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.

Keywords: density matrix embedding theory; hierarchical mean-field; infinite lattice; spin model

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

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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 superplaque 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. 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

$$H = J_1 \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j + J_2 \sum_{\langle\langle i,j \rangle\rangle} \mathbf{S}_i \cdot \mathbf{S}_j, \quad (1)$$

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

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

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 hardly 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 $|\tilde{\beta}_{\tau}\rangle$. In the original DMET [1], the impurity is considered to be embedded in a single particle mean-field environment, namely the states $|\tilde{\beta}_{\tau}\rangle$ 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 $|\tilde{\Psi}\rangle = \sum_{\tau}^T \lambda_{\tau} |\alpha_{\tau}\rangle |\tilde{\beta}_{\tau}\rangle_{BPS}$, where the $|\tilde{\beta}_{\tau}\rangle_{BPS}$ is a block product state, i.e.,

$|\tilde{\beta}_{\tau}\rangle_{BPS} = \prod_i \phi_{\tau}^i$ 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 $|\tilde{\beta}_1\rangle_{BPS}, \dots, |\tilde{\beta}_T\rangle_{BPS}$, 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 $|\tilde{\Psi}\rangle$ takes the form

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

where a state $|\tilde{\beta}_{\tau}\rangle_{BPS}^k$ ($k=1, \dots, K$) 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 the Ref. [9], by analyzing the environment states $|\tilde{\beta}_1\rangle_{BPS}, \dots, |\tilde{\beta}_T\rangle_{BPS}$, 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 $|\Phi\rangle = \prod_b |\tilde{\Psi}_{superblock}\rangle_b$, 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 the 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 $|\tilde{\beta}_{\tau}\rangle_{BPS}^k = \phi_{\tau,k}^1 \cdots \phi_{\tau,k}^8$, where the states $\phi_{\tau,k}^1, \dots, \phi_{\tau,k}^8$ 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 $|\tilde{\Psi}_{6 \times 6}\rangle$ 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

in 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) algorithm [27] based on the variational principle. The ground state can be obtained when the Rayleigh quotient

$$E = \langle \Phi | H | \Phi \rangle / \langle \Phi | \Phi \rangle \quad (4)$$

converges at minimum value. In the progress of optimizing, we just need to update one 6×6 state $|\tilde{\Psi}_{6 \times 6}\rangle$, and use it to replace others. For our method, the surrounding environment states

$|\tilde{\beta}_\tau\rangle_{BPS}^k$ can reach convergence with a rather small K . So it is a very efficient method. Our method has the advantage that the surrounding environment states $|\tilde{\beta}_\tau\rangle_{BPS}^k$ can reach convergence with a rather small K , thus it is a very efficient method. The ground state energy per site also can be calculated by using the method introduced in Ref. [9],

$$E_{per} = \frac{J_1}{2} \sum_{\langle \delta \rangle} \langle \mathbf{S}_i \cdot \mathbf{S}_{i+\delta} \rangle + \frac{J_2}{2} \sum_{\langle\langle \delta \rangle\rangle} \langle \mathbf{S}_i \cdot \mathbf{S}_{i+\delta} \rangle, \quad (5)$$

where i ($i \in A$) is the index of the sites in impurity A . The first (second) summation indicates the NN (NNN) sites of the square lattice.

3. Numerical tests

We should pay attention to the reduced density matrix of impurity A (2×2 cluster), which can be calculated from the ground state $|\Phi\rangle$ obtained by the variational method. The reduced density matrix can reflect the features of the ground state of the sites contained in the 2×2 impurity. The ground state energy per site can be calculated by Eq. (5), which takes the factor of environment into the consideration. Besides, we also can calculate the bond energies, magnetization, and the reduced fidelity. By using the translation invariant principle of the lattice, we can get the characteristics of the original H (Eq. (1)) of the $J_1 - J_2$ model. In the following calculation, we set $J_1 = 1$.

