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Monte Carlo diagonalization of many-body problems: Application to fermion systems

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Existing quantum Monte Carlo algorithms suffer from the so-called minus-sign problem. We propose a stochastic algorithm to compute ground-state properties of quantum lattice models that is free of minus-sign problems. Illustrative results for the two-dimensional Hubbard model are presented.

Numerical techniques to investigate models of interacting fermions employ either standard diagonalization algorithms or combine the Trotter-Suzuki (path-integral) product formula and the Metropolis Monte Carlo or a molecular-dynamics technique to study the system. The former approach yields numerically exact results for the ground state. It requires storage for at least two wave functions. These wave functions are represented as linear combinations of basis states, the number of which grows very fast with the system size. This characteristic feature limits the applicability of the diagonalization approach to small systems. In the latter approach, the quantum statistical problem involving very large ($>10^6\times10^6$, say) matrices is replaced by a multidimensional integral (or sum).[1,2] In principle, estimators of physical quantities can be obtained by the standard importance-sampling techniques used to study classical statistical-mechanical systems.[3] Unfortunately, when applied to quantum problems, the usefulness of these simulation techniques is reduced considerably. The most fundamental problem is that the integrand may become negative.[1,2] Conventional importance-sampling techniques require the integrand to be positive (see below). Moreover, the appearance of nonpositive distributions is a generic feature of the formalism and is not limited to fermion systems.[2] This fundamental problem is usually referred to as the minus-sign problem.[1,2,4]

Below we propose a different method for computing the ground state of (fermion) lattice models. Our method is numerically exact in the sense that it can be proven to yield the exact ground state, in principle. It collects states by means of importance sampling, is numerically stable, and is free of minus-sign problems. In addition, our method is sufficiently general to apply to a large class of quantum lattice problems.

Our scheme is based on the following considerations. If the exact ground state of a quantum system is a superposition of many (say, $>10^8$) basis states, the model may be considered as being numerically unsolvable if all these basis states are needed to obtain a good approximation to the ground state. As in previous work in this field, we adopt the basic assumption that an accurate representation of the ground state can be constructed by carefully selecting a limited set of basis states which are "important."[5] In quantum Monte Carlo (QMC) work one typically samples of the order of 10^5 states, most of which are not linearly independent.

Conventional importance-sampling techniques such as finite-temperature QMC,[1,2,4] projector QMC (PQMC),[2,4] and Green's-function Monte Carlo methods[6] use Markov matrices to generate a random walk in the (Hilbert) space of states.[7] The elements of the Markov matrix contain the ratio of the values of the integrand, appearing in the multidimensional integral, for two different states (or configurations).[7] In classical statistical mechanics this ratio is always positive. In this case the Perrón-Frobenius theorem[8] assets that the Markov process asymptotically generates states according to the probability distribution specified by the integrand. Then the importance-sampling method will work, at least in principle. For quantum systems in general, and for fermion models in particular, this ratio can take negative values.[1,2,4] This leads to the minus-sign problem, which renders simulations at low temperatures and/or for large systems extremely difficult.[1,9]

Instead of Markov matrices we propose to employ unitary (orthogonal in practice) matrices to perform the walk in Hilbert space and it is at this point that our approach is conceptually completely different from others. In the case of Markov-matrix-based methods there is no unique prescription to relate the "weight" function (the integrand) to a transition probability, i.e., a non-negative

matrix element, for going from one state to another.[10] This freedom is present in our case as well and we exploit it to devise an algorithm which can be used in practice.

Several criteria help eliminate candidates for unitary matrices which may perform the task of generating the ground state of the model Hamiltonian. Clearly any method which requires memory proportional to the dimension of the Hilbert space should be rejected because in that case the system sizes accessible would be too small and there already exist very efficient methods anyhow.[11] This in turn implies that the unitary matrices should have a simple representation, the simplest one being a sequence of two-by-two, plane rotation, matrices.[11] In practice this will allow us to calculate the effect of successive applications of unitary transformations in a very efficient manner. Finally we have to specify the plane rotation matrices.

