Counting world lines for many-fermion systems

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I explore a recursive enumeration of world-line diagrams as a numerical approach to simulating many-fermion lattice systems. Signs from fermion exchange are treated exactly. In addition, all values of the coupling constants are treated simultaneously. The method is computationally fast, although large-memory requirements restrict it to small spatial systems.

I. INTRODUCTION

Numerical simulations of quantum systems are a major industry in several subfields of physics. Lattice guage studies are giving first-principle results on hadronic processes, while calculations of many-electron systems are testing models of superconductivity. Despite many successes, the inclusion of fermionic degrees of freedom severely strains available computational resources. Furthermore, with a background baryon density in particle physics or away from half-filled bands in many-electron models, the problem becomes much more severe. Here the Monte Carlo approaches are hampered by the so-called "sign problem," wherein the measures encountered in the path integrals are not positive. Removing the signs from the measure yields expectation values with large fluctuations, requiring inordinately large statistics to extract meaningful results.

The fermion issue is often discussed in terms of the determinant of the matrix coupling the anticommuting fields to the bosonic fields of the problem. Expanding such a determinant in minors gives terms representing sets of fermionic loops. Each loop can be thought of as the world line for the fermion in question. In this paper, I work directly in this world line representation. I consider an enumeration of these loops in a recursive manner, finally expressing physical quantities in terms of this enumeration.

The concept of summing over world lines to study quantum mechanics goes back to Feynman.[1] Explicit evaluation of these path integrals by Monte Carlo methods has been advocated in Ref. 2. For many-fermion problems, Hirsch *et al.*[3] have presented a convenient world line formalism which I follow quite closely below.

I consider a recursive procedure essentially identical to one used for the Ising model in Ref. 4 to exactly solve small lattices and in Ref. 5 to find low-temperature series. Indeed, the extension of this method to fermions is suggested by the treatment of domain walls in the two-dimensional Ising model as fermion world lines.[6]

A complementary approach to the study of many-fermion systems is the direct diagonalization of the quantum Hamiltonian. While the relevant Hilbert space is exponentially large in the system volume, with nearest-neighbor couplings the Hamiltonian yields itself well to sparse matrix techniques. Here I also work with the full Hilbert space of states, and memory requirements of the enumeration process will be even larger than required for direct diagonalization. On the other hand, the approach presented here is computationally fast and simultaneously gives information on the model at all couplings. Although the size of the Hilbert space restricts me to rather small spatial systems, the limits on the temporal size are rather mild. Furthermore, the algorithm is not constrained by dimensionality beyond the fact that a given number of sites in a higher dimension inherently has a smaller linear extent.

I test the method on a simple Hubbard model[7] in two dimensions. This system has the essential problems associated with fermionic degrees of freedom, including a nonpositive fermion determinant when the system is away from half-filling. Furthermore, Ref. 3 has already set up a convenient world line formalism for this Hamiltonian. In this problem all the physics can be reduced to counting issues. It remains unclear how to generalize this when continuous fields are coupled to the fermions. In particular, I do not know how to generalize the method to lattice gauge theories. Possibly, this will require treating the bosonic fields via a similar counting technique.

II. WORLD LINE DIAGRAMS

The Hamiltonian that I study is

$$H=-K\sum_{\{i,j\},\sigma}(a^{\dagger}_{i,\sigma}a_{j,\sigma}+a^{\dagger}_{j,\sigma}a_{i,\sigma})+U\sum_{i}n_{i,\uparrow}n_{i,\downarrow}\ . \tag{2.1}$$

Here a ($a^{\dagger}$) denote the annihilation (creation) operators for electrons on a set of sites labeled by i and j. The index σ denotes the electron spin, which can be up or down ($\uparrow$ or $\downarrow$). The geometry of the system is determined by the set of nearest-neighbor pairs, denoted $\{i,j\}$. The number operator $a^{\dagger}_{i,\sigma}a_{i,\sigma}$ is denoted $n_{i,\sigma}$.

The fermion operators satisfy standard anticommutation relations

$$\begin{aligned}[a_{i,\sigma},a^{\dagger}_{j,\sigma'}]_{+}&\equiv a_{i,\sigma}a^{\dagger}_{j,\sigma'}+a^{\dagger}_{j,\sigma'}a_{i,\sigma}\\&=\delta_{i,j}\delta_{\sigma,\sigma'}\ ,\\ [a_{i,\sigma},a_{j,\sigma'}]_{+}&=0\ .\end{aligned} \tag{2.2}$$

The variable K controls how easily the fermions move around and is called the "hopping" parameter, and this term represents the "kinetic" energy. The coupling constant U measures the strength of the interaction for two electrons on the same site. This term is quartic in the creation and annihilation operators and represents the "potential" energy.

