Multilayer wave functions: A recursive coupling of local excitations

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Abstract – Finding a succinct representation to describe the ground state of a disordered interacting system could be very helpful in understanding the interplay between the interactions that is manifested in a quantum phase transition. In this work we use some elementary states to construct recursively an ansatz of multilayer wave functions, where in each step the higher-level wave function is represented by a superposition of the locally “excited states” obtained from the lower-level wave function. This allows us to write the Hamiltonian expectation in terms of some local functions of the variational parameters, and employ an efficient message-passing algorithm to find the optimal parameters. We obtain good estimations of the ground-state energy and the phase transition point for the transverse Ising model with a few layers of mean-field and symmetric tree states. The work is the first step towards the application of local and distributed message-passing algorithms in the study of structured variational problems in finite dimensions.

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Introduction. – In a wave function approach to the study of an interacting quantum system we usually resort to some physical and numerical insights to suggest a reasonable variational wave function that approximates the quantum state of the system. In fact, providing a succinct representation that well describes the physical state of the system means we know how to model the relevant quantum correlations in an efficient way. The number of variational parameters we need to characterize such a wave function could be of the order of the size of system, depending on the nature of quantum correlations captured by the wave function. Here it is essential to have an efficient optimization algorithm for minimizing the Hamiltonian expectation over the space of the variational parameters.

In this work we will use some ideas from the physics of quantum many-body systems, more specifically the matrix product states [1,2] and the coupled cluster method [3,4], to construct an ansatz of multilayer wave functions for a possibly disordered quantum system of interacting spins.

The matrix product states and the related generalizations [5,6], e.g. multiscale entanglement-renormalization [7,8] and projected entangled pair states [9,10], can be constructed by integrating over some auxiliary degrees of freedom interconnected in a specific manner to the physical variables to account for the entanglement in different parts of the system [11,12]. On the other hand, in the coupled cluster method one starts from an appropriate reference state, e.g. the Hartree-Fock wave function, and elaborates on the local excitations to obtain more accurate wave functions and estimations for the ground-state energy [13].

It is always useful in the study of interacting systems to start with the mean-field (MF) wave functions (or product states). More accurate wave functions are obtained by adding interactions between the variables [14–17]. Here, in general, we have to resort to some approximation algorithms, e.g. Monte Carlo [18], to compute efficiently the quantum expectations. In ref. [19] we proposed to estimate the expectations within the Bethe approximation, which allows us to write the Hamiltonian expectation in terms of some local functions of the

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variational parameters and the cavity marginals of the Bethe approximation; for a review of similar methods, see [20]. Note that the Bethe estimation of the Hamiltonian expectation is not necessarily an upper bound for the ground-state energy, unless the interaction graph defined by the trial wave function has a tree structure. Nevertheless, the same approximation offers efficient message-passing algorithms that have been proved useful in the study of random constraint satisfaction and optimization problems [21–23].

Symmetric wave functions with a tree structure provide us with another category of computationally tractable states which somehow complement the mean-field states; while the latter wave functions are good candidates for the state of the system in the ordered (ferromagnetic, or localized) phase, the symmetric states are more appropriate in the disordered (paramagnetic, or extended) phase. Moreover, in both the cases we can easily construct an orthonormal set of locally excited states that could be useful in the framework of the coupled cluster method [24]. We remark that the weighted graph states studied in quantum physics and information theory can be represented by application of some two-body unitary operators on initially mean-field states [25]. Similarly, we can obtain a weighted graph state with an initially tree wave function and still compute efficiently the quantum expectation of local observables.

In this study we use the mean-field and the symmetric tree wave functions to construct an ansatz of multilayer wave functions by a recursive coupling of the local excitations; we start from a reference wave function and in each step we construct a higher-level wave function by taking a superposition of the locally “excited states” obtained from the wave function in the previous step. In the last step we minimize the Hamiltonian expectation with respect to the variational parameters characterizing the reference state and the superposition functions. Note that we use the “excited state” for any state that is orthogonal to the trail wave function; in this sense, the average energy of an excited state could be less than that of the reference wave function as we minimize the energy over the whole set of the parameters only in the end of the process. The simple structure of the wave functions allows us to work with local energy functions of the variational parameters which is essential for utilizing distributed message-passing algorithms in the study of the optimization problem. In principle, the method can be implemented with more general wave functions for spin systems with an arbitrary interaction graph.

