Thermodynamics

Quantum statistical mechanics

$$\langle Q \rangle = \frac{1}{Z} \mathrm{Tr} \left\{ Q \mathrm{e}^{-H/T} \right\} \qquad Z = \mathrm{Tr} \left\{ \mathrm{e}^{-H/T} \right\} = \sum_{n=0}^{M-1} \mathrm{e}^{-E_n/T}$$

H (or block of H) diagonalized by transformation U

$$E = U^{-1} H U \quad \text{(diagonal matrix)}$$

$$\langle Q \rangle = \frac{1}{Z} \mathrm{Tr} \{ U^{-1} Q U U^{-1} \mathrm{e}^{-H/T} U \}$$

diagonal matrix

$$= \frac{1}{Z} \mathrm{Tr} \{ U^{-1} Q U \mathrm{e}^{-E/T} \}$$

For the trace, we only need the diagonal elements of the matrix

$$\langle Q \rangle = \frac{1}{Z} \sum_n \langle n | Q_U | n \rangle \mathrm{e}^{-E_n/T}, \quad Q_U = U^{-1} A U$$

$$U^{-1} = U^{T*}$$

U and E are delivered by the diagonalization function used

Example: Thermodynamics

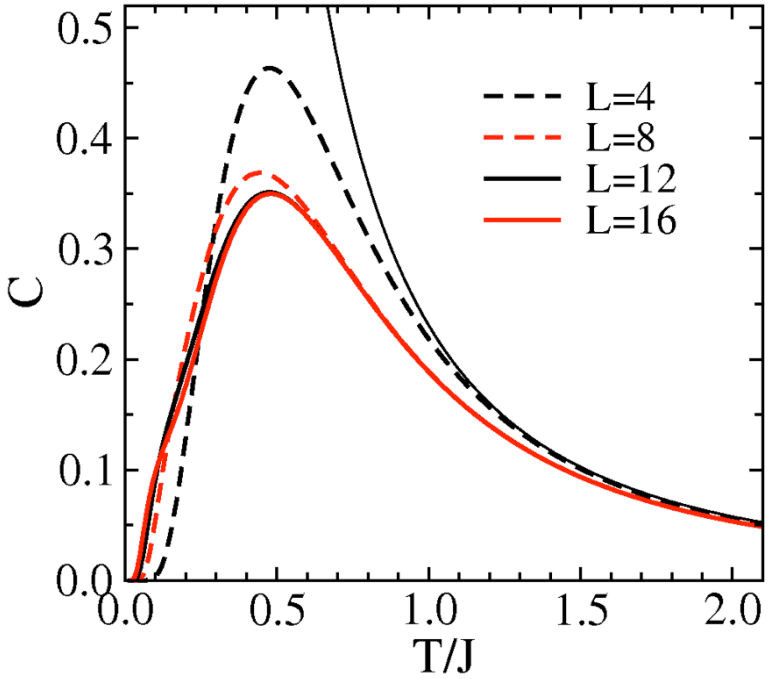
some quantities can be computed using only the magnetization m_z=0 sector

