Example: Thermodynamics

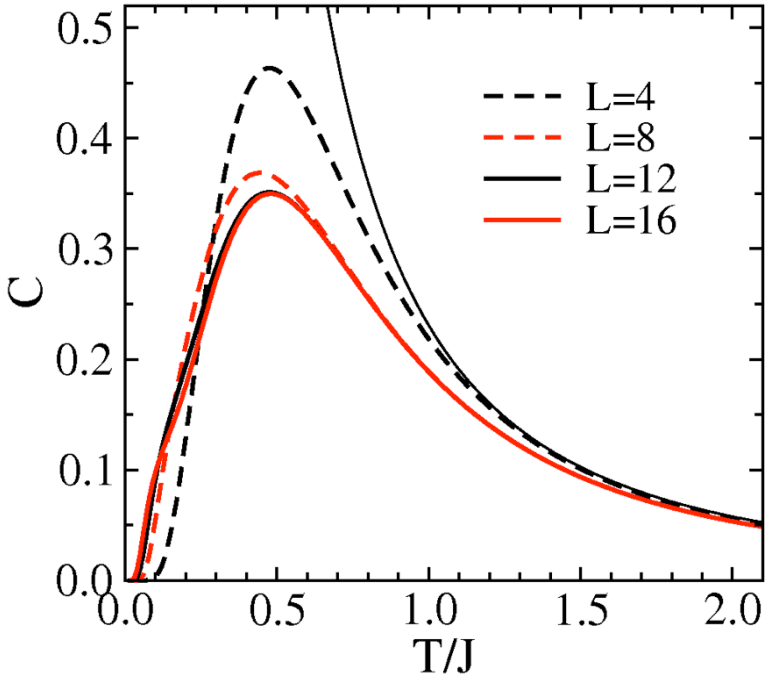
some quantities can be computed using only the magnetization m_z=0 sector

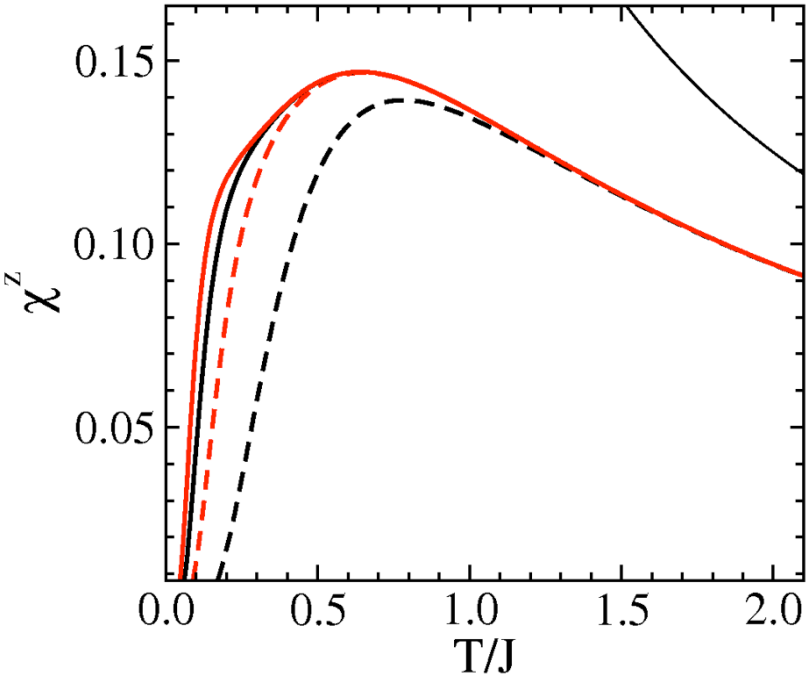
- spin-inversion symmetry can be used, smallest blocks
- spin-S state is **(2S+1)**-fold degenerate (no magnetic field) → weight factor
- possible spin dependence of expectation value → average over **m_z=–S,...,S**

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

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

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





Compared with leading high-T forms

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

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

The Lanczos method (review)

