New Stochastic Treatment of Fermions with Application to a Double Chain Polymer *
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#### Abstract

An extension of the stochastic algorithm as applied to Hamiltonian lattice field theories is developed. This new scheme will converge in problems that have intrinsic negative signs in the matrix elements. As an example, this scheme is applied to a two chain polymer problem with (spinless) fermions that have a pairwise interaction. Because of the multiple connected structure of the double chain, this problem has intrinsic minus signs. It cannot be transformed into a bosonic problem with only positive matrix elements. Numerical results from this application of the new algorithm are presented for the energy and certain correlation functions for moderately long chains. A discussion of a modification of the method which will allow the treatment of much larger systems is discussed.


## 1. Introduction

For large $\beta$, the operator $\exp (-\beta H)$ can be used to project onto the eigenstate of $H$ with the minimum eigenvalue. The available number of stochastic algorithms that can be utilized to perform this projection range over a virtual continuum. Starting from the population method, well described by Kalos and collaborators ${ }^{1}$ and Ceperley and Adler, ${ }^{2}$ they extend to the modified projector methods ${ }^{3,4}$ and on to the projector method. ${ }^{5}$

The algorithm to be described here is applicable to a large number of problems which possess negative matrix elements that cannot be interpreted as probabilities nor eliminated by a transformation such as is available for most onedimensional fermion models. The advantage of this method is that the evaluation of the fermion determinant (as found in conventional treatments of such problems) is avoided. Efficiency is thereby increased as well as accuracy, simplicity and generality (many non-local potentials can be directly treated). In this paper we will apply the algorithm to a simple but non-trivial example- a double chain spinless fermion system with 'Coulomb' interactions.

The Hamiltonian of the system of interest is (see Figure 1 for site labels and the definition of $x$ and $y$ )

$$
\begin{equation*}
H=K+V \tag{1.1}
\end{equation*}
$$

where both the hopping term K and the potential V can be broken up into terms operating in the $x$ and $y$ directions. The hopping terms are

$$
\begin{equation*}
K_{x}=-t_{x} \sum_{i \text { odd }} K(i, i+1) \tag{1.2}
\end{equation*}
$$

and

$$
\begin{equation*}
K_{y}=-t_{y} \sum_{i \text { odd }}[K(i, i+2)+K(i+1, i+3)], \tag{1.3}
\end{equation*}
$$

while the potential terms are

$$
\begin{equation*}
V_{x}=-v_{x} \sum_{i \text { odd }} N_{i} N_{i+1} \tag{1.4}
\end{equation*}
$$

and

$$
\begin{equation*}
V_{y}=-v_{y} \sum_{i \text { odd }}\left[N_{i} N_{i+2}+N_{i+1} N_{i+3}\right] \tag{1.5}
\end{equation*}
$$

where

$$
\begin{equation*}
K(i, j)=C_{i}^{\dagger} C_{j}+C_{j}^{\dagger} C_{i} \tag{1.6}
\end{equation*}
$$

and

$$
\begin{equation*}
N_{i}=C_{i}^{\dagger} C_{i} . \tag{1.7}
\end{equation*}
$$

The operators $C_{i}^{\dagger}$ and $C_{j}$ satisfy the usual anticommutation relations.
Following standard procedures, the Hamiltonian here is broken up into a linear checkerboard ${ }^{6}$ as shown in Figure 2. Each of the operators $H_{1}$ and $H_{2}$ is a sum of commuting Hamiltonians for a square. Since the $x$-terms must be shared (divided) between the two Hamiltonians, the Hamiltonian for each square is of the form

$$
\begin{equation*}
h=k+v \tag{1.8}
\end{equation*}
$$

where

$$
\begin{equation*}
k=-\frac{1}{2} t_{x}[K(1,2)+K(3,4)]-t_{y}[K(1,3)+K(2,4)] \tag{1.9}
\end{equation*}
$$

and

$$
\begin{equation*}
v=\frac{1}{2} v_{x}\left[N_{1} N_{2}+N_{3} N_{4}\right]+v_{y}\left[N_{1} N_{3}+N_{2} N_{4}\right] . \tag{1.10}
\end{equation*}
$$

