Summer research on grand canonical DMRG
A practical method to calculate bulk properties in thermodynamic limit use finite size

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Figure: Left: Magnetization curve of spin-1/2 kagome Heisenberg model calculated by ED; Right: Magnetization curve of spin-1/2 kagome Heisenberg model calculated by grand-canonical DMRG
Motivation

Figure: Left: Magnetization curve of spin-1/2 J1-J2 model calculated by DMRG without deformation
The model

The Hamiltonian of J1-J2 model is

$$\hat{H} = J_1 \sum_i S_i \cdot S_{i+1} + J_2 \sum_i S_i \cdot S_{i+2} \ (J_1 > 0, J_2 > 0).$$

(1)

We first study it on a spin chain. This model has already been realized on $SrCuO_2$, $(N_2H_5)CuCl_3$. [1]
Magnetization curve of the model

Figure: Magnetization curve of J1-J2 chain
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Infinite DMRG

Cut the system into left block and right block. Suppose \( \{ |i\rangle \} \) is basis for left block, and \( \{ |j\rangle \} \) is basis for right block.

\[
|\psi\rangle = \sum_{i,j} \psi_{i,j} |i\rangle |j\rangle
\] (2)

During the calculation, we want to set a maximum dimension of Hilbert space to avoid the ”dimension explosion problem”. The problem turns into how to choose a set of good basis states that can minimize the loss of information about ground state.
What basis is more important?

In numerical RG, they keep the basis with low eigenvalues, because, intuitively, we are going to calculate the ground state. However, we can also think density matrix is important. Because in experiment, what we get is observables. Suppose we have a local observable in the left block, \( O = \text{tr}(\hat{\rho}_A \hat{O}) \), where \( \rho_A \) is the left block reduced density matrix. So we want to keep those basis weighs more in reduced density matrix.
Grand-canonical DMRG

Infinite DMRG

Low rank approximation

Estimate $\tilde{\psi}$ when minimize $||\psi - \tilde{\psi}||_F$ subject to $\text{rank}(\tilde{\psi}) \leq m$.

Eckart-Young-Mirsky theorem

The low rank approximation problem has a analytical solution in terms of simple value decomposition of the matrix. An arbitrary matrix with dimension $D_A \times D_B$ can be factorized into $\psi = UDV^\dagger$, where $UU^\dagger = 1$, $VV^\dagger = 1$.

$$
|\psi\rangle = \sum_i^{D_A} \sum_j^{D_B} \sum_{\alpha}^{D_B} U_{i\alpha} \lambda_{\alpha} V^*_{\alpha j} |i\rangle |j\rangle \\
= \sum_{\alpha}^{D_B} \left( \sum_i^{D_A} U_{i\alpha} |i\rangle \right) \lambda_{\alpha} \left( \sum_j^{D_B} V^*_{\alpha j} |j\rangle \right) \\
= \sum_{\alpha}^{D_B} \lambda_{\alpha} |\alpha\rangle_A |\alpha\rangle_B
$$

(3)

$$
\rho_A = \sum_{\alpha} \lambda_{\alpha}^2 |\alpha\rangle_A A \langle \alpha|,
$$

(4)

$$
\rho_B = \sum_{\alpha} \lambda_{\alpha}^2 |\alpha\rangle_B B \langle \alpha|.
$$

(5)
Eckart-Young-Mirsky theorem

We see that the reduced density matrix share the same spectrum $\omega_\alpha = \lambda_\alpha^2$. If we sort the eigenvalues in descend order: $\omega_1, \omega_2, \ldots, \omega_m, \ldots, \omega_r$. The best low rank approximation is to choose the first $r$ eigenvectors with largest eigenvalue.

