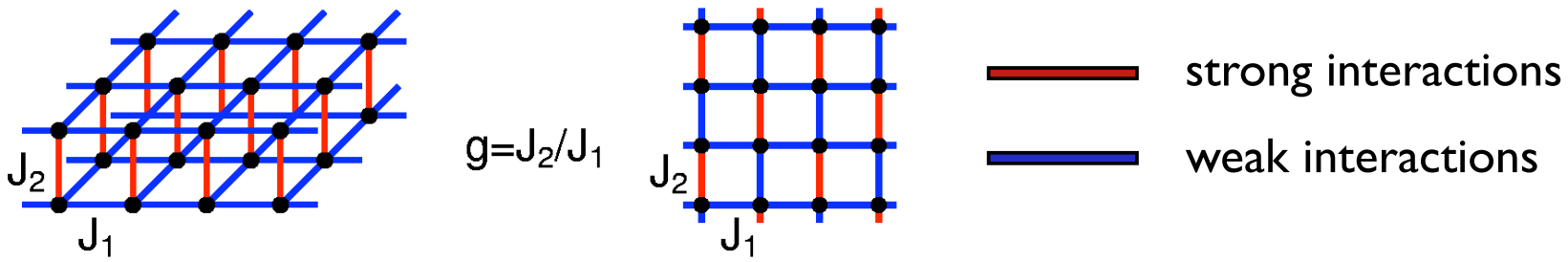
  - singlet-product state is exact for g=0.5 (Majumdar-Gosh point)



2D quantum-criticality (T=0 transition)

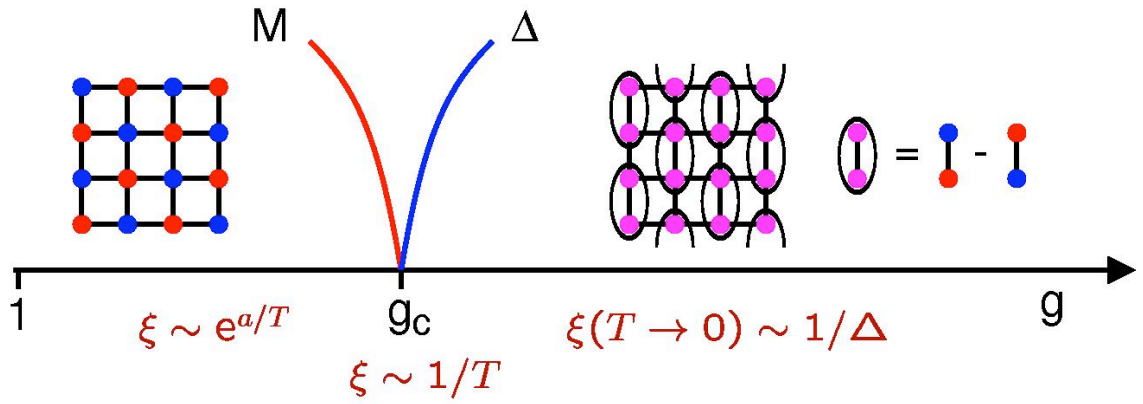
"Manually" dimerized S=1/2 Heisenberg models

Examples: bilayer, dimerized single layer



Singlet formation on strong bonds ➙ Neel - disordered transition

Ground state (T=0) phases



2D quantum spins map onto (2+1)D classical spins (Haldane)

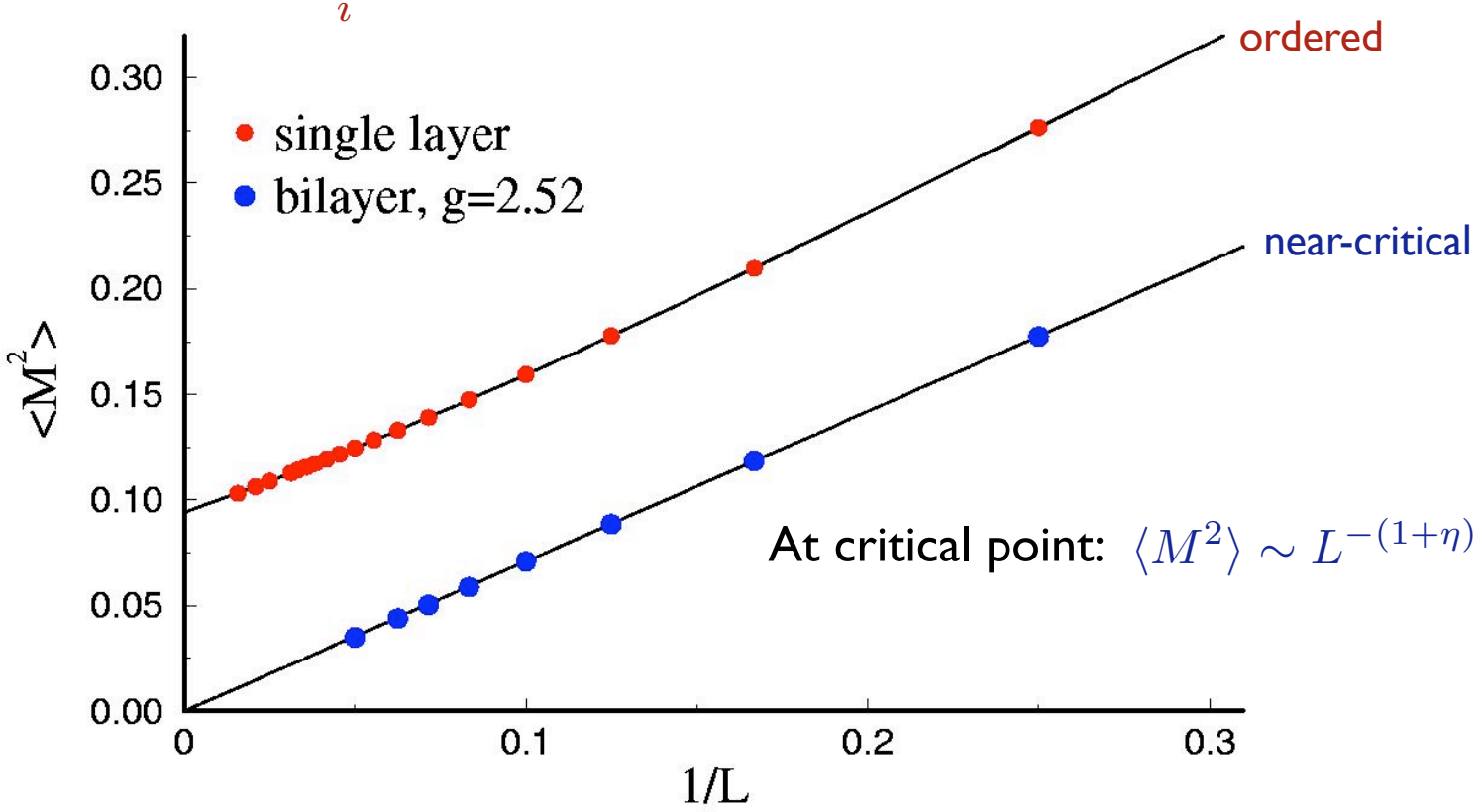
- Continuum field theory: nonlinear σ-model (Chakravarty, Halperin, Nelson)

⇒3D classical Heisenberg (O3) universality class expected

Example: 2D Heisenberg model (T→0) simulations
Finite-size scaling of the sublattice magnetization

$$\vec{M} = \frac{1}{N}\sum_i (-1)^{x_i+y_i}\vec{S}_i$$

In simulations we calculate <M^2>



At critical point: $\langle M^2 \rangle \sim L^{-(1+\eta)}$

Simulations & theory agree: O(3) universality class (e.g., η≈0.03)

[L. Wang, K. S. D. Beach, and A. W. Sandvik, PRB 73, 014431 (2006)]

- but staggered dimerization may (?) give another universality class

[S. Wenzel et al., PRL 101, 127202 (2008); F. C. Jiang, ArXiv:0911.0653]

Deconfined quantum criticality

$$H = J \sum_{\langle i,j \rangle} S_i \cdot S_j + g \times \cdots$$

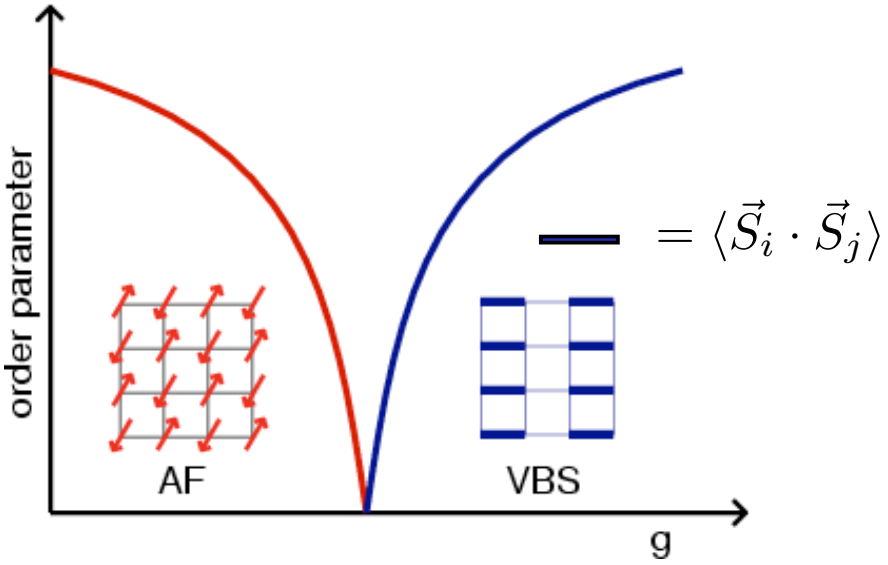
Senthil et al., Science 303, 1490 (2004)