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

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

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

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

- 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 Hamiltonian matrix is

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

Operator expectation values

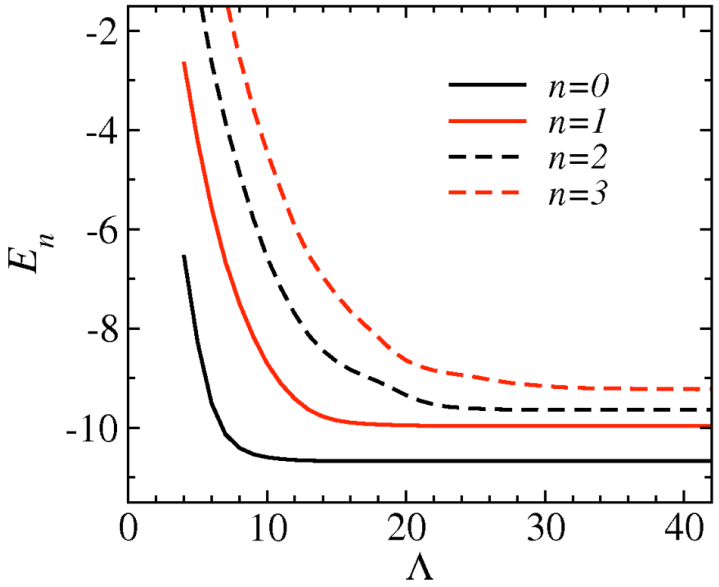
Diagonalizing the tri-diagonal matrix → eigenstates in the Lanczos basis

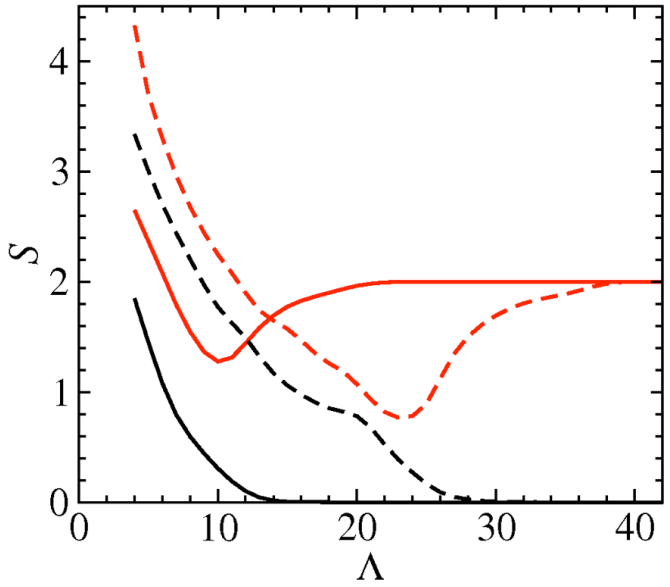
- eigenvectors v_n, energies E_n
- only some number of low-energy states (<< Λ) are correct eigenstates of H

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

Break-down of orthogonality

- will eventually happen for large m
- causes artificial degeneracies
- cured by re-orthogonalization
- all states have to be stored

