Using Matrix Product State to Solve Scale Invariant Hamiltonian in Efimov Physics

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Abstract

Matrix Product State (MPS) and Density Matrix Renormalization Group (DMRG) serve as effective variational techniques for investigating the low-energy states within quantum many-body systems, utilizing the underlying entanglement structures. By broadening the scope of MPS as a data representation framework, it becomes more adept at capturing intricate correlations within the system. Recent advancements have expanded the utility of this approach to efficiently address hydrodynamic equations, including the complex dynamics of phenomena like turbulence, and can compress data well[1] [5]. This study endeavors to adapt these methodologies to Efimov physics, which is characterized by unique universal properties and discrete scale invariance. Within this context, two new distinct approaches for generating the inverse of the required $\frac{1}{R^2}$ potential into MPS, thereby reproducing discrete scaling behavior, have been identified, alongside a detailed exploration of associated numerical challenges.

Introduction to MPS, MPO and DMRG

- Matrix product state (MPS):

$$|\psi\rangle = \sum_{\sigma_1\ldots\sigma_L} A^{\sigma_1}_{a_1} A^{\sigma_2}_{a_1,a_2}\ldots A^{\sigma_L}_{a_{L-1}}|\sigma_1\ldots\sigma_L\rangle \qquad (1)$$

where σ_i are called physical indices and a_i are called bond indices. MPS can be used to represent functions in binary fraction, an example is $f(x=\sum_{i=1}^{N}\frac{\sigma_i}{2^{N-i+1}})=x$ [4]

$$x=\sum_{i=1}^{N}\frac{\sigma_i}{2^{N-i+1}} = \begin{bmatrix}\frac{\sigma_1}{2^N} & 1\end{bmatrix}\begin{bmatrix}1 & 0\\ \frac{\sigma_2}{2^{N-1}} & 1\end{bmatrix}\cdots\begin{bmatrix}1 & 0\\ \frac{\sigma_{N-1}}{2^2} & 1\end{bmatrix}\begin{bmatrix}1\\ \frac{\sigma_N}{2^1}\end{bmatrix} \qquad (2)$$

where σ_i are 0 or 1. In this example, MPS compress the data from $2^N \to 8N$ parameters for N qubits. Unfortunately, most of functions need to do some approximation such as cross approximation to represent them into low bond dimension MPS.

- Matrix product operater (MPO):

$$\hat{O} = \sum_{(\sigma_1,\sigma_1')\ldots(\sigma_L,\sigma_L')} W^{\sigma_1,\sigma_1'}_{b_1} W^{\sigma_2,\sigma_2'}_{b_1,b_2}\ldots W^{\sigma_L,\sigma_L'}_{b_{L-1}}|\sigma_1\ldots\sigma_L\rangle\langle\sigma_1'\ldots\sigma_L'| \qquad (3)$$

MPO can be used to represent operator such as second order differential operator, it can write as the combination of raising($\hat{S}$) and lowering operator($\hat{S}^\dagger$)

$$\frac{\hat{S}-2\hat{I}+\hat{S}^\dagger}{\Delta x^2} \qquad (4)$$

$$\hat{S} = \begin{bmatrix}W^{\sigma_1,\sigma_1'}_1 & W^{\sigma_1,\sigma_1'}_2\end{bmatrix}\begin{bmatrix}W^{\sigma_2,\sigma_2'}_{1,1} & 0\\ W^{\sigma_2,\sigma_2'}_{2,1} & W^{\sigma_2,\sigma_2'}_{2,2}\end{bmatrix} \cdots \begin{bmatrix}W^{\sigma_{L-2},\sigma_{L-1}'}_{1,1} & 0\\ W^{\sigma_{L-2},\sigma_{L-1}'}_{2,1} & W^{\sigma_{L-2},\sigma_{L-1}'}_{2,2}\end{bmatrix}\begin{bmatrix}W^{\sigma_L,\sigma_L'}_1\\ W^{\sigma_L,\sigma_L'}_2\end{bmatrix} \qquad (5)$$

where $W^{\sigma_i,\sigma_i'}_{b_{i-1},b_i}$ are

$$\begin{cases} W^{0,1}_1 = W^{1,0}_2 = 1 & \text{for } i=1\\ W^{0,0}_{1,1} = W^{1,1}_{1,1} = W^{1,0}_{2,1} = W^{1,0}_{2,2} = 1 & \text{for } i=2 \text{ to } L-1\\ W^{0,0}_1 = W^{1,1}_1 = W^{0,1}_2 = 1 & \text{for } i=L \end{cases} \qquad (6)$$

This raising operator moves the function forward one unit.