In order to implement the stochastic method, the projection operator is usually simplified by using the above breakup of $H$. Then the first step is to subdivide $\beta$ into $J$ subintervals of width $\Delta=\beta / J$ and make the approximation

$$
\begin{equation*}
e^{-\beta H}=\left(e^{-\Delta\left(H_{1}+H_{2}\right)}\right)^{J}=(U)^{J}=(U(2) U(1))^{J} \tag{1.11}
\end{equation*}
$$

where $U(k) \equiv e^{-\Delta H_{k}}$. The accuracy of this approximation was studied in ref. 4 .
Since the Hamiltonian $H_{k}$ in $U(k)$ is a sum of independent blocks, the matrix elements of $U(k)$ are easy to evaluate in terms of the elements of the matrix $U$ for the four site square. A method for the accurate numerical evaluation of the four site matrix elements in terms of the simple two site problem is presented in Section 2 together with the resulting probabilities and scores. In this section we also give an algorithm for uniquely labeling all possible configurations of the system. In Section 3 we formulate the implementation of our new stochastic algorithm in the presence of negative scores, and describe how the corresponding measurements of energies and correlation functions are carried out. In Section 4 a modification of the basic method is described which allows one to treat larger systems with more degrees of freedom. Section 5 contains the results of the application of the method to the problem of two fully interacting chains. In the conclusion, Section 6, we discuss the advantages and limitations of the method and possible new applications.

## 2. Four Site Problem-Probabilities and Scores

## Matrix Elements:

In order to obtain numerical values of the non-vanishing matrix-elements for the problem of the square, it is convenient to use the Trotter product formula and let the computer do the work. ${ }^{7}$ Writing $h=k+v$, as defined above, we then approximate the general matrix element of $U(k)$ between the states $F$ and I by choosing a finite value for $s$ in the Trotter Product Formula:

$$
\begin{equation*}
\langle F| e^{-\Delta h}|I\rangle \cong\langle F|\left(e^{-(\Delta / 2 s) v} e^{-(\Delta / s) k} e^{-(\Delta / 2 s) v}\right)^{s}|I\rangle \tag{2.1}
\end{equation*}
$$

The basic matrix elements with $\Delta / s$ can be evaluated analytically and then the matrix multiplication necessary to raise it to the $s$ power can be carried out explicitly and easily by the computer. The states F and I are diagonal in fermion occupation numbers. The potential term $v$ is therefore also diagonal. The hopping terms will be split up and evaluated separately.

First define $\delta_{x}=\Delta t_{x} / 2 s$ and $\delta_{y}=\Delta t_{y} / s$ and then write to the same order as before

$$
\begin{equation*}
e^{-\delta k}=e^{\delta_{y}[K(1,3)+K(2,4)]} e^{\delta_{x}[K(1,2)+K(3,4)]} \tag{2.2}
\end{equation*}
$$

Each of these exponential operators factors exactly and can be easily evaluated. For example, the matrix elements of the $\mathrm{K}(1,2)$ term are symmetric and for the single particle move of $(1 \rightarrow 1)$

$$
\begin{equation*}
\langle | e^{\delta_{3} K(1,2)}| \rangle=\cosh \left(\delta_{x}\right) \tag{2.3}
\end{equation*}
$$

- 

while for the move ( $1 \rightarrow 2$ )

$$
\begin{equation*}
\langle | e^{\delta_{x} K(1,2)}| \rangle=\sinh \left(\delta_{x}\right) \tag{2.4}
\end{equation*}
$$

For the $y$-move $(1 \rightarrow 3)$, we find

$$
\begin{equation*}
\langle | e^{\delta_{y} K(1,3)}| \rangle=\sinh \left(\delta_{y}\right) . \tag{2.5}
\end{equation*}
$$

The above relations and approximations allow one to evaluate the necessary matrix elements in order to compute the probabilities for each possible move and its associated score. In numerical experiments, it was found that $s=8$ was sufficient to insure better than one part per million accuracy in all matrix elements. It is a simple matter to load up the matrix $\langle F| U(2) U(1)|I\rangle$ and raise it to the $8^{\text {th }}$ power by squaring it three times. However, first we must turn to the problem of labeling of states, since this will be necessary in order to implement the stochastic algorithm.