Explicit re-orthogonalization

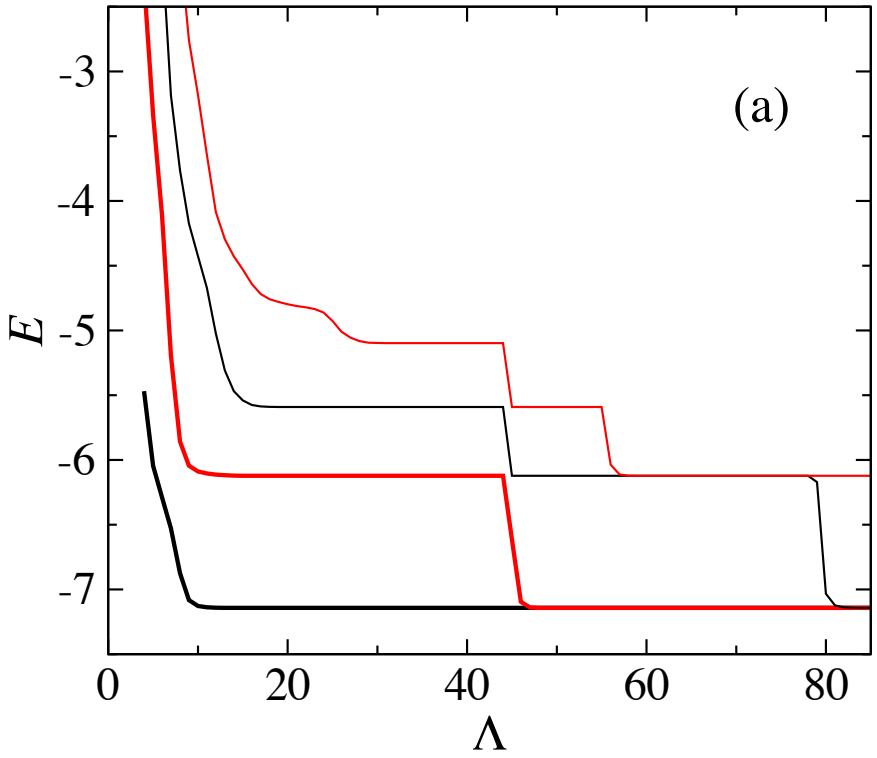
- after each Lanczos step (using the method with normalized states

$$|\phi_{m+1}\rangle \rightarrow \frac{|\phi_{m+1}\rangle - \sum_{i=0}^{m} q_i |\phi_i\rangle}{1 - \sum_{i=0}^{m} q_i^2}$$

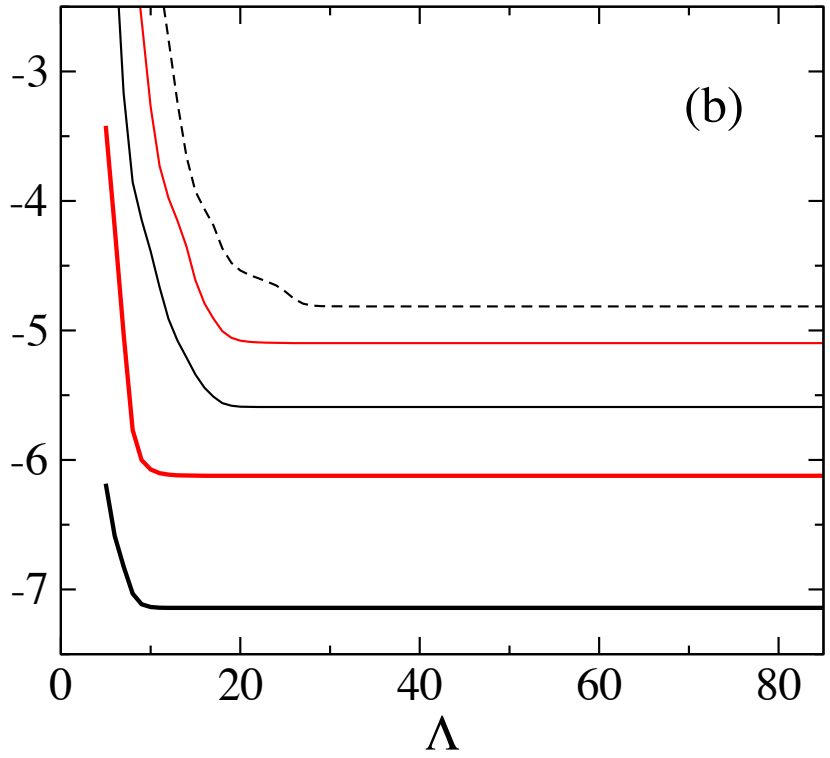
$$q_i = \langle \phi_i | \phi_{m+1} \rangle$$

