Semi-momentum states

Mix momenta +k and –k for k≠0,π. Introduce function

$$C_k^\sigma(r) = \begin{cases} \cos(kr), & \sigma = +1 \\ \sin(kr), & \sigma = -1. \end{cases}$$

Useful trigonometric relationships

$$\begin{aligned} C_k^{\pm}(-r) &= \pm C_k^{\pm}(r), \\ C_k^{\pm}(r+d) &= C_k^{\pm}(r)C_k^{+}(d) \mp C_k^{\mp}(r)C_k^{-}(d). \end{aligned}$$

Semi-momentum state

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

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

States with same k, different σ are orthogonal

$$\langle a^{-\sigma}(k)|a^\sigma(k)\rangle = \frac{1}{N_a} \sum_{r=1}^{R_a} \sin(kr)\cos(kr) = 0,$$

Normalization of semi-momentum states

$$N_a = \left(\frac{N}{R_a}\right)^2 \sum_{r=1}^{R_a} [C_k^\sigma(r)]^2 = \frac{N^2}{2R_a}$$

Hamiltonian: ac with H

$$H|a^\pm(k)\rangle = \sum_{j=0}^{N} h_a^j \sqrt{\frac{R_a}{R_{b_j}}} \Big(C_k^+(l_j)|b_j^\pm(k)\rangle \mp C_k^-(l_j)|b_j^\mp(k)\rangle \Big),$$

The matrix elements are

$$\langle b^\tau(k)|H_j|a^\sigma(k)\rangle = \tau^{(\sigma-\tau)/2} h_a^j \sqrt{\frac{N_{b_j}}{N_a}} C_k^{\sigma\tau}(l_j)$$

σ is mot a conserved quantum number

- H and T mix σ=+1 and σ=–1 states
- the H matrix is twice as large as for momentum states

Why are the semi-momentum states useful then?

Because we can construct a real-valued basis:

Semi-momentum states with parity

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

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

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

r	T^r		$T^r P$	
0	27	0 0 0 1 1 0 1 1	216	1 1 0 1 1 0 0 0
1	54	0 0 1 1 0 1 1 0	177	1 0 1 1 0 0 0 1
2	108	0 1 1 0 1 1 0 0	99	0 1 1 0 0 0 1 1
3	216	1 1 0 1 1 0 0 0	198	1 1 0 0 0 1 1 0
4	177	1 0 1 1 0 0 0 1	141	1 0 0 0 1 1 0 1
5	99	0 1 1 0 0 0 1 1	27	0 0 0 1 1 0 1 1
6	198	1 1 0 0 0 1 1 0	54	0 0 1 1 0 1 1 0
7	141	1 0 0 0 1 1 0 1	108	0 1 1 0 1 1 0 0

P,T transformations

example: N=8;note that

- **$T^5 P|a\rangle = |a\rangle$**

such P,T relationships will affect normalization and H-elements

Normalization: We have to check whether or not

$$T^m P|a\rangle = |a\rangle \quad \text{for some } m \in \{1,\ldots,N-1\}$$

Simple algebra gives

$$N_a^\sigma = \frac{N^2}{R_a} \times \begin{cases} 1, & T^m P|a\rangle \neq |a\rangle \\ 1 + \sigma p \cos(km), & T^m P|a\rangle = |a\rangle \end{cases}$$

In the latter case the σ=-1 and σ=+1 states are not orthogonal

Then only one of them should be included in the basis

- convention: **use σ=+1 if 1+*σp*cos(*km*)≠0, else σ=-1**

If both σ=+1 and σ=–1 are present:

- **we store 2 copies of the same representative**
- we will store the σ value along with the periodicity of the representative

Pseudocode: semi-momentum, parity basis construction

$$
\begin{array}{l}
\textbf{do } s = 0, 2^N - 1 \\
\quad \textbf{call checkstate}(s, R, m) \\
\quad \textbf{do } \sigma = \pm 1 \text{ (do only } \sigma = +1 \text{ if } k = 0 \text{ or } k = N/2) \\
\quad\quad \textbf{if } (m \neq -1) \textbf{ then} \\
\quad\quad\quad \textbf{if } \ (1 + \sigma p \cos(ikm2\pi/N) = 0) \ R = -1 \\
\quad\quad\quad \textbf{if } \ (\sigma = -1 \textbf{ and } 1 - \sigma p \cos(ikm2\pi/N) \neq 0); \ R = -1 \\
\quad\quad \textbf{endif} \\
\quad\quad \textbf{if } R > 0 \textbf{ then } a = a + 1; \ s_a = s; \ R_a = \sigma R; \ m_a = m \textbf{ endif} \\
\quad \textbf{enddo} \\
\textbf{enddo}
\end{array}
$$