Labeling of States:
A convenient way to label fermionic states is by the occupation numbers but expressed as a unique binary number. We define the label $L$ of our states to be

$$
\begin{equation*}
L=\sum_{i} 2^{i-1} n_{i} \tag{2.6}
\end{equation*}
$$

where the sum is over all sites and $n_{i}$ is the eigenvalue of $N_{i}$. The label L will be used to describe our complete lattice as well as the basic square. In this latter case, the label L can range from 0 to 15 exactly corresponding to the 16 possible fermionic states on four sites.

For example if there is a fermion on site 1 , then the move described in eqn.(2.5) will be written as

$$
-\quad\langle 4| e^{\delta_{y} K(1,3)}|1\rangle=\sinh \left(\delta_{y}\right)
$$

where $K(i, j)$ is labeled by sites and the state vectors by L. For the complete
lattice, the label $L$ cannot take on all possible values because the total number of fermions is conserved (approximately one out of four $L$ values is allowed for the cases to be discussed later).

Some Sample Labels:
In order to load a given initial configuration, it is necessary to compute the label $L$ for that arrangement of fermions. In this paragraph we will compute $L$ for some interesting states. One must simply choose the set of $n_{i}$ and evaluate the sum in eqn.(2.6) . We will restrict ourselves to the half-filled band only. With $N$ the number of rungs, and $M(=2 N)$ the total number of sites, then define the number $J=2^{N}$. The 'strong coupling' state (Coulomb repulsion) in which sites $1,4,5,8,9$, etc. are filled has the label

$$
\begin{equation*}
L_{1}=\frac{2}{5}\left(J^{2}-1\right) \tag{2.8}
\end{equation*}
$$

Its left-right reversed partner is

$$
\begin{equation*}
L_{2}=\frac{3}{5}\left(J^{2}-1\right) \tag{2.9}
\end{equation*}
$$

The reader should have no difficulty in proving that these labels are integers. The minimum and maximum label occurs when all the fermions are at the bottom or the top of the ladder. These labels are

$$
\begin{align*}
& L_{\min }=(J-1)  \tag{2.10}\\
& L_{\max }=J(J-1)
\end{align*}
$$

Finally, the labels for the states in which the fermions are all on the left or all
on the right side of the ladder are

$$
\begin{align*}
L_{\mathrm{left}} & =\frac{1}{3}\left(J^{2}-1\right) \\
L_{\mathrm{right}} & =\frac{2}{3}\left(J^{2}-1\right) \tag{2.11}
\end{align*}
$$

Probabilities and Scores:
The sum over intermediate states implicit in Eq. (1.11) is evaluated stochastically with importance sampling. We write

$$
\begin{equation*}
\langle F| U(\Delta, k)|I\rangle=S_{F I}(\Delta, k) P_{F I}(k) \tag{2.12}
\end{equation*}
$$

where F and I are the appropriate L labels and $S_{F I}$ is the score. The probability is denoted by $P_{F I}$, which satisfies

$$
\begin{equation*}
\sum_{F} P_{F I}(k)=1 \tag{2.13}
\end{equation*}
$$

The choice of the probabilities is not completely fixed. Once they are chosen however, the scores are computed via eqn(2.12). The probabilities should be chosen to minimize the fluctuations in the final measured quantity of interest, in part by "smoothing" out the breakup of $H$ into $H_{1}+H_{2}$. We will choose our probabilities to be those appropriate for the four site problem with 'trial' values for the hopping parameter and the Coulomb strength.