The ground state energy per site E_{per} as a function of J_2 is shown in Fig. 1, and we use $K=3$ for the surrounding environment states. As a comparison, we also show the extrapolation results of CCM [15]. Note that our results are not variational, therefore our energy curves are below or above the CCM_extr curves. As can be seen from this figure, our

ground state energy obtained by the superblock 6×6 is very close to that of the CCM_extr. An obvious cusp near $J_2 \approx 0.64$ is observed, which demonstrates a first-order phase transition and is close to the result of Cluster-DMET [9] near $J_2 = 0.62$. The inset shows the changes of E_{per} with different value of K for the surrounding environment states in the superblock 6×6 . In the region of $0.3 < J_2 < 0.64$, it has an obvious improvement from $K=1$ to $K=2$, and it changes a little from $K=2$ to $K=3$. In other regions, it almost has no change with K . This indicates our approximate environment states can converge with small K . Additionally, we also show the results obtained by the case of 4×4 superblock in this figure. The variational ground state of this case is obtained by our approximate HMF [18] approach, which is very close to the exact HMF [10] approach. We view the center 2×2 cluster of the superblock 4×4 as the impurity, and the E_{per} still is calculated by Eq. (5). In this case, the accuracy of the energy is lower, especially at the phase transition points. It means that it is not enough to take one neighbor site around the 2×2 impurity as the surrounding environment of the 2×2 impurity. However, the result is still satisfactory outside the phase transition points.

Fig. 1. The ground state energy per site E_{per} as a function of J_2 . Inset: the E_{per} for the environment states in the superblock 6×6 with $K=1$ (empty squares), 2 (empty triangles), and 3 (red triangles). As a comparison, squares denote the CCM_extr results.

In particular for the HAF at $J_2 = 0$, the ground state energy per site can be calculated according to the method in DMET (i.e. twice of the bond energy $2\langle S_i \cdot S_{i+1} \rangle$). The energy obtained by our method is -0.674 (-0.66) for the case of 6×6 (4×4) superblock. And the result of Cluster-DMET is -0.666942. If we calculate the ground state energy with the Eq. (5), in this way we obtain the energy with results of -0.665 (6×6) and -0.682 (4×4). The result

in the case of 6×6 superblock is consisted with the Cluster-DMET result -0.6659, and also is in good agreement with other methods for the HAF, such as the extrapolated CCM [14] and QMC techniques [13]. Compared with the best QMC estimated -0.6694, the accuracy reaches to 98.5% in the case of 4×4 superblock, and it is even higher in the case of 6×6 superblock which exceeds 99%. Anyway, our result is much better than that in the thermodynamic limit of HMF [10], with result of -0.64.

To reflect the features of our wavefunction, we calculate the bond energies within the 2×2 impurity A of a 6×6 superblock. Fig. 2 shows the bond energies calculated with $\langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle$, $i, j \in A$, and they are the NN or NNN single sites. The empty symbols are NN and NNN bond energies obtained by exact diagonalization (ED) for finite 40 spins lattice [20]. We can see that our NN and NNN bond energies have a discontinuous jump at the point $J_2 \approx 0.64$, signaling the first-order transition. Note that the shape of our bond energy curves resembles that obtained with the ED40 in the region $J_2 > 0.64$. But for $J_2 < 0.64$, the curves present different behaviors. Our results show that the bond energies increase with increasing J_2 , while the ED40 shows the decreases of the bond energies with J_2 . This indicates that the physical characterizations of the $J_1 - J_2$ model may be different in the infinite and finite size.

Fig. 2. The NN (squares) and NNN (cycles) bond energies versus J_2 . Solid (empty) symbols denote the bond energies obtained by our method (ED40).

In order to reveal the properties of our algorithm intuitively, we analyze the internal characteristics of the superblock 6×6 state. That is to investigate the impurity state and the surrounding environment state simultaneously, which is helpful for us to understand our methods. Fig. 3(a) shows the NN and NNN bond energies of the central 4×4 block inside the 6×6 superblock at the point $J_2 = 0.5$. Moreover, we numerically investigate the energy

E'_{per} of every site inside the 6×6 superblock which calculated by Eq. (5) (here the index i of this equation refers to the entire lattice sites). For simplicity, we only plot the results of the sites of one of the center lines at the points $J_2 = 0.1, 0.5, 0.8$, as shown in Fig. 3(b). We can see that the energy of the sites belonging to the impurity has higher accuracy than that of the surrounding environment. And the energy of the environment sites at the boundary of the superblock is close to the results of the HMF. For the sites between the impurity and the boundary, we can view them as the transition of the higher accuracy results to the mean-field results. Thus, our results demonstrate that we can still get a high accuracy results from the impurity sites, although the distant environment sites are dealt with at a mean-field level.