$$N = 16,\ k = 0,\ p = 1,\ z = 1$$

no orthogonalization



with orthogonalization



Spin correlations in the Heisenberg chain

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

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

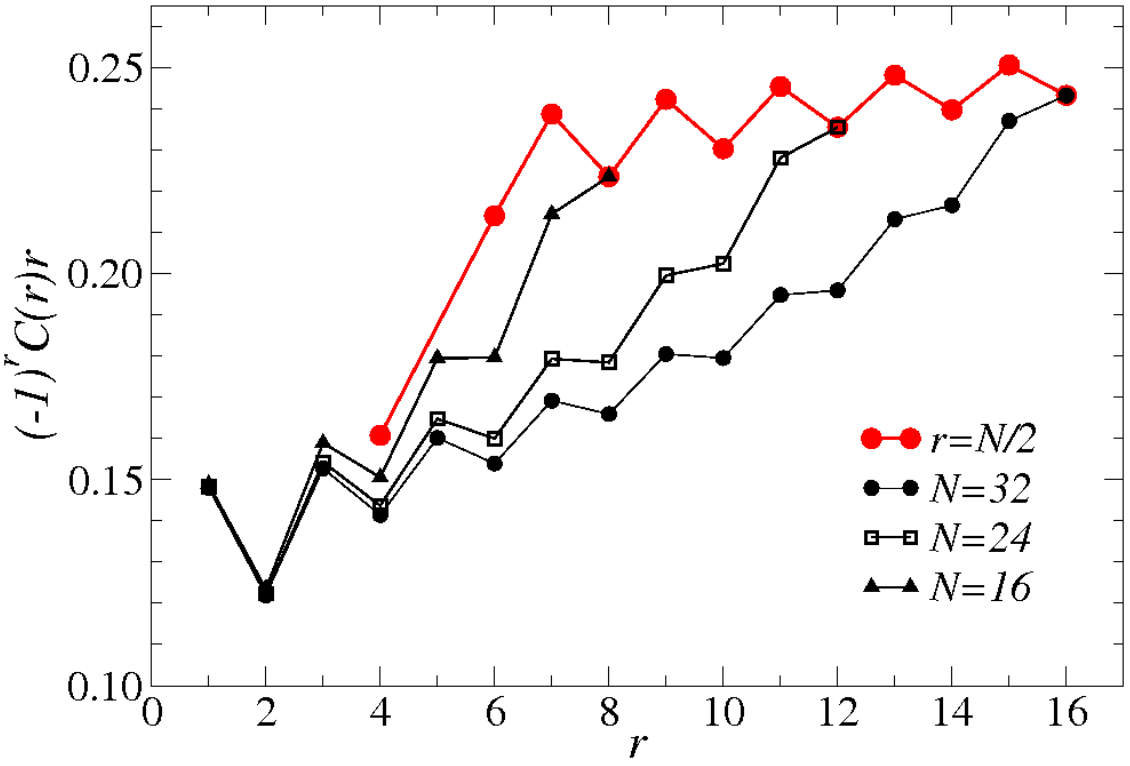
versus the distance r and at r=N/2 versus system size N

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

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

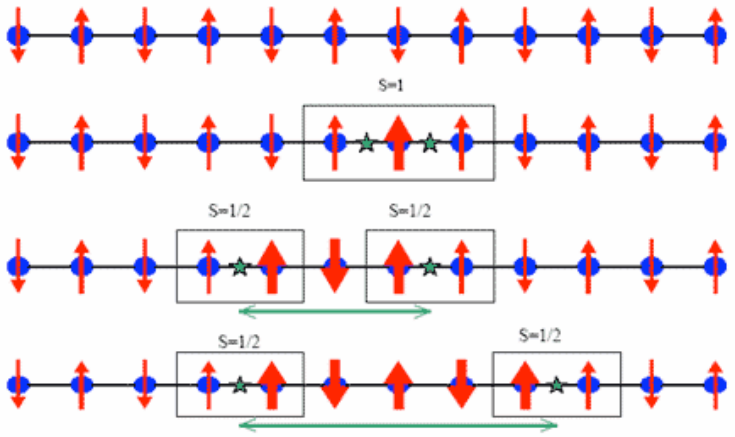
Plausible based on N up to 32
- other methods for larger N