## Configurations:

The generation of random configurations with the same score will be carried out essentially as described in ref. 4 but populations will not be generated and stored as separate entities. This cannot be done efficiently if there are negative signs in the scores. ${ }^{8}$

Our states of the full lattice will be written as

$$
\begin{equation*}
|\phi\rangle=\sum_{L} N(\phi, L)|L\rangle \tag{2.14}
\end{equation*}
$$

where $N(\phi, L)$ is the number of configurations with label L in the state $\phi$. These are the expansion coefficients for a general state $\phi$ in terms of the fermion position eigenstates. We will normally keep the total number of configurations,

$$
\begin{equation*}
N_{\mathrm{tot}}=\sum_{L} N(\phi, L) \tag{2.15}
\end{equation*}
$$

large, so that the fact the $N(\phi, L)$ is an integer will introduce a very small error. The states will be stored as an array of numbers $N(\phi, L)$, which as we shall see can be positive or negative.

Decoding the Labels:
The occupation numbers of the fermions can (and will) be decoded from $L$ by using modular arithmetic. Let us introduce a label $\mathrm{L}(\mathrm{I})$ that is the natural label starting from site I and going to M :

$$
\begin{equation*}
L(I)=\sum_{i=I}^{M} 2^{i-I} n_{i} \tag{2.16}
\end{equation*}
$$

Then the lattice label $L=L(1)$. Denoting an 'integer divide' by square brackets, we have

$$
\begin{equation*}
L(I+1)=\lfloor L(I) / 2] \tag{2.17}
\end{equation*}
$$

and hence

$$
\begin{equation*}
-\quad n_{I}=L(I)-2 L(I+1) \tag{2.18}
\end{equation*}
$$

Since an 'integer divide' by two is a shift, the process of decoding is very rapid.

## 3. Implementation

## The Algorithm:

Our stochastic algorithm proceeds in the following way. To proceed one further elemental time step, from the state $\phi$ to the state $\phi^{\prime}$, one operates on the configuration I a total of $N(\phi, I)$ (independent) times with the operator $U=U(2) U(1)$. One such application to $I$ leads to a final configuration $F$ with probability $P(F, I)$ and with score $S(F, I)$. The total probability and score (for the transition of the entire lattice) are products of the basic probabilities and scores for the moves carried out on each elemental square in $H_{1}$ and $H_{2}$. The score is accumulated as one goes through the lattice. The total score for every final state configuration generated is accumulated and stored; i.e. the total score for each is the algebraic sum of the scores from all initial states I that are hit and that lead to the particular configuration in question. Thus the final score for the configuration $F$ is

$$
\begin{equation*}
S(F) \equiv \sum_{I} S(F, I) \tag{3.1}
\end{equation*}
$$

Since some of the paths that lead to $F$ from the $I$ 's can interchange the order of fermions, minus signs will arise in the matrix elements. We see that this accumulated score allows the individual positive and negative scores to cancel as much and as accurately as possible (within statistics). The final task for this time step is to turn these accumulated scores into an integer population distribution.

We have chosen to do this as follows. Compute the total absolute score

$$
\begin{equation*}
S_{\mathrm{tot}}=\sum_{F}|S(F)| \tag{3.2}
\end{equation*}
$$

and form the ratio (which may be negative)

$$
\begin{equation*}
R(F)=\frac{S(F)}{S_{\mathrm{tot}}} \tag{3.3}
\end{equation*}
$$

Then the new integer population distribution for the next intermediate state $\phi^{\prime}$ is given by

$$
\begin{equation*}
N\left(\phi^{\prime}, F\right)=\text { Integer }\left[R(F) N_{\mathrm{tot}}\right], \tag{3.4}
\end{equation*}
$$

where the operation Integer can be performed several ways. We have chosen to throw a random number and to round the product $\left[R(F) N_{\text {tot }}\right]$ to the nearest integer accordingly. Note that the expansion coefficients $N\left(\phi^{\prime}, F\right)$ can be positive or negative.