To this end we need the following theorem: Let Ψ denote the eigenvector (ground state) of the Hamiltonian H corresponding to the lowest eigenvalue (ground-state energy) and let $\{\psi_i\}$, $i=1,\ldots,n$ be a complete set of states, with $\langle\psi_1|\Psi\rangle\neq 0$ and ordered such that

$$\langle\psi_1|H|\psi_1\rangle\leq\langle\psi_2|H|\psi_2\rangle\leq\cdots\leq\langle\psi_n|H|\psi_n\rangle . \quad (1)$$

For most systems of physical interest it is almost trivial to satisfy these two conditions. Assume there exists an index $j>1$ such that $\langle\psi_1|H|\psi_j\rangle\neq 0$. Application of the plane rotation R chosen such that $\langle\psi_1|R^{-1}HR|\psi_j\rangle=0$, yields

$$\langle\psi_1|R^{-1}HR|\psi_1\rangle<\langle\psi_1|H|\psi_1\rangle . \quad (2)$$

This process can be repeated, replacing H by the "rotated" Hamiltonian and taking different j's until all but the first element of the first row (or column) are zero. Then, under fairly general conditions, the first element of the first row converges to the ground-state energy and the ground state can be obtained from the product of plane-rotation matrices R_a:

$$|\Psi\rangle=\sum_{l=1}^{N}\left(\prod_{a=1}^{M}R_a\right)_{l,1}|\psi_l\rangle , \quad (3)$$

where M denotes the number of rotations carried out and $N\leq M$ is the number of basis states used.

From a theoretical viewpoint our method is an alternative procedure to separate the ground state from the rest of the spectrum, just as, for instance, the (inverse) power method or the Lanczos scheme.[11] Our scheme may be viewed as a variant of the Jacobi method for diagonalizing a real symmetric matrix.[11] The main difference is that we concentrate on the smallest eigenvalue (we could also concentrate on the largest eigenvalue, but from a physical point of view that is less interesting). This has important practical implications since our method, like the Lanczos method, allows one to handle very large matrices without having to store them.

The algorithm works as follows. First we choose a set of basis states $\{\psi_i\}$ for which the matrix elements of the Hamiltonian can be calculated efficiently and we order the states according to condition (1). At each iteration step we determine which element of the first row will yield the largest reduction of the first element of that row. We then apply to the matrix the plane rotation that reduces this nondiagonal matrix element to zero and repeat this procedure until the changes of the (1,1) matrix element drop below an acceptable level. The ground-state energy is then given by the first element of the first row. A straightforward generalization of this idea allows us to separate any (small) number of low-lying states. Instead of working on one row, we block diagonalize the matrix using the scheme outlined above and at the same time diagonalize the submatrix containing the low-lying states.

We have tested our algorithm on relatively small matrices ($<1000\times 1000$), comparing the outcome with results obtained by standard diagonalization routines. Once the correctness of the algorithm has been established the next step is to implement it as an importance-sampling scheme. This is done by enlarging the set of "important" states gradually during the iterating towards the ground state. A Monte Carlo process generates candidate basis states. To decide whether a basis state is important or not we calculate the effect on the (1,1) element of a plane rotation involving this state. If the reduction of the (1,1) element of the transformed Hamiltonian, i.e., the approximate ground-state energy, is sufficiently large the basis state is added to the current set of states. Note that by construction all of these states are linearly independent and our scheme is variational in the sense that it generates a strictly decreasing sequence of upperbounds to the exact ground state. In practice this scheme requires storage for the diagonal matrix elements, the first row of the transformed matrix, and the angles of the plane rotations. It scales linearly with the number of important basis states.

We have applied our method to the two-dimensional single-band Hubbard model, the reference system for testing methods for simulating fermions.[2,4] It describes some of the essential features of strongly correlated electrons systems and has attracted considerable attention in connection with the high-temperature superconductors.[12] The model is defined by the Hamiltonian

$$H=t\sum_{\langle i,j\rangle,\sigma}(c_{i,\sigma}^{\dagger}c_{j,\sigma}+c_{j,\sigma}^{\dagger}c_{i,\sigma})+U\sum_{i}n_{i\downarrow}n_{i\uparrow} , \quad (4)$$

where $c_{i,\sigma}^{\dagger}$ ($c_{i,\sigma}$) creates (annihilates) a fermion of spin $\sigma=\uparrow,\downarrow$ at site i, t is the hopping matrix element, U represents the on-site Coulomb interaction strength, and the sum over i and j is restricted to nearest neighbors. The linear size in the x (y) direction will be denoted by L_x (L_y). As usual, we adopt periodic boundary conditions. In practice we have chosen to work in the wave number instead of the real-space representation of model (1) to illustrate that our method does not rely on a particular choice of the representation. Depending on the model parameters it may, of course, be expedient to work in the most appropriate representation, in order to minimize the computational effort. Another appealing feature of our approach is that models, such as the t-J model, can be handled in exactly the same manner as (4).

