Approximating the ground state of fermion systems by multiple determinant states: Matching pursuit approach

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We present a simple and stable numerical method to approximate the ground state of a quantum many-body system by multiple determinant states. This method searches these determinant states one by one according to the matching pursuit algorithm. The first determinant state is identical to that of the Hartree-Fock theory. Calculations for a two-dimensional Hubbard model serve as a demonstration.

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Searching a single determinant state to approximate a quantum ground state, namely, the Hartree-Fock (HF) algorithm, plays an important role in the understanding of nuclear, atomic, and molecular structures. It is a long standing effort to extend the HF theory into a truly first principle method by searching multiple determinant states to span a quantum state, for recent examples, see Refs. [1–5], and references therein. The attracting feature is that this approach is very stable and free from the sign problem. It in principle can apply to a wide variety of systems. However, first principle calculation in terms of multiple determinant states is still a challenge. In fact, including multiple determinant states in the variational treatment, which is the common approach, often results in very complicated formulations. The computation cost is usually impractically demanding. Some realistic implementations impose restrictions on the determinant states. For example, the multiconfiguration Hartree-Fock theory [1], a time-dependent extension to the HF theory, requires single particle states to be orthogonal with each others. Here, we use an approach to approximate the quantum ground state via multiple determinant states.

Here, based on the matching pursuit (MP) algorithm [6–9], we show a numerical method to search determinant states to span the ground state of a fermion system. The determinant states are found one by one from all possible determinant states. Searching the first determinant state is identical to the Hartree-Fock theory. A significant feature of the current method is that several tens of basis determinant states are enough for reasonable result, and one can reach high accuracy by searching one or two thousands basis states. These numbers of basis states are several orders smaller than that of the stochastic diagonalization algorithm [5], which searches orthogonal determinant basis states stochastically to span a quantum wave function. In comparison with other algorithms of search determinant states to span a fermion ground state, such as the path-integral renormalization group (PIRG) algorithm [3,4], the current MP based method is quite simple and efficient.

The MP algorithm is originally designed for signal processing [6]. It is now popular on the engineering community for coding, analysis, and compression of video and audio data [7–9]. This algorithm searches some basis states from an overcomplete basis set to represent a sequence of data. The basis states are found one by one. The convergence of the MP algorithm is proved mathematically. For sufficient redundancy of the overcomplete basis set, the convergence can be exponential [9]. The MP algorithm is insensible to the dimension of the data, and thus promises applications in quantum many-body systems. In Ref. [10], the authors employ this algorithm to propagate quantum wave functions via split operator method in the Gaussian wave packet basis. An encouraging result is that several tens of Gaussian wave packets are able to accurately represent quantum wave function of a 20-dimensional model.

The goal of MP algorithm is to obtain a sparse representation of a signal. To represent a quantum many-body wave function ψ, the MP algorithm searches an overcomplete basis set and finds some basis states $\phi_1, \phi_2, \ldots, \phi_n$, such that the combination of the basis states $\psi_n = \alpha_1 \phi_1 + \cdots + \alpha_n \phi_n$ can best approach the state ψ. Mathematically, that is to require ψ_n has minimum distance with ψ, i.e., $|\psi - \psi_n|$ reaches minimum. The basis states are found one by one. At the kth step, the basis state ϕ_k is obtained such that the combination of the basis states $\psi_k = \alpha_1 \phi_1 + \cdots + \alpha_k \phi_k$ has minimum distance with the state ψ, i.e., $|\psi - \psi_k|$ has minimum for all possible choice of ϕ_k. Each more step brings the ψ_k closer to the target state ψ, i.e., the distance $|\psi - \psi_k|$ decreases with k.

The eigenvalue problem is equivalent to finding minimum values of the Rayleigh quotient

$$E = \langle \psi | H | \psi \rangle / \langle \psi | \psi \rangle, \tag{1}$$

where H is the Hamiltonian and ψ is the trial wave function. Calculation of the ground state by the MP algorithm is to search some basis states to span the ground state. The basis states are found one by one from an overcomplete basis set. Each searching process obtains one basis state such that the combination of this basis state and those already found minimizes the Rayleigh quotient for all possible choices of the current basis state. This process of finding a new basis state continues until convergence of E. Without loss of generality, in the following discussions, we focus on fermion systems, and use all possible Slater determinant states as an overcomplete basis set.

