Proof for an upper bound in fixed-node Monte Carlo for lattice fermions

D.F.B. ten Haaf, H.J.M. van Bemmel, J.M.J. van Leeuwen, and W. van Saarloos
Instituut-Lorentz, Leiden University, P.O. Box 9506, 2300 RA Leiden, The Netherlands

D.M. Ceperley
National Center for Supercomputing Applications, University of Illinois at Urbana-Champaign, 405 North Mathews Avenue, Urbana, Illinois 61801

We justify a recently proposed prescription for performing Green function Monte Carlo calculations on systems of lattice fermions, by which one is able to avoid the sign problem. We generalize the prescription such that it can also be used for problems with hopping terms of different signs. We prove that the effective Hamiltonian, used in this method, leads to an upper bound for the ground-state energy of the real Hamiltonian, and we illustrate the effectiveness of the method on small systems.

I. MOTIVATION

As is well known, exact Monte Carlo methods cannot be applied straightforwardly to fermionic systems. In such systems, the sign problem causes great difficulties in obtaining sufficient statistical accuracy,[1] particularly as the number of quantum particles increases. The reason is that, when sampling physical properties in configuration space, one collects large positive and negative contributions, due to the fact that a fermion wave function is of different sign in different regions of the configuration space. These contributions tend to cancel, giving a result that may be exponentially smaller than the positive and negative contributions separately.

Recently, some of us described a method to perform Green function Monte Carlo (GFMC) on a system of fermions on a lattice,[2] which is an extension of the fixed-node Monte Carlo method for continuum problems, developed by Ceperley and Alder.[3] In this method one avoids the sign problem, replacing the original Hamiltonian by an effective Hamiltonian, such that one obtains contributions of one sign only in the sampling procedure. The price one has to pay is in the fact that the ground-state energy E_{eff} of the effective Hamiltonian is, in general, not the same as the ground-state energy E_0 of the original Hamiltonian. It was claimed, however, that E_{eff} is a true upper bound for E_0, making the method variational.

The proof for this upper bound is less obvious than was suggested in Ref. 2, because an assumption was used about the form of the ground state of the effective Hamiltonian, which is not generally true [see the discussion following Eq. (17)]. It is possible, however, to give a general proof for the upper bound. In the process of deriving this proof, we found that our prescription can be generalized, such that also problems with a Hamiltonian containing hopping terms of different signs can be treated by this method. The aim of this paper is to give a general proof, illustrate the method on small systems, for which we diagonalize both the original and the effective Hamiltonians

exactly, and discuss the applicability of the method. We do not actually perform Monte Carlo simulations here.

II. EFFECTIVE HAMILTONIAN

We work in a configuration space $\{R\}$, where each R denotes a configuration of numbered fermions on a lattice. In this configuration space, the Hamiltonian $\mathcal{H}$ of our problem can be represented by a real symmetric matrix H with elements $\langle R|H|R'\rangle$. One is generally interested in finding the ground-state energy of this Hamiltonian subject to some symmetry constraints, for example, that the wave function be antisymmetric. We suppose that the ground state $|\psi_0\rangle$ of $\mathcal{H}$ is reasonably well approximated by a trial state $|\psi_T\rangle$, which is defined through its wave function in all possible configurations: $\psi_T(R) = \langle R|\psi_T\rangle$. We restrict ourselves to real trial wave functions, because the ground-state wave function can be taken real in this problem, and the sign of the trial wave function is one of the key ingredients for our method. Complex Hamiltonians and trial functions can be treated with the so-called *fixed-phase* method.[4] Typical examples of the Hamiltonians considered here are the Hubbard Hamiltonian or the Kondo lattice model, and the typical trial wave function is a determinant obtained by a mean-field approximation.

In general, a trial wave function divides the configuration space into *nodal regions*. A nodal region is a set of configurations in which the trial wave function has the same sign, and which are connected via the Hamiltonian. For an antisymmetric wave function, there is equivalence between the regions of positive and the regions of negative sign.