Quantum phase transition in a 2D model with one spin per unit cell

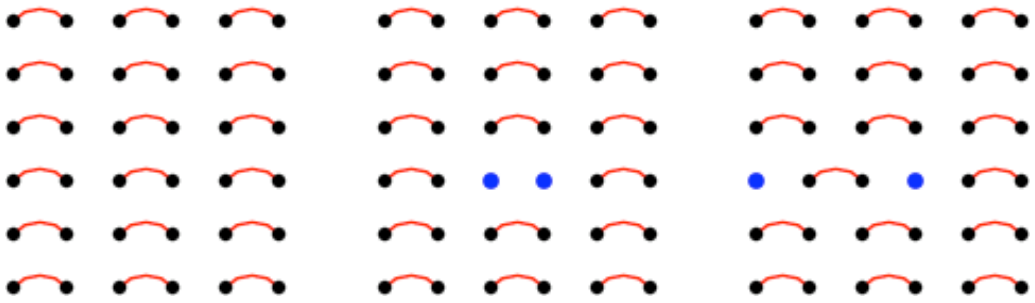
- antiferromagnetic for small g
- valence-bond solid (VBS) for large g (spontaneously broken symmetry)

Questions

- is the transition continuous?
  - normally order-order transitions are first order (Landau-Ginzburg)
  - theory of "deconfined" quantum critical points has continuous transition
- nature of the VBS fluctuations
  - emergent U(1) symmetry predicted



Spinon deconfinement upon approaching the critical point



Confinement inside VBS phase associated with new length scale and emergent U(1) symmetry

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Exact diagonalization

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Studies of small spin chains

Using basis states incorporating conservation laws (symmetries)

- magnetization conservation, momentum states, parity, spin inversion
- discussion without group theory
  - only basic quantum mechanics and common sense needed

Lanczos diagonalization (ground state, low excitations)

How to characterize different kinds of ground states

- critical ground state of the Heisenberg chain
- quantum phase transition to a valence-bond solid in a J_1-J_2 chain
- long-range interactions; continuous and first-order phase transitions

Numerical diagonalization of the hamiltonian

To find the ground state (maybe excitations, T>0 properties)
of the Heisenberg S=1/2 chain

$$H = J\sum_{i=1}^{N} \mathbf{S}_i \cdot \mathbf{S}_{i+1} = J\sum_{i=1}^{N} [S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + S_i^z S_{i+1}^z],$$

$$= J\sum_{i=1}^{N} [S_i^z S_{i+1}^z + \tfrac{1}{2}(S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+)]$$

Simplest way computationally; enumerate the states

- construct the hamiltonian matrix using bits

$$|0\rangle = |\downarrow,\downarrow,\downarrow,\ldots,\downarrow\rangle \quad (=0\ldots000)$$
$$|1\rangle = |\uparrow,\downarrow,\downarrow,\ldots,\downarrow\rangle \quad (=0\ldots001)$$
$$|2\rangle = |\downarrow,\uparrow,\downarrow,\ldots,\downarrow\rangle \quad (=0\ldots010)$$
$$|3\rangle = |\uparrow,\uparrow,\downarrow,\ldots,\downarrow\rangle \quad (=0\ldots011)$$

$$H_{ij} = \langle i|H|j\rangle$$
$$i,j = 0,\ldots,2^N-1$$

bit representation perfect for S=1/2 systems

- use >1 bit/spin for S>1/2, or integer vector
- construct H by examining/flipping bits

Diagonalizing the hamiltonian matrix

- on the computer
- gives the eigenvalues and eigenvectors

If U is the matrix whose columns are the eigenvectors of H, then

$$\langle n|A|n\rangle = [U^{T*}AU]_{nn}$$

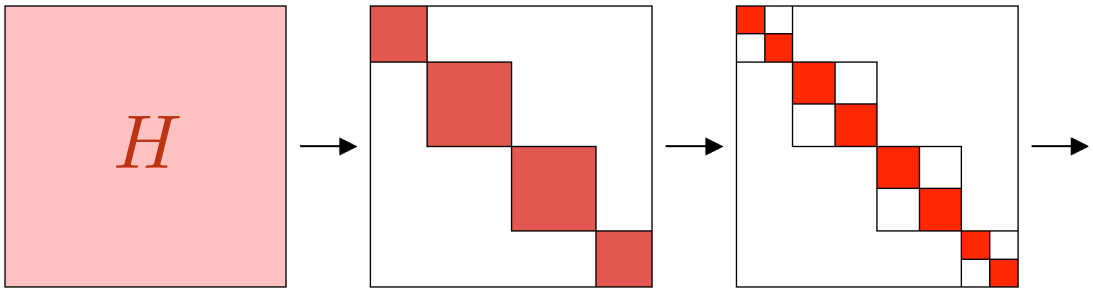
is the expectation value of some operator A in the n:th eigenstate

Problem: Matrix size $M=2^N$ becomes too large quickly

- maximum number of spins in practice; N≈20
- M^2 matrix elements to store, time to diagonalize $\propto M^3$

Using conservation laws (symmetries) for block-diagonalization

We can choose the basis in such a way that the H becomes block-diagonal



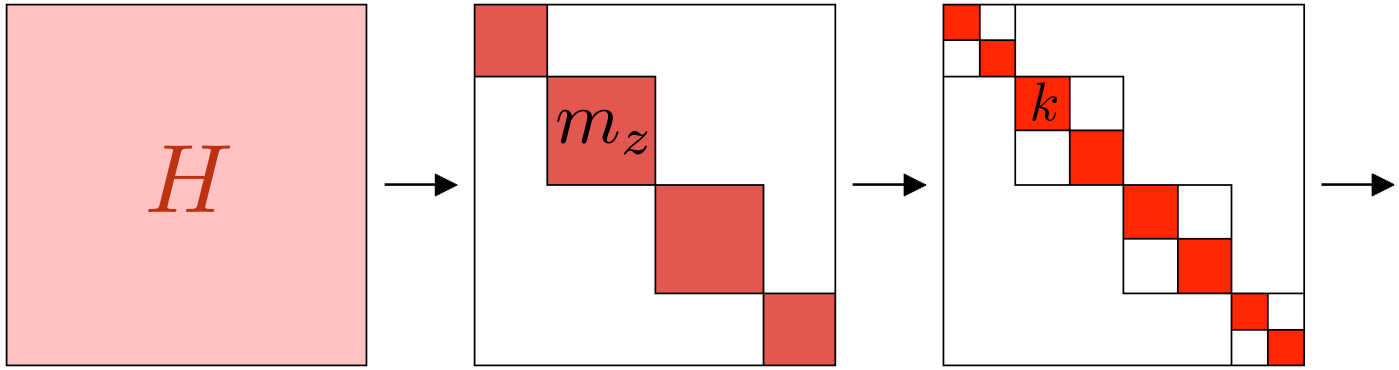
- the blocks can be diagonalized individually
- we can reach larger N (but not much larger, N≈40 is max)

Simplest example; magnetization conservation

$$m_z = \sum_{i=1}^{N} S_i^z$$

- blocks correspond to fixed values of m_z
- no H matrix elements between states of different m_z
- A block is constructed by only including states with a given m_z
  - corresponds to ordering the states in a particular way

Number of states in the largest block (m_z =0): $N!/[(N/2)!]^2$

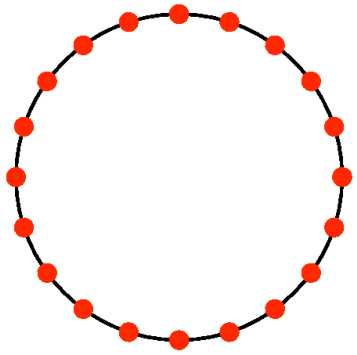


Other symmetries (conserved quantum numbers)

- can be used to further split the blocks
- but more complicated
  - basis states have to be constructed to obey symmetries
  - e.g., momentum states (using translational invariance)

Momentum states (translationally invariant systems)

A periodic chain (ring), translationally invariant



- the eigenstates have a momentum (crystal momentum) k

$$T|n\rangle = \mathrm{e}^{ik}|n\rangle \qquad k = m\frac{2\pi}{N}, \quad m = 0, \ldots, N-1,$$

The operator T translates the state by one lattice spacing

- for a spin basis state

$$T|S_1^z, S_2^z, \ldots, S_N^z\rangle = |S_N^z, S_1^z, \ldots, S_{N-1}^z\rangle$$

[T,H]=0 → momentum blocks of H

- can use eigenstates of T with given k as basis

A momentum state can be constructed from any **representative** state

$$|a(k)\rangle = \frac{1}{\sqrt{N_a}} \sum_{r=0}^{N-1} \mathrm{e}^{-ikr} T^r |a\rangle, \qquad |a\rangle = |S_1^z, \ldots, S_N^z\rangle$$

Construct ordered list of representatives
If Ia> and Ib> are representatives, then

$$T^r|a\rangle \neq |b\rangle \quad r \in \{1, \ldots, N-1\}$$

4-site examples
(**0011**)→(0110),(1100),(1001)
(**0101**)→(1010)

Convention: the representative is the one corresponding to the smallest integer

$$|a(k)\rangle = \frac{1}{\sqrt{N_a}} \sum_{r=0}^{N-1} \mathrm{e}^{-ikr} T^r |a\rangle, \qquad |a\rangle = |S_1^z, \ldots, S_N^z\rangle$$

The sum can contain several copies of the same state

- if $T^R|a\rangle = |a\rangle \quad \text{for some } R$
- the total weight for this component is

$$1 + \mathrm{e}^{-ikR} + \mathrm{e}^{-i2kR} + \ldots + \mathrm{e}^{-ik(N-R)}$$

- vanishes (state incompatible with k) unless kR=n2π
- the total weight of the representative is then N/R

$$kR = n2\pi \rightarrow \frac{mR}{N} = n \rightarrow m = n\frac{N}{R} \rightarrow \mathrm{mod}(m, N/R) = 0$$