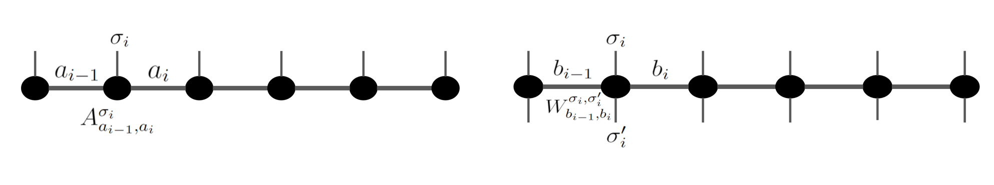

Figure 1: MPS (left) and MPO (right)

- Density Matrix Renormalization Group (DMRG):
DMRG attempts to search the minimum expectation value to find the ground state and ground state eigenvalue of the Hermitian operator, and used iterative methods such as Lanczos algorithm to solve the eigenvalue problem in each local site [6]

$$\tilde{H}_{(a_{i-1},a_i,\sigma_i),(a'_{i-1},a'_i,\sigma'_i)} v_{a'_{i-1},a'_i,\sigma'_i} = E v_{a'_{i-1},a'_i,\sigma'_i} \qquad (7)$$

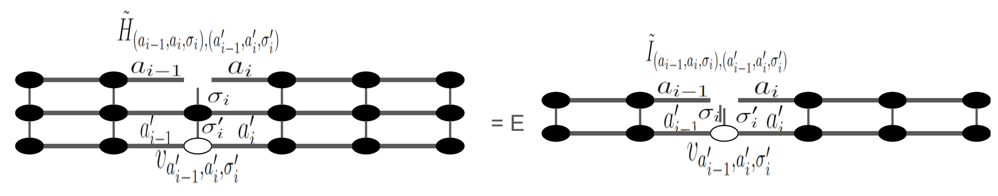

Figure 2: Sweeping site i by DMRG

Introduction to Efimov Physics

Efimov physics shows its three or more body bound states are not bound in its sub-systems, also these states are discrete scale invariance within a certain range[3] , and this property relates to limit cycle in renormalization group (RG)[2] , and their eigenvalues are in the ratio of $e^{-2\pi/s_0}$. Here, we will focus on solving the Differential equation in Efimov physics

$$\left(-\frac{\partial^2}{\partial R^2}+\frac{s_n^2-\frac{1}{4}}{R^2}-k^2\right)\sqrt{R}F_n(R)=0 \qquad (8)$$

with the only imaginary scaling factor $s_0 \approx 1.00624i$ that causes Efimov states in the case of three identical bosons.

Method1

Second-order differential operator act on a constant vector can be exact zero in finite difference representation if Neumann boundary condition is chosen, so a specific Hermitian operator can be established

$$-f(x)\frac{d^2}{dx^2}f(x) \qquad (9)$$

It's easy to see it has a zero eigenvalue with eigenvector $\frac{1}{f(x)}$. Therefore, if we know how to represent $f(x)$ into MPS, this operator can help us find MPS of its reciprocal function by DMRG. In addition, it's also a positive semi-definite matrix, so it can also ensure the zero eigenvalue is the ground state eigenvalue.

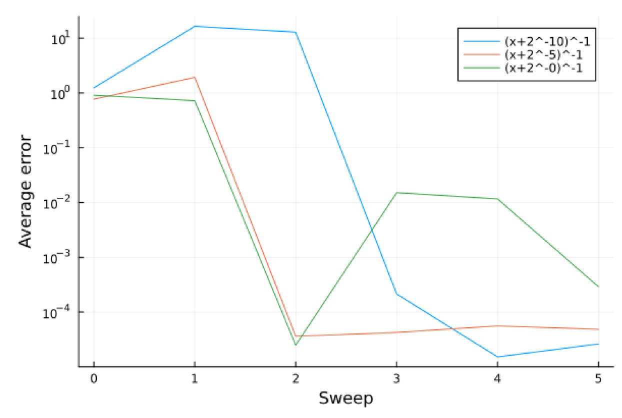

Figure 3: Average error compared to exact function for 20 qubits

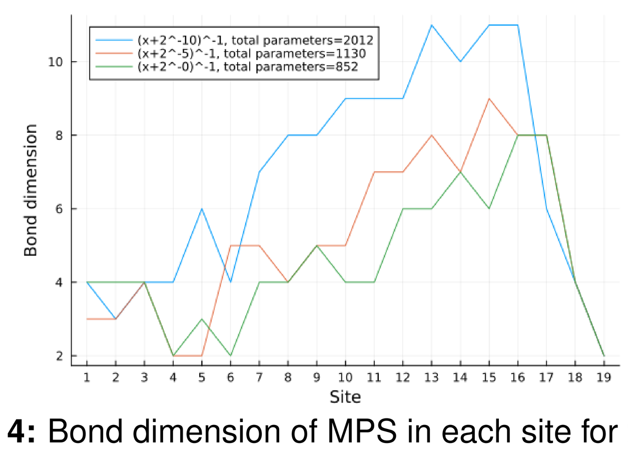

Figure 4: Bond dimension of MPS in each site for 20 qubits

Method2

If we change the coordinate from

$$x=\sum_i\frac{\sigma_i}{2^{N-i+1}} \to e^{\sum_i\frac{\sigma_i}{2^{N-i+1}}} \qquad (10)$$