Note that, for fermion systems, the first step is to find a Slater determinant state that minimizes the Rayleigh

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quotient. This is just the well known Hartree-Fock approximation. We employ an iterative method to search a new determinant state, including the first one. We denote the single particle basis states as $|i\rangle$ ($i=1,\ldots,n$) and a_i^+ (a_i) the operator for creation (annihilation) of the state $|i\rangle$, i.e., $|i\rangle = a_i^+|0\rangle$ with $|0\rangle$ the vacuum state. A determinant state can be expressed as

$$|\phi\rangle = \prod_{j=1}^{m} F_j^+|0\rangle, \quad (2)$$

where m is particle number and F_j^+ (F_j) is creation (annihilation) operator for single particle state $F_j^+ = c_{1j}a_1^+ + \cdots + c_{nj}a_n^+$. Searching for the determinant state $|\phi\rangle$ is equivalent to finding the coefficients $\{c_{ij}\}$ (or the operators $\{F_j^+\}$).

We use an iterative relaxation procedure to search the operators $\{F_j^+\}$. From an initial trial state in the form of Eq. (2) which can be chosen randomly, we optimize F_1^+, $F_2^+,\ldots,F_m^+$ consecutively. Each step of the optimization lowers the Rayleigh quotient. This iteration continues until the convergence of the Rayleigh quotient. Note that the determinant state (2) is a multilinear function of the coefficients $\{c_{ij}\}$. For a fixed j, $|\phi\rangle$ is just a linear function of $c_{1j},\ldots,c_{nj}$:

$$|\phi\rangle = \sum_i c_{ij}|\phi_{ij}\rangle, \quad (3)$$

where $|\phi_{ij}\rangle = \partial|\phi\rangle/\partial c_{ij}$. Thus an approximate ground state $\Psi_k = \sum_i \alpha_i \phi^{(i)} + \alpha\phi$ can be written as

$$\Psi_k = \sum_i \alpha_i \phi^{(i)} + \sum_i \alpha c_{ij}\phi_{ij}. \quad (4)$$

This means that we can improve Ψ_k and hence update the operator F_j^+ by finding the lowest eigenstate of the Hamiltonian in the subspace spanned by $\{|\phi_{ij}\rangle, i=1,\ldots,n\}$ and those previously found determinant states $|\phi^{(i)}\rangle$.

Such a relaxation procedure to update the operators F_j^+ is the key ingredient of this contribution. Supposing that we have already obtained $k-1$ determinant states $|\phi^{(i)}\rangle$, the searching process for kth determinant state $|\phi^{(k)}\rangle = |\phi\rangle$ in the form (2) involves the following iteration.

(1) Randomly generate a determinant state $|\phi\rangle$.

(2) For $j=1,2,\ldots,m$, do the following iteration loop to update $|\phi\rangle$:

(2a) calculate the matrix elements of the Hamiltonian in the subspace $\Xi_j^{(k)}$ spanned by $\{|\phi^{(1)}\rangle,\ldots,|\phi^{(k-1)}\rangle, |\phi_{1j}\rangle,\ldots,|\phi_{nj}\rangle\}$,

(2b) find the ground state Ψ_k^j of the Hamiltonian in the above subspace $\Xi_j^{(k)}$, $\Psi_k^j = \sum_i \alpha_i \phi^{(i)} + \sum_i \beta_{ij}^k \phi_{ij}$, and

(2c) update F_j^+ by setting $c_{ij} = \beta_{ij}^k$ ($i=1,\cdots,n$); then make $F_j^+|0\rangle$ orthogonal to other single particle states $\{F_l^+|0\rangle$, $l \neq j\}$, and restore $F_j^+|0\rangle$ to unit length by a normalization procedure.