Normalization of a state |*a*(k)> with periodicity R_a

$$\langle a(k)|a(k)\rangle = \frac{1}{N_a} \times R_a \times \left(\frac{N}{R_a}\right)^2 = 1 \rightarrow N_a = \frac{N^2}{R_a}$$

Basis construction: find all allowed representatives and their periodicities

(a_1, a_2, a_3, ..., a_M)
(R_1, R_2, R_3, ..., R_M)

The block size **M** is initially not known

- approximately 1/N of total size of fixed m_z block
- depends on the periodicity constraint for given k

The Hamiltonian matrix. Write $S = 1/2$ chain hamiltonian as

$$H_0 = \sum_{j=1}^{N} S_j^z S_{j+1}^z, \quad H_j = \tfrac{1}{2}(S_j^+ S_{j+1}^- + S_j^+ S_{j+1}^-), \quad j = 1, \ldots, N$$

Act with H on a momentum state

$$H|a(k)\rangle = \frac{1}{\sqrt{N_a}} \sum_{r=0}^{N-1} \mathrm{e}^{-ikr} T^r H|a\rangle = \frac{1}{\sqrt{N_a}} \sum_{j=0}^{N} \sum_{r=0}^{N-1} \mathrm{e}^{-ikr} T^r H_j|a\rangle,$$

$H_j|a\rangle$ is related to some representative: $H_j|a\rangle = h_a^j T^{-l_j}|b_j\rangle$

$$H|a(k)\rangle = \sum_{j=0}^{N} \frac{h_a^j}{\sqrt{N_a}} \sum_{r=0}^{N-1} \mathrm{e}^{-ikr} T^{(r-l_j)}|b_j\rangle$$

Shift summation index r and use definition of momentum state

$$H|a(k)\rangle = \sum_{j=0}^{N} h_a^j \mathrm{e}^{-ikl_j} \sqrt{\frac{N_{b_j}}{N_a}}|b_j(k)\rangle \qquad \rightarrow \text{matrix elements}$$

$$\langle a(k)|H_0|a(k)\rangle = \sum_{j=1}^{N} S_j^z S_j^z,$$

$$\langle b_j(k)|H_{j>0}|a(k)\rangle = \mathrm{e}^{-ikl_j} \frac{1}{2} \sqrt{\frac{R_a}{R_{b_j}}}, \qquad |b_j\rangle \propto T^{-l_j} H_j|a\rangle,$$

Reflection symmetry (parity)

Define a reflection (parity) operator

$$P|S_1^z, S_2^z, \ldots, S_N^z\rangle = |S_N^z, \ldots, S_2^z, S_1^z\rangle$$

Consider a hamiltonian for which [H,P]=0 and [H,T]=0; but note that [P,T]≠0

Can we still exploit both P and T at the same time? Consider the state

$$|a(k,p)\rangle = \frac{1}{\sqrt{N_a}} \sum_{r=0}^{N-1} \mathrm{e}^{-ikr} T^r (1 + pP)|a\rangle, \quad p = \pm 1$$

This state has momentum k, but does it have parity p? Act with P

$$P|a(k,p)\rangle = \frac{1}{\sqrt{N_a}} \sum_{r=0}^{N-1} \mathrm{e}^{-ikr} T^{-r} (P + p)|a\rangle$$

$$= p\frac{1}{\sqrt{N_a}} \sum_{r=0}^{N-1} \mathrm{e}^{ikr} T^r (1 + pP)|a\rangle \quad = p|a(k,p)\rangle \text{ if } k = 0 \text{ or } k = \pi$$

k=0,π momentum blocks are split into p=+1 and p=–1 sub-blocks

- [T,P]=0 in the k=0,π blocks
- physically clear because -k=k on the lattice for k=0,π
- we can exploit parity in a different way for other k →
- **semi-momentum states**

Semi-momentum states

Mix momenta +k and –k for k≠0,π

$$|a^\sigma(k)\rangle = \frac{1}{\sqrt{N_a}} \sum_{r=0}^{N-1} C_k^\sigma(r) T^r |a\rangle \qquad C_k^\sigma(r) = \begin{cases} \cos(kr), & \sigma = +1 \\ \sin(kr), & \sigma = -1. \end{cases}$$

$$k = m\frac{2\pi}{N}, \quad m = 1, \ldots, N/2 - 1, \quad \sigma = \pm 1$$

States with same k, different σ are orthogonal

Semi-momentum states with parity

This state has definite parity with p=+1 or p=–1 for any k

$$|a^\sigma(k,p)\rangle = \frac{1}{\sqrt{N_a^\sigma}} \sum_{r=0}^{N-1} C_k^\sigma(r)(1+pP)T^r|a\rangle.$$

- (k,–1) and (k,+1) blocks
- the basis is of the same size as the original k-blocks
- but these states are real, not complex ⇒ computational advantage
- For k≠0,π, the p=-1 and p=+1 states are degenerate

Spin-inversion symmetry

Spin inversion operator: $Z|S_1^z, S_2^z, \ldots, S_N^z\rangle = |-S_1^z, -S_2^z, \ldots, -S_N^z\rangle$

In the magnetization block $m^z=0$ we can use eigenstates of Z

$$|a^\sigma(k,p,z)\rangle = \frac{1}{\sqrt{N_a^\sigma}} \sum_{r=0}^{N-1} C_k^\sigma(r)(1+pP)(1+zZ)T^r|a\rangle,$$

$$Z|a^\sigma(k,p,z)\rangle = z|a^\sigma(k,p,z)\rangle, \quad z=\pm 1$$

Example: block sizes

$m_z=0$, k=0 (largest momentum block)

	$(p=\pm1, z=\pm1)$			
N	$(+1,+1)$	$(+1,-1)$	$(-1,+1)$	$(-1,-1)$
8	7	1	0	2
12	35	15	9	21
16	257	183	158	212
20	2518	2234	2136	2364
24	28968	27854	27482	28416
28	361270	356876	355458	359256
32	4707969	4690551	4685150	4700500

Total spin S conservation

- difficult to exploit
- complicated basis states
- calculate S using **$S^2=S(S+1)$**

$$\mathbf{S}^2 = \sum_{i=1}^{N}\sum_{j=1}^{N} \mathbf{S}_i \cdot \mathbf{S}_j$$

$$= 2\sum_{i<j} \mathbf{S}_i \cdot \mathbf{S}_j + \frac{3}{4}N$$

Example: Thermodynamics

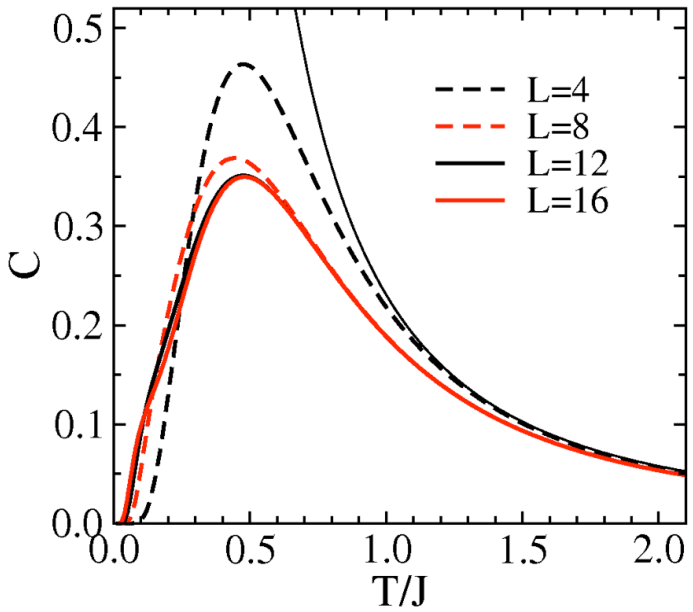
some quantities can be computed using only the magnetization m_z=0 sector

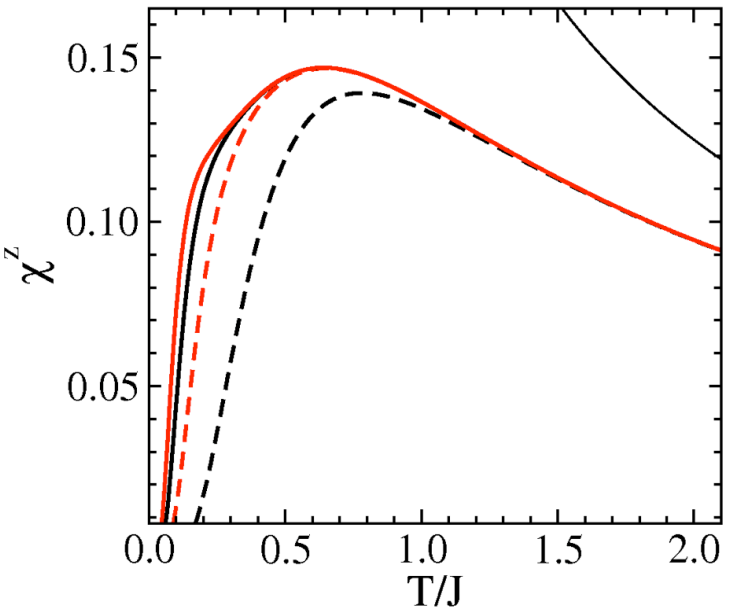
- spin-inversion symmetry can be used, smallest blocks
- spin-S state is **(2S+1)**-fold degenerate (no magnetix field) → weight factor
- possible spin dependence of expectation value → average over **m_z=–S,...,S**

$$C = \frac{d\langle H\rangle}{dt} = \frac{1}{T^2}\left(\langle H^2\rangle - \langle H\rangle^2\right)$$

$$\chi^z = \frac{d\langle m_z\rangle}{dh_z} = \frac{1}{T}\left(\langle m_z^2\rangle - \langle m_z\rangle^2\right)$$

$$\langle m_z\rangle = 0, \quad \langle m_z^2\rangle = \frac{\langle m_x^2 + m_y^2 + m_z^2\rangle}{3} = \frac{\langle S^2\rangle}{3} = \frac{S(S+1)}{3}$$





