

Selected Topics in Computational Quantum Physics

量子物理计算方法选讲

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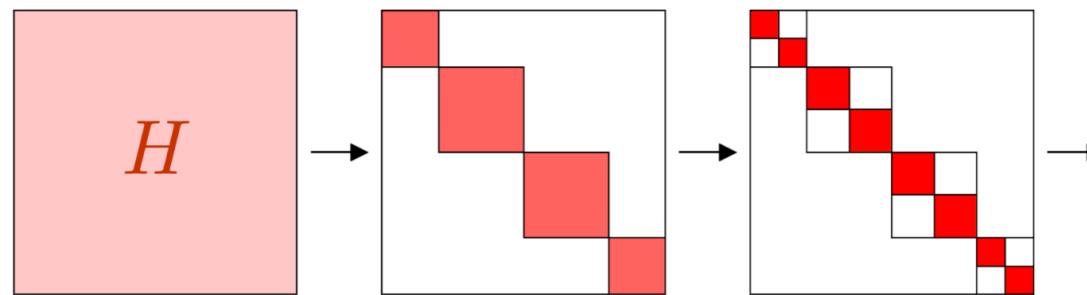
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Exact Diagonalization (ED)

$$H|\Psi\rangle = E|\Psi\rangle$$

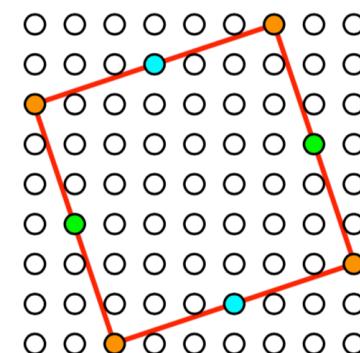
- main idea
- matrix representation of Hamiltonian
- implement symmetries
- Lanczos method
- time evolution
- finite temperature
- various applications

Symmetries

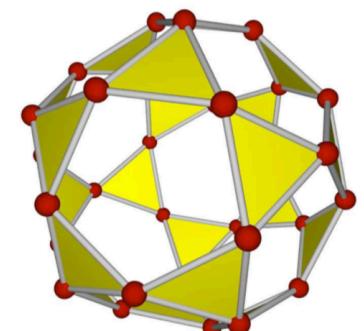


- $U(1)$ symmetry, particle number conservation
- translational symmetry, momentum space
- parity symmetry, reflection symmetry
- spin-inversion symmetry
- $SU(2)$ symmetry
- various spatial symmetry

40 sites square lattice
 $T \otimes PG = 40 \times 4$ elements



Icosidodecahedron (30 vertices)
 $I_h: 120$ elements

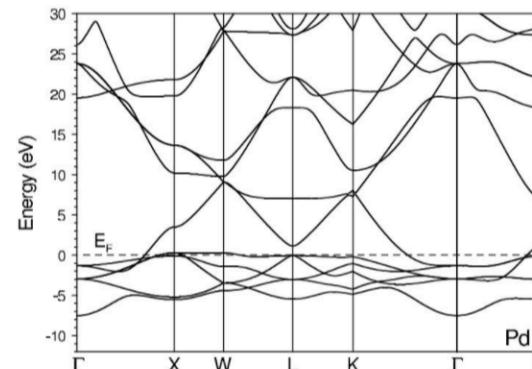
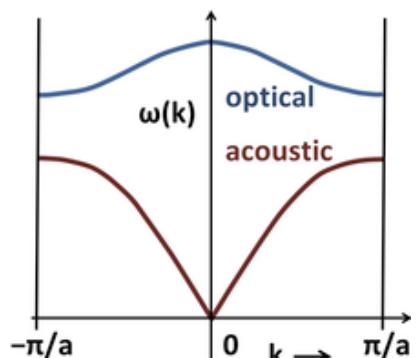


Dispersion relation

- total energy, momentum, and mass of particles are connected through the relativistic dispersion relation established by Paul Dirac

$$E^2 = (mc^2)^2 + (pc)^2$$

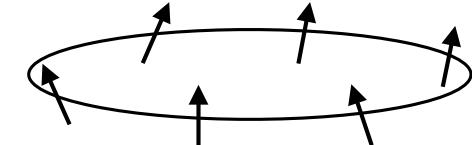
- in the ultra-relativistic limit is $E = pc$
in the non-relativistic limit is $E = p^2/2m$
- in the study of solids, the collection of all possible energies and momenta is known as the band structure of a material
properties of the band structure define whether the material is an insulator, semiconductor or conductor
- dispersion relation determines the properties of quasi particles