In GFMC with *importance sampling*, random walkers diffuse and branch through the configuration space in a stochastic way, guided by a trial wave function. The Hamiltonian is used to project out the lowest energy state. The process for a lattice model and its mathemati-

cal justification is described in more detail in Appendix A and Ref. 5. In the fixed-node approach, one ensures that the contribution of a specific walker is always positive, otherwise the negative signs will eventually interfere destructively. For completeness, and to indicate the connection with the sign problem in quantum Monte Carlo simulations, we expand on this point in Appendix A. If the off-diagonal terms in the Hamiltonian are all negative (as in the Hubbard model), a sign change only occurs when a walker goes from one nodal region to the other. More generally, a walker could collect an unwanted minus sign if there exists a pair of configurations R and R' such that

$$\langle R|H|R'\rangle\psi_T(R)\psi_T(R') > 0. \tag{1}$$

In order to prevent this from happening, we make an effective Hamiltonian which does not have such matrix elements.

The fixed-node method was developed for the case in which the electron coordinates are continuous variables.[6,3] There, one has to deal with kinetic terms of negative sign only, and the nodal surface of a trial wave function is uniquely defined as the set of configurations where it vanishes. The fixed-node constraint can be implemented by imposing the boundary condition that ψ must vanish on the nodal surface of ψ_T. In the limit of sufficiently small step sizes, we can make sure that Eq. (1) is never violated since R and R' become closer together and ψ_T will vanish. In this way, one obtains the lowest energy under the condition that the wave function has the same nodal structure as the trial wave function. This energy yields an upper bound to the true ground-state energy; in practice, very accurate estimates for the ground-state energy of continuum problems can be obtained.

On a lattice, one has to deal with discrete steps, and one has to treat the hops that cause a change of sign in a different way. In our implementation, we replace those unwanted hopping terms in the Hamiltonian by diagonal terms, that depend on the ratio of the trial wave function in the configurations R and R'. We thus construct an effective Hamiltonian $\mathcal{H}_{\text{eff}}$ as follows:

$$\langle R|H_{\text{eff}}|R'\rangle = \langle R|H|R'\rangle \quad \text{(if } \langle R|H|R'\rangle\psi_T(R)\psi_T(R') < 0)$$
$$= 0 \qquad \text{(otherwise)} \tag{2}$$

are the off-diagonal terms, and the diagonal terms are given by

$$\langle R|H_{\text{eff}}R\rangle = \langle R|H|R\rangle + \langle R|V_{\text{sf}}|R\rangle. \tag{3}$$

The last term in (3) is the *sign-flip potential* at R, which corrects for the contributions of the steps left out in H_{eff}. V_{sf} has only diagonal elements, which are defined by

$$\langle R|V_{\text{sf}}|R\rangle = \sum_{R'}^{\text{sf}} \langle R|H|R'\rangle \frac{\psi_T(R')}{\psi_T(R)}. \tag{4}$$

Here the summation is over all (neighboring) configurations R' of R for which (1) holds. Note that this is a sig-

nificant extension of the prescription presented in Ref. 2, where we only considered the case that all hopping terms are of negative sign, such that the sign-flipping hops would coincide exactly with the hops to a different nodal region. In the general case, we prefer to speak about sign-flipping steps instead of nodal-boundary steps, as the latter term may cause confusion.

Clearly, by this prescription, a hop that would induce a sign change is replaced by a positive diagonal potential. If instead one used only the truncated Hamiltonian as given by (2), with the original diagonal matrix elements $\langle R|H_{\text{eff}}|R\rangle = \langle R|H|R\rangle$, then the value of the wave function at the node would be too high and its energy too low. This was found in an earlier attempt to perform fixed-node Monte Carlo on lattice fermions by An and van Leeuwen.[7]

A somewhat similar procedure, called "model-locality," has been used by Mitas, Shirley, and Ceperley[8] in continuum problems with a nonlocal potential that arises from replacing atomic cores with pseudopotentials. As in a lattice system, they cannot solve the problem of crossing a node by making the step size of the walkers continuously smaller, because of the nonlocal potential that connects configurations at finite distances. In their approach, the unwanted off-diagonal terms are truncated, and replaced by diagonal contributions as in Eq. (4), but with the sum over all R', not just over sign-flip configurations. With the model-locality procedure, one does not obtain an upper bound for the ground-state energy.