(3) Check the convergence of the Rayleigh quotient. Repeat step (2) until reaching convergence.

In the case of $k=1$, the above searching process of finding the first determinant state is the same as the Hartree-Fock algorithm. A randomly generated initial trial state needs several tens of iteration rounds to converge. Each of the subsequent determinant states needs similar rounds of iteration. Here, the main numeric cost is step (2a) for the calculation of the matrix elements of the Hamiltonian between basis states. The step (2b) of finding the lowest eigenstate in the subspace can be implemented efficiently via an iteration algorithm [11,12] that needs only a small portion of the computation cost.

Starting from $k=2$, the number of iteration to obtain ϕ_k depends on the initial choice. If a trial state has large overlap with the state $(H-E_{k-1})|\Psi_{k-1}\rangle$, one may reach convergence by just a few rounds of iteration. Here, E_{k-1} and $\Psi_{k-1} = \sum_{i=1}^{k-1} \alpha_i \phi^{(i)}$ are the approximate ground-state energy and wave function obtained in the previous step. One can understand this property by considering minimization of the Rayleigh quotient in two-dimensional subspace spanned by Ψ_{k-1} and the trial state ϕ [5]. From this observation, we perform a preparing treatment of the trial state before step (2) of the above iteration procedure.

The preparing treatment of the initial trial state ϕ is to modify the state ϕ so that it has maximum overlap with the state $(H-E_{k-1})|\Psi_{k-1}\rangle$. This procedure is easy to carry out by exploiting the fact that state ϕ, or the overlap $\langle\phi|H-E_{k-1}|\Psi_{k-1}\rangle$, is a multilinear function of the coefficients c_{ij} (or the operators F_j^+). We maximize the overlap iteratively by updating the operators F_j^+, ($j=1,\ldots,m$), consecutively. Usually, three to five rounds of the iteration are enough. After such a preparing treatment, one usually needs about two to three iteration rounds of the searching process to minimize the Rayleigh quotient. Thus, such preparing treatment makes the overall procedure about five to ten times faster.

As an optional choice to achieve high accuracy, one can perform backward optimization after reaching convergence in the above procedure. This procedure updates the already found basis states one by one (one can also choose to update some selected basis states [7]). The operation to update a basis state is the same as searching for a new basis state. It is numerically expansive to perform the backward optimization. In fact, searching the basis states one by one is a kind of restriction on the determinant states, and the backward optimization means removing such constraints.

At first sight, the current method shares some features with the path-integral renormalization group (PIRG) algorithm [3,4]. However, based on different strategies, the PIRG and the current method are two different methods of searching basis determinant states. The PIRG filters out the ground state by repeatedly expanding $e^{-\tau H}|\psi\rangle$ into summation of determinant states and keeping some of the determinant states as new basis states to update the trial ground state $|\psi\rangle$. At each step, the PIRG must update whole basis states, while the current method only adds (or updates) one basis state via relaxation method and exploiting the multilinearity of the determinant states. Updating basis states in PIRG, i.e., choosing some determinant states from those that span the state $e^{-\tau H}|\psi\rangle$, involves diagonalization of many sizable matrices. The diagonalization in subspace is a major numeric cost of PIRG, while it takes only a small portion of numeric

TABLE I. Ground-state energies of some the 4×4 systems.

System	U/t	CPMC	SD	MP	N	Exact
10/16	4	−19.5808	−19.58	−19.5775	1874	−19.5808
14/16	4	−15.7296	−15.49	−15.7107	1865	−15.7446
16/16	4		−13.59	−13.5963	1622	−13.6219
10/16	8	−17.4800	−17.40	−17.4625	2000	−17.5104
14/16	8	−11.648		−11.6763	2000	−11.8688
16/16	8			−8.41565	1850	−8.46889
14/16	12	−9.696		−9.79500	2000	−10.0515
16/16	12			−5.95238	1950	−5.99222

TABLE II. Correlation functions of some the 4×4 systems.

