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Implementing the density matrix embedding theory with the hierarchical mean-field approach

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ABSTRACT

We show an implementation of density matrix embedding theory (DMET) for the spin lattice of infinite size. It is indeed a special form of hierarchical mean-field (HMF) theory. In the method, we divide the lattice into a small part and a large part. View the small part as an impurity, embedding in the large part, which is viewed as the environment. We deal the impurity with a high accuracy method. But treat the environment with a low-level method: the states of the environment nearby the impurity are expressed by a set of multiple block product states, while the distant parts are treated by mean-field consideration. Our method allows for the computation of the ground state of the infinite two-dimensional quantum spin systems. In the text, we take the frustrated Heisenberg model as an example to test our method. The ground state energy we calculated can reach a high accuracy. We also calculate the magnetization, and the fidelity to study the quantum phase transitions.

1. Introduction

Recently, the new DMET [1–5] provides a more simple way to deal with the quantum many-body systems. This new method has been successfully applied to solve the ground state of Hubbard model. The basic physics of DMET is analogous to the dynamical mean-field theory (DMFT) [6–8], which decomposes the system into two parts: the impurity and the environment. The impurity part of the system can be treated exactly, and the remaining part, i.e., environment is treated approximately. In DMFT, the observables related only to the impurity part, such as ground state energy per site, have high accuracy. The DMET reproduces the physics idea of the DMFT in a wavefunction method, which consider the impurity as embedding in a single particle mean-field environment. It calculates the density matrix, instead of the Green function. For the ground state, this method can reduce the cost substantially. A modification of the original DMET, called Cluster-DEMT [9] method, is capable to handle spin model with high accuracy results.

In numerical calculations, the original DMET uses a larger lattice to replace an infinite one. In our work, we develop a new way to handle the ground state of the real infinite lattice, which is a new implementation of the DMET and is inspired by the work of Ref. [9]. As mentioned in that paper, when solving the square lattice spin system with DMET, the impurity has strong correlation with the nearby environment, while the effect of distant parts of the environment is relatively weak (just a mean-field environment). Thus, we think of using the method of HMF [10] to implement the DMET: solve the impurity and nearby surroundings with a high-accuracy method, and treat the distant environment by mean-field consideration. In other words, we reformulate the DMET into the form of the HMF. Specifically, we consider the impurity and the surrounding environment as a superblock, corresponding to the superplaquette of the HMF, and identify such superblock as the relevant elementary degree of freedom [11,12]. Next we reformulate the variational wavefunction of this superblock in the spirit of the DMET. This is different to the HMF, in which the superblock state is exact. Then, apply a translationally invariant variational ansatz to the ground state of the entire lattice, the same as the HMF does. By this way, our method gets rid of the influence of the scaling effect of the lattice in the numerical calculations. The observables referring to the impurity are calculated with the reduced density matrix of the impurity. And the results of these observables can be extended to the infinite lattice according to the translational symmetry of the lattice. Compared with Cluster-DMET, we obtain the results which are more suitable to represent that of an infinite lattice. Moreover, we can reach high accuracy results at a mean-field computation cost.

In this paper, we show how the DMET works in the framework of the HMF, and analyze the properties of our algorithm.

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The Heisenberg model is the typical model to describe the quantum spin systems, which is studied by many methods, such as the quantum Monte Carlo (QMC) [13], couple cluster method (CCM) [14,15], variational method [16], Green's function method [17]. Aiming at illustrating the idea of our method, we use the normal $J_1 - J_2$ model (frustrated Heisenberg model) as an example. We primarily choose the 6×6 superblock as the elementary degree of freedom, which is a symmetry-preserving cluster (preserves the C_4 symmetry). For the environment states of this superblock, we use the multiple block product states to replace the single block product state of the Cluster-DMET, which can make an improvement to the ground state energy in the intermediate region. Meanwhile, we also show the ground state energy with the case of choosing the superblock size as 4×4. It can be directly calculated using the ground state obtained by the exact HMF [10] or our approximate HMF approach [18]. We compare our ground state energy to that of other methods, such as Cluster-DMET, CCM [14,15] and QMC [13]. Besides, we also use our method to investigate the quantum phase transition of the $J_1 - J_2$ model. Our results manifest that the magnetization disorder region is $0.41 \leq J_2/J_1 \leq 0.63$. Particularly, we use the reduced fidelity to observe the phase transition of this model, which can detect the position of transition points sensitively. Our article is organized as follows. In Section 2, we give the analytical derivation of our method. Section 3 shows our numerical results.