I consider applying $\exp(-\beta H)$ to some initial state $|\psi\rangle$. When β is large, this projects out the ground state, while, for smaller β, I speak of the "evolution" of the initial state. As iH is usually taken as the generator of translations in time, this evolution is formally in imaginary time.

To proceed, I break time up into N_T time slices and write

$$e^{-\beta H}=(e^{-\epsilon\beta H})^{N_T} , \tag{2.3}$$

where the temporal step size is $\epsilon=1/N_T$. At this point there are several ways to proceed; I follow Ref. 3 quite closely and break H up in a checkerboard fashion. Indeed, this section is essentially a review of that formalism. Temporarily restricting myself to one spatial dimensions, I write

$$H=T_1+T_2+V , \tag{2.4}$$

where T_1 includes hoppings between odd sites on the left and even sites on the right, T_2 involves the opposite parity bonds, and V represents the interaction term, proportional to U. I now assume ϵ is small and make the approximation[8]

$$e^{-\epsilon\beta H}=e^{-\epsilon\beta V/2}e^{-\epsilon\beta T_1}e^{-\epsilon\beta V/2}e^{-\epsilon\beta T_2}+O(\epsilon^2) . \tag{2.5}$$

For two spatial dimensions, I break the kinetic term of H into four pieces, representing the combinations of even or odd with x or y bonds.

With this breakup either T_1 or T_2 is a direct product of pieces coupling independent pairs of sites and involving no coupling between up and down spins. This makes diagonalization quite simple and gives the explicit matrix elements of $e^{-\epsilon\beta T_i}$. These elements have a simple diagrammatic interpretation used in the Monte Carlo simulations of Ref. 3 and form the basis of the counting algorithm presented below.

Consider the effect of, say, $e^{-\epsilon\beta T_1}$ on a single coupled pair of sites. If there are no electrons present, we just get a factor of unity. When a single electron is present, there are two nonvanishing matrix elements, representing the cases of whether the electron moves to the other site or not. The diagonal matrix element involving no motion is $\cosh(\epsilon\beta K)$, while if the electron hops I obtain a factor of $\sinh(\epsilon\beta K)$. Finally, if there are two electrons of the same spin present on both sites, the matrix is again diagonal and gives a factor of unity. For convenience I consider writing unity in the form $\cosh^2(\epsilon\beta K)-\sinh^2(\epsilon\beta K)$. In this way I can think of this term representing two processes, the first having the two electrons go forward in time without moving and the second representing an exchange, with the corresponding fermionic minus sign.

It is convenient to remove a factor of $\cosh^2(\epsilon\beta K)$ for each time step and each fermion present. Then any given diagram simply gives a factor of $\tanh(\epsilon\beta K)$ for every electron hopping. The remaining rule is that the potential term gives a factor of $e^{-\epsilon\beta U/2}$ every time an up and a down spin occupy the same lattice site.

When there are many fermions present, I need a convention to determine overall signs. This involves ordering the sites in some manner and then ordering up and down spins on the individual sites. Whenever a hop occurs, the sign is minus if an odd number of fermions are passed. Note that in two or more spatial dimensions this is a nonlocal evaluation. My convention is to place the sites in a sequence and put an up spins "on the left" of down ones on the same site. I always use periodic boundary conditions.

Now consider the matrix element

$$\langle\psi'|e^{-\beta H}|\psi\rangle , \tag{2.6}$$

where the initial and final states are eigenvectors of the occupation numbers $n_{i,\sigma}$; that is, I know where the initial and final electrons are. The result is a sum over all world line diagrams connecting the initial and final states. The world lines pass through the allowed squares of the checkerboard lattice, giving a factor of

$$t\equiv\tanh(\epsilon\beta K) \tag{2.7}$$

every time an electron hops and a factor of

$$v\equiv e^{-\epsilon\beta U/2} \tag{2.8}$$

whenever a site is doubly occupied by electrons of opposite spin. No site is permitted to have two or more world lines representing the same spin pass through it at the same time. Finally, count the number of fermion exchanges to determine the overall sign of the graph. Summing over all graphs gives the desired amplitude. This summarizes the world line diagrams as sampled by a Monte Carlo method in Ref. 3.

