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

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

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

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 → real basis (semi-momentum states, will not discuss here)

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

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

$$Z|\alpha(k,p,z)\rangle = z|\alpha(k,p,z)\rangle, \quad z = \pm 1$$

Example: block sizes

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

$(p=\pm 1, z=\pm 1)$

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 **$S^2=S(S+1)$**

$$\begin{aligned} \mathbf{S}^2 &= \sum_{i=1}^{N}\sum_{j=1}^{N} \mathbf{S}_i \cdot \mathbf{S}_j \\ &= 2\sum_{i<j} \mathbf{S}_i \cdot \mathbf{S}_j + \frac{3}{4}N \end{aligned}$$

Example: Thermodynamics

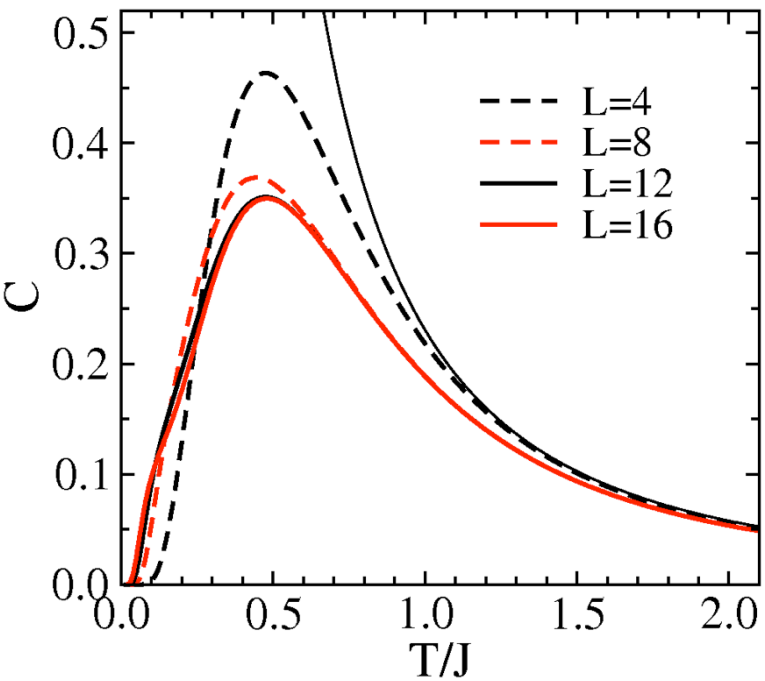
some quantities can be computed using only the magnetization m_z=0 sector

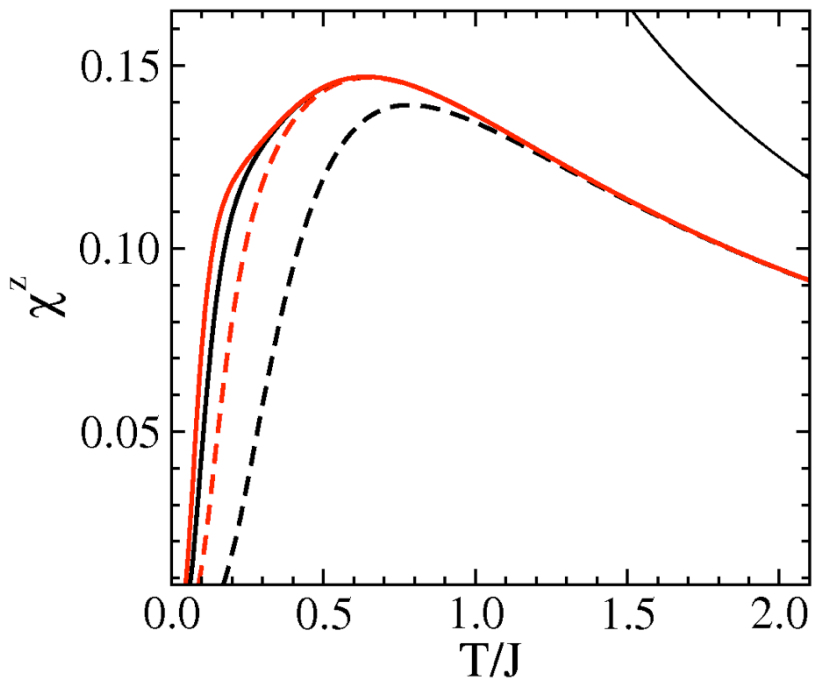
- spin-inversion symmetry can be used, smallest blocks
- spin-S state is **(2S+1)**-fold degenerate (no magnetix field) → weight factor
- possible spin dependence of expectation value → average over **m_z=−S,...,S**

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

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

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





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

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

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 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

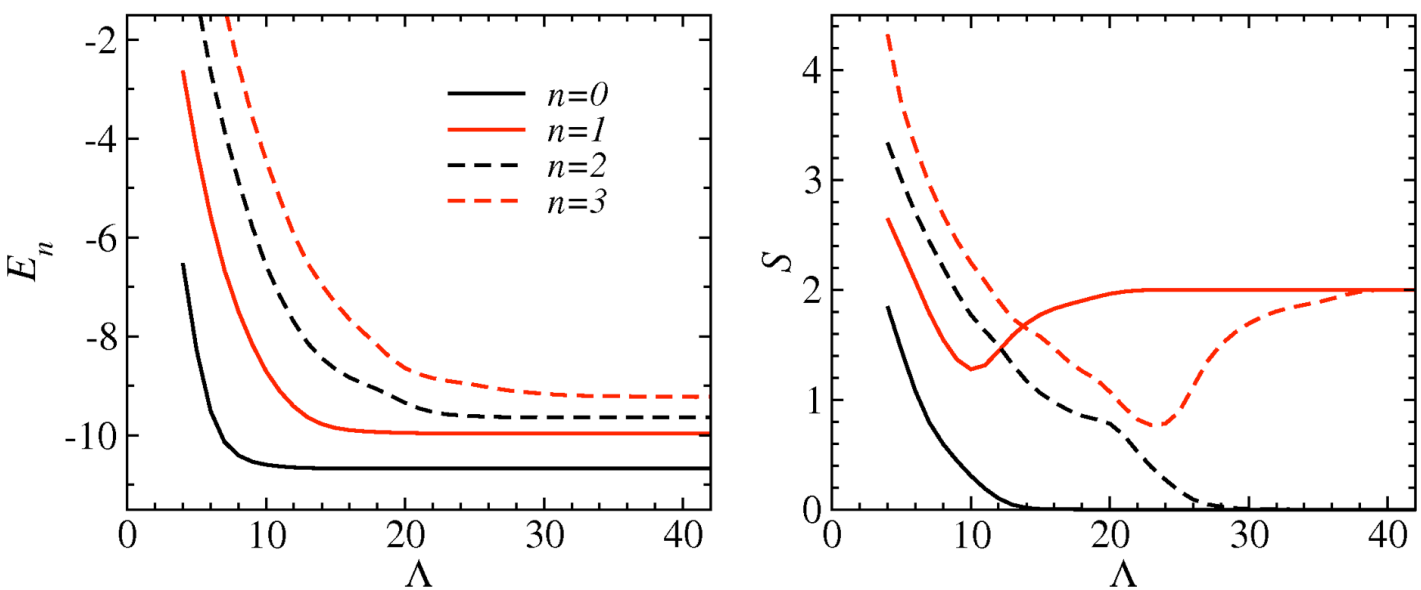
Diagonalizing the tri-diagonal matrix → eigenstates in the Lanczos basis

- 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

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

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

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