Lecture note on ED and DMRG

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Contents

1 Exact Diagonalization

1.1 Many body quantum system

I will briefly discuss many body quantum system and how to solve it at the basic level(directly diagonlize it)

A many body quantum system consist of a many body Hilbert space $\mathcal{V}_{tot}$ and a Hamiltonian $\mathcal{H}$.

We require the many-body Hilbert space to be tensor-product of local Hilbert space $\mathcal{V}_{tot} = \otimes_i \mathcal{V}_i$, thus a quantum states is a ray in the many-body Hilbert space $|\Psi\rangle = \Psi(m_1, m_2, \cdots, m_N)|m_1\rangle|m_2\rangle \cdots |m_N\rangle$ where $|m_i\rangle \in \mathcal{V}_i$

1.2 Examples

1.2.1 Hilbert space of 2 spins

Consider a coupled two spins system.

$$\mathcal{H} = J(\sigma_1^x \sigma_2^x + \sigma_1^y \sigma_2^y + \sigma_1^z \sigma_2^z) \tag{1.1}$$

- I will discuss how to write down the explicit form of the Hamiltonian in S_z basis
- I will discuss how to cast this Hamiltonian into a $U(1)$ conserved form and diagonalize it using $U(1)$ symmetry

1.2.2 Transverse field Ising model

Consider a spin chain with magnetic field.

$$H = -\sum_{i=1}^{L} \sigma_x^i \sigma_x^{i+1} + h \sum_{i=1}^{L} \sigma_z^i \tag{1.2}$$

- it's a $2^L \times 2^L$ Hamiltonian
- promote operator defined on single site into a many-particle Hilbert space $\sigma_z^i \longrightarrow I_1 \otimes I_2 \otimes \cdots \otimes \sigma_z^i \otimes I_{i+1} \otimes \cdots \otimes I_N$
- It straight forward to generate the Hamlitonian if we consider the binary coding of states(e.g. $|0010\rangle$ is the 2nd basis of the many body Hilbert space.)