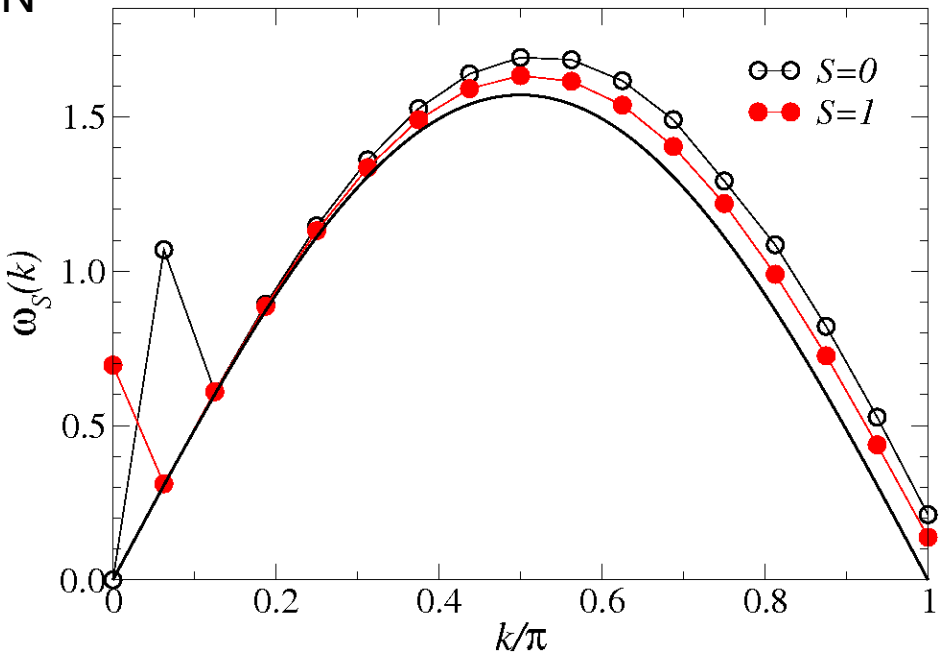
Power-law correlations are a sign of a "critical" state; at the boundary between
- ordered (antiferromagnetic)
- disordered (spin liquid)



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”