## Fermion Signs:

The problem of computing the signs of the relevant matrix element for a fermion move is a simple and local task. The signs that arise in most of the moves at a particular square are taken care of by the basic scores computed above. There is only one case that requires a special calculation of the fermionic sign in our site numbering system and that occurs when moves are carried out on the boundary square that connects the bottom to the top rung. This rung also feels the effect of the overall periodic or antiperiodic boundary conditions that have been imposed.

For this particular square, extra minus signs can arise when a fermion is moved from one of these rungs to the other. One must then count whether it bypassed an even or an odd number of (ordered) fermions during the move. Note however that the number of fermions that have been bypassed is given by the initial number loaded on the lattice minus the number in the boundary square. Thus it is a local algorithm and very easy and fast to implement.

## Measuring Energy:

In measuring the energy one can choose the final overlap state $\langle\chi|$ with a wide latitude ${ }^{9}$ so long as it has an overlap with most of the final generated configurations. The simplest choice in our case is probably

$$
\begin{equation*}
\langle x|=\sum_{F} \operatorname{sign}(S(F))\langle F|, \tag{3.5}
\end{equation*}
$$

which is inspired by the discussion in ref. 5 . The final formula for measuring the energy eigenvalue $E_{0}$ is

$$
\begin{equation*}
e^{-\Delta E_{0}}=\frac{\sum_{F}|S(F)|}{N_{\mathrm{tot}}} \tag{3.6}
\end{equation*}
$$

Other choices are possible, and for details see the arguments and discussion in ref. 4 .

## Measuring Correlation Functions:

It is not necessary but we will restrict our discussion to diagonal correlation functions. The three that we shall measure are:

$$
\begin{align*}
C_{x} & =\frac{1}{2}\left\langle N_{1} N_{2}+N_{3} N_{4}\right\rangle \\
C_{y} & =\frac{1}{2}\left\langle N_{1} N_{3}+N_{2} N_{4}\right\rangle  \tag{3.7}\\
C_{d} & =\frac{1}{2}\left\langle N_{1} N_{4}+N_{2} N_{3}\right\rangle
\end{align*}
$$

The correlation functions will be normalized per square, and they range between zero and one-half for a half filled band.
-Instead of measuring these correlation functions for each final configuration, they are computed beforehand and stored as functions of the final configuration label $F$ : i.e. $C_{x}(F), C_{y}(F)$, and $C_{d}(F)$. Then the correlation functions are
evaluated as

$$
\begin{equation*}
\left\langle C_{k}\right\rangle=\frac{\sum_{F} S(F)^{2} C_{k}(F)}{N_{\text {tot }}} \tag{3.8}
\end{equation*}
$$

Numerical results will be given later, but note that the eñergy and all of these diagonal correlation functions can be measured simultaneously.

## 4. Extension to Larger Systems

The array $N(\phi, L)$, which is used to store the distribution of the population, takes up memory space proportional to the number of basis states or to the total number of possible configuration labels. The rapid growth of this number with the number of sites in the system means that implementation of the above algorithm for very large systems is not possible. ${ }^{10}$ An alternative approach which avoids this problem in selected examples is suggested by considering Table 3. For the physically interesting regime of strong Coulomb repulsion, much of the array $N(\phi, L)$ is simply storing zero. The number of important configurations actually generated is considerably smaller than the number of permissible ones.Thus it seems reasonable to attempt to store only those states $L$ which do occur in the population.

We now consider a modified version of the algorithm which does exactly that, by replacing $N(\phi, L)$ by a pair of arrays $L(\phi, j)$ and $N_{s}(\phi, j)$, where $j$ runs from one to the size of the population. As before, $\phi$ specifies the state at a certain time step and is not an index that must be stored. However the index $j$ now only labels the individual members of the population. The information stored in $L(\phi, j)$ and $N_{s}(\phi, j)$ is the configuration label and the integer score of the $j^{\text {th }}$ configuration in the population. Thus, finite computer storage will imply limits
on the size of the populations that can be handled rather than limits on the size of the Hilbert space ( and hence lattice size ).