2. Numerical methods

We take the spin-1/2 frustrated Heisenberg antiferromagnetic (HAF) $J_1 - J_2$ model defined on a square lattice model to discuss our methods. The Hamiltonian reads

$$H = J_1 \sum_{\langle i,j \rangle} \boldsymbol{S}_i \cdot \boldsymbol{S}_j + J_2 \sum_{\langle\langle i,j \rangle\rangle} \boldsymbol{S}_i \cdot \boldsymbol{S}_j, \tag{1}$$

where J_1 is the nearest-neighbor (NN) and J_2 is the next-nearest-neighbor (NNN) antiferromagnetic interactions. In recent several decades, the ground state of this model has been investigated by using many numerical methods [10,15,17,19–24]. Thus, there are reliable data for comparison.

We divide the lattice into two parts: A and B. Part A is referred as an impurity in DMFT, and has a small number of degrees of freedom. Part B is the remaining part of the lattice, which can be viewed as the environment. According to the Schmidt decomposition [25,26], the ground state $|\Psi\rangle$ of H can be equally expressed as

$$|\Psi\rangle = \sum_{\tau}^{T} \lambda_\tau |\alpha_\tau\rangle |\beta_\tau\rangle, \tag{2}$$

where the $|\alpha_\tau\rangle$ and $|\beta_\tau\rangle$ are separately the states in the Hilbert space of the impurity A and environment B, and T is the dimension of the Hilbert space of A. Follow from this equation, the observables only containing the impurity's degrees of freedom can be obtained from the reduced density matrix of the impurity A. Since it is hard to get the exact $|\Psi\rangle$, the DMET provides an approximate method, namely, replace the exact environment states $|\beta_\tau\rangle$ with an approximate states $\left|\tilde{\beta}_\tau\right\rangle$. In the original DMET [1], the impurity is considered to be embedded in a single particle mean-field environment, namely the states $\left|\tilde{\beta}_\tau\right\rangle$ are single particle mean-field states. By direct using of this method on calculating the $J_1 - J_2$ model, however, it is unable to obtain the high accuracy results. The Cluster-DMET makes a modification on the original DMET. It expresses the approximate wavefunction of the lattice as $\left|\tilde{\Psi}\right\rangle = \sum_{\tau}^{T} \lambda_\tau |\alpha_\tau\rangle \left|\tilde{\beta}_\tau\right\rangle_{BPS}$, where the $\left|\tilde{\beta}_\tau\right\rangle_{BPS}$ is a block product state, i.e., $\left|\tilde{\beta}_\tau\right\rangle_{BPS} = \prod_i \phi_\tau^i$ with the ϕ_τ^i being the state of a small block. We see that the approximate environment state in Cluster-DMET [9] is expressed by the T block product states $\left|\tilde{\beta}_1\right\rangle_{BPS}, \ldots, \left|\tilde{\beta}_T\right\rangle_{BPS}$, which is beyond the simple single particle mean-field environment. In this work, we make further improvement for the environment state based on this block product states environment. We replace the state $|\beta_\tau\rangle$ of Eq. (2) with a superposition of K block product states, namely with a superposition of multiple block product states. Our approximate wavefunction $\left|\tilde{\Psi}\right\rangle$ takes the form