In the following we will specify the wave functions and the local excitations that we are going to work with in the multilayer wave functions. Then we present the message-passing algorithm that is used to minimize the Hamiltonian expectation, and report some preliminary results for the ferromagnetic transverse Ising model in one and two spatial dimensions. The reader can find more on details of the calculations in [26].

Definitions. – Consider the transverse Ising model with Hamiltonian

$$H = - \sum_{(ij) \in E_q} J_{ij} \sigma_i^x \sigma_j^x - \sum_i h_i \sigma_i^z,$$

where $i = 1, \ldots, N$ labels the sites in the quantum interaction graph $E_q$. The $\sigma_i^{x,y,z}$ are the standard Pauli matrices. And we use the orthonormal set of the standard Pauli matrices. And we use the orthonormal set of the states $|\sigma_1, \ldots, \sigma_N\rangle$ with $\sigma_i = \pm 1$ in the $\sigma_i^z$ representation.

Starting from a reference wave function $|\Psi_0\rangle = \sum_{\sigma} \psi_0(\sigma; P^0(1))|\sigma\rangle$ characterized by the variational parameters $P^0$, we construct the orthonormal set of excited states $S_0 = \{|\Psi_0,s_0\rangle|s_0 = 0, \ldots, N_0\rangle\}$, where $|\Psi_0,0\rangle \equiv |\Psi_0\rangle$. Then a higher-level wave function is obtained by taking a superposition of the excited states $|\Psi_1\rangle = \sum_{s_0} \psi_1(s_0; P^1(1))|\Psi_0,s_0\rangle$. Note that $|\Psi_1\rangle$ depends also $P^0$ through the $|\Psi_0,s_0\rangle$. The process can be repeated for $t$ steps to construct a $(t+1)$-layer wave function. At layer $t$ we have $|\Psi_t\rangle = \sum_{s_{t-1}} \psi_t(s_{t-1}; P^t)|\Psi_{t-1},s_{t-1}\rangle$ with the orthonormal set of excited states $S_{t-1} = \{|\Psi_{t-1},s_{t-1}\rangle|s_{t-1} = 0, \ldots, N_{t-1}\rangle\}$ and $|\Psi_{t-1},0\rangle \equiv |\Psi_{t-1}\rangle$. The aim is to minimize the Hamiltonian expectation over the variational parameters,

$$E_0 = \min_{\{P^0, \ldots, P^t\}} \langle \Psi_t | H | \Psi_t \rangle,$$

for some succinct representation of the variational states characterized by the parameters and the nature of excitations in the excited states. We recall that by the “excited state” we mean any state that is orthogonal to the trial wave function, and that is not necessarily an eigenstate of the Hamiltonian.

One can write the excited states at layer $l > 0$ as $|\Psi_{t,s_l}\rangle = \sum_{s_{t-1}} \psi_t(s_{t-1}, s_l; P^t)|\Psi_{t-1},s_{t-1}\rangle$. Notice that $\psi_t(s_{t-1}; P^t) = \psi_1(s_{t-1}, 0; P^t)$ as defined above. Moreover, by the orthogonality of the excited states we have $\sum_{s_{t-1}} \psi_t^* (s_{t-1}, s_l^*; P^t) \psi_t (s_{t-1}, s_l; P^t) = \delta_{s_l^*,s_l}$. This results in the following wave function at layer $t$:

$$|\Psi_t\rangle = \sum_{s_{t-1} \ldots s_2, s_1, \sigma} \psi_t(s_{t-1}; P^t) \psi_{t-1}(s_{t-2}, s_{t-1}; P^{t-1}) \ldots \psi_1(s_0, s_1; P^1) \psi_0(\sigma, s_0; P^0) |\sigma\rangle.$$