$$||\psi - \tilde{\psi}||_F = \sum_{m+1}^r \omega_i$$

(6)
Truncation

We use the eigenvectors \{\ket{\alpha}\}, \{\ket{\beta}\} of the left and right reduced density matrix. When we add a site \(i + 1\) to the left block and a site \(i + 2\) to the right block, the new basis are: \{\ket{\alpha_i} \otimes \ket{s_{i+1}}\}, \{\ket{s_{i+2}} \otimes \ket{\beta_{i+3}}\}. The new basis states of left and right block are related to previous step as:

\[
\ket{\alpha_{i+1}} = \sum_{s_{i+1}, \alpha_i} \langle \alpha_i s_{i+1} | \alpha_{i+1} \rangle \alpha_i s_{i+1} = \sum_{s_{i+1}, \alpha_i} (U_L)_{\alpha_i s_{i+1}, \alpha_{i+1}} \ket{\alpha_i s_{i+1}} \tag{7}
\]

\[
\ket{\beta_{i+2}} = \sum_{s_{i+2}, \beta_{i+3}} \langle s_{i+2} \beta_{i+3} | \beta_{i+2} \rangle \ket{s_{i+2} \beta_{i+3}} = \sum_{s_{i+2}, \beta_{i+3}} (U_R)_{s_{i+2} \beta_{i+3}, \beta_{i+2}} \ket{s_{i+2} \beta_{i+3}} \tag{8}
\]
Truncation

$U_L$, and $U_R$ are the truncation matrix. The operator can be transformed into new basis representation using them. For example, an operator $O$ acting on a site in left block:

\[
\langle O \rangle_{\alpha_{i+1}, \alpha'_{i+1}} = \langle \alpha_{i+1} | \hat{O} | \alpha'_{i+1} \rangle
\]

\[
= \sum_{\alpha_i,s_{i+1}} \sum_{\alpha'_i,s'_{i+1}} \langle \alpha_{i+1} | \alpha_i s_{i+1} \rangle \langle \alpha_i s_{i+1} | \hat{O} | \alpha'_i s'_{i+1} \rangle \langle \alpha'_i s'_{i+1} | \alpha'_{i+1} \rangle 
\]

\[
= \sum_{\alpha_i,s_{i+1}} \sum_{\alpha'_i,s'_{i+1}} (U_L^\dagger)_{\alpha_{i+1}, \alpha_i} (O_L,i)_{\alpha_i s_{i+1}, \alpha'_i} (U_L)_{\alpha'_i s'_{i+1}, \alpha'_{i+1}}
\]
Why finite DMRG?

Problem with infinite DMRG

Infinite DMRG shares the same potential problem with Numerical RG. The problem is that configuration with lowest energy at infinite size will not also be the low energy configuration at finite size. Also the Hamiltonian changes at each step. There is no self-consistent loop.

Strength of finite DMRG

The Hamiltonian will not change once the system size is achieved. We can improve the accuracy step by step, and this works like a self-consistent loop.
Finite DMRG

- First, we use the infinite DMRG method to grow the system to a desire size. This process is called "warm-up".
- Then, we do the sweep process as Fig. 4 shows, until the energy or some observables converges.

**Figure:** sweep process
DMRG with $U(1)$ symmetry

Because the Hamiltonian commute with total spin z operator, Hamiltonian should be block diagonalized. Thus, the things we need to store are final quantum number, initial quantum number and corresponding block matrix. In this new representation, wave-function is also stored as left quantum number, right quantum number, and corresponding block matrix.

\[
H = \begin{array}{ccc}
3 & 2 & 1 \\
3 & \text{hatched} & \text{hatched} \\
2 & \text{hatched} & \text{hatched} \\
1 & \text{hatched} & \text{hatched} \\
\end{array}
\]
DMRG with $U(1)$ symmetry

Using idea of objective oriented programming (OOP), we only need to redefine the class of matrix and reload corresponding functions of that class. Of all functions, doing kronecker product of two matrices is tricky.
Grand-canonical DMRG

Intuition of grand-canonical DMRG

From Fig. 5(a), we can see that the normal open boundary condition DMRG will give rise to small plateaus when calculating magnetization curve due to the finite size effect. It is natural to think that if we deform the Hamiltonian and make the boundary less important and into a heat bath, the bulk property can be reflected from the several central sites.