Implement translational symmetry

- using translational symmetry can further reduce the Hilbert space dimension

$$[T, H] = 0$$



T is the translational operator

$$T^0|0011\rangle = |0011\rangle, T^1|0011\rangle = |0110\rangle, T^2|0011\rangle = |1100\rangle, T^3|0011\rangle = |1001\rangle$$

- commuting operators have the same eigenstates

idea: we first construct the eigenstates of the translational operator T , and then write down H on the basis of these eigenstates, so that H is further block-diagonalized

- the eigenstates of T can be constructed using the projector

$$P_k = \frac{1}{N} \sum_{j=0}^{N-1} e^{i\frac{2\pi}{N}kj} T^j$$

where $k = 0, 1, \dots, N - 1$

Eigenstate projector

- N -site ring, translating N steps brings the spins back to their original state

$$T^N = 1$$

- for a given state $|r\rangle$, the state $P_k|r\rangle$ is an eigenstate of T

$$TP_k|r\rangle = T \left[\frac{1}{N} \sum_{j=0}^{N-1} e^{i\frac{2\pi}{N}kj} T^j \right] |r\rangle = e^{-i\frac{2\pi}{N}k} \left[\frac{1}{N} \sum_{j=0}^{N-1} e^{i\frac{2\pi}{N}k(j+1)} T^{(j+1)} |r\rangle \right] = e^{-i\frac{2\pi}{N}k} P_k |r\rangle$$

the corresponding eigenvalue is $e^{-i\frac{2\pi}{N}k} = e^{-iK}$

$K = 2\pi k/N$ is the discrete lattice momentum

- P_k has the following properties

$$P_k^\dagger = \frac{1}{N} \sum_{j=0}^{N-1} e^{-i\frac{2\pi}{N}kj} T^{-j} = \frac{1}{N} \sum_{j'=0}^{N-1} e^{i\frac{2\pi}{N}kj'} T^{j'} = P_k$$

$$P_k^2 = P_k^\dagger P_k = \frac{1}{N^2} \sum_{l,j=0}^{N-1} e^{i\frac{2\pi}{N}k(l-j)} T^{(l-j)} = \frac{1}{N} \sum_{j'=0}^{N-1} e^{i\frac{2\pi}{N}kj'} T^{j'} = P_k$$

Example: $N = 4$

- for a given state $|r\rangle$, the state $P_k|r\rangle = \frac{1}{N} \sum_{j=0}^{N-1} e^{i\frac{2\pi}{N}kj} T^j |r\rangle = 0$ for some special k

	$ r\rangle$	$T^0 r\rangle$	$T^1 r\rangle$	$T^2 r\rangle$	$T^3 r\rangle$	$P_{k=0} r\rangle$	$P_{k=1} r\rangle$	$P_{k=2} r\rangle$	$P_{k=3} r\rangle$
$\#(\uparrow) = 0$	$ 0000\rangle$	✓	✗	✗	✗				
$\#(\uparrow) = 1$	$ 0001\rangle$	$ 0001\rangle$	$ 0010\rangle$	$ 0100\rangle$	$ 1000\rangle$	✓	✓	✓	✓
$\#(\uparrow) = 2$	$ 0011\rangle$	$ 0011\rangle$	$ 0110\rangle$	$ 1100\rangle$	$ 1001\rangle$	✓	✓	✓	✓
	$ 0101\rangle$	$ 0101\rangle$	$ 1010\rangle$	$ 0101\rangle$	$ 1010\rangle$	✓	✗	✓	✗
$\#(\uparrow) = 3$	$ 0111\rangle$	$ 0111\rangle$	$ 1110\rangle$	$ 1101\rangle$	$ 1011\rangle$	✓	✓	✓	✓
$\#(\uparrow) = 4$	$ 1111\rangle$	✓	✗	✗	✗				

$$P_{k=1}|0101\rangle = \frac{1}{4} \left(e^{i\frac{2\pi}{4} \times 1 \times 0} |0101\rangle + e^{i\frac{2\pi}{4} \times 1 \times 1} |1010\rangle + e^{i\frac{2\pi}{4} \times 1 \times 2} |0101\rangle + e^{i\frac{2\pi}{4} \times 1 \times 3} |1010\rangle \right) = 0$$