If a state $L$ occurs $l$ times in the population, we can allocate $l$ values of the index $j$ to this state or combine all occurrences of the state into ane value of $j$. As with the previous method, we will use the latter strategy so that negative weights are cancelled against positive weights; a bonus of this scheme is an improvement in accuracy in that important configurations will not use storage which would otherwise be available for smaller terms. Thus $L(\phi, j) \neq L(\phi, j \prime)$ if $j \neq j \prime$. The number $N_{s}(\phi, j)$ is then the cumulative integer score for the state $j$.

It is precisely this consolidation of states and the associated combining of scores that differentiates this algorithm from the usual (see Refs. 1 and 2 ) population method. The thinning of configurations with negative scores is an essential feature in our algorithm.

Now we will describe the application of our stochastic algorithm to populations stored in this way. ${ }^{11}$ To apply the operator $U$ to the population $\phi$, operate on the state with label $I=L(\phi, 1)$ a number of times given by $\left|N_{s}(\phi, 1)\right|$. The result of each of these operations is a potentially different state and the transition to a final configuration $F$ occurs with probability $P(F, I)$. As each of the final states are generated from the $\left|N_{s}(\phi, 1)\right|$ initial states, their configuration labels and associated scores are written separately into a temporary work area. No care is taken at this point to combine separate instances of any particular final state. One continues to step through the entire population in this way, acting on each configuration the appropriate number of times.

The final population consists of $\sum_{I}\left|N_{s}(\phi, I)\right|$ states with their associated labels and scores, all written into a temporary work area. The final step is to
consolidate the separate occurrences of particular final states and their scores, and write this information back into the arrays $L(\phi 1, j)$ and $N_{s}(\phi 1, j)$. To accumulate this nondegenerate population, there are several sorting methods which can be used. We have implemented several different versions which will be described in detail elsewhere.

The length of time required to apply the operator $U$ to the population and write the results into the temporary work area is proportional to the size of the population. However, the length of time required to perform the sorting and consolidating grows as the square of the population. Techniques have been implemented for decreasing the contribution of this latter factor to the running time by binning the configurations as they are being stored in the temporary work area. This decreases the number in each bin that must be sorted. The introduction of $B$ bins results in a decrease in the coefficient of the quadratic term in the running time on the order of $1 / B$, and a concomitant slight increase in the linear part. Overall time for this algorithm is comparable to but larger than that required by the earlier algorithm, in the regime where the size of the population is roughly the same as the size of Hilbert space.

For the same population and parameter set, the statistical fluctuations should be the same in this method and the one previously described. However, it is clear that this second version can be applied to larger systems for which the earlier algorithm is not applicable due to computer memory restrictions.

## 5. Numerical Results

In order to test the algorithm we first compute the energy density in the absence of a Coulomb interaction, as a function of $t_{\boldsymbol{z}}$ for fixed $t_{y}$ for systems containing $M=4,8$, and 16 sites using both periodic and antiperiodic boundary conditions. This problem can be solved exactly by Fourier transform for any value of $t_{x}$ and $t_{y}$. In particular, for zero transverse hopping ( $t_{x}=0$ ), the problem separates into two independent linear chains of length $N=M / 2$, and by relabelling, one could eliminate all negative matrix elements. The comparison of the energy density for different values of the hopping parameters with the exact result in the absence of a Coulomb repulsion is a severe test of our method. Table 1 shows the values of the energy density $E / M$ for $t_{x}=0,0.5$, and 1.0 for fixed $t_{y}=$ 1.0. The results for periodic and antiperiodic boundary conditions are given. Table 2 shows the values of the energy density $E / M$ for $t_{x}=0.5$ and $t_{y}=1.0$ for $M=4,8$, and 16 sites, again for both periodic and antiperiodic boundary conditions.