Fig. 3. The internal characteristics of a superblock 6×6 state. (a) The NN (black lines) and NNN (green lines) bond energies in the superblock at the point $J_2 = 0.5$. We show only the central 4×4 range of this superblock. A small red dot denotes a spin. (b) The ground state energy E'_{per} of the sites on one of the center lines of the superblock at the points

$J_2 = 0.1, 0.5, 0.8$; The isolated symbols are the results obtained by HMF 2×2 at the points $J_2 = 0.1$ (triangular), 0.5 (star), 0.8 (square).

It is widely accepted that there are two phase transitions in the ground state of the $J_1 - J_2$ model (Eq. (1)). There are the Néel like magnetic phase and the collinear magnetic phase, corresponding to small and large J_2 , respectively. These two phases are separated by the intermediate quantum paramagnetic phase. Next we use the magnetic orders to study the magnetization and detect the quantum critical points of the $J_1 - J_2$ model with our method. We calculate the staggered and collinear (along horizontal direction) magnetizations, defined as $M_{s,c} = \frac{1}{4} \sum_{i \in A} \langle (-1)^{\varepsilon_i} S_i^z \rangle$ according to Eq. (14) of Ref. [10]. The M_s is the staggered magnetization with $\varepsilon_i = i_x + i_y$, and M_c is the collinear magnetization with $\varepsilon_i = i_x$. The (i_x, i_y) is the coordinate of site i . Fig. 4 shows the magnetization M . As a comparison, we also show the magnetization of a spin at the center of a 4×4 block (cluster), i.e., $\langle S_i^z \rangle$, which is obtained by the cluster mean-field theory (CMFT) [23]. We can clearly see that there exist two phase transition points. At the small J_2 side, the staggered magnetization M_s is not zero. This denotes a Néel order phase that is characterized by an anti-parallel spin orientation of nearest neighbors. As J_2 increases, the Néel order is smoothly suppressed and continuously vanishes at the point $J_2 \approx 0.41$, signaling the occurrence of a second-order phase transition. The Cluster-DMET gives this type of phase transition at point $J_2 \approx 0.42$. It is worthy of being mentioned, if we use $K=1$ for the environment states, it is cannot catch this type of phase transition. From the large J_2 side, the magnetization has nonzero M_c , which indicates that the spin orientation of nearest neighbors is anti-parallel in horizontal direction and parallel in vertical direction. It is so-called collinear order phase. As J_2 decreases, the collinear order also decreases smoothly. At $J_2 \approx 0.64$, the M_c suddenly jump to zero, indicating the occurrence of a first-order transition. In the region $0.41 \leq J_2 \leq 0.63$, the order parameter M is always zero, and there is no magnetic order.

This is the quantum paramagnetic phase.

Fig. 4. The staggered and collinear (along horizontal direction) magnetizations. The comparison is the magnetization of a spin $\langle S_i^z \rangle$ at the center of a superblock 4×4 , obtained by the CMFT [23]. PM denotes paramagnetic.

We also numerically investigate the fidelity and the fidelity susceptibility to observe the quantum phase transitions in the ground state of the $J_1 - J_2$ model. The fidelity is defined by the modulus of the overlap between two states (see Ref. [28] for a view). It is not related to the concept of Landau-Ginzburg-Wilson spontaneous symmetry-breaking phase transitions theory. Thus, maybe it can detect the phase transition points which cannot be described by the traditional local order parameters method. Recently, there are many papers have used the fidelity to study the problem of quantum phase transitions for various systems [29-35]. These works manifest that the fidelity is a good indicator of quantum phase transitions. In our methods, the impurity A is a part (here use $\bar{A}$ to label the remaining part) of the entire lattice, which state described by a reduced density matrix. Thus we can use the strategy of reduced fidelity [36,37] to study the phase transitions of the $J_1 - J_2$ model. The reduced fidelity is defined as