- after translating R steps, obtaining the original state $T^R|r\rangle = |r\rangle$
the allowed k satisfies $kR = \text{integer} \times N$ for spin systems
 $\text{mod}(kR, N) = 0$

Get properties of every configuration

- for each configuration, we need to know
 - (1) whether it is a representative configuration
 - (2) its corresponding representative configuration $|r\rangle$
 - (3) how many translation steps can convert it to the representative configuration

Check	0	1	2
0	1	0	0
1	1	1	0
2	0	1	1
3	1	3	0
4	0	1	2
5	1	5	0
6	0	3	1
7	1	7	0
8	0	1	3
9	0	3	3
10	0	5	1
11	0	7	3
12	0	3	2
13	0	7	2
14	0	7	1
15	1	15	0

- we write a code to generate a list called $\text{Check}[i, :]$
- 0th column: whether the configuration is a representative configuration, 1 for yes, 0 for no
 - 1st column: the corresponding representative configuration
 - 2nd column: the translation step R
- for example, $8 = 1000$ is obtained from the representative configuration $1 = 0001$ through 3 translation steps so that $\text{Check}[8,0] = 0$, $\text{Check}[8,1] = 1$, $\text{Check}[8,2] = 3$

Normalization and Hamiltonian matrix

- the normalized basis for each fixed-momentum Hilbert space is

$$|r_k\rangle = \frac{P_k|r\rangle}{\sqrt{\langle r|P_k^\dagger P_k|r\rangle}} = \frac{P_k|r\rangle}{\sqrt{\langle r|P_k|r\rangle}}$$

- we discard those $|r\rangle$ with $P_k|r\rangle = 0$
- since $[T, H] = 0$, we have $[P_k, H] = 0$
- we calculate the Hamiltonian matrix for a given k sector
the matrix element between two state $|r_k\rangle$ and $|r'_k\rangle$ is given by

$$\langle r'_k | H | r_k \rangle = \frac{\langle r' | P_k^\dagger H P_k | r \rangle}{\sqrt{\langle r' | P_k | r' \rangle \langle r | P_k | r \rangle}} = \boxed{\frac{\langle r' | P_k H | r \rangle}{\sqrt{\langle r' | P_k | r' \rangle \langle r | P_k | r \rangle}}}$$

- we need to apply the projector only once after we applied H to the representative $|r\rangle$
repeating the procedure for all representative $|r\rangle$, we obtain the matrix for a given k

Example: $N = 4$

- using translational symmetry can further block-diagonalized the Hamiltonian

$ 0000\rangle$	$\#(\uparrow) = 0$																			
$ 0001\rangle$																				
$ 0010\rangle$				$\#(\uparrow) = 1$																
$ 0100\rangle$																				
$ 1000\rangle$																				
$ 0011\rangle$																				
$ 0101\rangle$																				
$ 0110\rangle$								$\#(\uparrow) = 2$												
$ 1001\rangle$																				
$ 1010\rangle$																				
$ 1100\rangle$																				
$ 0111\rangle$													$\#(\uparrow) = 3$							
$ 1011\rangle$																				
$ 1101\rangle$																				
$ 1110\rangle$														$\#(\uparrow) = 4$						
$ 1111\rangle$																				

$ 0000_{k=0}\rangle$	$k = 0$																			
$ 0001_{k=0}\rangle$		$k = 0$																		
$ 0001_{k=1}\rangle$			$k = 1$																	
$ 0001_{k=2}\rangle$				$k = 2$																
$ 0001_{k=3}\rangle$					$k = 3$															
$ 0011_{k=0}\rangle$						$k = 0$														
$ 0101_{k=0}\rangle$							$k = 0$													
$ 0011_{k=1}\rangle$								$k = 1$												
$ 0011_{k=2}\rangle$									$k = 2$											
$ 0101_{k=2}\rangle$										$k = 3$										
$ 0011_{k=3}\rangle$											$k = 0$									
$ 0111_{k=0}\rangle$											$k = 1$									
$ 0111_{k=1}\rangle$												$k = 2$								
$ 0111_{k=2}\rangle$													$k = 3$							
$ 0111_{k=3}\rangle$														$k = 0$						
$ 1111_{k=0}\rangle$															$k = 1$					