The code and resulting spectrum is(adapted from Xiao Gang Wen's PPT)

```
X=sparse([0,1;1,0]); Z=sparse([1,0;0,-1]);
XX=kron(X,X); L=13; h=1.0; J=1.0
H=-kron(kron(X, speye(2^(L-2)) ),X);
for i=1:L-1
  H=H - kron( speye(2^(i-1)), kron(J*XX, speye(2^(L-1-i)))) ;
end
for i=1:L
  H=H - kron( speye(2^(i-1)), kron(h*Z, speye(2^(L-i)))) ;
end
eigs( H , 10, 'sa') # compute the lowest 10 eigenvalues
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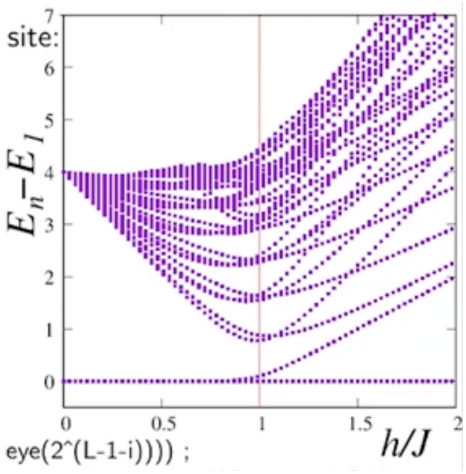

1.3 Thermodynamics using ED

We can obtain all the eigenvalues and eigenvectors of a many-body Hamiltonian using ED.

The finite temperature properties of a small cluster of sites could also been determined

- $$\langle \mathcal{O} \rangle = \frac{1}{Z} \sum_n e^{-\beta \epsilon_n} \langle n | \mathcal{O} | n \rangle, \tag{1.3}$$

1.4 advantages and disadvantages

- we know all about the systems(e.g. ground state and finite temperature, response to the pertubation)
- highest prevision, no truncation error
- impose symmetry could facilitate the computation, make it faster($U(1), Z(N), SU(2), SU(N)$). People use $U(1)$ charge conservation and momentum conservation in moire system
- restricted ED in a small portion of Hilbert space(projected ED on a isolated band, Configuration interaction in quantum chemistry, CIS and CISD)
- exponential increase of computational complexity(exponential wall)

2 Coarse graining scheme of Steven White: Density matrix renormalization group

I will introduce the original version of DMRG invented by Steven White in a phenomelogical way[1].

2.1 'Heterogeneous' Hilbert space

Can we use the ED result in small size to approximate ground state of larger system? We start with 2-spin system

$$\mathcal{H} = J(\sigma_1^x\sigma_2^x + \sigma_1^y\sigma_2^y + \sigma_1^z\sigma_2^z) \tag{2.1}$$

Diagonalizing it, we obtain the ground state and the density matrix.

$$|\Psi\rangle = \sum \Psi_{a_1a_2}|a_1\rangle|a_2\rangle \tag{2.2}$$

$$\hat{\rho} = \sum \Psi_{a_1a_2}\Psi^*_{a_3a_4}|a_1\rangle|a_2\rangle\langle a_3|\langle a_4| \tag{2.3}$$

$\hat{\rho}$ is a 4×4 matrix, which is faithfully discribed by $|\Psi\rangle$, who has 4 orthogonal components.

Some components is more important than others, this could be done using SVD

$$\hat{\rho} = \sum_i \lambda_i|i\rangle\langle i| \tag{2.4}$$

The 'weight' of those components is determined by value of λ_i

Let build the basis of 3 spin system using the coarse grained result of two spin system $|i\rangle$ and newly added degrees of freedom $|s_3\rangle$, And diagonlize the Hamiltonian using the 'Heterogeneous' Hilbert space

$$|\Psi\rangle = \sum \Psi_{mn}|i_m\rangle|s_n\rangle \tag{2.5}$$

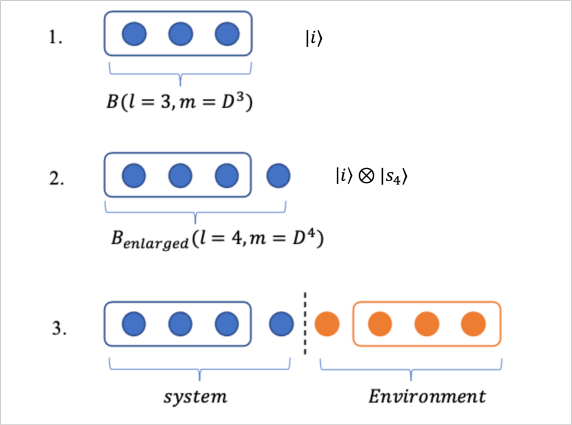

Figure 1: Coarse graining scheme, the 3 site rectangled is coarse grained and is represented by $|i\rangle$

This is the minimal example of Steven white's coarse idea I think(of course this protocol could be doubled to avoid even-odd effect)

2.2 evaluating hamiltonian in this basis

The Hamiltonian defined in this variational space could be written as

$$H_e = H_B \otimes I_d + \frac{J}{2}(S_b^+ \otimes S_d^- + S_b^- \otimes S_d^+) + J_z S_b^z \otimes S_d^z, \tag{2.6}$$

2.3 Truncation error

- These two sections will be taught along with DMRG notebook

3 Haldane gap

The Haldane gap refers to a phenomenon in quantum spin chains, which is a one-dimensional spin system with neighboring interaction.

In 1983, **F. Duncan M. Haldane** made a conjecture[2, 3] about the nature of low-energy excitations in such systems:

- Consider the antiferromagnetic Heisenberg spin chain, where neighboring spins prefer to be anti-aligned.
- The Hamiltonian is: $H = J\sum_i \mathbf{S}_i \cdot \mathbf{S}_{i+1}$, $J > 0$ for antiferromagnetism.

Haldane predicted:

- Integer spin chains (e.g., spin-1, spin-2) have a finite energy gap between the ground state and the first excited state — this is the Haldane gap.
- Half-integer spin chains (e.g., spin 1/2, spin-3/2) are gapless — their excitation spectrum goes down to zero energy.

This conjecture is important because the **Spin-1** chain serves as an early(maybe the first) example of topological effects in condensed matter physics. integer vs. half-integer spins correspond to different topological sectors in the Nonlinear σ model, which lead to the development of topological order concepts.

Although the theoretical argument could be tough, now we can directly examine it using numerical tools.

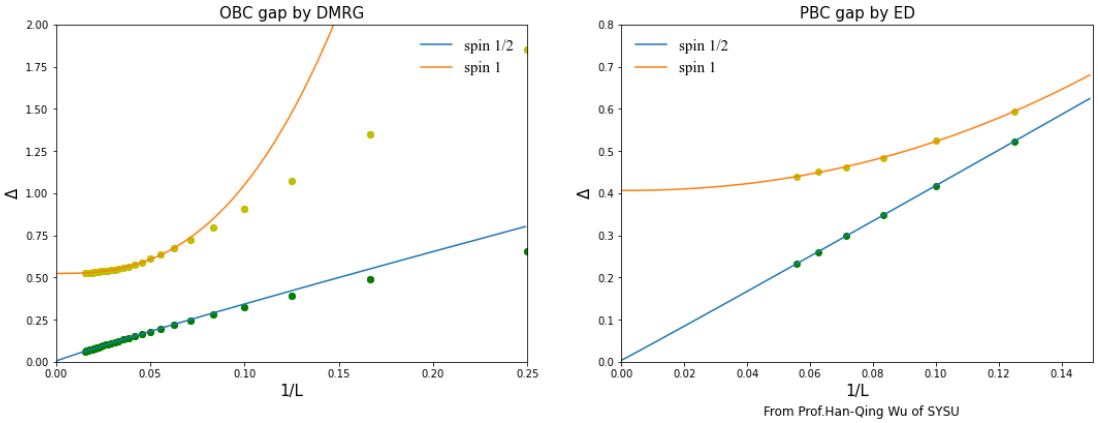

Figure 2: Haldane gap, finite size scaling of energy gap of spin-1 and spin 1/2 chains using ED and DMRG

Numerical calculation directly verifies Haldane's conjecture without diving into sophisticated analytics.

References

[1] U. Schollwöck, The density-matrix renormalization group in the age of matrix product states, Annals of Physics **326** (2011) 96–192.

[2] F.D.M. Haldane, O(3) nonlinear sigma model and the topological distinction between integer- and half-integer-spin antiferromagnets in two dimensions, Physical Review Letters **61** (1988) 1029–1032.

[3] Y. Zhou, K. Kanoda and T.-K. Ng, Quantum spin liquid states, Reviews of Modern Physics **89** (2017) .