III. UPPER BOUND

We want to show that the prescription given above for $\mathcal{H}_{\text{eff}}$ leads to an upper bound for the ground-state energy of $\mathcal{H}$. In order to do so, we define a truncated Hamiltonian $\mathcal{H}_{\text{tr}}$, and a *sign-flip* Hamiltonian $\mathcal{H}_{\text{sf}}$, by

$$\mathcal{H} = \mathcal{H}_{\text{tr}} + \mathcal{H}_{\text{sf}}, \tag{5}$$
$$\mathcal{H}_{\text{eff}} = \mathcal{H}_{\text{tr}} + \mathcal{V}_{\text{sf}}, \tag{6}$$

where the diagonal elements of H_{tr} are

$$\langle R|H_{\text{tr}}|R\rangle = \langle R|H|R\rangle, \tag{7}$$

and its off-diagonal elements are given by

$$\langle R|H_{\text{tr}}|R'\rangle = \langle R|H_{\text{eff}}|R'\rangle. \tag{8}$$

$\mathcal{V}_{\text{sf}}$ is the sign-flip potential, for which the matrix elements are given by (4), and H_{sf} contains only the off-diagonal elements of H, which are put to zero in the effective Hamiltonian. We now take *any* state

$$|\psi\rangle = \sum_R |R\rangle\psi(R), \tag{9}$$

and we compare its energy with respect to $\mathcal{H}$ and to $\mathcal{H}_{\text{eff}}$:

$$\Delta E = \langle\psi|(\mathcal{H}_{\text{eff}} - \mathcal{H})|\psi\rangle$$
$$= \langle\psi|(\mathcal{V}_{\text{sf}} - \mathcal{H}_{\text{sf}})|\psi\rangle. \tag{10}$$

ΔE can be written explicitly in terms of the matrix elements of $V_{\rm sf}$ and $H_{\rm sf}$:

$$\Delta E = \sum_R \psi(R)^* \left[\langle R|V_{\rm sf}|R\rangle \psi(R) - \sum_{R'} \langle R|H_{\rm sf}|R'\rangle \psi(R') \right].$$

(11)

We rewrite this expression in terms of the matrix elements of H:

$$\Delta E = \sum_R \psi(R)^* \left[\sum_{R'}^{\rm sf} \langle R|H|R'\rangle \frac{\psi_T(R')}{\psi_T(R)} \psi(R) \right.$$

$$\left. - \sum_{R'}^{\rm sf} \langle R|H|R'\rangle \psi(R') \right].$$

(12)

In this double summation each pair of configurations R and R' occurs twice. We combine these terms and rewrite (12) as a summation over pairs:

$$\Delta E = \sum_{(R,R')}^{\rm sf} \langle R|H|R'\rangle \left[|\psi(R)|^2 \frac{\psi_T(R')}{\psi_T(R)} \right.$$

$$+ |\psi(R')|^2 \frac{\psi_T(R)}{\psi_T(R')}$$

$$\left. - \psi(R)^* \psi(R') - \psi(R')^* \psi(R) \right].$$

(13)

Denoting by $s(R,R')$ the sign of the matrix element $\langle R|H|R'\rangle$, and using the fact that for all terms in this summation the condition (1) is satisfied, we can finally write ΔE as

$$\Delta E = \sum_{(R,R')}^{\rm sf} |\langle R|H|R'\rangle| \left| \psi(R) \sqrt{\left|\frac{\psi_T(R')}{\psi_T(R)}\right|} - s(R,R')\psi(R') \sqrt{\left|\frac{\psi_T(R)}{\psi_T(R')}\right|} \right|^2.$$

(14)

Note that we do not have to worry about configurations R, where $\psi_T(R) = 0$: they do not occur in this summation. Obviously, ΔE is positive for any wave function ψ. Thus, the ground-state energy of $\mathcal{H}_{\rm eff}$ is an upper bound for the ground-state energy of the original Hamiltonian $\mathcal{H}$.