- only $U(1)$ symmetry: $1 + 4 + 6 + 4 + 1 = 16$
- both $U(1)$ and translational symmetry:

$$1 + (1 + 1 + 1 + 1) + (2 + 1 + 2 + 1) + (1 + 1 + 1 + 1) + 1 = 16$$
- only translational symmetry:

$$(1 + 1 + 2 + 1 + 1) + (1 + 1 + 1) + (1 + 2 + 1) + (1 + 1 + 1) = 16$$

Be careful about fermion sign

- T translates spin-up and spin-down configurations at the same time
 T may introduce an additional sign

spin- \downarrow	spin- \uparrow	decimal	basis
0011	0101	53	$C_{0\uparrow}^\dagger C_{2\uparrow}^\dagger C_{0\downarrow}^\dagger C_{1\downarrow}^\dagger 0\rangle$
$T \leftarrow$ 0110	1010	106	$C_{1\uparrow}^\dagger C_{3\uparrow}^\dagger C_{1\downarrow}^\dagger C_{2\downarrow}^\dagger 0\rangle$
$T \leftarrow$ 1100	0101	197	$C_{2\uparrow}^\dagger C_{4\uparrow}^\dagger C_{2\downarrow}^\dagger C_{3\downarrow}^\dagger 0\rangle = C_{2\uparrow}^\dagger C_{0\uparrow}^\dagger C_{2\downarrow}^\dagger C_{3\downarrow}^\dagger 0\rangle = -C_{0\uparrow}^\dagger C_{2\uparrow}^\dagger C_{2\downarrow}^\dagger C_{3\downarrow}^\dagger 0\rangle$
$T \leftarrow$ 1001	1010	154	$C_{3\uparrow}^\dagger C_{5\uparrow}^\dagger C_{3\downarrow}^\dagger C_{4\downarrow}^\dagger 0\rangle = C_{3\uparrow}^\dagger C_{1\uparrow}^\dagger C_{3\downarrow}^\dagger C_{0\downarrow}^\dagger 0\rangle = C_{1\uparrow}^\dagger C_{3\uparrow}^\dagger C_{0\downarrow}^\dagger C_{3\downarrow}^\dagger 0\rangle$

- therefore, we need to reconsider the allowed momentum k for a given representative configuration

make sure $|r_k\rangle = \frac{P_k|r\rangle}{\sqrt{\langle r|P_k|r\rangle}}$ does not vanish

KR may not be a multiple of N any more

How to get good quantum number?

- given a 1D finite system with translational symmetry, $[T, H] = 0$
the crystal momentum k is a good quantum number,
how to get E vs k in practice?
- use the aforementioned method, construct momentum basis by hand
Good: Hilbert space is smaller; Bad: sometimes coding is a headache
- for fermionic and bosonic systems, use Fourier transformation to transform the whole Hamiltonian into momentum space
NOT work for spin systems, why?
- get the matrix representation of T , diagonalize T to get the momentum basis
- first diagonalize H , then calculate T (diagonalize T in case of degeneracy)
- get energy and momentum simultaneously by diagonalizing HT , giving Ee^{ik}

Another possible way

- solve the eigenvalue problem

$$(H - \alpha e^{-ik}T) |\psi\rangle = \lambda |\psi\rangle$$

for the eigenvalue $\lambda = \omega - \alpha$ with the most negative real part

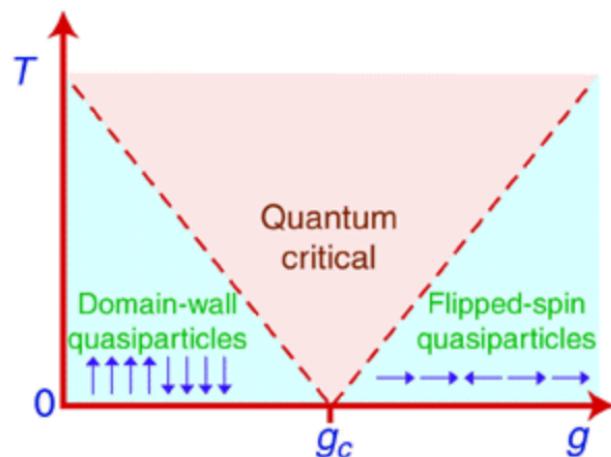
- it would be more elegant to consider the operator $H - \alpha e^{-ik}T - \alpha e^{ik}T^\dagger$ such that the eigenvalue problem remains Hermitian
in practice, adding the hermitian conjugate may not be needed
- when α is sufficiently large and translation symmetry is sufficiently well captured, this eigenvalue should indeed be real and correspond to an eigenstate with momentum k and energy value ω
- we need to further verify whether $|\psi\rangle$ is an eigenvector of H and remove the artificial ones