Compared with leading high-T forms

$\chi = (1/4)/T$

$C = (3/13)/T^2$

The Lanczos method

If we need only the ground state and a small number of excitations
- can use "Krylov space" methods, which work for much larger matrices
- basis states with 10^7 states or more can be easily handled (30-40 spins)

The Krylov space and "projecting out" the ground state

Start with an arbitrary state $|\psi\rangle$
- it has an expansion in eigenstates of H; act with a high power Λ of H

$$H^\Lambda|\Psi\rangle = \sum_n c_n E_n^\Lambda |n\rangle = E_0^\Lambda \left(c_0|0\rangle + c_1 \left(\frac{E_1}{E_0}\right)^\Lambda |1\rangle + \ldots \right)$$

For large Λ, if the state with largest $|E_n|$ dominates the sum
- one may have to subtract a constant, using *H–C*, to ensure ground state
- even better to use linear combination of states generated for different Λ

$$|\psi_a\rangle = \sum_{m=0}^{\Lambda} \psi_a(m) H^m |\Psi\rangle, \quad a = 0, \ldots, \Lambda$$

- diagonalize H in this basis

In the **Lanczos basis**, H is tridiagonal, convenient to generate and use
- Normally M=50-200 basis states is enough; easy to diagonalize H

Constructing the Lanczos basis

First: construct **orthogonal but not normalized basis $\{f_m\}$.** Define

$$N_m = \langle f_m | f_m \rangle, \quad H_{mm} = \langle f_m | H | f_m \rangle$$

The first state $|f_0\rangle$ is arbitrary, e.g., random. The next one is

$$|f_1\rangle = H|f_0\rangle - a_0|f_0\rangle$$

Demand orthogonality

$$\langle f_1 | f_0 \rangle = \langle f_0 | H | f_0 \rangle - a_0 \langle f_0 | f_0 \rangle = H_{00} - a_0 N_0 \quad \rightarrow \quad a_0 = H_{00}/N_0$$

All subsequent states are constructed according to

$$|f_{m+1}\rangle = H|f_m\rangle - a_m|f_m\rangle - b_{m-1}|f_{m-1}\rangle$$

$$a_m = H_{mm}/N_m, \quad b_{m-1} = N_m/N_{m-1}$$

Easy to prove orthogonality of all these states ($\langle f_{m+1}|f_m\rangle = 0$ is enough)

The hamiltonian in the Lanczos basis

Rewrite the state generation formula

$$H|f_m\rangle = |f_{m+1}\rangle + a_m|f_m\rangle + b_{m-1}|f_{m-1}\rangle$$

Because of the orthogonality, the only non-0 matrix elements are

$$\begin{aligned}
\langle f_{m-1}|H|f_m\rangle &= b_{m-1}N_{m-1} = N_m \\
\langle f_m|H|f_m\rangle &= a_m N_m \\
\langle f_{m+1}|H|f_m\rangle &= N_{m+1}
\end{aligned}$$

But the f-states or not normalized. The normalized states are:

$$|\phi_m\rangle = \frac{1}{\sqrt{N_m}}|f_m\rangle$$

In this basis the H-matrix is

$$\begin{aligned}
\langle \phi_{m-1}|H|\phi_m\rangle &= \sqrt{b_{m-1}} \\
\langle \phi_m|H|\phi_m\rangle &= a_m \\
\langle \phi_{m+1}|H|\phi_m\rangle &= \sqrt{b_m}
\end{aligned}$$

Alternative way

generate the normalized basis directly

• start with $|\phi_0\rangle$ arbitrary, normalized, and then

$$|\phi_1\rangle = \frac{1}{N_1}\big(H|\phi_0\rangle - a_0|\phi_0\rangle\big).$$

$$|\phi_{m+1}\rangle = \frac{1}{N_{m+1}}\big(H|\phi_m\rangle - a_m|\phi_m\rangle - N_m|\phi_{m-1}\rangle\big) = \frac{|\gamma_m\rangle}{N_{m+1}}$$

The definition of N_m is different, and no b_m:

$$\begin{aligned} a_m &= \langle\phi_m|H|\phi_m\rangle \\ N_m &= \langle\gamma_m|\gamma_m\rangle^{-1/2} \end{aligned}$$

Generate $|\gamma_m\rangle$ first, normalize to get N_{m+1}

The H-matrix is

$$\begin{aligned} \langle\phi_{m-1}|H|\phi_m\rangle &= N_m \\ \langle\phi_m|H|\phi_m\rangle &= a_m \\ \langle\phi_{m+1}|H|\phi_m\rangle &= N_{m+1} \end{aligned}$$

Operator expectation values

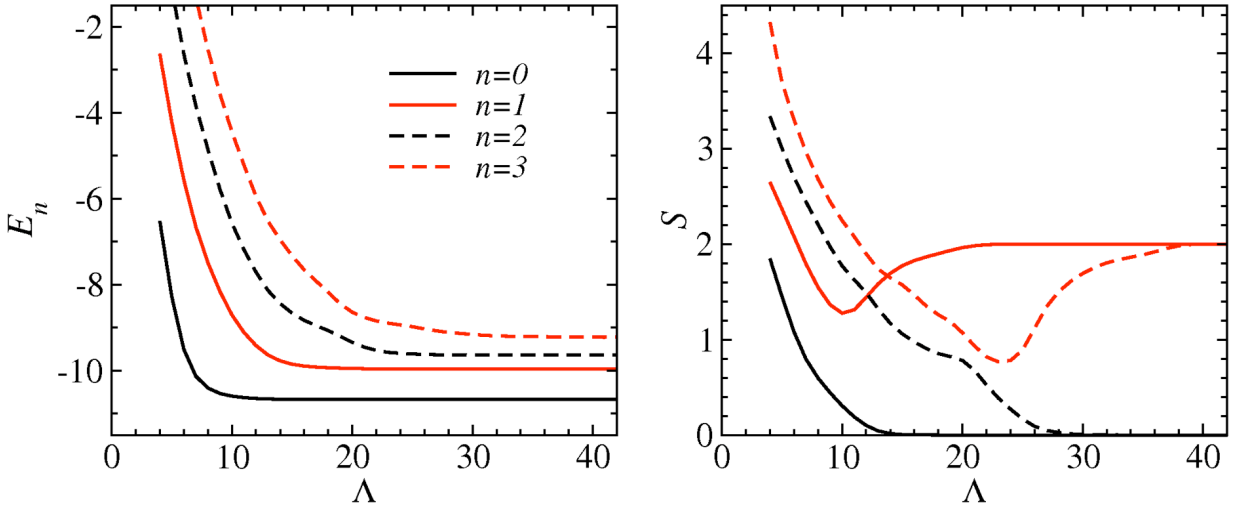
Diagonalizing the tri-diagonal matrix → eigenstates in the Lanczos basis

- eigenvectors v_n, energies E_n
- only some number of low-energy states (<< Λ) are correct eigenstates of H

To compute expectation values we go back to the original basis

$$\psi_n(a) = \sum_{m=0}^{\Lambda} v_n(m)\phi_m(a), \qquad a = 1, \ldots, M$$

Convergence properties of the Lanczos method



Example; 24-site chain
m_z = 0, k = 0, p = 1, z= 1
block size M=28416

Total spin S extracted assuming that

$$\langle S^2 \rangle = S(S+1)$$

Ground state converges first, then successively excited states

Spin correlations in the Heisenberg chain

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

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

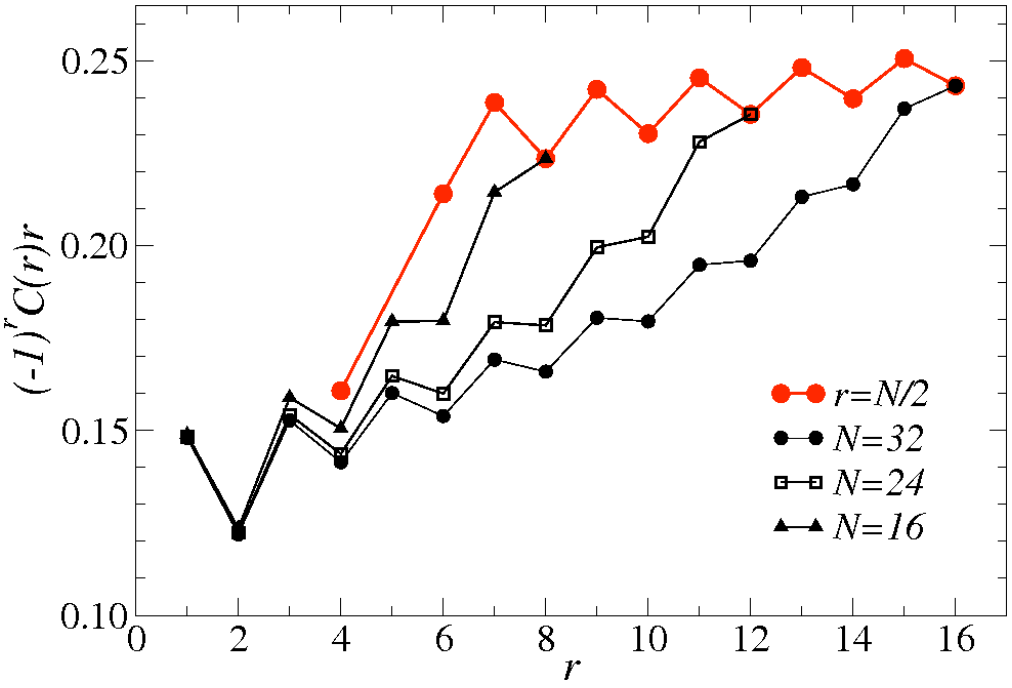
versus the distance r and at r=N/2 versus system size N