Now the GFMC method can calculate the exact ground-state energy $E_{\rm eff}$ of $\mathcal{H}_{\rm eff}$, without any sign problem. Assuming the trial function ψ_T has the correct symmetry (for example is antisymmetric), then $\psi_{\rm eff}$ will carry the same symmetry[9] and hence: $E_{\rm eff} \geq \langle \psi_{\rm eff}|\mathcal{H}|\psi_{\rm eff}\rangle \geq E_0$, where the second inequality follows from the usual variational principle. Hence the fixed-node energy is an upper bound to the true ground-state energy. One can easily verify that $\mathcal{H}|\psi_T\rangle = \mathcal{H}_{\rm eff}|\psi_T\rangle$, and thus one can be sure that the GFMC procedure improves on the energy of the trial wave function: $E_{\rm eff} \leq \langle \psi_T|\mathcal{H}_{\rm eff}|\psi_T\rangle = \langle \psi_T|\mathcal{H}|\psi_T\rangle$.

IV. VARIATION OF THE TRIAL STATE

Let us consider the situation where we use the exact ground state $|\psi_0\rangle$ of $\mathcal{H}$, with energy E_0, as trial state. Obviously, for the method to be useful, it is desirable that in that case the effective Hamiltonian has the same ground-state energy E_0, and the same ground state $|\psi_0\rangle$, as would make it possible to find the true ground state by varying the trial wave function in some way. In Eq. (14) we substitute ψ_0 for ψ_T. In order to have ΔE equal to zero, each individual term in the summation (14) has to vanish, thus leading to

$$\psi(R) \sqrt{\left|\frac{\psi_0(R')}{\psi_0(R)}\right|} - s(R,R')\psi(R') \sqrt{\left|\frac{\psi_0(R)}{\psi_0(R')}\right|} = 0, \quad (15)$$

or

$$\frac{\psi(R)}{\psi(R')} = s(R,R') \left|\frac{\psi_0(R)}{\psi_0(R')}\right| = \frac{\psi_0(R)}{\psi_0(R')}, \quad (16)$$

for all sign-flipping pairs (R,R'). This condition is trivially fulfilled for $\psi = \psi_0$. Thus, the true ground-state energy can be reached by variation of the trial wave function. One can further extend this result to show that as $\psi_T \to \psi_0$ the error in the fixed-node energy will be second order in the difference, $\psi_T - \psi_0$, with the coefficient positive.

The original contention in Ref. 2 was that the wave function, obtained through this effective Hamiltonian, would have exactly the same ratio at each sign-flipping pair R and R' as the trial wave function, i.e.,

$$\frac{\psi_{\rm eff}(R)}{\psi_{\rm eff}(R')} = \frac{\psi_T(R)}{\psi_T(R')}. \quad (17)$$

This, however, is, in general, not the case, as one can see from considerations about the symmetry of the wave function. An example for a small system, which illustrates this point, is given in Appendix B. Note that our proof for the upper bound does not rely on the assumption (17), and that the conclusion we put forward in Ref. 2 about the variational principle, remains unchanged. In fact, because the ground state of $\mathcal{H}_{\rm eff}$ is found in a much less restricted space of states than those satisfying (17), the resulting estimate for the ground-state energy is much better than was anticipated.

There is an important difference between the lattice and continuum fixed-node method. In the continuum method, it is only the sign of the trial function that matters. If the nodes are correctly placed, one will obtain the exact energy regardless of the magnitude of the trial function. Clearly this does not hold with the lattice fixed-node procedure: the sign of the trial function and the relative magnitudes of the trial function in configu-

rations that are connected by a sign flip must be correct. For example, in the continuum the exact result would be obtained for a one-dimensional (1D) problem since the nodal surface are the coincident hyperplanes. One does not nessecarily get the exact result for a 1D lattice model as one of the following examples shows.

