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A generalization of Handscomb's quantum Monte Carlo scheme—application to the 1D Hubbard model

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Abstract. A recently introduced generalization of Handscomb's quantum Monte Carlo scheme is further developed. Expressions for expectation values of various observables are studied in detail. A more efficient algorithm for importance sampling in a space of state vectors and operator strings is constructed, using the 1D Hubbard model as an illustrative example. As a test of the method, 32-site rings at band fillings $\frac{1}{4}$, $\frac{3}{8}$ and $\frac{1}{2}$ are studied at a low temperature. Results for spin- and charge-density structure factors and static susceptibilities are presented.

1. Introduction

Quantum Monte Carlo simulation is a powerful non-perturbative method for studies of lattice models in condensed-matter physics. A host of simulation techniques have been developed, such as the Suzuki–Trotter [1–5] and Handscomb's [6–9] schemes for spin systems and world-line [10] and determinant [11–13] methods for interacting-fermion systems. Apart from the so-called 'sign problem' [14], which restricts the class of models which can be efficiently studied, a limiting factor is the very long computation times required for large systems at low temperatures, where the interesting physics takes place. Thus there is continued interest in algorithm development. In this paper we further develop the generalization of Handscomb's scheme introduced in [15], and apply it to the 1D Hubbard model.

Consider the thermal expectation value of an operator $\hat{A}$ at temperature $T = 1/\beta$,

$$\langle \hat{A} \rangle = \frac{1}{Z} \mathrm{Tr}\{ \hat{A} \mathrm{e}^{-\beta \hat{H}} \} \tag{1.1}$$

for a system described by a Hamiltonian

$$\hat{H} = \sum_{i=1}^{M} \hat{H}_i \,. \tag{1.2}$$

In Handscomb's simulation scheme [6] $\mathrm{e}^{-\beta \hat{H}}$ is Taylor-expanded and the powers of $\hat{H}$ are written as sums of products of the operators $\hat{H}_i$, i.e.

$$\langle \hat{A} \rangle = \frac{1}{Z} \sum_{n=0}^{\infty} \sum_{S_n} \frac{(-\beta)^n}{n!} \mathrm{Tr}\left\{ \hat{A} \prod_{i=1}^{n} \hat{H}_{l_i} \right\} \tag{1.3}$$

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where S_n denotes an index sequence $l_1, \ldots, l_n$ with $1 \leqslant l_i \leqslant M$. The partition function is similarly written as

$$Z = \sum_{n=0}^{\infty} \sum_{S_n} \frac{(-\beta)^n}{n!} \mathrm{Tr}\left\{ \prod_{i=1}^{n} \hat{H}_{l_i} \right\} = \sum_{n=0}^{\infty} \sum_{S_n} W(S_n) . \tag{1.4}$$

If all the traces in (1.3) and (1.4) can be rapidly evaluated, expectation values can be estimated sampling the sequences S_n using the magnitude of $W(S_n)$ as the relative probability of generating a sequence S_n. However, the traces are generally not easy to evaluate, and the method is essentially applicable only to the $s = \frac{1}{2}$ Heisenberg model, for which the traces can be evaluated analytically in any number of dimensions [6]. In [15] a generalization was developed in which instead of the traces above, matrix elements $\langle \alpha | \prod H_{l_i} | \alpha \rangle$ are used in the weights. The sampling space is thus extended to also include a complete set of basis states so that a 'configuration' is specified by an index sequence and a state vector. This scheme is applicable to a much wider class of models. In the present study the method is further improved on. Specifically, a new procedure for generating configurations is developed and general expressions for various expectation values are studied in detail. The method is applicable to spin systems and interacting fermion and boson systems. In the case of fermions the sign problem is likely to limit the use to one-dimensional systems. As a demonstration of the method, a study of the one-dimensional Hubbard model is included.

In section 2 the general formalism of the method is introduced and in section 3 expressions for operator averages of interest are derived. In section 4 a scheme for generating configurations is developed, using the 1D Hubbard model as an illustrative example. Results of test runs on this model are compared with exact data for small systems in section 5, where results of simulations of larger systems at various band fillings are also presented.