The ground state energy density for the case $t_{x}=t_{y}=1.0$ as a function of the strength of the Coulomb interaction, $v_{x}=v_{y}$ with symmetric and antisymmetric boundary conditions is shown in Figures 3 and 4 . In Figure 5 we show the variation of the energy density as both $t_{x}$ and $v_{x}=v_{y}$ are varied with $t_{y}$ fixed.

In Figure 6 , we plot the three correlation functions, defined in Eqn.(3.7) as functions of the Coulomb coupling $v_{x}=v_{y}$. The approach to the strong coupling limit ( $C_{x}=C_{y}=0 ; C_{d}=0.5$ ) is clear.

Finally, Table 3 shows the variation of the number $N_{c}$ of distinct configurations in the ground state wave function as generated by our stochastic method for different values of the hopping parameters and the Coulomb coupling. The rapid
decrease of $N_{c}$ with increasing $v_{x}=v_{y}$ and decreasing $t_{x}$ (for fixed $t_{y}$ ) should be noted. This suggests that the method may be applicable to larger systems without a drastic increase in the number of configurations that must be included, at least for the case of a small interchain hopping parameter and a large Coulomb interaction.

## 6. Discussions and Conclusions

The method presented in this paper provides an extension of stochastic Monte Carlo methods to the study of fermion systems in slightly more than one-dimension. Even though the infamous minus signs in the matrix elements or weighting functions cannot be eliminated in this case, the method seems to converge well. Its main advantages and limitations are:

1. It is simple to implement, requiring only local operations and a small number of memory lookups.
2. The square (four site) matrix elements are computed essentially exactly with the Coulomb terms present. These are then used to determine accurately the probabilities and scores.
3. The splitting of the Hamiltonian into $H_{1}$ and $H_{2}$, chosen so that they can be applied independently as a direct product, does not introduce any significant errors.
4. Each sweep through the set of configurations in the population produces an improved trial wave function which is closer to the exact ground state solution. One may then take two possible approaches to improve the accuracy and limit the statistical fluctuations of measurements:
(a) In the first one starts with a population of $N_{\text {tot }}$ strong coupling configurations and applies the $U$ projection operator $L+\Delta L$ times. Measurements are carried out only during the last $\Delta L$ time steps. This is then repeated by starting with the same initial population, thereby generating a set of statistically independent averages.
(b) In the second approach one does not start the repetition of the process by reloading the initial population but retains the distribution of configurations that has been generated.
5. Even for values of $t_{x}$ comparable to $t_{y}$, where there are sizable cancellations, the measured values given by the accumulated score method converge well in the presence of fermionic minus signs. However, to obtain reasonably accurate results, one must use populations that are sufficiently large. Indeed, for no Coulomb interaction, the number must be of the order of the maximum possible number of configurations $\sim(2 N)!/(N!)^{2}$. This number becomes unmanageable for lattices only slightly larger than the $\sim 16$ total sites treated here. While this is indeed a serious drawback of the first method as implemented in this paper, this criticism does not apply to the second method as discussed in Section 5. However the necessary sorting requires additional computer time.
6. One can see from Table 3 that the number of distinct configurations that are generated stochastically decreases markedly in certain regions of parameter space. This can be used as the starting point for several different implementations of the basic algorithm. The reduction in the number of important configurations in the Coulomb regime means that the modified algorithm can be applied effectively. We have found that by starting the
system off with a strong Coulomb term and reducing it in steps as the Monte Carlo proceeds, one gets good results without a large increase in the number of configurations generated. This feature in turn will permit the treatment of much larger systems without a prohibitive increase in the necessary computer memory or in the population required to get statistically significant results (and hence the computing time required).

In summary, we have found that double fermionic chains can be treated by our new algorithm. The accumulated score method as implemented here seems to converge well even in the presence of fermionic minus signs. The numerical fluctuations are reasonable and measurements can be performed quite efficiently ${ }^{12}$ for both energies and correlation functions. An application of the method described here to determine the ground state properties of the Periodic Anderson Model is presently underway, and results will be reported elsewhere.