Transverse field Ising model

$$H = -J \sum_{i=1}^N \left(g\sigma_i^x + \sigma_i^z\sigma_{i+1}^z \right) \quad J, g \geq 0$$

$$\sigma^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \sigma^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

- the simplest exactly solvable model with quantum phase transition
- quantum phase transition
 - phase transitions at zero temperature, which occur when some parameter in the Hamiltonian is varied
- ground states in two limits
$$|G\rangle = \begin{cases} |\uparrow\uparrow\dots\uparrow\rangle \text{ or } |\downarrow\downarrow\dots\downarrow\rangle & g = 0 \\ |\rightarrow\rightarrow\dots\rightarrow\rangle & g \rightarrow \infty \end{cases}$$
- $g_c = 1$ is the phase transition point
- see the book “Quantum phase transition” by Sachdev, chapter 4.2 for details



Exact solution

- Step 1: Jordan-Wigner transformation

very powerful mapping between spin-1/2 spins and spineless fermions

we introduce $\sigma_i^z = -\prod_{j=1}^{i-1} (1 - 2C_j^\dagger C_j) (C_i + C_i^\dagger)$, $\sigma_i^x = 1 - 2C_i^\dagger C_i$.

then $H = -J \sum_{i=1}^N (g\sigma_i^x + \sigma_i^z \sigma_{i+1}^z)$

$$= -J \sum_{i=1}^N g (1 - 2C_i^\dagger C_i) - J \sum_{i=1}^{N-1} (C_i^\dagger - C_i) (C_{i+1} + C_{i+1}^\dagger) + JP (C_N^\dagger - C_N) (C_1 + C_1^\dagger)$$

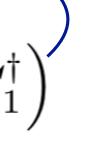
where $P = \prod_{i=1}^N \sigma_i^x = \prod_{j=1}^N (1 - 2C_j^\dagger C_j) = \exp(i\pi M)$, $M = \sum_{i=1}^N C_i^\dagger C_i$

- when M is odd, $P = -1$ periodic boundary condition

$$H = -J \sum_{i=1}^N g (1 - 2C_i^\dagger C_i) - J \sum_{i=1}^{N-1} (C_i^\dagger - C_i) (C_{i+1} + C_{i+1}^\dagger)$$


- when M is even, $P = +1$

anti-periodic boundary condition

$$H = -J \sum_{i=1}^N g (1 - 2C_i^\dagger C_i) - J \sum_{i=1}^{N-1} (C_i^\dagger - C_i) (C_{i+1} + C_{i+1}^\dagger) + J (C_N^\dagger - C_N) (C_1 + C_1^\dagger)$$


Exact solution

- Step 2: Fourier transformation

we introduce

$$C_k = \frac{1}{\sqrt{N}} \sum_{j=1}^N C_j \exp(-ikj), \quad k = 2\pi n/N,$$

if we choose n as

$$n = \begin{cases} \text{integer} & \text{when } M \text{ is odd} \\ \text{half-integer} & \text{when } M \text{ is even} \end{cases}$$

the Hamiltonian can be written in a general form

$$H = J \sum_k \left[2(g - \cos k) C_k^\dagger C_k + i \sin k (C_{-k}^\dagger C_k^\dagger + C_{-k} C_k) - g \right].$$