2. General formalism

Writing the trace in (1.3) as a sum over diagonal matrix elements, the thermal expectation value of an operator $\hat{A}$ can be written

$$\langle \hat{A} \rangle = \frac{1}{Z} \sum_{\alpha} \sum_{n=0}^{\infty} \sum_{S_n} \frac{(-\beta)^n}{n!} \left\langle \alpha \left| \hat{A} \prod_{i=1}^{n} \hat{H}_{l_i} \right| \alpha \right\rangle \tag{2.1}$$

where the states $|\alpha\rangle$ form a complete set. We define a weight function for configurations (α, S_n) as

$$W(\alpha, S_n) = 3 \frac{(-\beta)^n}{n!} \left\langle \alpha \left| \prod_{i=1}^{n} \hat{H}_{l_i} \right| \alpha \right\rangle . \tag{2.2}$$

Given that a function $A(\alpha, S_n)$ can be found, such that (2.1) can be written

$$\langle \hat{A} \rangle = \frac{\sum_{\alpha} \sum_{n=0}^{\infty} \sum_{S_n} A(\alpha, S_n) W(\alpha, S_n)}{\sum_{\alpha} \sum_{n=0}^{\infty} \sum_{S_n} W(\alpha, S_n)} \tag{2.3}$$

the average can be estimated using importance sampling in the space $\{|\alpha\rangle\} \otimes \{S_n, n = 0, 1, \ldots, \infty\}$. In [15] a maximum length of the sequences was chosen in a self-consistent fashion and unit operators were introduced in the operator products shorter than the maximum length, so that the simulation scheme could be formulated in a space with fixed length of the index sequences. Here we will put no upper bound, however, and there are no intrinsic approximations in the method. As in Handscomb's scheme, the contributions from different lengths of the sequences will be determined by the temperature and the energy and the heat capacity of the system [6]. Only a limited range of lengths will give significant contributions. Thus the fact that the sampling space includes index sequences of all lengths will pose no problem in practice (except perhaps close to a phase transition).

We will work under the assumption that a positive-definite weight can be constructed, so that an expectation value is given by

$$\langle \hat{A} \rangle = \langle A(\alpha, S_n) \rangle_W \tag{2.4}$$

where $\langle \cdots \rangle_W$ indicates the arithmetic average with the configurations generated using W as a relative weight. We choose a basis $\{|\alpha\rangle\}$ in which the Hamiltonian can be written as a sum of operators $\hat{H}_i$ such that

$$\hat{H}_i|\alpha\rangle = h(i, \alpha)|\alpha'\rangle \qquad |\alpha\rangle, |\alpha'\rangle \in \{|\alpha\rangle\} \tag{2.5}$$

i.e. the result of $\hat{H}_i$ operating on a basis vector is proportional to a basis vector (or zero). Typically, for spin systems the basis chosen is the basis $\{|S_1^z, \ldots, S_N^z\rangle\}$ of eigenstates of the z-component of the spin at all sites and for tight-binding models the basis $\{|n_1, \ldots, n_N\rangle\}$ of eigenstates of the number operators for all sites. We define a propagated state $|\alpha(p)\rangle$,

$$|\alpha(p)\rangle = r \prod_{i=1}^{p} \hat{H}_{l_i}|\alpha\rangle \qquad |\alpha(0)\rangle = |\alpha\rangle \tag{2.6}$$

where r is a normalization factor. The matrix element in (2.2) is then

$$\left\langle \alpha \middle| \prod_{i=1}^{n} \hat{H}_{l_i} \middle| \alpha \right\rangle = \begin{cases} \prod_{i=1}^{n} h[l_i, \alpha(i-1)] & \text{if } |\alpha(n)\rangle = |\alpha(0)\rangle \\ 0 & \text{otherwise.} \end{cases} \tag{2.7}$$

In a Monte Carlo simulation a configuration $(\alpha', S'_{n'})$ is tentatively generated from a configuration (α, S_n) by a small change in the latter. The probability of accepting the new configuration involves the ratio of the weight factors,

$$R = \frac{W(\alpha', S'_{n'})}{W(\alpha, S_n)}. \tag{2.8}$$

The updating scheme should be constructed such that the part of the product in (2.7) affected by a change can be easily isolated and the ratio rapidly evaluated. Before such a scheme is constructed in section 4, we turn our attention to general expressions for a number of expectation values of interest.