$$\left|\tilde{\Psi}\right\rangle = \sum_{\tau}^{T} |\alpha_\tau\rangle \left(\lambda_\tau^1 \left|\tilde{\beta}_\tau\right\rangle_{BPS}^1 + \cdots + \lambda_\tau^K \left|\tilde{\beta}_\tau\right\rangle_{BPS}^K\right), \tag{3}$$

where a state $\left|\tilde{\beta}_\tau\right\rangle_{BPS}^k$ $(k = 1, \ldots, K)$ is a block product state, and the λ_τ^k are the superposition coefficients. In the case of $K = 1$, our state is equivalent to that in Ref. [9]. And the accuracy of the environment B states increases with increasing K.

In Ref. [9], by analyzing the environment states $\left|\tilde{\beta}_1\right\rangle_{BPS}, \ldots, \left|\tilde{\beta}_T\right\rangle_{BPS}$, it finds that those states of the distant parts of the environment B are close to the mean-field result. Thus, we can directly treat the distant parts of the environment at a same mean-field level. Simultaneously, we make an improvement on the treatment of the near parts of the environment. This technique can be implemented with the HMF approach. We consider the impurity and the surrounding sites which cannot be treated with the mean-field as a superblock, and choose it as our elementary degree of freedom. The wavefunction of this superblock is written in the form of Eq. (3), and it is invariant under translations. We apply the translationally invariant conditions to get the entire lattice state $|\Phi\rangle$, which is expressed as $|\Phi\rangle = \prod_b \left|\tilde{\Psi}_{superblock}\right\rangle_b$, where b is the index of superblocks. It is apparent that our wavefunction is a formulation of HMF. Thus, our method can be applied to carry the numerical calculation on the infinite lattice.

In the concrete calculation for the $J_1 - J_2$ model in Ref. [9], it shows that only two nearby sites around a 2×2 impurity are not mean-field environment. So we choose a 6×6 superblock as the superblock of the HMF. Symmetric covering of the square lattice with this superblock can reproduce the original Bravais lattice, and more the C_4 lattice symmetry is also preserved. We use this 6×6 superblock to illustrate our method. First, we divide the superblock into nine 2×2 clusters (small blocks). Consider the center 2×2 cluster as the impurity A, and the basis states of this impurity are $|\alpha_\tau\rangle$. The remaining eight clusters are the surrounding environment of this impurity. For this environment, we have $\left|\tilde{\beta}_\tau\right\rangle_{BPS}^k = \phi_{\tau,k}^1 \cdots \phi_{\tau,k}^8$, where the states $\phi_{\tau,k}^1, \ldots, \phi_{\tau,k}^8$ correspond to the eight clusters, and the state $\phi_{\tau,k}^i = c_{\tau,k}^{i,0} |\downarrow\downarrow\downarrow\downarrow\rangle + \cdots + c_{\tau,k}^{i,15} |\uparrow\uparrow\uparrow\uparrow\rangle$. Then, according to Eq. (3), we can easily get the state $\left|\tilde{\Psi}_{6\times6}\right\rangle$ of the 6×6 superblock. For such superblock, the 2×2 impurity states are exact, and the states of the surrounding environment (eight 2×2 clusters) are treated by K multiple block product states. Finally, the wavefunction $|\Phi\rangle$ of the entire lattice is the products of the 6×6 superblock states, with each superblock having the same wavefunction. Actually, in the case of smaller superblocks, such as 4×4 superblock, one can easily treat it exactly with the HMF approach. There is no need for using the approximation as mentioned above. For using the Schmidt decomposition, we can decompose the superblock state obtained by the HMF 4×4 into the form of DMET.

We optimize our state $|\Phi\rangle$ to the ground state with the method in Ref. [18], which has been used to optimize the state given by our approximate HMF method. In a word, this optimizing method is to optimize the state $|\Phi\rangle$ with the matching pursuit (MP)