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

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

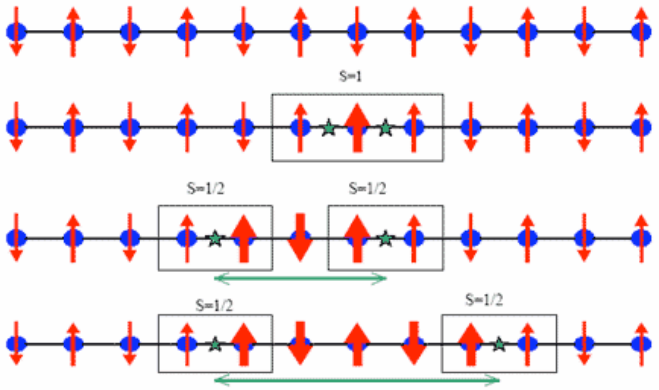
Plausible based on N up to 32
- other methods for larger N

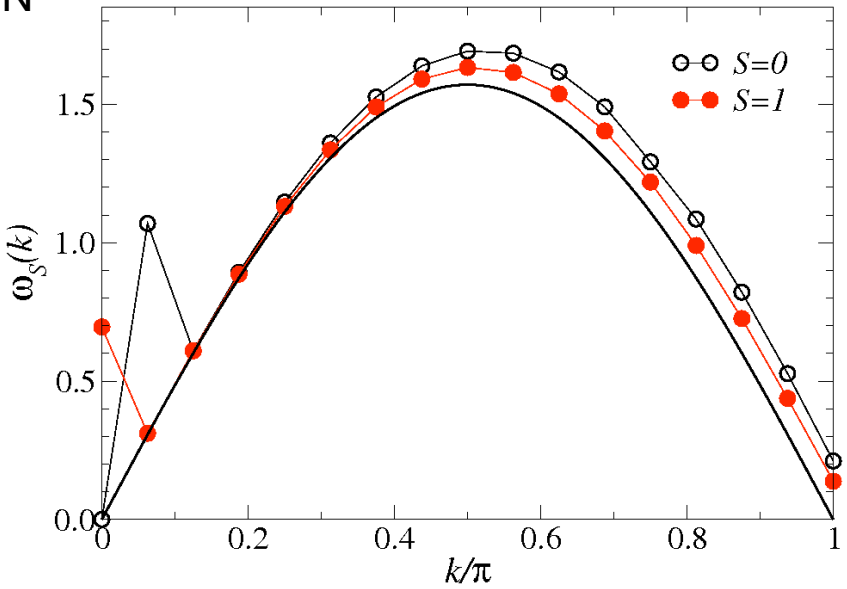
Power-law correlations are a sign of a "critical" state; at the boundary between
- ordered (antiferromagnetic)
- disordered (spin liquid)



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”

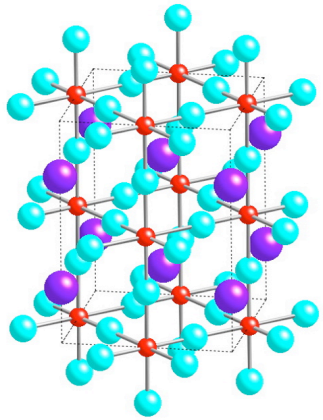


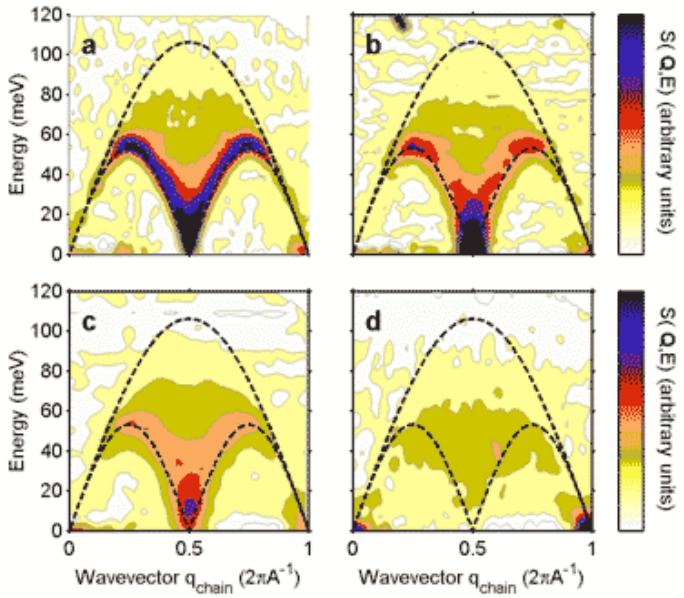


Neutron scattering experiments

- quasi-one-dimensional $KCuF_3$

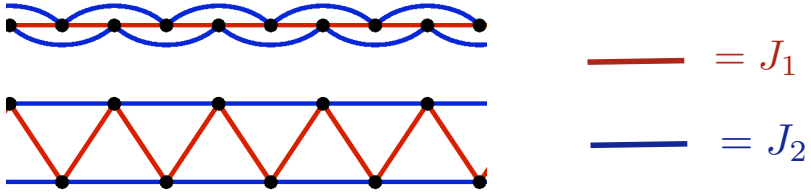
B. Lake et al., Nature Materials 4 329-334 (2005)





Heisenberg chain with frustrated interactions

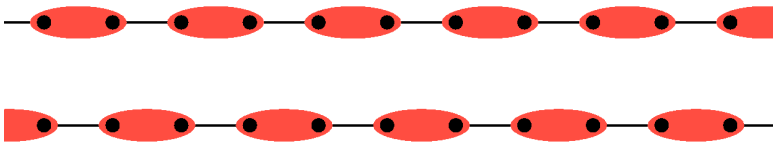
$$H = \sum_{i=1}^{N} \left[J_1 \mathbf{S}_i \cdot \mathbf{S}_{i+1} + J_2 \mathbf{S}_i \cdot \mathbf{S}_{i+2} \right]$$



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

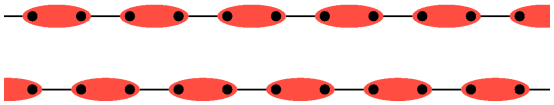
The symmetry is not broken for finite N

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

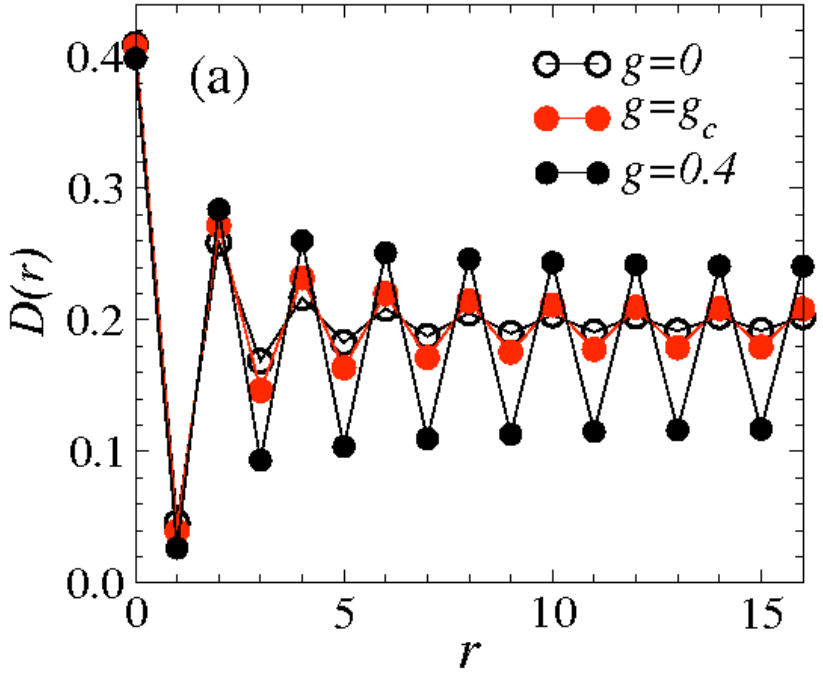
$$|\Psi_0\rangle \sim |\Psi_A\rangle + |\Psi_B\rangle, \qquad |\Psi_1\rangle \sim |\Psi_A\rangle - |\Psi_B\rangle$$

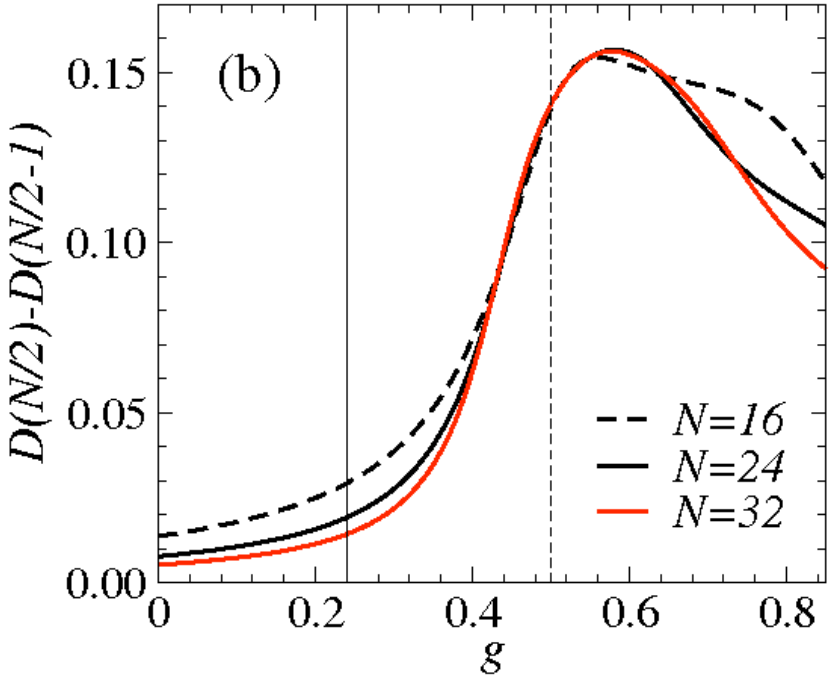
The VBS state can be detected in finite systems using “dimer” correlations