Then the average value of a local operator $O$ with matrix elements $O_{\sigma^*\sigma} \equiv \langle \sigma^*|O|\sigma\rangle$ can be computed in a recursive way by

$$\langle O \rangle_t = \sum_{s_{t-1}} |\psi_t(s_{t-1}; P^t)|^2 \times \left( \sum_{s_{t-1}} \psi_t^* (s_{t-1}; P^t) O^*_{\sigma^*s_{t-1}^*} \psi_t^* (s_{t-1}; P^t) \right).$$
where

\[ [O]_{ll}^{s_{l-1} s_l} \equiv \sum_{s_{l-1}} |\psi(s_{l-1}, s_l; P_l)|^2 \times \left( \sum_{s_{l-1}} \frac{|\psi_l'(s_{l-1}, s'_l; P'_l)|}{|\psi_l(s_{l-1}, s_l; P_l)|} (O)_{ll-1}^{s_{l-1} s'_l} \right), \tag{5} \]

setting \( s_{-1} \equiv \sigma \) and \( [O]_{-1} \equiv O \). Obviously, to compute the Hamiltonian expectation efficiently we have to limit ourselves to simple enough wave functions and excitations.

**Characterizing the wave functions.** – A trial wave function \( |\Psi| = \sum_\sigma \psi(\sigma; P)|\sigma| \) is characterized by the structure of the coefficients and the set of parameters \( P \).

In the study of multilayer wave functions we will use the mean-field and the symmetric tree states. The mean-field states can in general be represented by

\[ \psi(\sigma; B) = e^{i \Theta(\sigma)} \prod_i \left( \frac{e^{B_i \sigma_i/2}}{\sqrt{\cosh(B_i)}} \right), \tag{6} \]

with an arbitrary real phase \( \Theta(\sigma) \) and complex fields \( B_i = B_i^R + i B_i^I \). We call such a state mean-field because the probability measure \( \mu(\sigma; B) \equiv |\psi(\sigma; B)|^2 \) represents a classical system of independent variables. On the other hand we have the symmetric tree states:

\[ \psi(\sigma; K) = \frac{e^{i \Theta(\sigma)}}{\sqrt{2^N}} \prod_{ij \in T} \left( \frac{e^{K_{ij} \sigma_i \sigma_j/2}}{\sqrt{\cosh(K_{ij}^R)}} \right), \tag{7} \]

for some tree interaction graph \( T \) and complex couplings \( K_{ij} = K_{ij}^R + i K_{ij}^I \). Here the associated probability measure has a tree structure and is symmetric under \( \sigma \rightarrow -\sigma \). In both the cases we will write the phase in terms of some local interactions: \( \Theta(\sigma) = \sum_i \Lambda_i \sigma_i/2 + \sum_{ij \in E} \Gamma_{ij} \sigma_i \sigma_j/2 \). Note that besides the variational parameters we need to specify the interaction graphs \( T \) and \( E \). Here to maximize the gain from the interactions in the wave functions we follow the quantum interaction graph \( E_q \); i.e. we prefer to have interactions between the nearest neighbors in \( E_q \), and then between the next nearest neighbors and so on.

**Characterizing the excitations.** – In this section we will take the mean-field and the symmetric tree states to illustrate the nature of the local excitations that we are going to exploit in constructing the multilayer wave functions.

**Local excitations in the mean-field states.** Consider the mean-field state \( \psi(\sigma; B) \) defined in eq. (6). We define a set of orthonormal mean-field states \( |i_1 \ldots i_n\rangle \) for \( n = 1, \ldots, N \) with the same phase \( \Theta(\sigma) \) but different fields \( B_i \). The state \( |i_1 \ldots i_n\rangle \) is orthogonal to \( |\Psi| \) at sites \( \{i_1 \ldots i_n\} \); that is \( \hat{B}_i^R = -B_i^R \) and \( \hat{B}_i^I = B_i^I + \pi \) for \( i \in \{i_1 \ldots i_n\} \), otherwise \( \hat{B}_i = B_i \). We can represent all the above states in the occupation number representation by \( |s\rangle \equiv |s_1, \ldots, s_N\rangle \), with \( s_i \in \{0, 1\} \) to show the presence of a local excitation at site \( i \). Note that the state \( |0\rangle \) gives the original mean-field state, and \( \psi(\sigma; s; B) = \langle \sigma | s \rangle \) a higher-level wave function is obtained by a superposition of the locally excited states.