Figure: (a): Magnetization of twisted three-leg spin tube[3]; (b): Grand-canonical DMRG
Deformation of Hamiltonian

Consider a 1D lattice general Hamiltonian consisting of \( L \) sites.

\[
\hat{H} = \sum_{i=1}^{L} u(i) + \sum_{l} \sum_{i=1}^{L-l} h_l(i) \quad (10)
\]

\[
\hat{H}_{\text{deform}} = \sum_{i=1}^{L} f_0(i) u(i) + \sum_{l} \sum_{i=1}^{L-l} f_l(i) h_l(i) \quad (11)
\]

The given function \( f_l(i) \) should smoothly vary from the maximum value near the center to zero at both ends so as to gradually scale down the energy.

Sine-square deformation (SSD)

\[
f_l(i) = \sin^2\left(\frac{\pi(i + (l - 1)/2)}{L}\right) \quad (12)
\]
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Magnetization

Figure: Magnetization curve calculated using SSD deformation
How do we get the magnetization curve using grand-canonical DMRG

Procedure

- Choose one deformation which can smoothly scale down the boundary energy
How do we get the magnetization curve using grand-canonical DMRG

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- Choose one deformation which can smoothly scale down the boundary energy
- Given an approximate total spin $z M_{\text{given}}$
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- Choose one deformation which can smoothly scale down the boundary energy
- Given an approximate total spin $z M_{\text{given}}$
- Do the grand-canonical DMRG
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- Choose one deformation which can smoothly scale down the boundary energy
- Given an approximate total spin $z M_{\text{given}}$
- Do the grand-canonical DMRG
- Get the average $Sz$ of sites near the center, and it stands for the $Sz$ in the thermal dynamic limit
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**Procedure**

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**Questions**

- Is the deformation unique?
How do we get the magnetization curve using grand-canonical DMRG

Procedure

- Choose one deformation which can smoothly scale down the boundary energy
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Questions

- Is the deformation unique?
- Is the result sensitive to $M_{\text{given}}$?
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Procedure

- Choose one deformation which can smoothly scale down the boundary energy
- Given an approximate total spin \( z M_{\text{given}} \)
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Questions

- Is the deformation unique?
- Is the result sensitive to \( M_{\text{given}} \)?
- Can result near the center stand for thermodynamic limit?
How do we get the magnetization curve using grand-canonical DMRG

Procedure

- Choose one deformation which can smoothly scale down the boundary energy
- Given an approximate total spin $z M_{\text{given}}$
- Do the grand-canonical DMRG
- Get the average $S_z$ of sites near the center, and it stands for the $S_z$ in the thermal dynamic limit

Questions

- Is the deformation unique?
- Is the result sensitive to $M_{\text{given}}$?
- Can result near the center stand for thermodynamic limit?
The effect of deformation

The deformation is not unique, as long as it scales down the boundary energy.

Figure: Figure from PRB 86.041108
The effect of $M_{\text{given}}$ 

The result is not sensitive to $M_{\text{given}}$. 

![Graph showing the effect of $M_{\text{given}}$]
The effect of $M_{\text{given}}$

The result is not sensitive to $M_{\text{given}}$.

Figure: Heisenberg chain
**Thermodynamic limit**

Figure: J1-J2 1D chain. h/J1=0.15. The configuration on the 1/3 magnetic plateau. Left: calculated with SSD deformation, total site: 50; Right: calculated without deformation, total site: 200.
Conclusion

- Grand-canonical DMRG is an effective method to calculate the bulk property with a finite size.
- The method is robust against $M_{\text{given}}$
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[1] M. Matsuda and K. Katsumata

[2] Kouichi OKUNISHI and Takashi TONEGAWA
Magnetic Phase Diagram of the S=1/2 Antiferromagnetic Zigzag Spin Chain in the Strongly Frustrated Region: Cusp and Plateau

Ground state phase diagram of twisted three-leg spin tube in magnetic field
Thanks Hongchen and Shenxiu for many discussions. Thanks Tom for hosting me in the group. Thanks everyone for the happy time during summer!
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Phase diagram

Figure: D: dimer gapped phase; P: 1/3 plateau; TL1: one component TL liquid; TL2: two component TL liquid; EO: even-odd behavior branch[2]