$$F = \text{Tr} \sqrt{\sqrt{\rho_A(J_2)} \rho_A(J_2 + \Delta) \sqrt{\rho_A(J_2)}} , \quad (8)$$

where $\rho_A(J_2)$ and $\rho_A(J_2 + \Delta)$ are the reduced density matrices of the impurity A at the points J_2 and $J_2 + \Delta$, respectively. The reduced density matrix $\rho_A = \text{Tr}_{\bar{A}}(|\Phi\rangle\langle\Phi|)$ is obtained by tracing other degrees of freedom from the state of the system. The corresponding fidelity susceptibility is given by

$$\chi_F = \lim_{\Delta \rightarrow 0} \frac{-2 \ln F}{\Delta^2} , \quad (9)$$

which is the second derivative of the reduced fidelity.

We calculate the reduced fidelity and corresponding fidelity susceptibility between two

reduced states $\rho_A(J_2)$ and $\rho_A(J_2 + \Delta)$ with fixed $\Delta=0.01$, as shown in Fig. 5. As expected, there are clearly two sudden drops of the value of the reduced fidelity, i.e. the points $J_2=0.41$ and $J_2=0.64$, for which the fidelity susceptibility is divergent. This demonstrates two phase transition points of the $J_1 - J_2$ model, which is consistent with the traditional order parameters method.

Fig. 5. (Upper panel) The reduced fidelity of impurity A state. The points with minimum value are the critical points. (Lower panel) The corresponding fidelity susceptibility, which converges at the two critical points. We take the separation $\Delta=0.01$ in the figures.

4. Conclusions

We have shown an implementation of the DMET in the framework of the HMF theory, which is tested on the infinite $J_1 - J_2$ model. Our method combines the merits of the DMET and HMF approach. In the concrete calculations, we use multiple block product states to express the surrounding environment states of the impurity, which makes a significant improvement to the ground state energy in the intermediate region. The numerical results show that our ground state energy is in good agreement with the CCM method, and the accuracy of the energy is much higher than the conventional HMF. The quantum states which are calculated by our method also can correctly describe the quantum phase transitions, which occurs at the points $J_2 \approx 0.41$ and $J_2 \approx 0.64$. Thus, our method is efficient in calculating the ground states of the infinite spin system.

Acknowledgments

We thank Jin Huang and Liang-Liang Zhang for beneficial discussions and comments. This work has been supported by the National Science Foundation of China (Grant No.10875087).

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Fig. 1. The ground state energy per site E_{per} as a function of J_2 . Inset: the E_{per} for the environment states in the superblock 6×6 with $K=1$ (empty squares), 2 (empty triangles), and 3 (red triangles). As a comparison, squares denote the CCM_extr results.

Fig. 2. The NN (squares) and NNN (cycles) bond energies versus J_2 . Solid (empty) symbols denote the bond energies obtained by our method (ED40).

Fig. 3. The internal characteristics of a superblock 6×6 state. (a) The NN (black lines) and NNN (green lines) bond energies in the superblock at the point $J_2 = 0.5$. We show only the central 4×4 range of this superblock. A small red dot denotes a spin. (b) The ground state energy E'_{per} of the sites on one of the center lines of the superblock at the points $J_2 = 0.1, 0.5, 0.8$; The isolated symbols are the results obtained by HMF 2×2 at the points $J_2 = 0.1$ (triangular), 0.5 (star), 0.8 (square).

Fig. 4. The staggered and collinear (along horizontal direction) magnetizations. The comparison is the magnetization of a spin $\langle S_i^z \rangle$ at the center of a superblock 4×4 , obtained by the CMFT [21]. PM denotes paramagnetic.

Fig. 5. (Upper panel) The reduced fidelity of impurity A state. The points with minimum value are the critical points. (Lower panel) The corresponding fidelity susceptibility, which converges at the two critical points. We take the separation $\Delta = 0.01$ in the figures.