3. Expressions for expectation values

Since

$$W(\alpha, S_n) = W[\alpha(p), S_n(p)] \tag{3.1}$$

where $S_n(p)$ is the index sequence $l_{p+1}, \ldots, l_n, l_1, \ldots, l_p$, obtained by cyclically permuting S_n p times, an equivalent expression for the average (2.4) is

$$\langle \hat{A} \rangle = \left\langle \frac{1}{n} \sum_{p=0}^{n-1} A[\alpha(p), S_n(p)] \right\rangle_W . \tag{3.2}$$

The use of the averaged A improves on the statistics of the simulation and also, as will be seen below, allows for some formal simplifications.

If the operator $\hat{A}$ is diagonal in the basis used, i.e.

$$\hat{A}|\alpha\rangle = a(\alpha)|\alpha\rangle \tag{3.3}$$

we clearly have $A(\alpha, S_n) = a(\alpha)$, or

$$\langle \hat{A} \rangle = \left\langle \sum_{p=0}^{n-1} a[\alpha(p)] \right\rangle_W . \tag{3.4}$$

For non-diagonal operators the situation is more complicated. In principle an expression for an expectation value of any operator $\hat{A}$ can be constructed if $\hat{A}$ can be written as a sum of products of the operators $\hat{H}_i$ in the Hamiltonian. Consider $\hat{A} = \hat{H}_k$. Then

$$\langle \hat{A} \rangle = \langle \hat{H}_k \rangle = \frac{1}{Z} \sum_{\alpha} \sum_{n=0}^{\infty} \sum_{S_n} \frac{(-\beta)^n}{n!} \left\langle \alpha \left| \hat{H}_k \prod_{i=1}^{n} \hat{H}_{l_i} \right| \alpha \right\rangle . \tag{3.5}$$

For a given state $|\alpha\rangle$ there is a one-to-one correspondence between the contributing sequences of length $m-1$ above and sequences of length m which give a non-zero weight (2.2) and which have k as their last element ($l_m = k$). Thus, defining

$$A(\alpha, S_n) = \begin{cases} -n/\beta & l_n = k \\ 0 & l_n \neq k \end{cases} \tag{3.6}$$

we get (3.5) when summing $A(\alpha, S_n) W(\alpha, S_n)$. Using (3.2) the average is obtained sampling the number $N(k)$ of indices k in the sequences

$$\langle \hat{H}_k \rangle = -\frac{1}{\beta} \langle N(k) \rangle_W . \tag{3.7}$$

Thus the energy is given by the average length of the sequences

$$E = -\frac{1}{\beta} \langle n \rangle_W . \tag{3.8}$$

The heat capacity is obtained taking the derivative with respect to the temperature of the above expression. The result is

$$C = \langle n^2 \rangle_W - \langle n \rangle_W^2 - \langle n \rangle_W \,. \tag{3.9}$$

For a product of m operators $\hat{H}_{k_1}, \ldots, H_{k_m}$ we get

$$\left\langle \prod_{i=1}^{m} \hat{H}_{k_i} \right\rangle = \frac{1}{(-\beta)^m} \left\langle \frac{(n-1)!}{(n-m)!} N(k_1, \ldots, k_m) \right\rangle_W \tag{3.10}$$

where $N(k_1, \ldots, k_m)$ denotes the number of ordered sub-sequences $k_1, \ldots, k_m$ in S_n. The form of (3.10) indicates that it will be difficult to obtain good estimates of products of a large number of operators.