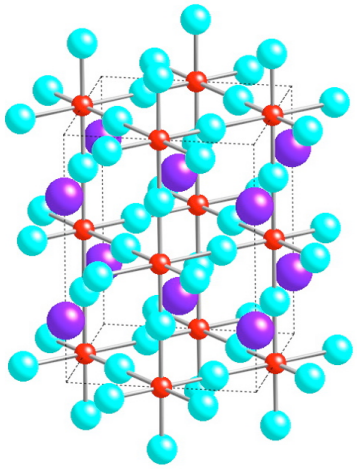


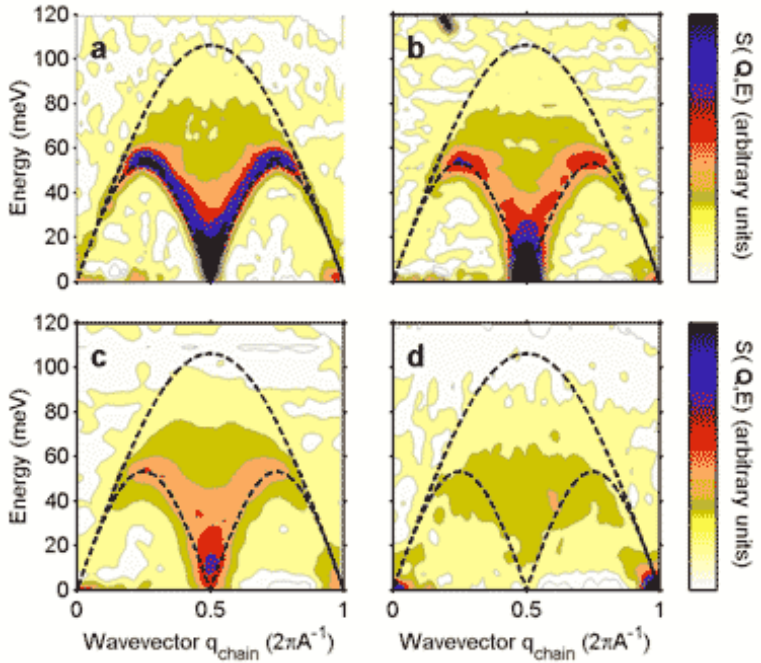


Neutron scattering experiments

- quasi-one-dimensional $KCuF_3$

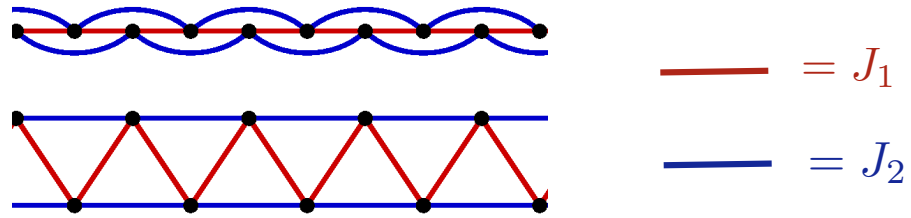
B. Lake et al., Nature Materials 4 329-334 (2005)





Heisenberg chain with frustrated interactions

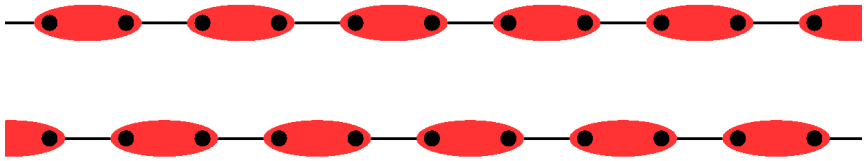
$$H = \sum_{i=1}^{N} \left[J_1 \mathbf{S}_i \cdot \mathbf{S}_{i+1} + J_2 \mathbf{S}_i \cdot \mathbf{S}_{i+2} \right]$$



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

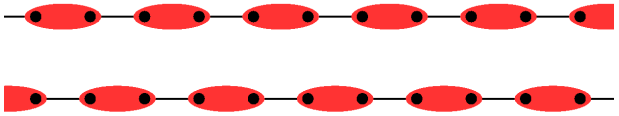
The symmetry is not broken for finite N

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

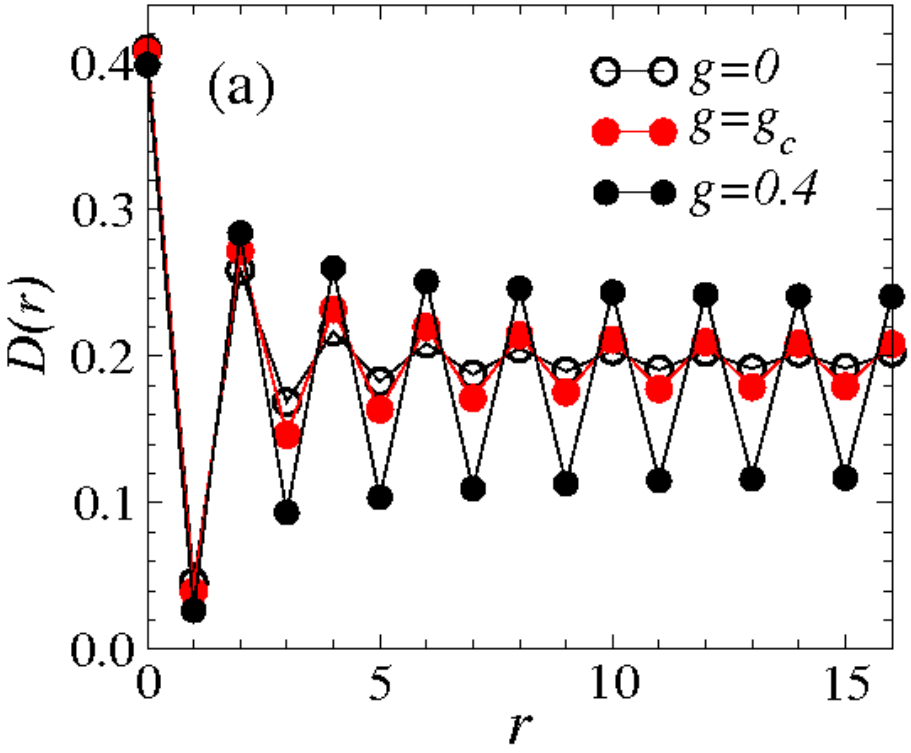
$$|\Psi_0\rangle \sim |\Psi_A\rangle + |\Psi_B\rangle, \qquad |\Psi_1\rangle \sim |\Psi_A\rangle - |\Psi_B\rangle$$