Exact solution

- Step 3: Bogoliubov transformation

we introduce

$$\begin{aligned} C_k &= u_k \gamma_k + i v_k \gamma_{-k}^\dagger, & C_{-k} &= u_k \gamma_{-k} - i v_k \gamma_k^\dagger \\ C_k^\dagger &= u_k \gamma_k^\dagger - i v_k \gamma_{-k}, & C_{-k}^\dagger &= u_k \gamma_{-k}^\dagger + i v_k \gamma_k \end{aligned}$$

where u_k, v_k are real numbers, satisfying

$$u_k^2 + v_k^2 = 1, \quad u_{-k} = u_k, \quad v_{-k} = -v_k$$

now the Hamiltonian becomes

$$H = J \sum_k \left\{ \begin{array}{l} \gamma_k^\dagger \gamma_k [2(g - \cos k) u_k^2 + 2 \sin k u_k v_k] - g \\ + (1 - \gamma_k^\dagger \gamma_k) [2(g - \cos k) v_k^2 - 2 \sin k u_k v_k] \\ + (\gamma_k^\dagger \gamma_{-k}^\dagger - \gamma_{-k} \gamma_k) [2(g - \cos k) (i u_k v_k) - i \sin k (u_k^2 - v_k^2)] \end{array} \right\}$$

Exact solution

- Step 4: final step

we choose

$$u_k = \cos\left(\frac{\theta_k}{2}\right), \quad v_k = \sin\left(\frac{\theta_k}{2}\right), \quad \tan\theta_k = \frac{\sin k}{g - \cos k}$$
$$2u_kv_k = \sin\theta_k = \frac{\sin k}{\sqrt{(g - \cos k)^2 + \sin^2 k}}, \quad u_k^2 - v_k^2 = \cos\theta_k = \frac{g - \cos k}{\sqrt{(g - \cos k)^2 + \sin^2 k}}$$

we finally have

$$H = 2J \sum_k \sqrt{1 + g^2 - 2g \cos k} \left(\gamma_k^\dagger \gamma_k - \frac{1}{2} \right)$$
$$= 2J \sum_k \sqrt{1 + g^2 - 2g \cos k} \gamma_k^\dagger \gamma_k - J \sum_k \sqrt{1 + g^2 - 2g \cos k} = \boxed{\sum_k \epsilon_k \gamma_k^\dagger \gamma_k - \epsilon_0}$$

ϵ_k is the spectrum of a non-interacting single particle $\gamma_k^\dagger \gamma_k$

question: how to get many-particle eigen-energies?

show that they agree with the eigenvalues from the spin model.

Build many-particle spectrum

- $g = 2, P = +1, M$ is even, n is half-integer

$$k_{-1.5} = \frac{2\pi}{4} \times (-1.5), k_{-0.5} = \frac{2\pi}{4} \times (-0.5), k_{0.5} = \frac{2\pi}{4} \times (0.5), k_{1.5} = \frac{2\pi}{4} \times (1.5)$$

$$\epsilon_{-1.5} = 5.59587, \epsilon_{-0.5} = 2.94725, \epsilon_{0.5} = 2.94725, \epsilon_{1.5} = 5.59587$$

$$\epsilon_0 = \frac{1}{2} \times (5.59587 + 2.94725 + 2.94725 + 5.59587) = 8.54312$$

Numerical results in $P = +1$ subspace	momentum of occupied quasi-particles	constructed many-particle eigen-energies
-8.54312	all levels empty	-8.54312
-2.64861	(-0.5), (0.5)	$2.94725 + 2.94725 - 8.54312 = -2.64861$
0	(-1.5), (0.5)	$5.59587 + 2.94725 - 8.54312 = 0$
0	(-1.5), (-0.5)	$5.59587 + 2.94725 - 8.54312 = 0$
0	(1.5), (-0.5)	$5.59587 + 2.94725 - 8.54312 = 0$
0	(1.5), (0.5)	$5.59587 + 2.94725 - 8.54312 = 0$
2.64861	(-1.5), (1.5)	$5.59587 + 5.59587 - 8.54312 = 2.64861$
8.54312	(-1.5), (-0.5), (0.5), (1.5)	$5.59587 + 2.94725 + 2.94725 + 5.59587 - 8.54312 = 8.54312$