Method	System	U/t	$\rho(2,1)$	$S_m(\pi,\pi)$	$S_d(\pi,\pi)$
CPMC	10/16	4	−0.0556	0.731	0.504
MP(800)	10/16	4	−0.0559	0.7315	0.5089
Exact	10/16	4	−0.0556	0.73	0.506
QL	16/16	4	−0.0363	3.42	0.3946
MP(437)	16/16	4	−0.0478	3.490	0.3888
Exact	16/16	4	−0.0475	3.64	0.385
CPMC	10/16	8	−0.0462	0.761	0.4403
MP(800)	10/16	8	−0.0493	0.7645	0.4412
Exact	10/16	8	−0.0485	0.75	0.443

operations in the current method. The current method only calculates matrix elements of the Hamiltonian between determinant states; this is much easier and more efficient than expanding $e^{-\tau H}|\psi\rangle$ (or $H|\psi\rangle$) into summation of determinant states.

We test the above method via the two dimensional fermionic Hubbard mode on a $N=L\times L$ square lattice with periodic condition. The Hamiltonian reads

$$H = -t\sum_{\langle ij\rangle} (c_{i\sigma}^+ c_{j\sigma} + c_{j\sigma}^+ c_{i\sigma}) + U\sum_i n_{i\uparrow} n_{i\downarrow}. \qquad (5)$$

Here $c_{j\sigma}^+$ ($c_{j\sigma}$) is the creation (annihilation) operator of an electron with spin σ at the jth site and $n_{j\sigma}=c_{j\sigma}^+ c_{j\sigma}$. U is the on-site Coulomb energy. The summation $\langle ij\rangle$ runs over nearest-neighbor sites.

Table I shows ground-state energies (in the unit of t) of some 4×4 systems. The column "system" indicates the number of electrons versus the lattice number. N is number of basis determinant states to span the ground state of the current method (MP). We list the results of the constrained path quantum Monte Carlo (CPMC) [13], stochastic diagonalization (SD) [5], and exact diagonalization [14–17] for comparison. The accuracy of our method is almost unchanged for various interaction strength U and filling number. This demonstrates the stability of the method. All initial trial states for searching basis determinant states are randomly generated without any symmetry consideration. We use the convergence rate $\epsilon=2|E_n-E_{n-1}|/|E_n+E_{n-1}|$ to determine the number of basis states, where E_n and E_{n-1} are ground-state energies obtained with n and $n-1$ basis states, respectively. The searching for basis states stops if ϵ is smaller than a criteria ϵ_0, or maximum acceptable number of basis states is reached. Usually, $\epsilon_0=10^{-5}$ is enough to obtain quite reasonable result. At this setting, one usually needs several hundreds of basis states which increases slowly with U. If $\epsilon_0=10^{-6}$, one needs several thousands of basis states for convergence. Roughly speaking, the result from about 100 basis states is quite good. The interesting point is that the beginning several tens of determinant states, usually less than 60 basis states, make dominant contributions. The first one, i.e., the HF approximation, contributes the most. The number of dominant basis states increases slowly with the interaction strength U. After the dominant basis states, the contribution from each of the following ones drops rapidly.

Table II shows ground state's correlation functions of some 4×4 systems. The comparing results of CPMC, quantum Langevin (QL), and exact diagonalization are from Refs. [13], [17], and [14,17], respectively. Here S_m and S_d are magnetic and density structure factors [13], respectively; and $\rho(\mathbf{r})$ is the one body density matrix. The number in the column "method" is the number of basis states of our method (MP). The current method obtains the ground-state energy and wave function at the same time. Then calculation of the correlation functions and other related quantities is a trivial task that simply reads the wave function. In comparison with the exact result, we see that the wave functions are almost in the same accuracy as the correspondent energies. Again, the beginning several tens of basis states make major contributions. To demonstrate this property, as indicated in the parentheses, we use only several hundred basis states to calculate the correlation functions in Table II. Since our program does not perform any symmetry treatment, we can only compare nondegenerated ground states with the exact result. In fact, the present method can take symmetries into account. After the searching process of finding basis determinant states, the resultant wave function is usually a combination of ground states with different symmetries. One may employ, e.g., the project technique [18] to filter out the target symmetry. This may further improve the accuracy.