**Local excitations in the symmetric tree states.** Consider the symmetric tree state \( \psi(\sigma; K) \) defined in eq. (7). We define a set of orthonormal symmetric tree states \( |(i_1) \ldots (i_n)\rangle \) for \( n = 1, \ldots, N - 1 \) with the same phase \( \Theta(\sigma) \) but different couplings \( K_{ij} \). The state \( |(i_1) \ldots (i_n)\rangle \) is orthogonal to \( |\Psi| \) at edges \( \{(i_1) \ldots (i_n)\} \); that is \( K_{ij}^R = -K_{ij}^R \) and \( K_{ij}^I = K_{ij}^I + \pi \) for \( (ij) \in \{(i_1) \ldots (i_n)\} \), otherwise \( K_{ij} = K_{ij} \). Again, we represent all the above states in the occupation number representation by \( |s\rangle \), with \( s_{ij} \in \{0, 1\} \) to show the presence of a local excitation at edge \( (ij) \). So the state \( |0\rangle \) represents the original tree state.

Note that instead of having excitations on the edges we could have the excitations on the nodes; here a local excitation on node \( i \) is defined by modifying the parameters on all the edges emanating from the node and is represented by the occupation number \( s_i \). But, since the number of edges is one less than the number of nodes, we have to use only \( N - 1 \) node variables to represent the orthogonal set of locally excited states.

**Optimization algorithm.** – In this section we briefly describe the optimization algorithm we will use to minimize the Hamiltonian expectation. Let us assume we write the energy as \( \langle H \rangle = \sum_\sigma E_\sigma(P_\sigma) \) where \( P_\sigma \) is the set of variational parameters \( P_i \) that appear in the local energy function \( E_\sigma \). To say something about the optimal parameters we can study the following statistical physics problem \( Z = \sum_\sigma e^{-\beta E_\sigma} \sum_\sigma E_\sigma \). For finite \( \beta_{opt} \), we use the Bethe approximation to write the cavity marginals \( M_{a \rightarrow v}(P_a) \) and \( M_{v \rightarrow a}(P_v) \) of the variational parameter \( P_v \). The former messages are sent from the local energy functions to the parameters and give the probability of having the parameter \( P_v \) in the absence of the other energy functions involving the parameter. The latter messages are sent from the parameters to the local energy functions. These messages give the probability of having the parameter \( P_v \) in the absence of the interaction \( E_a \). The equations governing the above cavity marginals are called belief propagation (BP) equations [23,27].

But we are interested in the limit \( \beta_{opt} \rightarrow \infty \) where the probability distribution of the variational parameters is concentrated on the optimal ones. Taking the scaling \( M_{a \rightarrow v}(P_v) = e^{-\beta_{opt} M_{a \rightarrow v}(P_v)} \) and similarly for \( M_{v \rightarrow a}(P_v) \), we get

\[ M_{a \rightarrow v}(P_v) = \min_{\{P_u | u \in \partial a \setminus v\}} \left\{ E_\sigma(P_\sigma) + \sum_{u \in \partial a \setminus v} M_{u \rightarrow a}(P_u) \right\}, \tag{8} \]

\[ M_{v \rightarrow a}(P_v) = \sum_{b \in \partial v \setminus a} M_{b \rightarrow v}(P_v). \tag{9} \]
These are the so-called minsum equations [27]. Here \( \partial v \) is the set of interactions depending on \( P_v \). Solving the equations by iteration, one finds an estimation of the optimal parameters by

\[
P_v^{\text{min}} = \arg \min_{P_v} \sum_{\alpha \in \partial v} M_{\alpha \rightarrow v}(P_v).
\]