III. RECURSIVE COUNTING

The above formalism gives the diagrammatic sum

$$\langle\psi'|e^{-\beta H}|\psi\rangle\propto\sum_d t^{N_t(d)}v^{N_v(d)}s_d , \tag{3.1}$$

where t and v are defined above for notational simplicity an overall constant factor of $\cosh^2(\epsilon\beta K)$ per fermion per time slice has been dropped. The sum is over all diagrams d, and $N_t(d)$ and $N_v(d)$ denote the number of hoppings and number of doubly occupied sites in the respective diagram. The number of fermion crossings determines $s_d\in\{\pm1\}$, the overall sign of the diagram. I now rearrange this to a sum over the number of hoppings and coupling terms:

$$\langle\psi'|e^{-\beta H}|\psi\rangle\propto\sum_{N_t,N_v}N(N_t,N_v,\psi',\psi)t^{N_t}v^{N_v} . \tag{3.2}$$

Here $N(N_t,N_v,\psi',\psi)$ is an integer which counts the number of diagrams having N_t hoppings and N_v interaction terms. The world lines start at the occupied sites of the state ψ and end at those of ψ'. In this counting the sign of the diagram is included; that is, N represents the number of positive diagrams minus the number of negative

ones. Here I explicitly write the dependence on the initial and final states, as this will be used for the recursion discussed below.

All information about this discretized system is contained in the table of integers $N(N_t,N_v,\psi',\psi)$. I now consider constructing part of this table explicitly by recursively building up the space-time lattice one square at a time. To initialize the procedure, when the time height of my lattice is zero, there can be no hoppings and thus all counts vanish unless ψ' and ψ are the same, in which case the count is 1.

After initialization the procedure is recursive. Assume that I have the counts for a partially constructed lattice. Now add one new active square of the checkerboard lattice. By active I mean one of the squares on which hopping is allowed. There are at most four forms this added square can take, and thus one count for the new lattice is a sum of up to four terms depending on the electron occupations of the covered sites.

As the lattice is being built up, at intermediate stages the temporal top of the system will be "ragged," in the sense that some sites will be one time step ahead of the others. Nevertheless, the top layer always has the same number of sites, and the space of states is unchanged. In adding a new square to a checkerboard, the two old sites should have the same time coordinate. This can be assured by having an even number of sites in a one-dimensional system and corresponding constraints on higher dimensions. In the following examples, I always take an even number of sites and for two dimensions I work with them arranged in a helix with an odd shift to the neighbors in the second direction.

The total number of possible counts grows as the square of the volume of the Hilbert space restricted to fixed numbers of spin-up and spin-down particles. This results from the dependence on both the top and bottom layers. In practice, this is uncomfortably large, and so I restrict myself to a fixed bottom layer. This allows larger systems to be studied, but precludes calculations where many initial states are needed, as for traces. I still need all elements of the Hilbert space on the top layer. This is because any of these states may be needed as intermediate states later in the recursion.

As many different counts are needed for each state, the algorithm uses a lot of memory, indeed, even more than required for exact diagonalization methods, which just keep a few numbers per state. On the other hand, the recursion is quite fast, as any new count depends on at most four of the old ones.

One trick to save considerable memory is to only enumerate for half the required time slices and then stack an inverted copy of the lattice on itself. Summing over the enclosed slice gives the counts from the initial state to itself the full time later, up to an unimportant switch in the even-odd checkerboard convention at the halfway point. On a periodic lattice this can be generalized by shifting the states before the folding process to give the counts from the initial state to any shift of itself. This doubling trick, however, is limited to obtaining the diagram counts where the final state is related to the initial one by some symmetry.

IV. SOME "EXPERIMENTS"

In Fig. 1 I consider a single electron on a periodic one-dimensional 26-site spatial lattice. I iterated the counting procedure for 25 time steps to obtain a 26×50 checkerboard. As discussed at the end of the last section, this is doubled on top of itself, resulting in a 26×100 checkerboard lattice. In the figure I show the number of paths from a fixed initial site to the same site on the final time slice as a function of the number of hoppings along the path. Since there are no paths that return to the same site after an odd number of hoppings, I only plot paths for an even number of hoppings and connect the points to form the smooth curve. A similar table of numbers is generated for each final state of the system.