In the repulsive case $U>0$ and for a non-half-filled band all known simulation methods suffer from severe minus-sign problems,[2,4] especially at low temperature. In particular for band-fillings (excluding the half-filled band case) corresponding to open-shell situations, it can be extremely difficult to obtain reliable results for the ground-

TABLE I. Comparison between ground-state energies as obtained from the Monte Carlo diagonalization (MCD) method proposed in this paper, from exact numerical diagonalization (Exact), and from projector quantum Monte Carlo (PQMC) simulation.

(L_x,L_y)	U	$(n_\uparrow,n_\downarrow)$	Exact	PQMC	MCD
3×3	4	(3,4)	−7.915		−7.915
3×3	20	(3,4)	−6.122		−6.120
3×3	4	(4,5)	−6.210		−6.203
3×3	8	(4,5)	−3.545		−3.545
4×4	4	(2,2)	−11.53		−11.53
4×4	4	(3,3)	−15.14		−15.14
4×4	4	(4,4)		−17.3	−17.53
4×4	4	(5,5)	−19.58[a]	−19.6	−19.57
4×4	4	(6,6)			−17.70
4×4	4	(7,7)	−15.74[a]	−15.7	−15.45
4×4	4	(8,8)	−13.62[a]	−13.6	−13.42
4×4	−4	(5,5)		−32.6	−32.64
4×4	−4	(8,8)		−45.4	−45.35
4×4	4	(1,13)	−7.063		−7.063
8×8	3	(5,5)		−34.5	−34.49
8×8	4	(5,5)		−34.3	−34.31
8×8	6	(5,5)		−34.1	−34.03
8×8	4	(9,9)		−54.6	−54.37
8×8	4	(13,13)			−66.05

[a]Reference 15.

state properties. For the attractive model $U<0$ the integrand is positive and accurate quantum Monte Carlo results can be obtained.

To illustrate the power of our method we have performed Monte Carlo diagonalizations for systems of various sizes, fillings, and interactions U ($t=1$ in our numerical work). A comparison of our results and those obtained from exact numerical diagonalization and projector quantum Monte Carlo simulation is given in Table I. In general, good agreement is found. The error on the MCD and PQMC results is of the same order of magnitude ($\approx 1\%$). The difference between the exact diagonalization and MCD data is less than 2.5%. The number of important basis states gathered by our method never exceeded 70000. This suggests that the crucial assumption, namely, that good results can be obtained with a (small) fraction of all basis states, may hold. To appreciate the importance-sampling aspect of our scheme it is of interest to consider the number of states involved. Disregarding reductions due to symmetry a 4×4 lattice with five spin-up and five spin-down electrons has more than 19×10^6 states. A 4×4 lattice with eight spin-up and eight spin-down electrons has more than 16×10^7 states. The former corresponds to the closed-shell situation, the latter to an open-shell case, the number of degenerate Fermi seas being 56. Apparently our method is able to select the most important states out of this large number. The data of Table I further suggest that to reach the same level of accuracy, open-shell systems require more basis states than closed-shell cases. To investigate the effect of the degeneracy in the noninteracting case we have also implemented a block-diagonalization variant of our algorithm. We found that our technique has no problems dealing with highly degenerate matrices, a feature which it seems to share with the Jacobi method.[11]

At the end of the calculation, the many-body ground-state wave function can be reconstructed from the sequence of plane rotations.[11] Thus, any correlation function of interest can be computed. For model (4) we have computed the momentum distribution and the s-wave pairing correlation function. Our method reproduces PQMC results[13,14] for the on-site s-wave pairing correlation function, supporting the idea that the repulsive single-band Hubbard model exhibits no superconductivity in this channel. As our method directly yields the ground state, the argument that the temperature used in quantum Monte Carlo simulations work may be too high does not apply.

To summarize, we have presented a Monte Carlo scheme to determine ground-state properties of quantum systems. It uses a sequence of orthogonal transformation to perform a walk on the space of basis states, collects important basis states during the walk, and does not suffer from minus-sign problems. We have demonstrated that our algorithm can be used to study quantum systems which are not amenable to exact numerical diagonalization.

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