V. ILLUSTRATIONS

We illustrate the effect of the effective Hamiltonian for the single-band Hubbard model by exact calculations on two small systems: a loop of four lattice sites on the corners of a square, and a graph consisting of eight points on the corners of a cube. We use the well-known Hamiltonian,

$$\mathcal{H} = -t \sum_{\langle i,j \rangle, \sigma} c_{i\sigma}^{\dagger} c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}, \qquad (18)$$

containing nearest-neighbor hopping with strength t and a local interaction between electrons of opposite spin with strength U. We consider the square with two electrons with spin up and two with spin down, and the cube with four up and one down and with four up and four down, respectively. In all cases, we use the results of self-consistent mean-field calculations as trial wave functions, and we compare the mean-field energy (MF), the lowest energy of the effective Hamiltonian (FN, for fixed node), and the exact ground-state energy, for different values of the interaction parameter U. We use different restrictions on the average number of electrons with spin up and down per site, in order to obtain different types of self-consistent mean-field wave functions. Writing $\langle n_{i\sigma} \rangle = \langle n_{\sigma} \rangle + (-1)^{\sigma} q_{i\sigma}$ for the average number of spin-σ particles on site i, we denote $q_{i\sigma} = 0$ by H (homogeneous), and $q_{i\sigma} = (-1)^i q_{\sigma}$, with q_{σ} a constant, by AF (antiferromagnetic, or Néel order favored). In the case of the cube with four up and one down spins (i.e., off half filling), the self-consistent mean-field solution with lowest energy turns out to have a symmetry different from both H and AF. As the exact ground state of $\mathcal{H}$, as well as of $\mathcal{H}_{\text{eff}}$, is not degenerate in these cases, it cannot have broken symmetry for $\langle n_{i\sigma} \rangle$. Note that, for $U = 0$, the mean-field approximation yields the exact ground state, and we checked that also the fixed-node result equals the exact ground-state energy in that case. The results are presented in Table I.

As one can see, the fixed-node approach on these small systems yields a significant improvement on the upper bound for the ground-state energy, compared to the mean-field approximations. One may note the fact that the mean-field wave function with lowest energy does, in general, not give the best fixed-node result. In a real problem, one would want to find the best possible trial wave function as input for the fixed-node procedure, and it is clear from these results that "best" does *not* mean "having the lowest variational energy" here. The sign of the trial wave function and its behavior at the nodal boundary determine how good the fixed-node energy will be.

TABLE I. Comparison of the energies obtained for three different systems by means of self-consistent mean-field (MF), fixed-node (FN), and exact calculations (Ref. 10). All values are given in units of t.

System	U	Trial type	Energies		
			MF	FN	Exact
Square	0		-4	-4	-4
2↑ 2↓	1	AF	-3.2855	-3.3172	-3.3409
Cube	0		-9	-9	-9
4↑ 1↓	1	H	-8.5	-8.5419	-8.5420
	6	H	-6	-7.2508	-7.2533
	6		-6.0701	-7.2424	-7.2533
	10	H	-4	-6.8400	-6.8442
	10	AF	-4.2551	-6.7476	-6.8442
	10		-5.3271	-6.7637	-6.8442
Cube	0		-12	-12	-12
4↑ 4↓	1	H	-10	-10.1148	-10.1188
	2.5	H	-7	-7.7257	-7.7510
	2.5	AF	-7.0061	-7.6942	-7.7510
	10	H	8	-2.6597	-2.8652
	10	AF	-2.3113	-2.6382	-2.8652

VI. CONCLUSIONS AND OUTLOOK

This method can be applied to any lattice model provided that only the Hamiltonian and a trial wave function with the proper symmetry are given. It is supervariational, in the sense that it always yields an upper bound for the energy, which is the lowest possible value consistent with the imposed constraint. By varying the the effective Hamiltonian through the trial wave function, in principle, the exact ground-state energy can be obtained.

Note that we have not used the symmetries of the trial state as input for our method. This means that it is possible to use this method for models of frustrated spins on a lattice and, via the appropriate mappings, for systems of bosons as well, or for excited states which are ground states of a given symmetry. In a forthcoming publication, possibilities to do so will be presented and discussed.

Note further that the *nodal relaxation* method, as described in Ref. 3 for continuum problems, is also applicable on the lattice. In this method, one uses the fixed-node approach to improve on the trial wave function. When this has been done, one removes the sign-flip constraint, and allows the walkers to move through the whole configuration space. If the fixed-node result is close enough to the ground state, one can sample the exact ground-state energy before the sign problem destroys the accuracy.

In the near future, we plan to use this method for Monte Carlo studies on some of the systems mentioned above, in order to find more comparisons of the fixed-node approach with known results, to check the effectiveness of the method, and to tackle some new problems as well.