The counts in Fig. 1 range from 1 for 0 or 100 hoppings to approximately 8.5×10^{27} for 50 jumps. These numbers were obtained exactly using high-precision integer arithmetic. Tests with storing the counts with floating-point numbers indicate that this exact treatment is not essential for systems of the sizes considered here. Nevertheless, the exact approach provides extra confidence in allowing for arbitrary cancellations when different sign contributions are added with several fermions present.

Figure 2 uses these counts and similar ones obtained with a shift in the final state to show the spreading of the electron distribution. I display the wave function as a function of position on the lattice. The curves are all normalized to unit maximum. The final state is obtained after applying $e^{-\beta H}$ to the initial electron, located at site 0. From bottom up the curves represent β of 2, 8, 32, and 128, respectively. Here and for all following figures, the hopping parameter K is set to unity. As in Fig. 1, the lattice is a doubled one of 50 times slices; thus I have a

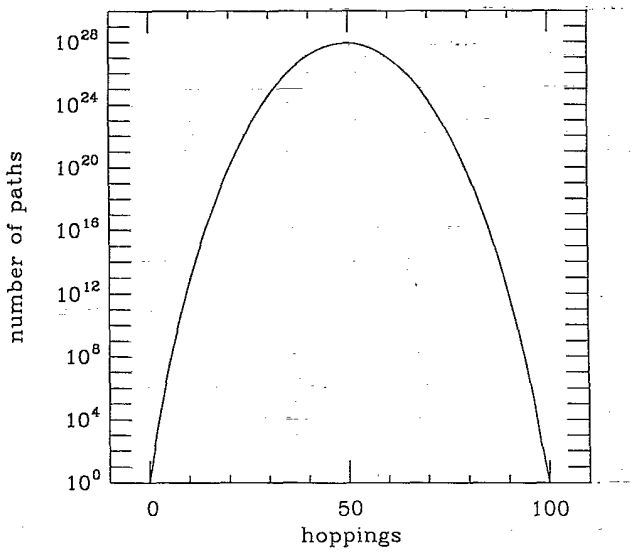

FIG. 1. Raw counts for the number of paths from a given spatial site to itself as a function of the number of hoppings on the path. The lattice is a one-dimensional ring of 26 spatial sites, and time has been divided into 50 slices, each of which is two checkerboard squares deep. Only even numbers of hoppings appear.

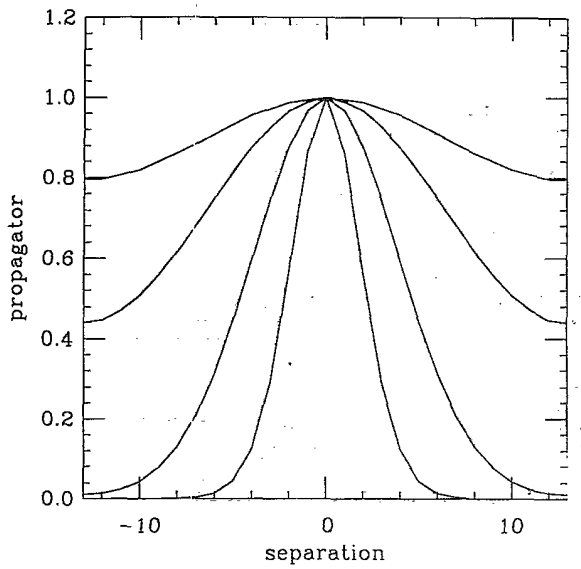

FIG. 2. Spreading of a one-electron wave function on a 26-site, one-dimensional ring. All curves come from the same set of counts and are normalized to unity at the peak. With unit hopping parameter, the curves from bottom up represent the final state after applying $e^{-\beta H}$ for $\beta=2$, 8, 32, and 128. The initial electron position was at site 0.

26×100 checkerboard. All curves in this figure are generated from the same table of counts; the only difference is how the counts are weighted. This is one of the main advantages of the method: All couplings are studied at once.

The approach does not depend on how the spatial sites are connected. Figure 3 again represents wave-function spreading, but now on a two-dimensional lattice. Here I have arranged the same 26 spins in a periodic helix, with successive turns of the helix 5 sites apart. Thus site 0 is a nearest neighbor to sites 1, 5, 21, and 25. Note the fast leakage of the wave function to these points. Also note that the wave function smooths out much faster than in Fig. 1 because the sites are more closely connected.