**Multilayer wave functions of mean-field states.** –

The one-dimensional model. We start from a one-dimensional mean-field wave function \( \psi_0(\sigma; B_0) \propto e^{i\theta_0(\sigma) + B_0 \sigma_i^x/2} \) and couple the local excitations by another one-dimensional mean-field state \( \psi_1(s_0; B_1) \propto e^{ix_1(\sigma_1) + B_1 \sigma_i^x/2} \) as shown in fig. 1. For the phases we assume \( \Theta(\sigma) = \sum \hat{\Gamma}_{i} \sigma_i \sigma_{i+1}/2 \) with some interactions along the quantum interaction graph, and similarly for \( \Theta_1(s_0) \). We can still compute exactly the average energies \( \langle \epsilon_i \rangle = -h \langle \sigma_i^x \rangle \) and \( \langle \epsilon_i, \epsilon_{i+1} \rangle = -J_{i, i+1} \langle \sigma_i^z \sigma_{i+1}^z \rangle \), depending locally on the subset of the parameters \( \{B_0, B_1, \Gamma_0, \Gamma_1, \Gamma_2, \Gamma_3, \Gamma_4, \Gamma_5, \Gamma_6, \Gamma_7, \Gamma_8, \Gamma_9, \Gamma_{10} \} \). Notice that by these average energies we couple the neighboring parameters in different layers. This defines a bipartite interaction graph \( G_v \), where each local energy function \( \langle \epsilon_i \rangle \), represented by node \( a \), depends on the parameters \( P_{\partial a} \) in its neighborhood subset \( \partial a \), and each parameter \( P_v \in \{B_0, B_1, \Gamma_0, \Gamma_1, \Gamma_2, \Gamma_3, \Gamma_4, \Gamma_5, \Gamma_6, \Gamma_7, \Gamma_8, \Gamma_9, \Gamma_{10} \} \), represented by node \( v \), appears in the subset of interactions \( \partial v \). Given the local energy functions and the dependency graph of the variational parameters we can use the minsum algorithm to minimize the Hamiltonian expectation.

In the same way, we can continue by coupling the local excitations in layer \( t = 1 \) by another mean-field wave function. In fig. 2 we display the results obtained with a few layers of mean-field states for the transverse Ising model in one dimension. The relative error in the ground-state energy \( \delta e(h) \equiv (E_0/E_0^{\text{exact}} - 1) \) computed at the critical point \( h = 1 \) reads \( \delta e_{\text{MF}}(1) = 0.01825(t = 0), 0.00499(t = 1), 0.00262(t = 2) \). For \( h = 1 \) the MF-MF-MF-\( t = 0 \) and \( h = 1 \) the MF-MF-MF-\( t = 2 \) ground states obtained by the minsum algorithm were used. The arrow shows the exact phase transition point. Note that the mean-field states (MF) work better than the symmetric states (S) in the ordered phase, and the symmetric states result in smaller energies in the disordered phase.

Higher dimensions. It is straightforward to work with the multilayer wave functions of mean-field states in higher spatial dimensions. Obviously, the number of variational parameters involved in the quantum expectation of a local observable is of order \( (t + 1)^{d+1} \) in \( d \) dimensions. Consequently, the computation time grows exponentially with \( (t + 1)^{d+1} \). Note that this complexity is due to the (imaginary) interactions in the phase \( \Theta \); in fact if the interaction graph defined by the \( \Gamma_{ij} \) is a tree we can compute the quantum expectation of any product operator in a time of
order \( NC_{\max}[2^{2(t+1)}]^2 \). Here \( C_{\max} \) is the maximum connectivity of the nodes in the tree, and \( 2(t+1) \) is the length of binary string \((\sigma, s_0, i \ldots s_{t-1}, i; \sigma', s'_0, i \ldots s'_{t-1}, i)\) located at each site of the interaction graph. Figure 3 shows the results we obtain by a two-layer wave function of mean-field states in the two-dimensional transverse Ising model.