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



Results from Lanczos diagonaization; different coupling ratios ***g=J₂/J₁***

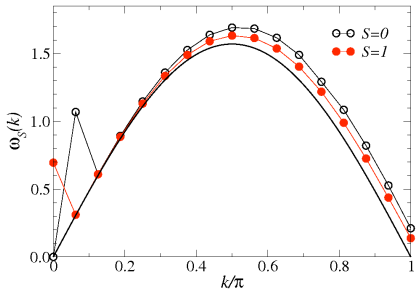




It is not easy to detect the transition this way

- 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)]

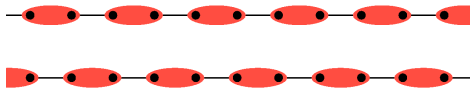
Determining the transition point using level crossings



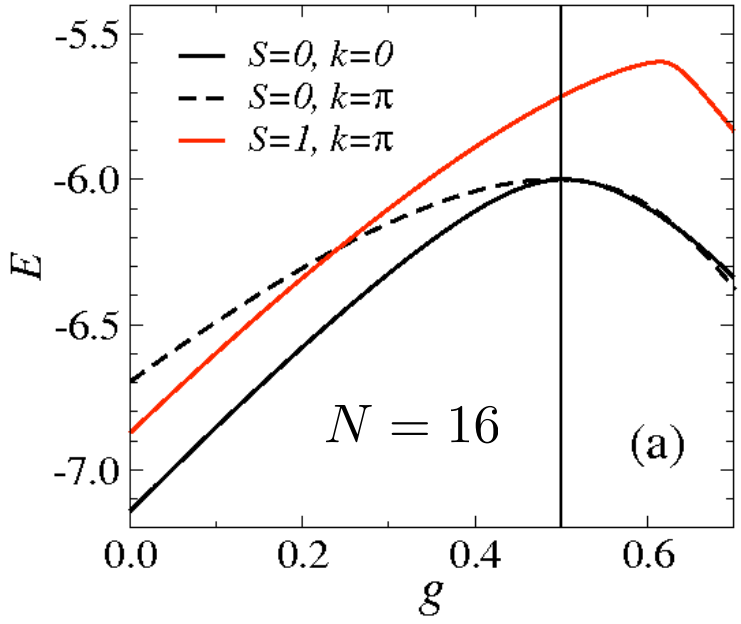
Lowest excitation for the g=0 Heisenberg chain is a triplet
- this can be expected for all $g<g_c$

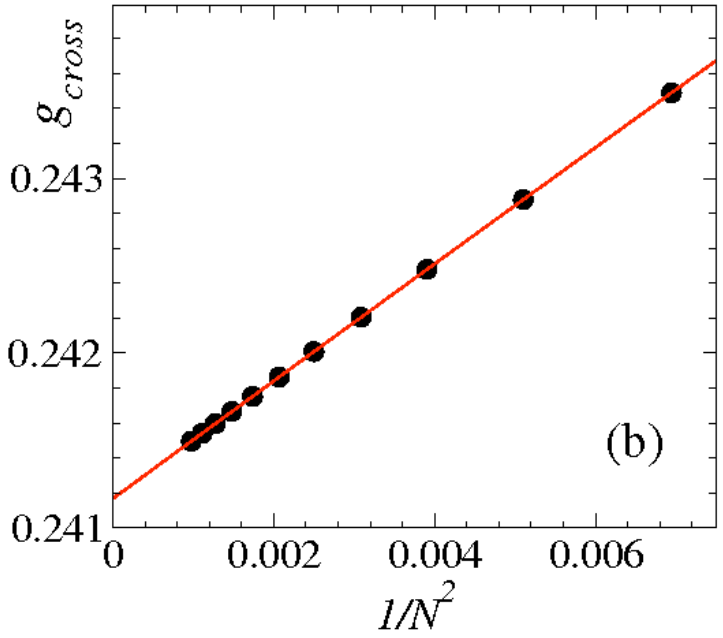
The VBS state is 2-fold degenerate for infinite N
- and for any N at g=1/2
- these two states are singlets
- gap between them closes exponentially as $N\to\infty$
- the lowest excitation is the second singlet

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



The two lowest excited states 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)]

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

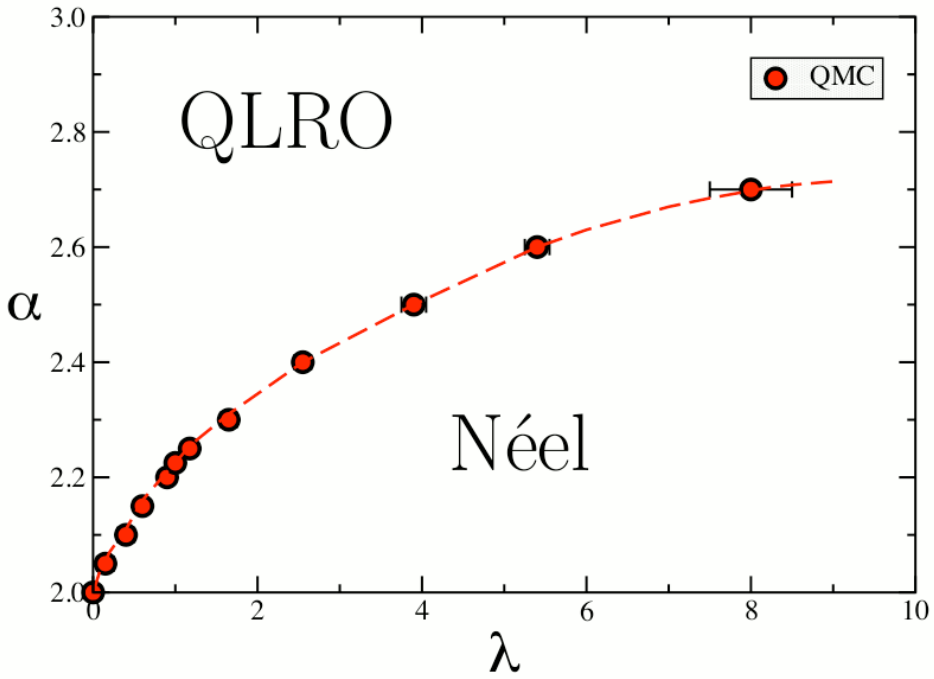
Phase transition between

- critritical 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

[A. W. S., unpublished work in progress]

Un-frustrated power-law decaying J_r, frustrating J_2

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

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

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

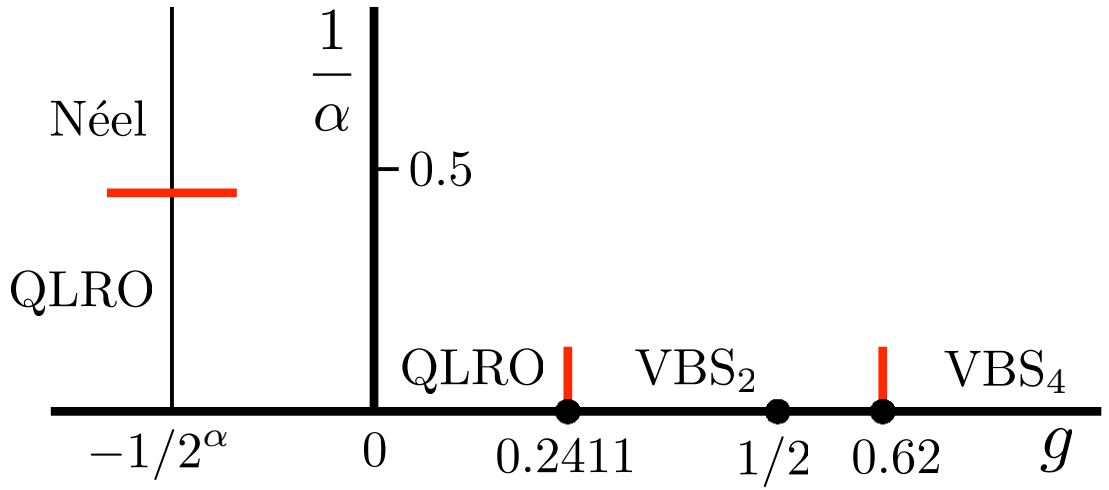
For $\alpha \to \infty$ the system reduces to the J_1-J_2 chain with $g = J_2/J_1$

(g,α) phase diagram

- two lines known
- other phases?
- Néel - VBS transition?