The helical lattices used here have previously been advocated for various reasons. In Ref. 5 a system of 18 sites with a helical period of 5 was used to give each neighbor 6 sites from his periodic neighbor, thus mimicking a 6×6 lattice. A lattice of 10 sites with period 3 is the so called "$\sqrt{10}\times\sqrt{10}$" lattice used, for instance, in Ref. 9. For two spatial dimensions the temporal checkerboard should be generalized; I consider hoppings consecutively between even-x bonds, odd-x bonds, even-y bonds, and odd-y bonds. This choice is arbitrary, but should be irrelevant for small time steps.

I now turn to the interacting system and start with the state $|\psi_0\rangle$ of one spin-up and one spin-down electron on adjacent sites of an eight-site helix with period 3. I work with unit hopping parameter and a coupling $U=5$. Figure 4 shows the relaxation of the system energy as a function of time. Here the three solid curves, from asymptotically lowest to highest, represent a total number of time slices of 8, 10, and 12, respectively. The dashed line represents an extrapolation from the last two solid curves to an infinite number of time slices, with the assumption that corrections are proportional to the inverse of the timelike lattice spacing. This extrapolation appears stable and will be used henceforth. There are several ways to extract the energy from the counts; I find it from the change in the norm of $e^{-\beta H}|\psi_0\rangle$ before and after the last time step.

On each curve in this figure, the time to each point is divided into the respective number of slices; thus the effective timelike lattice spacing is not constant, but proportional to the time at which the energy is being measured. In other words, each curve is in its entirety obtained from the counts before and after the final slice, with only the expansion parameters changing as one

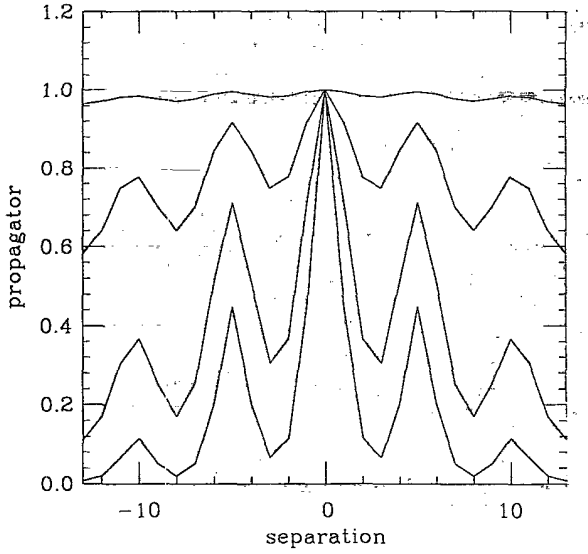

FIG. 3. Wave-function spreading on a 26-site periodic helix with 5 sites per turn. Here $e^{-\beta H}$ is applied to the initial states for $\beta=1$, 2, 4, and 8.

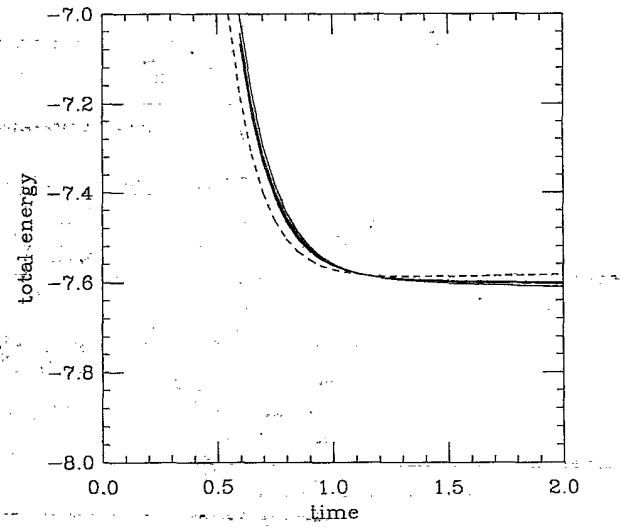

FIG. 4. Energy relaxation for a spin-up-spin-down pair on an 8-site, period-3 helix. The three curves represent 8, 10, and 12 time slices, and the dashed curve represents an extrapolation to zero temporal lattice spacing. The coupling U is 5, and the hopping parameter K is 1.0.

moves along the curve. This idea of maintaining a constant number of slices rather than a constant lattice spacing is novel to this counting approach.