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8. For background, see the discussion in refs. 1 and 2 .
9. See the discussion in refs. 4 and 5 .
10. For example, for the case treated in Section $5, M=16$, the total number of possible configurations for a half filled band is only 12,870 . However, a modest increase to $M=20$ would require several megabytes of computer memory.
11. For contrast, see the description of the Ensemble Projector Monte Carlo by T. A. DeGrand and J. Potvin, Phys. Rev. D91, 871 (1985).
12. All our data presented in this paper were obtained in $\sim 2$ hours on the SLAC 8 MIPS IBM3081K machine. A typical set of parameters for 16 sites is $\beta=8, T=32$ (which was more than adequate for convergence), and $N_{t o t}=16,000$. A complete measurement of the energy and the correlation functions ran in less than two minutes.

Table 1

| Periodic Boundary Condition |  |  | Antiperiodic Boundary Condition |  |
| :---: | :---: | :---: | :---: | :---: |
| $t_{\boldsymbol{x}}$ | E/M | Exact | E/M | Exact |
| 0 | $-0.605(2)$ | -0.6036 | $-0.656(1)$ | -0.6533 |
| 0.5 | $-0.667(3)$ | -0.6661 | $-0.659(2)$ | -0.6533 |
| 1 | $-0.732(3)$ | -0.7286 | $-0.721(2)$ | -0.7119 |

Stochastic and exact energy densities for 16 sites and for selected $t_{x}$ values. This data is for no Coulomb interaction and $t_{y}=1.0$. A conservative estimate of the statistical uncertainties of the last digits are given in the parentheses.

Table 2

| $M$ | E/M Periodic | Exact | E/M Antiperiodic | Exact |
| :---: | :---: | :---: | :---: | :---: |
| 4 | $-1.001(3)$ | -1.0000 | $-0.248(3)$ | -0.2500 |
| 8 | $-0.625(4)$ | -0.6250 | $-0.712(3)$ | -0.7071 |
| 16 | $-0.667(3)$ | -0.6660 | $-0.659(2)$ | -0.6533 |

Size dependence of the stochastic and exact energy densities for no Coulomb term, $t_{x}=0.5$, and $t_{y}=1.0$. A conservative estimate of the statistical uncertainties in the last digit is given in the parentheses.

Table 3

| $t_{x}$ | $v_{x}=x_{y}$ | $N_{c}$ |
| :---: | :---: | :---: |
|  | 0 | 7490 |
| 1 | 4 | 3178 |
|  | 8 | 1104 |
|  | 0 | 5182 |
| 0.5 | 4 | 1962 |
|  | 8 | 791 |
|  | 0 | 3598 |
| 0 | 4 | 1255 |
|  | 8 | 487 |

The number of distinct configurations $N_{c}$ generated for 16 sites at various values of $t_{z}$ and $v_{z}=v_{y}$, with $t_{y}$ fixed at 1.0. The maximum possible value of $N_{c}$ is 12870 .

## FIGURE CAPTIONS

1. The double chain and the labeling of sites. The total number of sites is $M$, and the total number of rungs is $N(=M / 2)$.
2. The double chain and the breaking up into Hamiltonians $H_{1}$ and $H_{2}$.
3. Plot of the energy per site as a function of the Coulomb coupling $v_{x}=v_{y}$ for a lattice of size $M=16$ sites with symmetric boundary conditions.
4. Same plot as Fig. 3 but with antisymmetric boundary conditions.
5. Plot of the energy per site as a function of the transverse hopping parameter $t_{z}$ with the longitudinal $t_{y}$ fixed, and as a function of the Coulomb coupling $v_{x}=v_{y}$ for symmetric boundary conditions.
6. A plot of the three correlation functions defined in the text is given as a function of the Coulomb coupling $v_{x}=v_{y}$. The hopping parameters are both fixed at one.


Fig. 1


Fig. 2


Fig. 3


Fig. 4


Fig. 5


Fig. 6


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