In the subroutine **checkstate**(), we now find whether

$$T^m P|a\rangle = |a\rangle \ \text{ for some } m \in \{1, \ldots, N-1\}$$

m=–1 if there is no such transformation

if m≠-1, then the σ=+1 and σ=-1 states are not orthogonal

- use only the σ=+1 state if it has non-zero normalization
- use the σ=-1 state if σ=+1 has normalization=0
- R=–1 for not including in the basis

the subroutine **checkstate**()
is modified to gives us:

- periodicity R (R=–1 if incompatible)
- m>0 if $T^m P|s\rangle = |s\rangle$
- m=–1 if no such relationship

check all translations of |s> →

construct reflected state P|s> →

check all translations of P|s> →

```
subroutine checkstate(s, R, m)
R = −1
if (∑_i s[i] ≠ n_↑) return
t = s
do i = 1, N
    t = cyclebits(t, N)
    if (t < s) then
        return
    elseif (t = s) then
        if (mod(k, N/i) ≠ 0) return
        R = i; exit
    endif
enddo
t = reflectbits(s, N); m = −1
do i = 0, R − 1
    if (t < s) then
        R = −1; return
    elseif (t = s) then
        m = i; return
    endif
    t = cyclebits(t, N)
enddo
```

Hamiltonian : Act with an operator H_j on a representative state:

$$H_j|a\rangle = h_a^j P^{q_j} T^{-l_j} |b_j\rangle$$

We can write H acting on a basis state as

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

Using the properties (trigonometry) of the C-functions:

$$H|a^\sigma(k,p)\rangle = \sum_{j=0}^{N} h_a^j(\sigma p)^{q_j} \sqrt{\frac{N_{b_j}^\sigma}{N_a^\sigma}} \times$$

$$\left(\cos(kl_j)|b_j^\sigma(k,p)\rangle - \sigma\sqrt{\frac{N_{b_j}^{-\sigma}}{N_{b_j}^\sigma}} \sin(kl_j)|b^{-\sigma}(k,p)\rangle\right)$$

If, for some m, $T^m P|b_j\rangle = |b_j\rangle$ then

$$\sqrt{\frac{N_{b_j}^{-\sigma}}{N_{b_j}^\sigma}} = \sqrt{\frac{1-\sigma p\cos(km)}{1+\sigma p\cos(km)}} = \frac{|\sin(km)|}{1+\sigma p\cos(km)}$$

$$\langle b_j^\mp(k,p)|b_j^\pm(k,p)\rangle = -p$$

else the ratio is one and the + and – states are orthogonal

The matrix elements are

diagonal in σ

$$\langle b_j^\sigma(k,p)|H_j|a^\sigma(k,p)\rangle = h_a^j(\sigma p)^{q_j}\sqrt{\frac{N_{b_j}^\sigma}{N_a^\sigma}} \times$$

$$\begin{cases} \cos(kl_j), & P|b_j\rangle \neq T^m|b_j\rangle \\ \frac{\cos(kl_j)+\sigma p\cos(k[l_j-m])}{1+\sigma p\cos(km)}, & P|b_j\rangle = T^m|b_j\rangle \end{cases}$$

off-diagonal in σ

$$\langle b_j^{-\sigma}(k,p)|H_j|a^\sigma(k,p)\rangle = h_a^j(\sigma p)^{q_j}\sqrt{\frac{N_{b_j}^{-\sigma}}{N_a^\sigma}} \times$$

$$\begin{cases} -\sigma\sin(kl_j), & P|b_j\rangle \neq T^m|b_j\rangle, \\ \frac{-\sigma\sin(kl_j)+p\sin(k[l_j-m])|}{1-\sigma p\cos(km)}, & P|b_j\rangle = T^m|b_j\rangle, \end{cases}$$

Pseudocode: semi-momentum, parity hamiltonian

If 2 copies of the same representative, σ=−1 and σ=+1:

- do both in the same loop iteration
- examine the previous and next element
- carry out the loop iteration only if representative found for the first time

```
do a = 1, M
    if (a > 1 and s_a = s_{a-1}) then
        cycle
    elseif (a < M and s_a = s_{a+1}) then
        n = 2
    else
        n = 1
    endif
    ...
enddo
```

n is the number of copies of the representative

```
do i = a, a + n - 1
    H(a, a) = H(a, a) + E_z
enddo
```

diagonal matrix elements

- **E_z** = diagonal energy

```
s = flip(s_a, i, j)
call representative(s, r, l, q)
call findstate(r, b)
if (b ≥ 0) then
    if (b > 1 and s_b = s_{b-1}) then
        m = 2; b = b - 1
    elseif (b < M and s_b = s_{b+1}) then
        m = 2
    else
        m = 1
    endif
    do j = b, b + m - 1
    do i = a, a + n - 1
        H(i, j) = H(i, j) + helement(i, j, l, q)
    enddo
    enddo
endif
```

construct off-diagonal matrix elements

helement() computes the values based on

- stored info
- and l,q

```
subroutine representative(s, r, l, q)
...
t = reflectbits(s, N); q = 0
do i = 1, N - 1
    t = cyclebits(t, N)
    if (t < r) then r = t; l = i; q = 1 endif
enddo
```

find the representative r of s

- translation and reflection numbers l,q

Using spin-inversion symmetry

Spin inversion operator: $Z|S^z_1,S^z_2,\ldots,S^z_N\rangle = |-S^z_1,-S^z_2,\ldots,-S^z_N\rangle$

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

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

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

Normalization: must check how a representative transforms under Z,P,T

$$\begin{array}{llll}
1) & T^mP|a\rangle \neq |a\rangle, & T^mZ|a\rangle \neq |a\rangle & T^mPZ|a\rangle \neq |a\rangle \\
2) & T^mP|a\rangle = |a\rangle, & T^mZ|a\rangle \neq |a\rangle & T^mPZ|a\rangle \neq |a\rangle \\
3) & T^mP|a\rangle \neq |a\rangle, & T^mZ|a\rangle = |a\rangle & T^mPZ|a\rangle \neq |a\rangle \\
4) & T^mP|a\rangle \neq |a\rangle, & T^mZ|a\rangle \neq |a\rangle & T^mPZ|a\rangle = |a\rangle \\
5) & T^mP|a\rangle = |a\rangle, & T^nZ|a\rangle = |a\rangle & \Rightarrow T^{m+n}PZ|a\rangle = |a\rangle
\end{array}$$

For cases 2,4,5 only σ=+1 or σ=−1 included

$$N_a^\sigma = \frac{2N^2}{R_a}\times\begin{cases} 1, & 1) \\ 1+\sigma p\cos(km), & 2) \\ 1+z\cos(km), & 3) \\ 1+\sigma pz\cos(km), & 4) \\ [1+\sigma p\cos(km)][1+z\cos(kn)], & 5) \end{cases}$$

Hamiltonian: acting on a state gives a transformed representative

$$H_j|a\rangle = h_a^j P^{q_j} Z^{g_j} T^{-l_j} |b_j\rangle$$

$$q_j \in \{0,1\}, \quad g_j =\in \{0,1\}, \quad l_j = \{0,1,\ldots,N-1\}$$

After some algebra .... we can obtain the matrix elements

diagonal in σ

$$\langle b_j^\sigma(k,p)|H_j|a^\sigma(k,p)\rangle = h_a^j(\sigma p)^{q_j} z^{g_j} \sqrt{\frac{N_{b_j}^\tau}{N_a^\sigma}} \times$$

$$\begin{cases} \cos(kl_j), & 1),3) \\ \frac{\cos(kl_j)+\sigma p\cos(k[l_j-m])}{1+\sigma p\cos(km)}, & 2),5) \\ \frac{\cos(kl_j)+\sigma pz\cos(k[l_j-m])}{1+\sigma pz\cos(km)}, & 4) \end{cases}$$

off-diagonal in σ

$$\langle b_j^{-\sigma}(k,p)|H_j|a^\sigma(k,p)\rangle = h_a^j(\sigma p)^{q_j} z^{g_j} \sqrt{\frac{N_{b_j}^\tau}{N_a^\sigma}} \times$$

$$\begin{cases} -\sigma\sin(kl_j), & 1),3) \\ \frac{-\sigma\sin(kl_j)+p\sin(k[l_j-m])}{1-\sigma p\cos(km)}, & 2),5) \\ \frac{-\sigma\sin(kl_j)+pz\sin(k[l_j-m])}{1-\sigma pz\cos(km)}, & 4) \end{cases}$$

Example: block sizes

k=0, m_z=0 (largest block)

N	$(+1,+1)$	$(+1,-1)$	$(-1,+1)$	$(-1,-1)$
	$(p=\pm 1, z=\pm 1)$			
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