The method appears to be also useful for continuum problems, where one has a nonlocal potential. For example, one can modify the model-locality approach of Ref. 8 so that it does yield an upper bound. Essentially one must allow nonlocal moves which do not change the sign

and add terms to the effective Hamiltonian corresponding to discarded moves.

We finally note that another promising avenue for further development of the conceptual basis of our approach is given by the observation by Martin that the use of an effective Hamiltonian can be couched in the language of density functional theory.[11] This makes it possible to apply a number of well-known results for the behavior of the energy functional under variation of both the effective Hamiltonian and the trial state $|\psi_T\rangle$.

ACKNOWLEDGMENTS

APPENDIX A: THE SIGN PROBLEM IN MONTE CARLO

In this appendix, we clarify the origin of the sign problem for a specific way of performing Green function Monte Carlo on lattice fermions, and we explain how one is able to circumvent this problem, using the fixed-node approach. More details of this version of GFMC as applied to lattices are given in Ref. 5.

In a GFMC simulation, one tries to obtain information about the properties of the ground state of a given Hamiltonian $\mathcal{H}$. Starting from a trial state, one can obtain (a stochastic representation of) the ground state by repeatedly applying a projection (or diffusion) operator. On a lattice it is simplest to use an operator that is linear in $\mathcal{H}$, and that can be viewed as the first-order expansion of an exponential diffusion operator in imaginary time:

$$\mathcal{F} = 1 - \tau(\mathcal{H} - w), \tag{A1}$$

where w is a parameter that should be chosen close to the ground-state energy in order to keep the wave function normalized. The parameter τ is taken small enough to ensure that the diagonal terms of this operator are positive. The off-diagonal elements in the matrix representation for $\mathcal{F}$ are, up to a factor $-\tau$, the same as those for $\mathcal{H}$. The nth approximation of the ground state is given by

$$|\psi^n\rangle = \mathcal{F}^n |\psi_T\rangle. \tag{A2}$$

One can check that, if the trial state has some overlap with the ground state, $|\psi^n\rangle$ will converge exponentially fast to the ground state for large n.

The ground-state energy can be calculated as

$$E_n = \frac{\langle \psi_T | \mathcal{H} | \psi^n \rangle}{\langle \psi_T | \psi^n \rangle}. \tag{A3}$$

We rewrite this expression as a summation over paths in configuration space:

$$E = \frac{\sum_{\mathcal{R}} E(R_n) \langle \psi_T | R_n \rangle \prod_{i=1}^{n} \langle R_i | F | R_{i-1} \rangle \langle R_0 | \psi_T \rangle}{\sum_{\mathcal{R}} \langle \psi_T | R_n \rangle \prod_{i=1}^{n} \langle R_i | F | R_{i-1} \rangle \langle R_0 | \psi_T \rangle}, \tag{A4}$$

where $E(R) \equiv \langle \psi_T | H | R \rangle \langle \psi_T | R \rangle^{-1}$ is the local energy at R, and $\mathcal{R} = \{R_0, R_1, R_2, ..., R_n\}$ denotes a path in configuration space.

In a GFMC procedure this expression is sampled stochastically by constructing paths $\mathcal{R}$ in configuration space, and calculating the energy from the contributions of those paths. Importance sampling is used to reduce the fluctuation of those paths by modifying $\mathcal{F}$. The sign problem arises from the fact since the fermion trial wave function is antisymmetric, its sign will vary. Also, the matrix elements $\langle R | F | R' \rangle$ between different R and R' need not be always positive. Thus, when performing a random walk to obtain a path $\mathcal{R}$, starting from a configuration R_0, where the trial wave function $\psi_T(R_0)$ is of specific sign, one may end up in a configuration R_n, where the trial function is of the opposite sign, or one may have collected an odd number of negative $\langle R | F | R' \rangle$ in the path. For large n, one obtains about as many positive as negative contributions; the difference is used to determine the energy. One can easily show that the "signal-to-noise" ratio must decrease exponentially in n once negative contributions are allowed. Intuitively, it is easy to understand that this will give rise to an inaccurate result. In practice, this severely limits the applicability of quantum Monte Carlo methods to fermion problems.