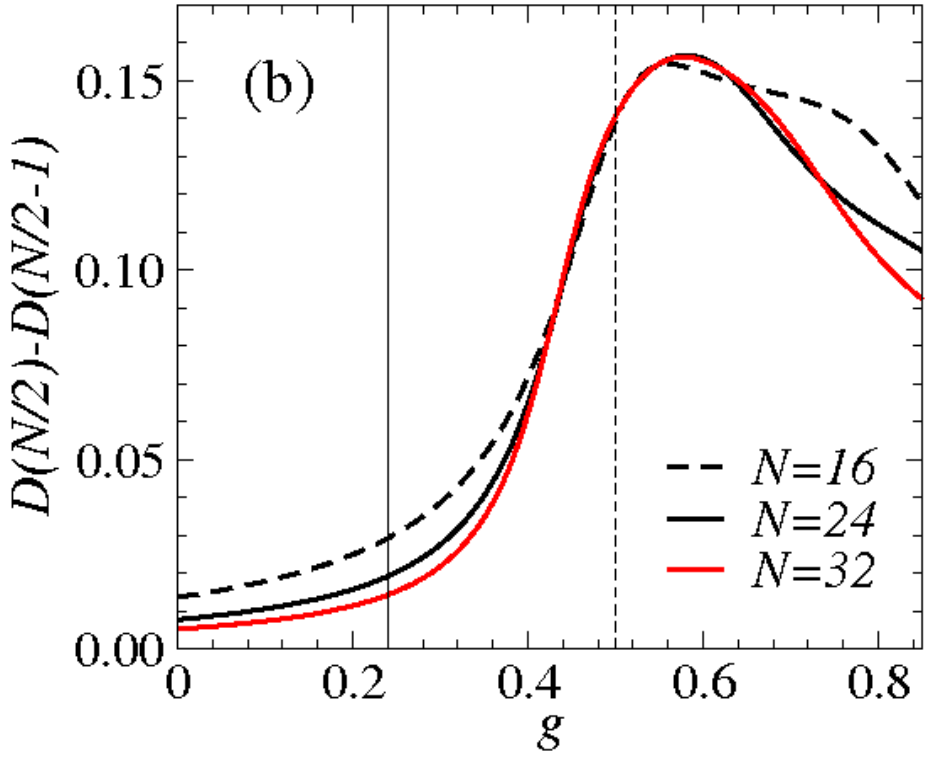
The VBS state can be detected in finite systems using “dimer” correlations

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



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

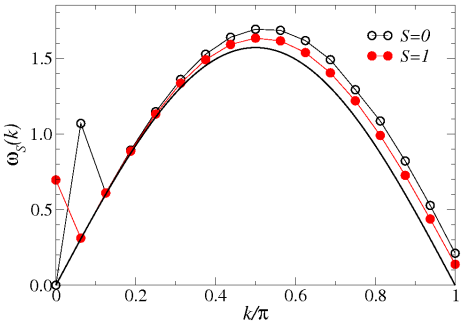




It is not easy to detect the transition this way

- 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)]

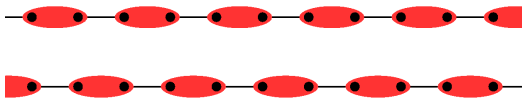
Determining the transition point using level crossings