Figure 5 shows the energy relaxation for several values of the interaction U. These curves all use the same extrapolation to vanishing time step as gave the dashed line in Fig. 4. From bottom to top, the solid curves represent U of -5, 0, 5, and 10, respectively. At $U=0$ the curve relaxes to the exact value of -8 for the energy.

The dashed curve in Fig. 5 represents a direct simulation of the infinite-U limit. For this purpose only paths where the electrons did not simultaneously pass through the same site were considered. In addition, the spin-up and down electrons were not allowed to cross each other on the same bond at the same time step. These rules dramatically reduce the scope of the world line counting and allow the study of considerably larger systems.

Since full information on the wave function is available, one can study any physical parameter desired. In Fig. 6 I show, as a function of U, the probability that the spin-up and- down electron on this eight-site lattice lie on the same site. The cross at $U=0$ represents the exact value $\frac{1}{64}$ for the ground state of noninteracting particles. For this figure I measure the pair density after applying $e^{-1.5H}$ to the initial state. I again extrapolate from time divided into 10 and 12 slices. The pair density is calculated at each site, giving rise to eight curves which are superposed and mostly indistinguishable. Note that at negative U these curves are beginning to fan out, showing that with an attractive interaction the system takes longer to spread into its spatially uniform ground state. While there are in principle eight curves plotted here, the upper curve represents the equal densities on the sites where the electrons started, and the lower curve is the superposition of the results for the other six sites, all of which are nearest neighbors to one of the initial sites. The latter curves are not all exactly degenerate, but close enough to appear so on the graph.

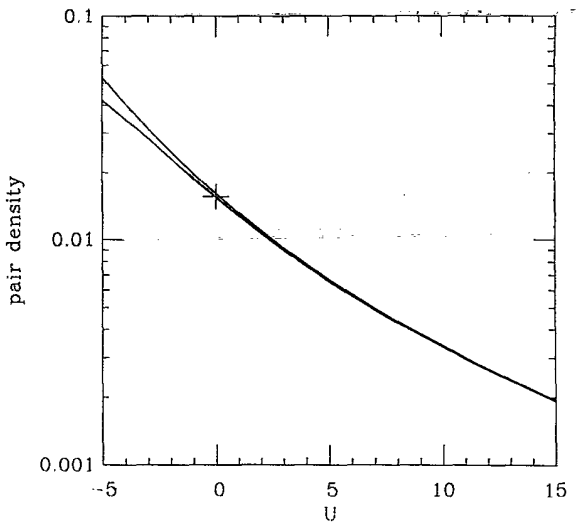

FIG. 6. Pair density for two electrons of opposite spin as a function of the interaction U on an 8-site period-3 helical lattice. The fanning of the curves at negative U represents insufficient time for relaxation. The cross at $(0, \frac{1}{64})$ marks the exact solution for the free theory.

For Fig. 7, I return to the infinite-U limit and plot the total energy as a function of time for a variety of fillings. This is on the same 8-site period-3 helix used above. Note that the half-filled case, with 4 spin-up and 4 spin-down particles, is stuck at zero energy. Indeed, in the infinite-U limit this case is peculiar, with no net motion of the particles allowed. With one electron less, that is, for the (4,3) case, the graph shows a rather slow convergence compared to the lower curves. For one electron the curve relaxes to the exact value of -4 for the energy. The interaction of the second electron raises the (1,1)

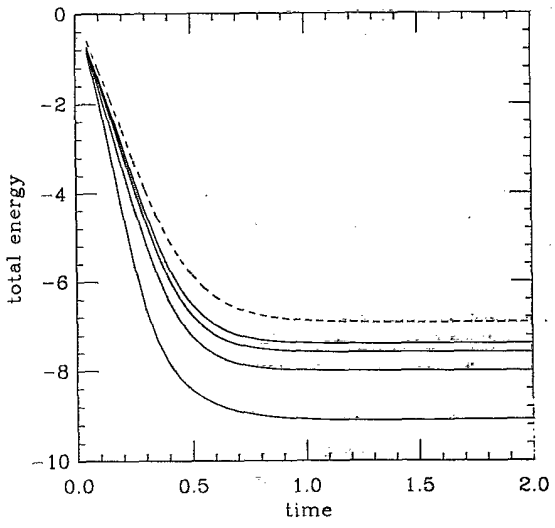

FIG. 5. Relaxation to the ground state of two electrons of opposite spin for various values of the interaction parameter U. From bottom up the curves represent $U=-5$, 0, 5, 10, and infinity, respectively.