Now consider an *imaginary-time-dependent product*

$$\hat{A}_2(\tau)\hat{A}_1(0) = \mathrm{e}^{\tau \hat{H}} \hat{A}_2 \mathrm{e}^{-\tau \hat{H}} \hat{A}_1 \,. \tag{3.11}$$

Taylor-expanding the exponentials, the ensemble average can be written

$$\langle \hat{A}_2(\tau)\hat{A}_1(0) \rangle = \frac{1}{Z} \sum_{\alpha} \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} \frac{(\tau-\beta)^n (-\tau)^m}{n!m!} \langle \alpha | \hat{H}^n \hat{A}_2 \hat{H}^m \hat{A}_1 | \alpha \rangle \,. \tag{3.12}$$

Changing to a summation over index sequences and a sum over all positions of $\hat{A}_2$ in the operator product results in

$$\langle \hat{A}_2(\tau)\hat{A}_1(0) \rangle = \frac{1}{Z} \sum_{\alpha} \sum_{n=0}^{\infty} \sum_{m=0}^{n} \sum_{S_n} \frac{(-\tau)^m (\tau-\beta)^{n-m}}{(n-m)!m!}$$
$$\times \left\langle \alpha \left| \prod_{i=m+1}^{n} \hat{H}_{l_i} \hat{A}_2 \prod_{j=1}^{m} \hat{H}_{l_j} \hat{A}_1 \right| \alpha \right\rangle . \tag{3.13}$$

Consider first the case of $\hat{A}_1$, $\hat{A}_2$ diagonal. We then get, comparing with the weight function (2.2) and using (3.2),

$$\langle \hat{A}_2(\tau)\hat{A}_1(0) \rangle = \left\langle \sum_{p=0}^{n-1} \sum_{m=0}^{n} \frac{\tau^m (\beta-\tau)^{n-m}}{\beta^n} \frac{(n-1)!}{(n-m)!m!} a_1[\alpha(p)] a_2[\alpha(p+m)] \right\rangle_W . \tag{3.14}$$

The propagated states $|\alpha(p)\rangle$ are periodic for all allowed configurations, so that with an index sequence of length n, $|\alpha(n+p)\rangle = |\alpha(p)\rangle$. For $\hat{A}_1$, $\hat{A}_2$ not necessarily diagonal, consider the simplest case $\hat{A}_1 = \hat{H}_{k_1}$, $\hat{A}_2 = \hat{H}_{k_2}$. We then get

$$\langle \hat{H}_{k_2}(\tau)\hat{H}_{k_1}(0) \rangle = \left\langle \sum_{m=0}^{n-2} \frac{\tau^m (\beta-\tau)^{n-m-2}}{\beta^n} \frac{(n-1)!}{(n-m-2)!m!} N(k_1, k_2; m) \right\rangle_W \tag{3.15}$$

where $N(k_1, k_2; m)$ is the number of times the indices k_1, k_2 appear in the sequence S_n in the given order and separated by m positions.

Integrating $\langle \hat{A}_2(\tau)\hat{A}_1(0)\rangle$ from 0 to β gives a Kubo integral. Using the periodicity of the propagated states gives in the diagonal case

$$\int_0^\beta d\tau \langle \hat{A}_2(\tau)\hat{A}_1(0)\rangle = \left\langle \frac{\beta}{n(n+1)} \left[\left(\sum_{p=0}^{n-1} a_1[\alpha(p)] \right) \left(\sum_{p=0}^{n-1} a_2[\alpha(p)] \right) + \sum_{p=0}^{n-1} a_1[\alpha(p)] a_2[\alpha(p)] \right] \right\rangle_W . \tag{3.16}$$