Table III shows ground-state energies for large system size that exact diagonalization is impossible. Here N is the number of basis states of the current method (MP). Our re-

TABLE III. Ground-state energies (in the unit of t) of some large systems with $U=4t$.

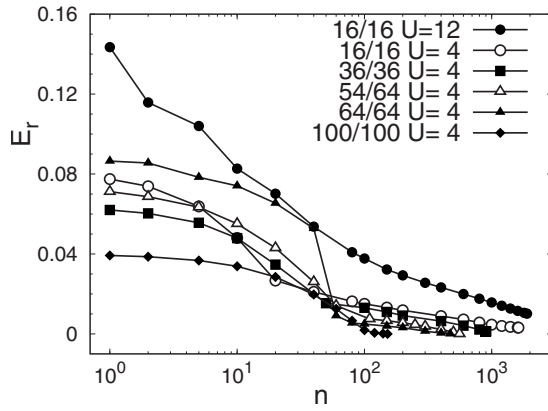| system	QMC	VMC	SD	MP	N
26/6×6	−42.32		−40.77	−41.0757	400
34/6×6	−33.30	−32.76		−32.7323	940
36/6×6	−30.96	−30.384		−30.5166	905
50/8×8	−72.80		−67.00	−68.5029	630
54/8×8	−67.55			−63.8981	560
62/8×8	−57.70			−55.5255	490
64/8×8	−55.23			−53.583	472
100/10×10	−86.70			−82.9549	152

FIG. 1. Relative error E_r versus number of basis states n for various filling numbers and system sizes.

sult is quite close to that of the SD [5], and the variational quantum Monte-Carlo (VMC) [4]. It is worth noting that the number of basis states of our method is several orders smaller than that of the SD algorithm. As a consequence, our method needs much less memory, and there is no need for external storage. There are several percent of discrepancy with the quantum Monte Carlo (QMC) result [19]; this disagreement increases with the system size. This needs further investigations. The discrepancy between QMC result and the strict variational result is also found by other authors, see, e.g., Refs. [3,4,18]. For practical applications, the extrapolation method introduced in PIRG's implementation is an useful tool to handle the discrepancy with QMC results [3,18]. Similar to the 4×4 cases, the beginning several tens of basis states make dominant contribution. For a fixed interaction strength U, the contribution from the dominant basis states increases with the system size. This means that one needs less basis states for larger system size. On the other hand, the computation cost to search a basis state scales about quadratically with the system size. The role of preparing step for searching a basis state is more significant for larger system size. Without this preparing step, after several tens of dominant basis states, the overlap between a randomly generated trial state ϕ and the state $(H-E_{k-1})|\Psi_{k-1}\rangle$ almost vanishes. One must substantially increase accuracy requirement for following steps, which in turn increases numeric cost. The computation cost scales about quadratically with the number of basis states.

Figure 1 shows the relative error $E_r=|(E_n-E_0)/E_0|$ versus the number of basis states n, where E_n is the ground-state energy obtained with n basis states, and E_0 is the converged ground-state energy (or exact ground-state energy if available). This illustrates the overall properties of the method. The first basis state makes the most important contribution. It accounts for about 80 to 95 % of the ground-state energy depending on system size and correlation strength. Roughly speaking, the mean field effect increases with the system

size, and decreases with the correlation between electrons of the system. For system size $N_0=4 \times 4$ with $U=12t$, the contribution of the first basis state is about 80%. As the system size reaching $N_0=10 \times 10$ with $U=4t$, the contribution of the first basis state is more than 90%. As a consequence, for a same accuracy requirement, the number of necessary basis states decreases with system size. The convergence rate is fast for the beginning several tens of dominant basis states. These basis states contribute more than 95% to the ground state for moderate correlation. Then contribution from each of the following basis states drops rapidly. However, the major computation cost for Fig. 1 is to search the remaining basis states. In practical calculations, one usually needs several tens of basis states for a reasonable accuracy.