Multilayer wave functions of symmetric tree states. –

The one-dimensional model. – We consider the symmetric states in the one-dimensional system as shown in fig. 1. We take the symmetric wave function \( \psi_0(\sigma; K^0) \propto e^{J_{0}(\sigma) + \sum K^0_{i,i+1} \sigma_i \sigma_{i+1}/2} \) and couple the local excitations by another symmetric state \( \psi_1(s_0; K^1) \propto e^{J_{1}(s_0) + \sum K^1_{i,i+1} (2s_{i-1} - 1)(2s_{i+1} - 1)/2} \), where we used \( s_0,i \) for the variable on edge \((i,i+1)\). For the phases we assume \( \Theta_0(\sigma) = \sum \lambda_i^0 \sigma_i / 2 \) and similarly for \( \Theta_1(s_0) \). The average local energies \( \langle e_i \rangle \), \( \langle e_{i,i+1} \rangle \) can still be computed exactly for such a wave function. Note that the quantum expectation of any local observable would depend on a local subset of the parameters, thanks to the factorization property of the symmetric tree states and orthogonality of the excited states. Given the local energy functions we use the above min-summation equations to find the optimal variational parameters. Figure 2 shows how such wave functions work by increasing the number of layers. The data in the figure have been obtained for \( \Lambda_t = 0, \pm \pi/2 \) and \( K^t_{ij} = 0 \); we did not observe significant improvement by changing these parameters, at least for the two-layer wave function. Here the relative error computed at the critical point reads \( \delta E_{\mathrm{MF}}(1) = 0.01825(t = 0), 0.00542(t = 1), 0.00540(t = 2) \) for the \((t+1)\)-layer wave functions. In the ordered phase for \( h = 0.9 \) we obtain \( \delta E_{\mathrm{MF}}(0.9) = 0.0314(t = 0), 0.0111(t = 1), 0.0024(t = 2) \), to be compared with the mean-field one \( \delta E_{\mathrm{MF}}(0.9) = 0.0021(t = 1) \). However, in the disordered phase \( \delta E_{\mathrm{MF}}(1.1) = 0.00261(t = 1) \), which is much smaller than the error obtained by the mean-field wave functions for \( t = 2 \).

Higher dimensions. – Using the tree wave functions in higher dimensions is not so straightforward. Here we briefly describe a possible way of utilizing the tree states in two dimensions and leave more investigations for future studies; see also [30]. Let us partition the system into pairs of spins represented by orthonormal states \( |s^x_s^y \rangle = \sum s^x_s^y \alpha \sigma_i^x \sigma_j^y |s_i^x s_j^y \rangle \) with binary variables \( s^x_s^y \in \{-1, +1\} \). Clearly, the mapping can be represented by any unitary transformation of the states \( |\sigma_i^x \sigma_j^y \rangle \). The transformation from the physical variables \( (\sigma_i^x, \sigma_j^y) \) to the auxiliary variables \( (s^x_s^y) \) serves to reduce the entanglement between the two sets of \( x \) and \( y \) variables [7,8]. Then we proceed by coupling the auxiliary variables in the two sets by a symmetric state:

\[
|\Psi\rangle = \sum_{s^x, s^y} e^{i\Theta(s^x, s^y)} \prod_{(\alpha, \beta) \in T} \left( e^{K_{\alpha, \beta}^x s^x_\alpha s^x_\beta / 2} / \cosh(K_{\alpha, \beta}^x) \right) \prod_{(\alpha, \beta) \in T} \left( e^{K_{\alpha, \beta}^y s^y_\alpha s^y_\beta / 2} / \cosh(K_{\alpha, \beta}^y) \right) |s^x s^y\rangle. \tag{10}
\]

And the phase can be represented by \( \Theta(s^x, s^y) \).

Conclusion. – We proposed an ansatz of multilayer wave functions based on the recursive coupling of the local excitations in the mean-field and the symmetric tree states. This allows us to compute exactly (for small number of layers) the quantum expectation of local observables, and employ an efficient message-passing algorithm to minimize the Hamiltonian expectation over the space of the variational parameters. Here we worked with the mean-field and the symmetric tree states, but the method can in principle be implemented with more complicated states after a proper characterization of the local excitations. It is the nature of these states and the local excitations that determines the minimal number of layers.
we need to approximate reasonably the ground state of the system; and that is important because the computational complexity grows exponentially with the number of layers. The problem is more difficult in the fermionic systems due to the global nature of the fermion sign, and it would be interesting to extend the method to deal with the non-local string interactions [31].

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