For the product $\langle \hat{H}_{k_2}(\tau)\hat{H}_{k_1}(0)\rangle$ considered above, the Kubo integral becomes

$$\int_0^\beta d\tau \langle \hat{H}_{k_2}(\tau)\hat{H}_{k_1}(0)\rangle = \frac{1}{\beta} \left\langle \sum_{m=0}^{n-2} N(k_1, k_2; m) \right\rangle_W \tag{3.17}$$

which can be written in the simple form

$$\int_0^\beta d\tau \langle \hat{H}_{k_2}(\tau)\hat{H}_{k_1}(0)\rangle = \frac{1}{\beta} \langle N(k_1)N(k_2)\rangle_W . \tag{3.18}$$

4. Application to the 1D Hubbard model

In this section a simulation scheme for the 1D Hubbard model in the canonical ensemble is constructed. The Hamiltonian is

$$\hat{H} = -t \sum_{i=1}^{N} \sum_{\sigma=\uparrow,\downarrow} (c_{i,\sigma}^+ c_{i+1,\sigma} + c_{i+1,\sigma}^+ c_{i,\sigma}) + U \sum_{i=1}^{N} n_{i\uparrow} n_{i\downarrow} \tag{4.1}$$

where the operators refer to the position basis, with basis states

$$|\alpha\rangle = |n_{1\uparrow}, \ldots, n_{N\uparrow}\rangle \otimes |n_{1\downarrow}, \ldots, n_{N\downarrow}\rangle . \tag{4.2}$$

As we work in the canonical ensemble the sum in (2.1) is over all states with given numbers of particles with spin up and down. We define the operators

$$\begin{aligned} \hat{H}_{1,i} &= c_{i,\uparrow}^+ c_{i+1,\uparrow} + c_{i+1,\uparrow}^+ c_{i,\uparrow} \\ \hat{H}_{2,i} &= c_{i,\downarrow}^+ c_{i+1,\downarrow} + c_{i+1,\downarrow}^+ c_{i,\downarrow} \\ \hat{H}_{3,i} &= 1 - n_{i\uparrow} n_{i\downarrow} \\ \hat{H}_{4,i} &= 1 . \end{aligned} \tag{4.3}$$

In terms of these operators the Hamiltonian, with t set to 1, can be written

$$\hat{H} = -\sum_{i=1}^{N}(\hat{H}_{1,i} + \hat{H}_{2,i} + U\hat{H}_{3,i} + \hat{H}_{4,i}) + N(U+1)\,. \tag{4.4}$$

The unit operators are included in $\hat{H}_{3,i}$ in order to make the weight function positive-definite. The unit operators $\hat{H}_{4,i}$ are added to the Hamiltonian for the purposes of the updating scheme. The constant $N(U+1)$ only sets the zero of the energy and is neglected in the simulation.

We adopt the phase conventions

$$\begin{aligned} c^{+}_{i,\uparrow}|\ldots, n_{i\uparrow} = 0, \ldots\rangle &= (-1)^{n^{<}_{i\uparrow}}|\ldots, n_{i\uparrow} = 1, \ldots\rangle \\ c^{+}_{i,\downarrow}|\ldots, n_{i\downarrow} = 0, \ldots\rangle &= (-1)^{n_{\uparrow}+n^{<}_{i\downarrow}}|\ldots, n_{i\downarrow} = 1, \ldots\rangle \end{aligned} \tag{4.5}$$

where $n^{<}_{i\sigma}$ denotes the number of spin-σ particles on sites with position numbers less than i and $n_{\uparrow}$ is the total number of spin-$\uparrow$ particles. For $c_{i,\uparrow}$ and $c_{i,\downarrow}$ similar phase relationships hold. With antiperiodic boundary conditions,

$$\begin{aligned} c^{+}_{N+1,\sigma} &= -c^{+}_{1,\sigma} \\ c_{N+1,\sigma} &= -c_{1,\sigma} \end{aligned} \tag{4.6}$$

it follows that if both $n_{\uparrow}$ and $n_{\downarrow}$ are even, any $\hat{H}_{a,b}$ gives the phase $+1$ when operating on a basis vector. A positive-definite weight function is thus ensured.