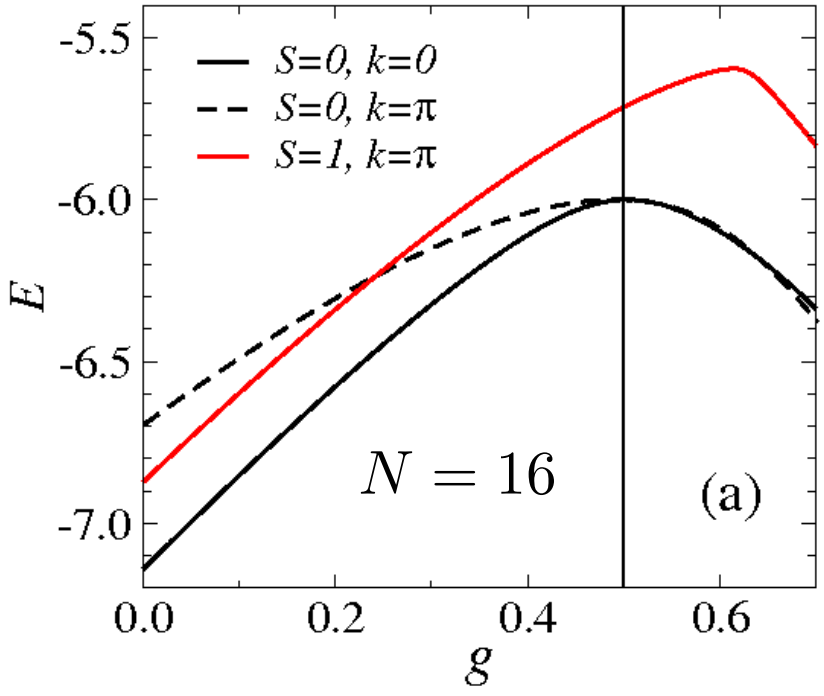
Lowest excitation for the g=0 Heisenberg chain is a triplet
- this can be expected for all $g<g_c$

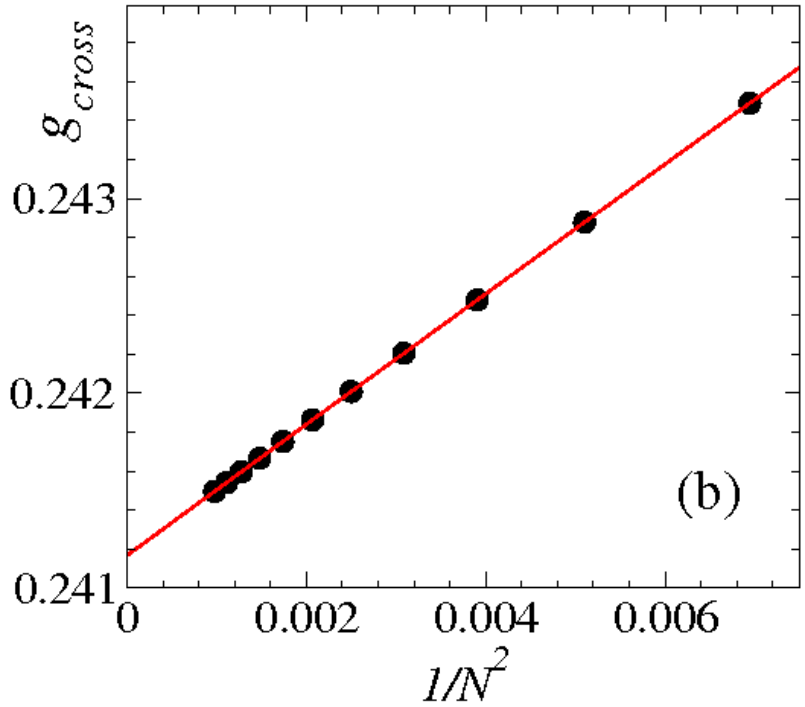
The VBS state is 2-fold degenerate for infinite N
- and for any N at g=1/2
- these two states are singlets
- gap between them closes exponentially as N→∞
- the lowest excitation is the second singlet

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



The two lowest excited states should cross at g_c





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