We perform backward optimization for some cases to improve the accuracy. There is very limited improvement from the backward optimization if the MP method is converged. The improvement is usually less than 0.5%. If backward optimization is performed before the convergence of MP process, the improvement can be more than 1.5% for some cases.

Our calculation is performed on a single PC [AMD Opteron(TM) Processor 248]. Parallel implementation is easy for the current method. Since the major numeric cost is the computation of the matrix elements of the Hamiltonian during the search of the basis states, parallel implementation can be easily realized by requiring each node to handle some matrix elements of the Hamiltonian.

There are many possible ways to improve the current method. For example, it is worth exploring other types of basis states. In the present form, our method is an extension to the mean-field HF approximation. Mathematically, the redundancy of the overcomplete basis states is crucial for the convergence speed of the MP algorithm [9]. By increasing the redundancy of the overcomplete basis states, i.e., enlarging the searching space, it is possible to speed up the convergence of MP method for searching the basis states. On the other hand, for particles moving in 3D space, storage of a single particle state needs sizable memory, one may choose the basis states for single particles as product of one-dimensional wave functions. In principle, this method is able to compute the exited states. With some modifications, it may be feasible to calculate the low-lying exited states.

In summary, the current method is stable and free from the sign problem. It can apply to any system that can apply Hartree-Fock algorithm, and can be regarded as an extension to the Hartree-Fock algorithm. Several tens of determinant states are usually enough for meaningful result. This method may offer an alternative to explore quantum effects of many-body systems.

[1] M. Nest, R. Padmanaban, and P. Saalfrank, J. Chem. Phys. **126**, 214106 (2007); M. Nest, T. Klamroth, and P. Saalfrank, *ibid.* **122**, 124102 (2005); M. H. Beck and H.-D. Meyer, *ibid.* **114**, 2036 (2001).

[2] G. Beylkin, M. J. Mohlenkamp, and F. Prez, e-print arXiv:0708.2896v1[math-ph].

[3] M. Imada and T. Kashima, J. Phys. Soc. Jpn. **69**, 2723 (2000); T. Kashima and M. Imada, *ibid.* **70**, 2287 (2001).

[4] T. Yanagisawa, Phys. Rev. B **75**, 224503 (2007).

[5] H. De Raedt and M. Frick, Phys. Rep. **231**, 107 (1993).

[6] S. Mallat and Z. Zhang, IEEE Trans. Signal Process. **41**, 3397 (1993).

[7] L. Rebollo-Neira and D. Lowe, IEEE Signal Process. Lett. **9**, 137 (2002); M. Andrle, L. Rebollo-Neira, and E. Sagianos, *ibid.* **11**, 705 (2004).

[8] P. Huggins and W. Zucker, IEEE Trans. Signal Process. **55**, 3760 (2007).

[9] R. Gribonval and P. Vandergheynst, IEEE Trans. Signal Process. **52**, 255 (2006).

[10] Y. Wu and V. S. Batista, J. Chem. Phys. **118**, 6720 (2003); **121**, 1676 (2004).

[11] F. Andreozzi, A. Porrino, and N. L. Iudice, J. Phys. A **35**, L61 (2002).

[12] Q. Jie and D. Liu, Phys. Rev. E **68**, 056706 (2003).

[13] S. Zhang, J. Carlson, and J. E. Gubernatis, Phys. Rev. Lett. **74**, 3652 (1995); Phys. Rev. B **55**, 7464 (1997).

[14] A. Parola, S. Sorella, M. Parrinello, and E. Tosatti, Phys. Rev. B **43**, 6190 (1991).

[15] H. Q. Lin, Phys. Rev. B **44**, 7151 (1991).

[16] G. Fano, F. Ortolani, and A. Parola, Phys. Rev. B **42**, 6877 (1990).

[17] A. Parola, S. Sorella, R. Car, M. Parrinello, and E. Tosatti, Physica C **162–164**, 771 (1989).

[18] T. Mizusaki and M. Imada, Phys. Rev. B **69**, 125110 (2004).

[19] N. Furukawa and M. Imada, J. Phys. Soc. Jpn. **61**, 3331 (1992).