Under this new coordinate, the functions that can be exactly represented in low bond dimension MPS have also changed

- x coordinate: x^n, e^{kx} and $\cos(kx)$
- e^x coordinate: $(\log(x))^n$, x^k, and $\cos(k\log(x))$

for any k and positive integer n. Moreover, it changes the way to represent operator into its MPO, and the second order differential operator becomes

$$\frac{d}{dx}\frac{d}{dx} \to \frac{d}{de^x}\frac{d}{de^x} = e^{-x}\frac{d}{dx}e^{-x}\frac{d}{dx} \qquad (11)$$

Now, it becomes non-Hermitian, but DMRG requires Hermitian operator. However, if we transform $\psi \to e^{-0.5x}\psi$, and rewrite the Schrödinger equation

$$\left(-e^{0.5x}\frac{d}{de^x}\frac{d}{de^x}e^{-0.5x}+V(e^x)\right)\psi(e^x)=E\psi(e^x) \qquad (12)$$

The new operator $-e^{0.5x}\frac{d}{de^x}\frac{d}{de^x}e^{-0.5x}$ becomes Hermitian again, this also can see in finite difference representation

$$f''(x_i)=\frac{f(x_{i+1})-2f(x_i)+f(x_{i-1})}{d^2}\to$$
$$e^{0.5x_i}f''(e^{x_i})e^{-0.5x_i}=2\frac{e^{\frac{1.5}{2N}}f(x_{i-1})-(e^{\frac{1}{2N}}+1)f(x_i)+e^{\frac{0.5}{2N}}f(x_{i+1})}{(e^{\frac{1}{2N}}-1)^2(e^{\frac{1}{2N}}+1)e^{2\frac{i}{2N}}} \qquad (13)$$

where x_i is the position and d is the distance between x_i and x_{i+1}. Notice that changing to other coordinate except e^x is difficult to represent in Hermitian MPO, due to the fact that differentiate other type of functions are not same to do the finite difference, they are not just an overall factor difference like e^x, and the approximation may break the Hermitian property.

Result

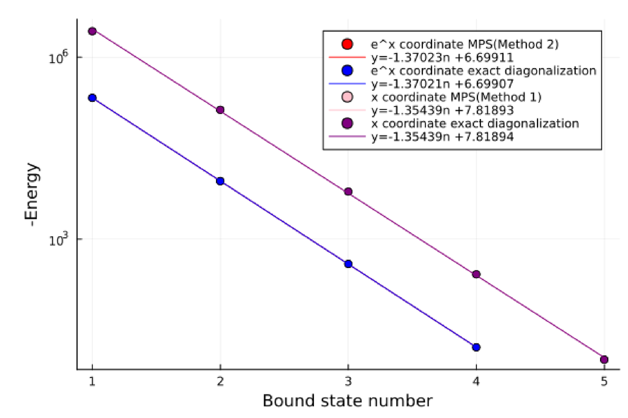

Figure 5: Efimov energy with $s_0 = 2i$ using 10 qubits.

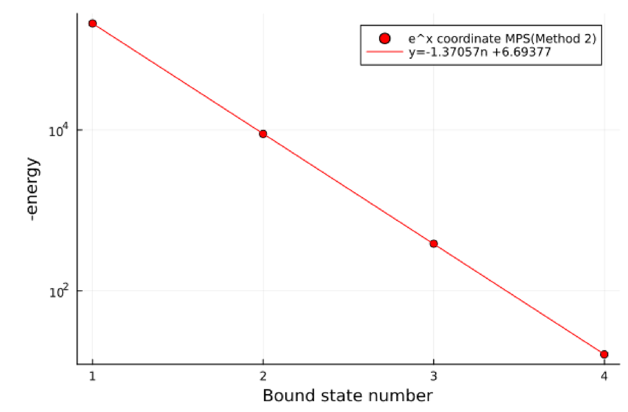

Figure 6: Efimov energy with $s_0 = 2i$ using 20 qubits.

Conclusions & Discussion

- Method1 in current situation can build $\frac{1}{x+2^{-10}}$ for 20 qubits with good enough compression and precision, but still can't solve Eq. 9 even at higher s_0. In the future, we will also compare this method with the cross approximation.
- Method1 have many kinds of deformation, such as using periodic boundary condition or using high order differential operator, but it's not so important to compare them in our case, because the bond dimension is not high here, but it may be very different in other cases.
- Method2 gives the exact $\frac{1}{x}$ by changing the coordinate to e^x, and this method works better than Method1, although it may have less bound states.
- Method2 is also very suitable to do the scaling transformation, and we hope we can use this property to see limit cycle in Efimov states in the future.

References

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