In the fixed-node approach, one wants to avoid that contributions of different sign can be obtained. In order to ensure this, one demands that *at every individual step* along a path, only positive contributions are allowed. Thus, all steps satisfying Eq. (1) have to be discarded. The prescription (2–4) for the effective Hamiltonian takes care of this constraint. Finally, we remark that this prescription fits very well with the way we perform importance sampling. When using the trial wave function as a guiding function for the random walks, at any point in the walk one needs to know the value of the trial wave function, and one can use this value at the same time for guiding the walks and for the implementation of the fixed-node effective Hamiltonian. Note that the summation needed to define the effective potential in Eq. (4) only grows linearly with the size of the system for a Hamiltonian such as the Hubbard model. Thus, it does not appreciably slow the calculation.

APPENDIX B: EXAMPLE OF FIXED-NODE PROCEDURE

In this appendix, we give an illustration of how the effective Hamiltonian is created, and what its effect is, on a very simple small system. All steps can be straightforwardly generalized to more complicated systems.

Consider the Hamiltonian

$$\mathcal{H} = -t \sum_{\langle i,j \rangle, \sigma} c_{i\sigma}^{\dagger} c_{j\sigma} \qquad (B1)$$

on a loop of four sites with two spinless fermions. We define *configurations of labeled fermions* $[i_1 i_2]$, where particle j ($1 \le j \le 2$) sits on site i_j ($1 \le i_j \le 4$). We number the sites, as follows:
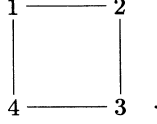
A valid (i.e., antisymmetric) fermion wave function ψ must satisfy $\psi([ij]) = -\psi([ji])$. The configuration space of this system consists of 12 configurations, and can be depicted as follows:
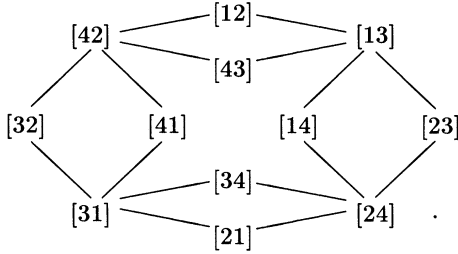
The lines (or bonds) represent valid hops in this space. The matrix elements $\langle [ij]|H|[kl] \rangle$ of the Hamiltonian for this system are $-t$ if there is a bond between $[ij]$ and $[kl]$ (in that case $i = k$ or $j = l$ must hold), or 0 otherwise. The ground state of this Hamiltonian is symmetric under exchange of the particles, and we have to restrict the wave function explicitly to be antisymmetric in order to find a valid fermion wave function. To obtain a Hamiltonian $\underline{H}$, which describes the fermion problem only, we define *antisymmetric states* $[\underline{ij}]$, which are antisymmetrized combinations of the configurations:

$$[\underline{ij}] = \frac{1}{\sqrt{2}} \left([ij] - [ji] \right). \qquad (B2)$$

In this way, each pair of configurations $[ij]$ and $[ji]$ produces two states, $[\underline{ij}]$ and $[\underline{ji}]$, which only differ by their sign. One has the freedom to choose one of these states to obtain only one state per pair of configurations, and one can calculate the resulting Hamiltonian for the $[\underline{ij}]$:

$$\langle [\underline{ij}]|\underline{H}|[\underline{kl}] \rangle = \frac{1}{2} \sum_{\Pi_1} \sum_{\Pi_2} \mathrm{sg}(\Pi_1)\mathrm{sg}(\Pi_2) \langle \Pi_1[ij]|H|\Pi_2[kl] \rangle$$
$$= \mathrm{sg}(\Pi)\langle [ij]|H|\Pi[kl] \rangle, \qquad (B3)$$

where Π_1 and Π_2 denote permutations of the two particles, sg gives the sign of a permutation, and $\Pi[kl]$ is the permutation of $[kl]$ that can be reached by one hop from $[ij]$, such that $\langle [ij]|H|\Pi[kl] \rangle = -t$. We can again denote the Hamiltonian in a picture, representing matrix