Build many-particle spectrum

- $g = 2, P = -1, M$ is odd, n is integer

$$k_{-2} = \frac{2\pi}{4} \times (-2), k_{-1} = \frac{2\pi}{4} \times (-1), k_0 = \frac{2\pi}{4} \times (0), k_1 = \frac{2\pi}{4} \times (1), k_2 = \frac{2\pi}{4} \times (2)$$

$$\epsilon_{-2} = 6, \epsilon_{-1} = 4.47214, \epsilon_0 = 2, \epsilon_1 = 4.47214, \epsilon_2 = 6$$

since $N = 4$, we can choose 4 momenta at most, either $\{k_0, k_1, k_{-1}, k_{-2}\}$ or $\{k_0, k_1, k_{-1}, k_2\}$

$$\epsilon_0 = \frac{1}{2} \times (6 + 4.47214 + 2 + 4.47214) = 8.47214$$

Numerical results in $P = -1$ subspace	momentum of occupied quasi-particles	constructed many-particle eigen-energies
-6.47214	[0]	$2 - 8.47214 = -6.47214$
-4	[-1]	$4.47214 - 8.47214 = -4$
-4	[1]	$4.47214 - 8.47214 = -4$
-2.47214	[-2]	$6 - 8.47214 = -2.47214$
2.47214	[-1], [0], [1]	$4.47214 + 2 + 4.47214 - 8.47214 = 2.47214$
4	[-2], [-1], [0]	$6 + 4.47214 + 2 - 8.47214 = 4$
4	[-2], [1], [0]	$6 + 4.47214 + 2 - 8.47214 = 4$
6.47214	[-1], [1], [-2]	$4.47214 + 4.47214 + 6 - 8.47214 = 6.47214$

Build many-particle spectrum

- $g = 0.5, P = +1, M$ is even, n is half-integer

$$k_{-1.5} = \frac{2\pi}{4} \times (-1.5), k_{-0.5} = \frac{2\pi}{4} \times (-0.5), k_{0.5} = \frac{2\pi}{4} \times (0.5), k_{1.5} = \frac{2\pi}{4} \times (1.5)$$

$$\epsilon_{-1.5} = 2.79793, \epsilon_{-0.5} = 1.47363, \epsilon_{0.5} = 1.47363, \epsilon_{1.5} = 2.79793$$

$$\epsilon_0 = \frac{1}{2} \times (2.79793 + 1.47363 + 1.47363 + 2.79793) = 4.27156$$

Numerical results in $P = +1$ subspace	momentum of occupied quasi-particles	constructed many-particle eigen-energies
-4.27156	all levels empty	-4.27156
-1.32431	(-0.5), (0.5)	$1.47363 + 1.47363 - 4.27156 = -1.32431$
0	(-1.5), (0.5)	$2.79793 + 1.47363 - 4.27156 = 0$
0	(-1.5), (-0.5)	$2.79793 + 1.47363 - 4.27156 = 0$
0	(1.5), (-0.5)	$2.79793 + 1.47363 - 4.27156 = 0$
0	(1.5), (0.5)	$2.79793 + 1.47363 - 4.27156 = 0$
1.32431	(-1.5), (1.5)	$2.79793 + 2.79793 - 4.27156 = 1.32431$
4.27156	(-1.5), (-0.5), (0.5), (1.5)	$2.79793 + 1.47363 + 1.47363 + 2.79793 - 4.27156 = 4.27156$

- $g = 0.5, P = -1, M$ is odd, n is integer

$$k_{-2} = \frac{2\pi}{4} \times (-2), k_{-1} = \frac{2\pi}{4} \times (-1), k_0 = \frac{2\pi}{4} \times (0), k_1 = \frac{2\pi}{4} \times (1), k_2 = \frac{2\pi}{4} \times (2)$$

$$\epsilon_{-2} = 3, \epsilon_{-1} = 2.23607, \epsilon_0 = 1, \epsilon_1 = 2.23607, \epsilon_2 = 3$$

since $N = 4$, we can choose 4 momenta at most, either $\{k_0, k_1, k_{-1}, k_{-2}\}$ or $\{k_0, k_1, k_{-1}, k_2\}$

$$\epsilon_0 = \frac{1}{2} \times (3 + 2.23607 + 1 + 2.23607) = 4.23607$$

Numerical results in $P = -1$ subspace	momentum of occupied quasi-particles	constructed many-particle eigen-energies
-4.23607	all levels empty	-4.23607
-1	[−1], [0]	$2.23607 + 1 - 4.23607 = -1$
-1	[1], [0]	$2.23607 + 1 - 4.23607 = -1$
-0.23607	[−2], [0]	$3 + 1 - 4.23607 = -0.23607$
0.23607	[−1], [1]	$2.23607 + 2.23607 - 4.23607 = 0.23607$
1	[−1], [2]	$2.23607 + 3 - 4.23607 = 1$
1	[1], [−2]	$2.23607 + 3 - 4.23607 = 1$
4.32607	[−1], [0], [1], [2]	$2.23607 + 1 + 2.23607$ $+3 - 4.23607 = 4.32607$