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

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

Full diagonalization; expectation values

shorthand block label: **j=(m_z,k,p)** or **j=(m_z=0,k,p,z)**

$$D_j^{-1} H_j D_j = E_j, \quad \langle n_j | A | n_j \rangle = [D_j^{-1} A D_j]_{nn}$$

T>0: sum over all blocks j and states in block n=0,M_j–1

$$\langle A \rangle = \frac{1}{Z} \sum_j \sum_{n=0}^{M_j-1} \mathrm{e}^{-\beta E_{j,n}} [D_j^{-1} A_j U_j]_{nn}, \qquad Z = \sum_j \sum_{n=0}^{M_j-1} \mathrm{e}^{-\beta E_{j,n}}$$

E_j = diagonal (energy) matrix, $E_{j,n}$ = energies, n=0,...,M_j–1

Full diagonalization limited to small N; N=20-24

Example: Thermodynamics

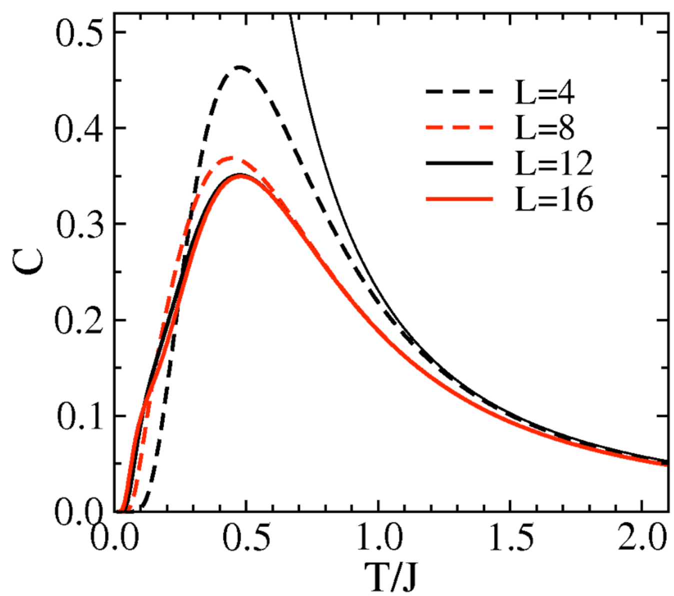
some quantities can be computed using only the magnetization m_z=0 sector

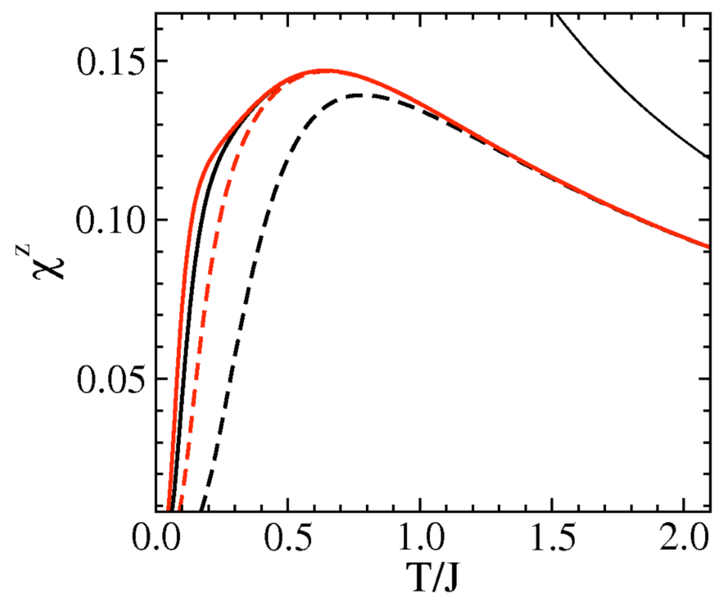
- spin-inversion symmetry can be used, smallest blocks
- spin-S state is **(2S+1)**-fold degenerate (no magnetix field) → weight factor
- possible spin dependence of expectation value → average over **m_z=–S,...,S**

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

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

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





Compared with leading high-T forms
$\chi = (1/4)/T$
$C = (3/13)/T^2$

The Lanczos method

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, *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

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

The next state and its overlaps with the previous states

$$|f_2\rangle = H|f_1\rangle - a_1|f_1\rangle - b_0|f_0\rangle$$

$$\langle f_2|f_1\rangle = H_{11} - a_1 N_1, \quad \langle f_2|f_0\rangle = N_1 - b_0 N_0$$

For orthogonal states

$$a_1 = H_{11}/N_1, \quad b_0 = N_1/N_0$$

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

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