Technically challenging

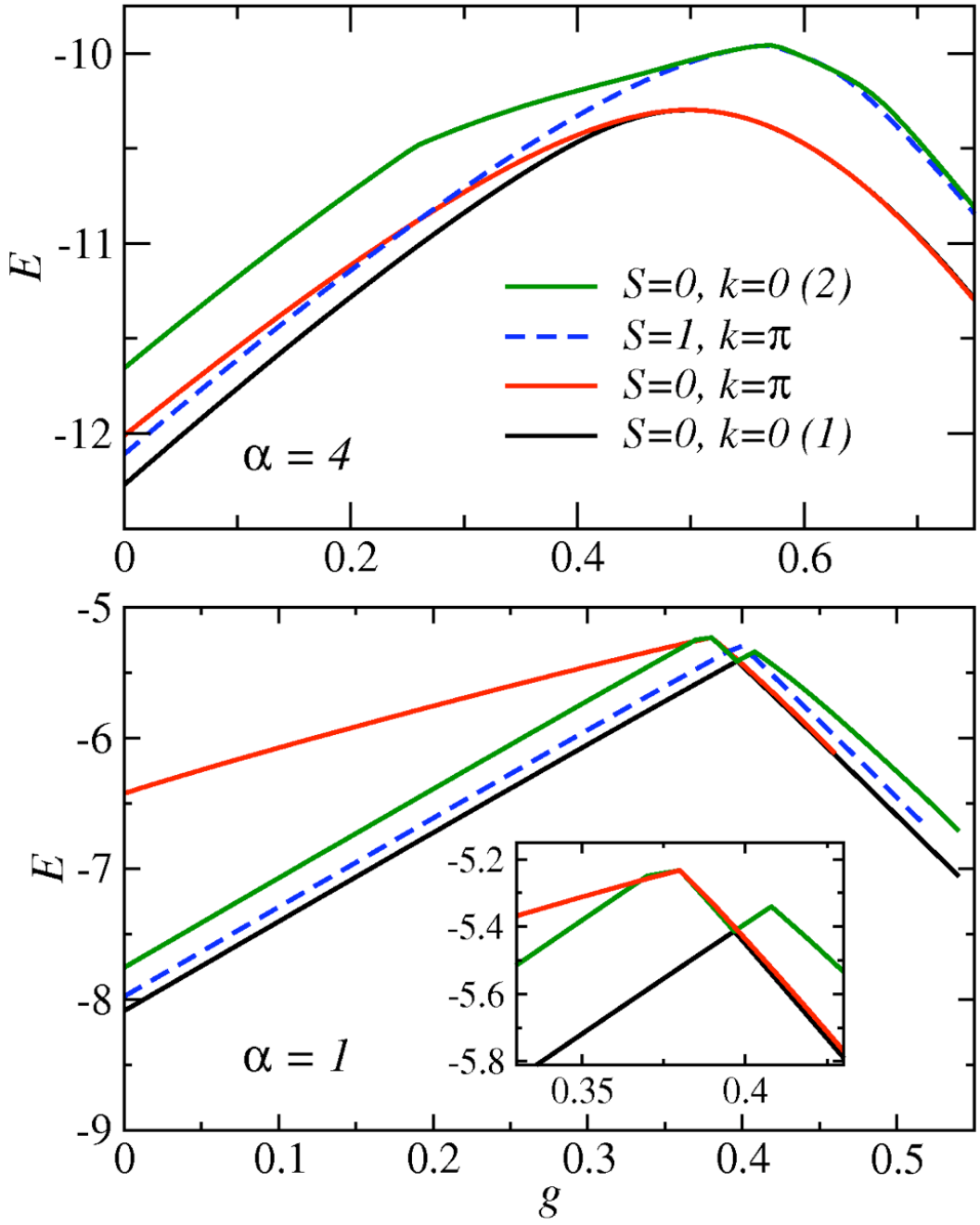
- QMC sign problem
- long-range interactions
  - DMRG difficulties
- What can exact diag tell?



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

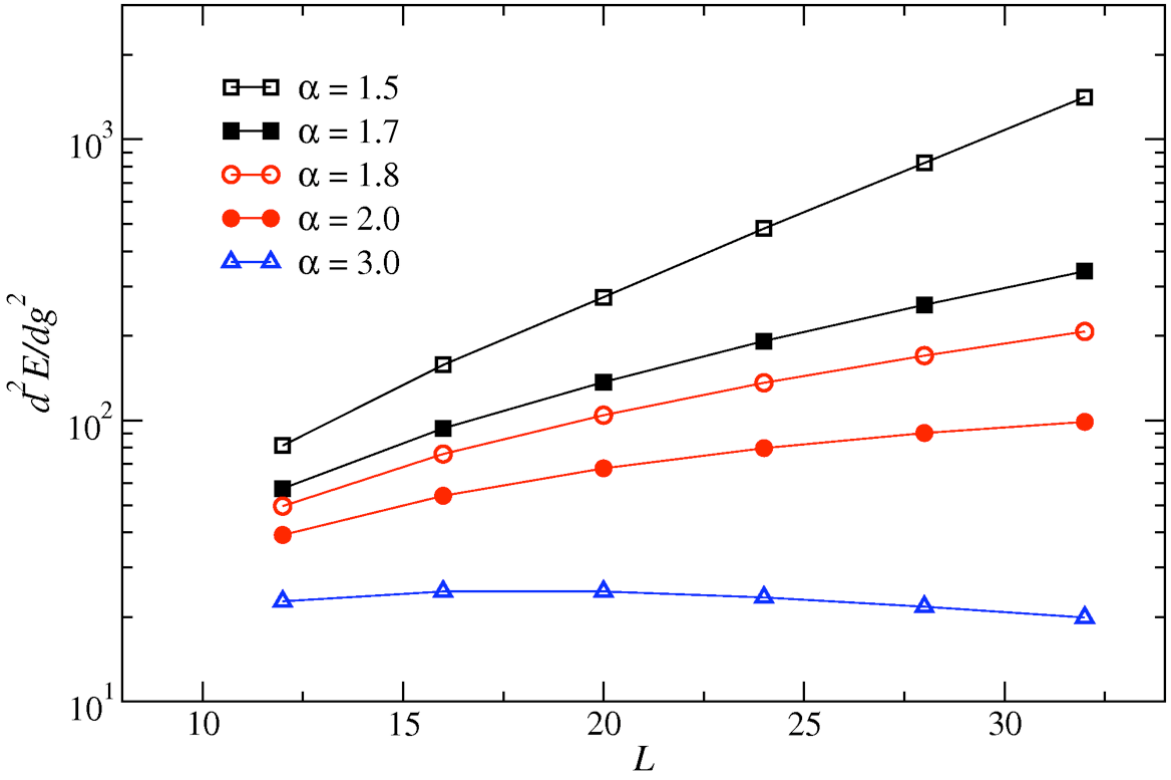
Different curve shapes for small α (<2)
- sharp breaks
- avoided level crossings
- indicative of 1st order phase transition