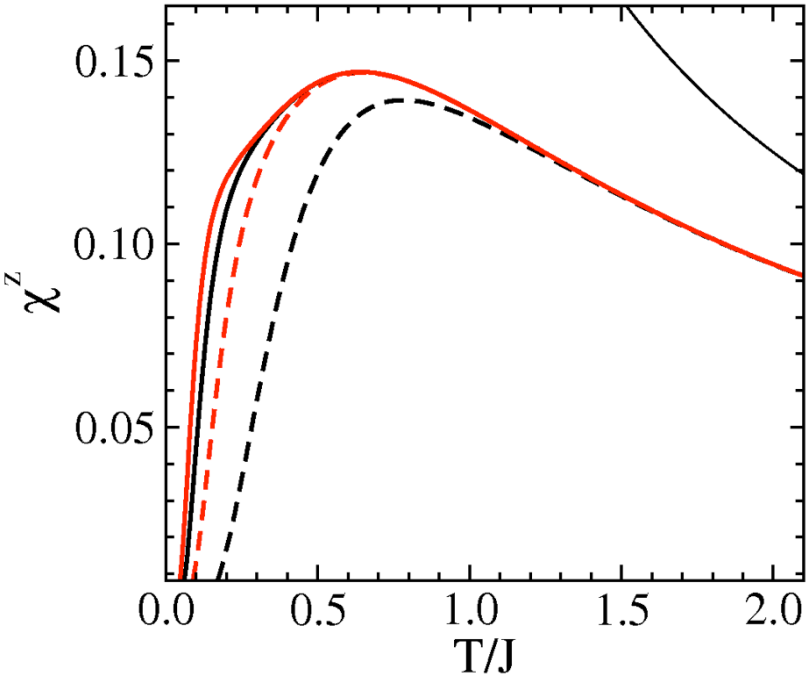
- spin-inversion symmetry can be used, smallest blocks
- spin-S state is **(2S+1)**-fold degenerate (no magnetic field) → weight factor
- possible spin dependence of expectation value → average over **m_z=–S,...,S**

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

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

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





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

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

As we discussed before, there is also a slightly different method that works with orthogonal states from the outset; recommended

Operator expectation values

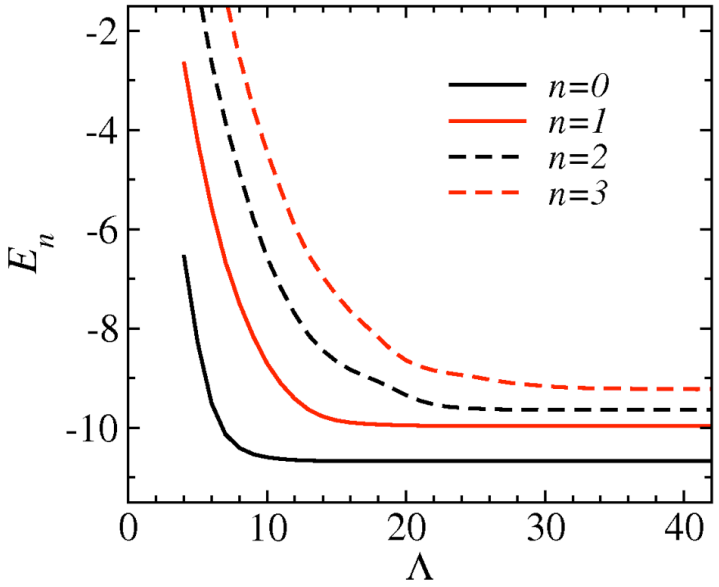
Diagonalizing the tri-diagonal matrix → eigenstates in the Lanczos basis

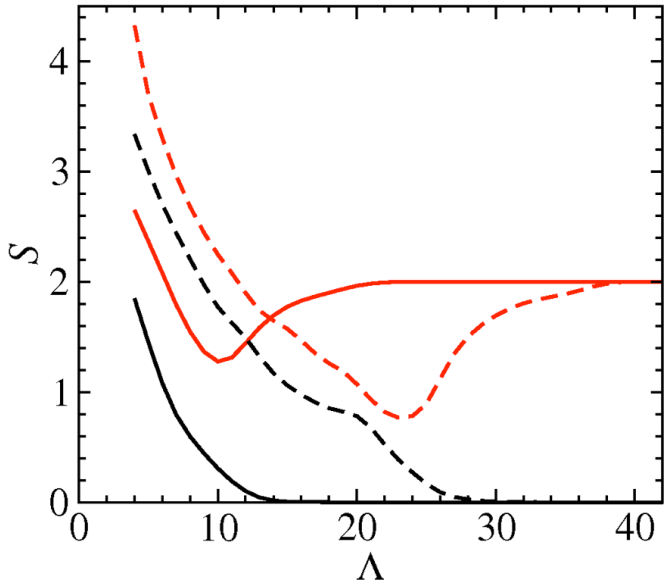
- eigenvectors v_n, energies E_n
- only some number of low-energy states (<< Λ) are correct eigenstates of H

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

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

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

- normalize after

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