elements $-t$ by thin lines and $+t$ by thick lines (we choose the $[\underline{ij}]$ with $i < j$; other choices give different pictures but the same results):
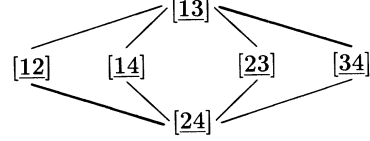
This structure fully contains the antisymmetry, and the corresponding Hamiltonian gives all the information there is on the fermion problem. Its ground state is degenerate, with energy $-2t$, and possible ground states are

$$|\psi_0\rangle = \frac{1}{2} \left| [\underline{13}] + [\underline{14}] + [\underline{23}] + [\underline{24}] \right\rangle, \qquad (B4)$$

and

$$|\psi_0'\rangle = \frac{1}{2} \left| [\underline{12}] + [\underline{13}] - [\underline{24}] - [\underline{34}] \right\rangle. \qquad (B5)$$

It is easy to generalize this procedure for any system of lattice fermions.

Let us now consider a trial state, and calculate the effective Hamiltonian according to our fixed-node prescription. The trial wave function defines the *nodal regions* through its sign in all states, and, because we are working with negative hopping terms, the sign-flip constraint reduces to sign changes of the wave function only. We take a very simple trial state

$$|\psi_T\rangle = \frac{1}{\sqrt{6}} \left| [\underline{12}] + [\underline{13}] + [\underline{14}] + [\underline{23}] + [\underline{24}] + [\underline{34}] \right\rangle, \qquad (B6)$$

purposely chosen such that we only have to slightly adapt the previous picture to denote the effective Hamiltonian:
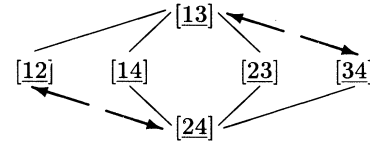
Here, the thin lines are still matrix elements $-t$. The thick lines have been cut (we do not allow these hops in the effective Hamiltonian) and replaced by arrows, indicating diagonal matrix elements, which in this simple case all become $+t$, because we have chosen equal weights for all the states in the trial wave function. The (nondegenerate) ground state of this effective Hamiltonian is

$$|\psi_0^{\mathrm{eff}}\rangle = |0.165([\underline{12}] + [\underline{34}])$$
$$+ 0.448([\underline{13}] + [\underline{24}]) + 0.523([\underline{14}] + [\underline{23}]))\rangle, \qquad (B7)$$

with energy $-1.709t$. Note that, e.g., the states $[\underline{12}]$ and $[\underline{24}]$ do *not* have the same wave function in this ground state, while they do in the trial state. As one could have expected from symmetry considerations, the wave function is the same in states that have an equivalent position

in the picture, i.e., occur symmetrically in the effective Hamiltonian. States that are connected via the boundary do not, in general, have such symmetry, and thus there is no reason to expect that they would obey (17). Note also that the energy of the effective ground state is above the ground-state energy of the true problem, as it should be according to our proof that it is an upper bound for that energy.

[1] For a review and recent references, see, e.g., W. von der Linden, Phys. Rep. **220**, 53 (1992); or H. de Raedt and W. von der Linden, in *The Monte Carlo Method In Condensed Matter Physics*, edited by K. Binder (Springer Verlag, Berlin, 1992).

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[9] Note that one can, in principle, construct a total antisymmetric wave function from the wave function that one has constructed in one nodal region of the trial wave function by extending it to the other regions antisymmetrically. One can do this because the (effective) Hamiltonian commutes with such an antisymmetrization operator. However, in practice, one in fact samples the properties of the wave function, rather than constructing the wave function itself. For a more elaborate discussion on symmetry see, e.g., P.J. Reynolds, D.M. Ceperley, B.J. Alder, and W.A. Lester, Jr., J. Chem. Phys. **77**, 5593 (1982).

[10] The FN and exact results have been obtained by means of numerical routines to exactly diagonalize a matrix of dimension 36×36 (for the square with $2\uparrow$ and $2\downarrow$), 560×560 (cube with $4\uparrow$, $1\downarrow$), and 4900×4900 (cube with $4\uparrow$, $4\downarrow$), respectively. In the latter case, group theory was used to reduce the matrix to blocks of 1896×1896 or smaller.

[11] R.M. Martin (private communication).