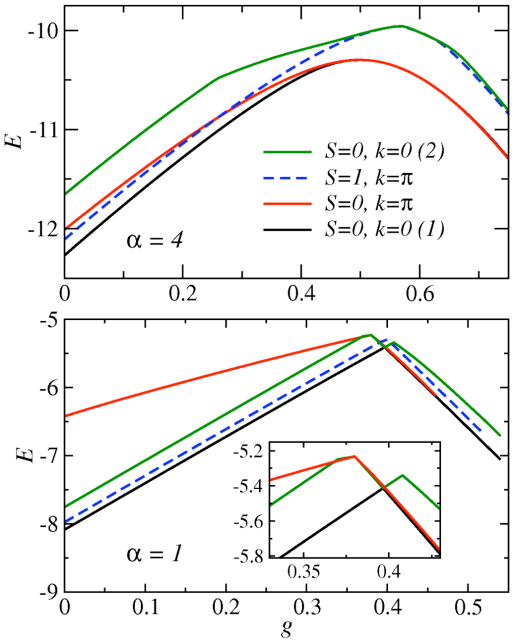


Analysis of the ground state energy curve $E_0(g)$

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

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

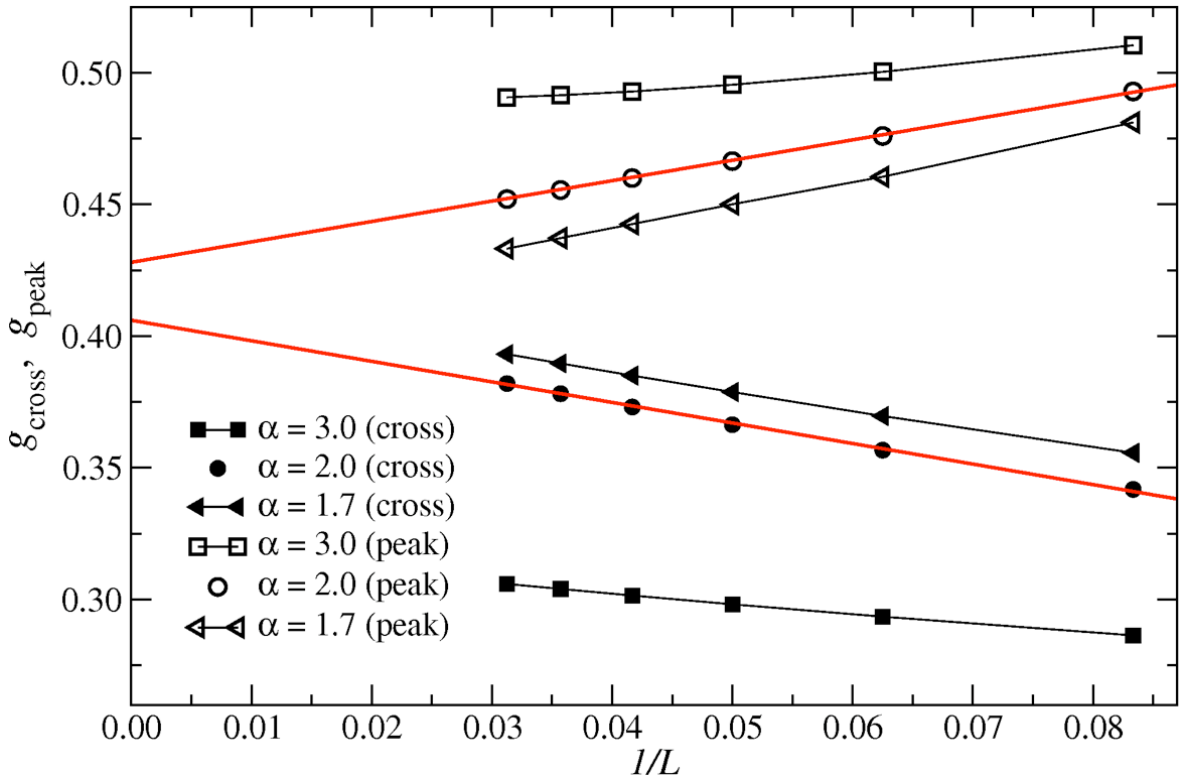




Exponentially divergent peak curvature for α<2

- 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

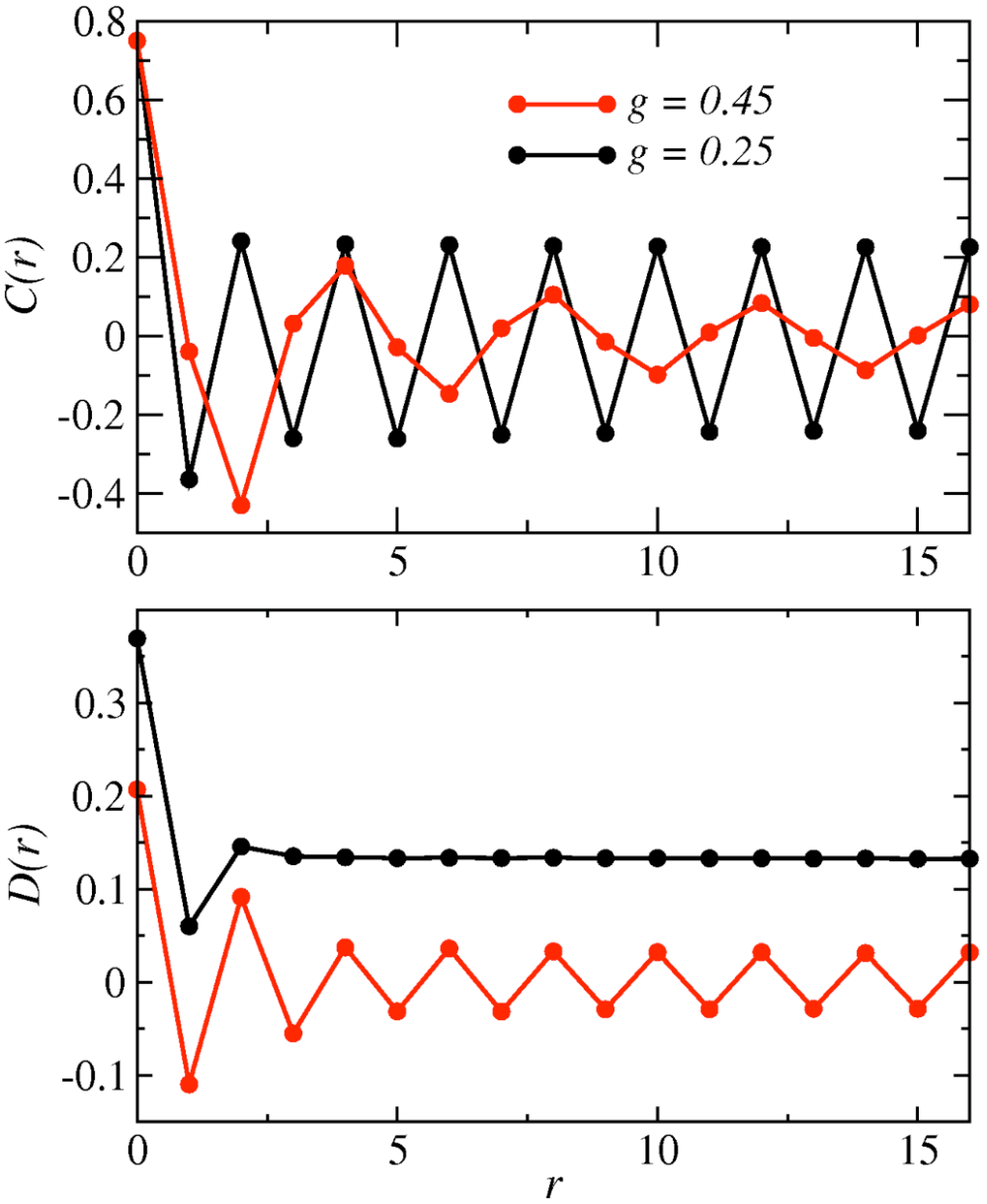
For α<1.8

- 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?

Correlations

Spin correlations C(r)
- staggered (Neel) for $g<g_c$
- period 4 for $g>g_c$

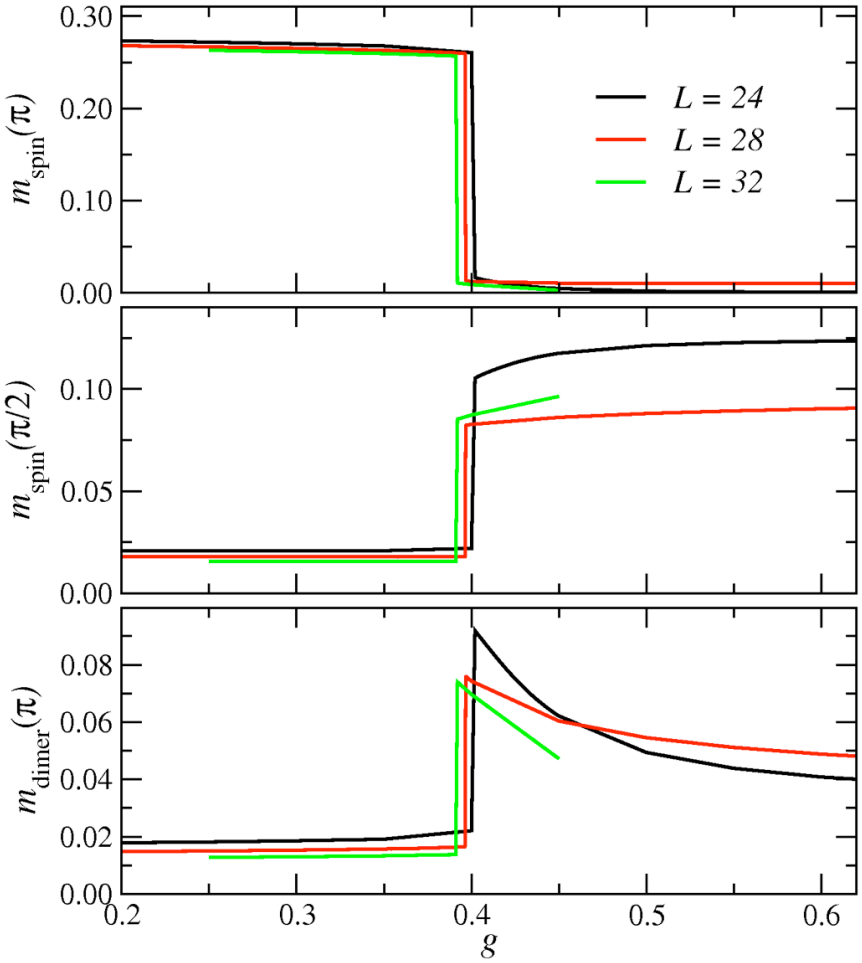
Dimer correlations D(r)
- short-ranged for $g<g_c$
- period-2 VBS for $g>g_c$



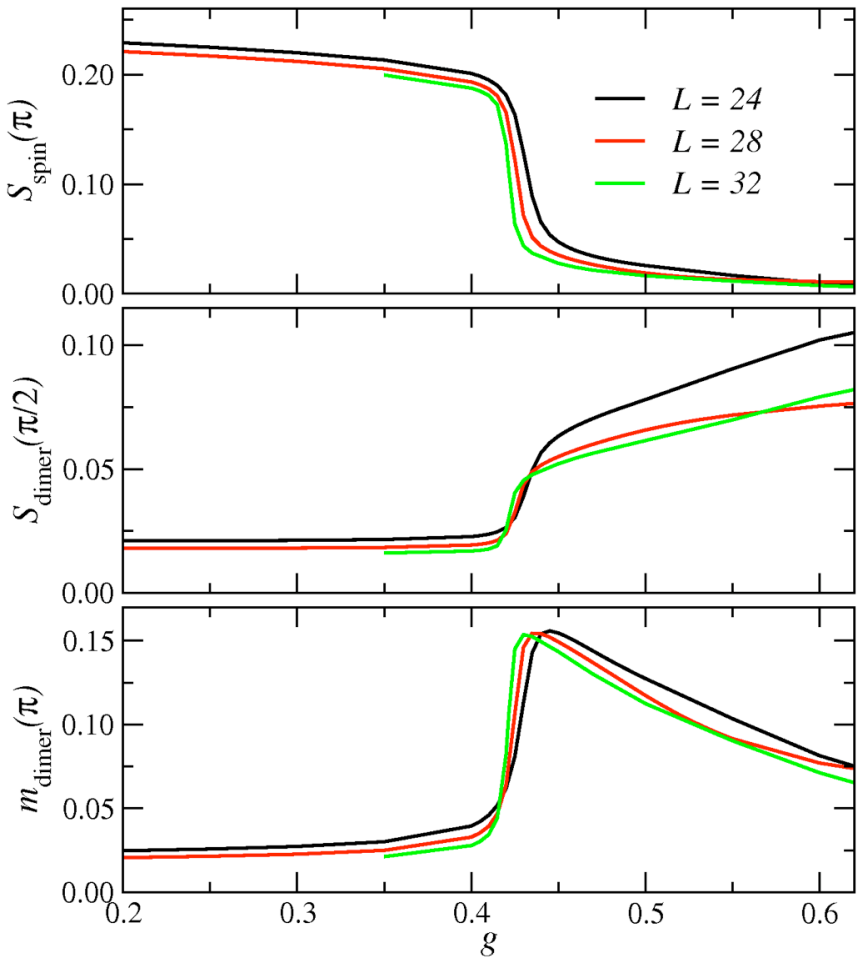
Order parameters

$$m(q) = \frac{1}{N} \sum_{r=0}^{N-1} \mathrm{e}^{-iqr} C(r)$$

$\alpha = 1.0$



$\alpha = 1.5$



The VBS may have long-range period-4 (q=π/2) spin order
• a kind of spin-super-solid

More work needed to settle details of the phase diagram