Homework rules

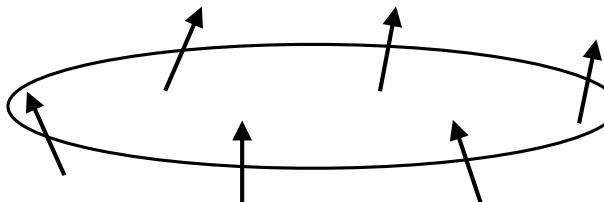
- this homework has one task
please submit through <http://learn.tsinghua.edu.cn>
- please submit **source code** and a **detailed note** to explain your code and results
- **deadline** is Oct 20, 23:00
- if you submit after the deadline, you will have less points
- if you are an expert in exact diagonalization, this homework may be waived
please contact me in person and submit something you have done before

Homework

- consider the 1D spin model on a N -site ring
please take parameters: $g = 1$, $J = 1$, $h = 1$

$$H = - \sum_j \left(g\sigma_{j-1}^z \sigma_j^y \sigma_{j+1}^z + J\sigma_j^z \sigma_{j+1}^z + h\sigma_j^x \right)$$

where σ^x , σ^y , and σ^z are Pauli matrices



- write a code to calculate the dispersion relation $E(k)$ of this model
show the eigenvalues in each momentum sector for $N = 8$
- calculate the ground state energy E per site and the magnetization per site $\langle \sigma_i^z \rangle$ and $\langle \sigma_i^x \rangle$ using the true ground state

Sample output

- please note the input parameters are **different** from homework

Case: g= 1 J= 1 h= 1.2 Ns= 6

```
(1)_Momentum_Sector_ki= 0 : [-9.6871158 -9.35916998 -6.67892917 -5.47466807 -3.13404403 -0.80328314  
 0.3865042 1.20960813 2. 2.54105608 2.74203618 4.48321614  
 8.58816183 9.18662763]  
(1)_Momentum_Sector_ki= 1 : [-6.99254762 -5.49321515 -3.42237678 -0.50509985 0.3877056 1.24801119  
 2.33479699 4.77600193 5.66672369]  
(1)_Momentum_Sector_ki= 2 : [-6.65776694 -4.32572458 -2.87321219 -2.15188254 -0.77579702 -0.32347021  
 0.27409269 2.72558454 3.39083412 4.91944974 7.79789239]  
(1)_Momentum_Sector_ki= 3 : [-4.75608342 -4.1176038 -3.7094474 -2. -2. 0.32957255  
 2.02823755 3.7094474 5.76674783 8.74912928]  
(1)_Momentum_Sector_ki= 4 : [-6.65776694 -4.32572458 -2.87321219 -2.15188254 -0.77579702 -0.32347021  
 0.27409269 2.72558454 3.39083412 4.91944974 7.79789239]  
(1)_Momentum_Sector_ki= 5 : [-6.99254762 -5.49321515 -3.42237678 -0.50509985 0.3877056 1.24801119  
 2.33479699 4.77600193 5.66672369]  
(2)_Ground_State_energy_per_site= -1.6145193003964797  
(2)_Ground_State_sigmax_per_site= (0.6029072339605066+0j)  
(2)_Ground_State_sigmaz_per_site= (-2.146431180941969e-15+0j)
```

Grading of this homework

- academic integrity [+50]
completing assignments independently, creating and expressing your own ideas, DON'T copy answers from others or allow others to copy your answers
- the source code can be executed [+10] and can provide correct results [+10]
the source code has high readability [+10]
- there is a detailed note file to explain the basic principle, source code and results [+10]
the note file is well-written and easy to understand [+10]
- did not show the eigenvalues in each momentum sector [-20]
did not show the magnetization [-20]
- time-dependent score: after DDL: [-1 per day]
- self-motivation score: new ideas or extra results [+10]