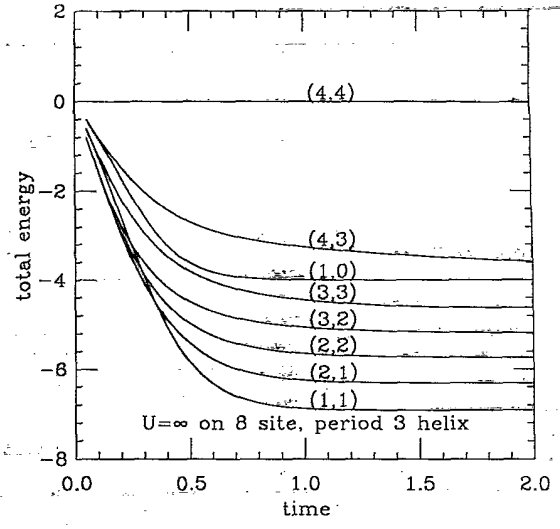

FIG. 7. Relaxation of the total energy of the infinite U model as a function of time for various fillings of an 8-site period-3 helical lattice. The curves are labeled by pairs of numbers representing the numbers of spin-up and -down electrons, respectively.

curve above the free value of -8. As further electrons are added, the energy continues to rise, partly because of the interaction and partly because of the fermionic nature of the particles forcing them into higher levels. Indeed, a similar experiment for the free case with $U=0$ shows successive particles going into higher states.

V. MEMORY ISSUES

The primary disadvantage of this counting method is the huge amounts of computer memory required. Indeed, I work with the entire Hilbert space for the quantum system, and for each state I keep a large number of counts. Thus the memory requirements are larger than required for exact diagonalization using sparse matrix techniques. On the other hand, the method is complementary in the information it provides, enabling all values of the couplings to be studied at once.

Some memory could be saved by using a translation-invariant initial state. Then the counts to all translations of a given final state would be equal and need not be stored. Indeed, this trick was essential to obtaining interesting expansions for Ref. 5. On the other hand, here the gain is reduced by a factor of 2 by the checkerboard lattice. This trick inherently involves a substantial speed loss because now an entire layer must be added at once, rather than a single lattice square. Then the loop over states becomes double loop over the Hilbert space. Furthermore, a translation-invariant state eliminates the ability to watch some interesting phenomena such as the wave function spreading seen in Figs. 2 and 3. Thus here I have opted against using translation-invariant initial states.

Another way to reduce memory needs is to give up the exact integer arithmetic for floating-point accumulation of the counts. Simple tests indicate little loss for the results presented here, but the gain is limited in light of the exponential growth in memory needs inherent in the algorithm. Also, cancellations may become dangerous for larger systems as the sign problem becomes increasingly severe. This issue needs more investigation.

VI. CONCLUDING REMARKS

I have presented a method for simulating lattice fermion systems. The approach is quite fast, but requires large amounts of computer memory. The method has several compelling advantages. Primarily, there is no sign problem; all fermionic antisymmetrization is taken care of exactly. Indeed, this is true for arbitrary lattice geometry. Second, all values of the couplings are done simultaneously. Third, not being a Monte Carlo simulation, there are no statistical errors; in particular, once a run is done, it is finished and no knowledge is gained without going to a different size system. Finally, because only a single pass is made through the system, the net amount of computer time required is quite modest.

Here I have worked directly in the Hilbert space with a fixed number of fermions. Thus issues such as an applied magnetic field or chemical potential merely involve comparing results with different fillings. In particle physics the filled Dirac sea should be explicitly included; that is, for zero chemical potential one should work with the fermion states half-filled.

For Monte Carlo approaches a half-filled lattice is often the easiest case to treat because the determinant can be made positive via a symmetry between spin-down holes and spin-up electrons. For the method discussed here, in contrast, it is low fillings which are preferred because the Hilbert space is smaller. Indeed, the half-filled case has the most states and thus is the most difficult.

An important unresolved question is how to adapt the method to fermions coupled to continuous bosonic fields, in particular to gauge fields. As the basis of the method is a counting procedure, one perhaps should treat the other fields similarly. This resembles a computer evaluation of the strong-coupling expansion and may provide interesting challenges for non-Abelian theories.

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