Now, let S_n denote a sequence of index pairs $\binom{a_1}{b_1}, \ldots, \binom{a_n}{b_n}$, with $a_i = 1,2,3,4$, and $b_i = 1, \ldots, N$. We will also use the notation $\binom{a}{b}_i$ and call this object an a-operator acting on the state $|\alpha(i)\rangle$, as if it were the actual operator $\hat{H}_{a,b}$.

The weight function can now be written

$$W(\alpha, S_n) = \frac{\beta^n U^{n_3}}{n!} M(\alpha, S_n) \tag{4.7}$$

where n_3 is the number of 3-operators in S_n and M is the matrix element

$$M(\alpha, S_n) = \left\langle \alpha \middle| \prod_{i=1}^{n} \hat{H}_{a_i,b_i} \middle| \alpha \right\rangle . \tag{4.8}$$

With the definitions (4.3) M is always equal to 0 or 1.

We now construct an algorithm for a random walk in the space $\{|\alpha\rangle\} \otimes \{S_n, n = 1,2,\ldots,\infty\}$, satisfying the detailed balance principle,

$$\frac{P[(\alpha, S_n) \to (\alpha', S'_{n'})]}{P[(\alpha', S'_{n'}) \to (\alpha, S_n)]} = \frac{W(\alpha', S'_{n'})}{W(\alpha, S_n)} \tag{4.9}$$

where $p[(\alpha, S_n) \to (\alpha', S'_{n'})]$ is the probability of making a transition from (α, S_n) to $(\alpha', S'_{n'})$. Starting from a configuration with non-zero weight, the weight function ratio is

$$R = \frac{W(\alpha', S'_{n'})}{W(\alpha, S_n)} = \frac{n!}{n'!}\frac{\beta^{n'}}{\beta^n}\frac{U^{n'_3}}{U^{n_3}} M(\alpha', S'_{n'}). \tag{4.10}$$

As $M(\alpha', S'_{n'})$ is either zero or one, all acceptance probabilities can be calculated under the assumption that it actually is equal to unity. Then M need only be evaluated in case a change has been (tentatively) accepted and the change finally accepted if M remains equal to one and rejected otherwise. This allows for considerable time savings, since the most time-consuming step is the evaluation of M.

The updating scheme consists of a number of Monte Carlo moves which together ensure ergodicity. The length of the index sequence is changed by inserting and removing 4-operators, which can appear anywhere in the sequence, independently of the state $|\alpha\rangle$. All other moves are made with the length of the sequence fixed. The number of 3-operators is changed in moves of the type $\binom{4}{b}_p \leftrightarrow \binom{3}{b'}_p$. Any 3-operator can be removed from a sequence, whereas $\binom{3}{b}$ cannot be inserted at position p if site b in the state $|\alpha(p-1)\rangle$ is doubly occupied. Changes in the number of 1- and 2-operators must involve (at least) two operators in order to maintain a non-zero weight. Moves of the types $\binom{4}{b}_{p_1}\binom{4}{b}_{p_2} \leftrightarrow \binom{t}{b}_{p_1}\binom{t}{b}_{p_2}$, $t = 1, 2$, are sufficient to generate all allowed sequences for an open chain. With periodic boundary conditions additional moves changing the 'winding number' must be included, at least for small N and when boundary conditions are important. In moves involving 1- or 2-operators at positions p_1 and p_2, the states $|\alpha(k)\rangle$, $k = p_1, \ldots, p_2 - 1$ (alternatively $k = p_2, \ldots, p_1 - 1$), are affected (the position indices are periodic with period n). The move results in a zero matrix element M if an operator $\binom{t}{b}_p$ acts on a state $|\alpha(p-1)\rangle$ with $n_{b\uparrow}(p-1) = n_{b+1\uparrow}(p-1)$ or $n_{b\downarrow}(p-1) = n_{b+1\downarrow}(p-1)$ and $t = 1, 2$ respectively. The move can also result in a 3-operator acting on a doubly occupied site, which again gives a zero M. For the moves involving 1- or 2-operators the index sequence is split into $N/2$ sub-sequences, with the kth sub-sequence containing all operators acting on either the two sites $2k$, $2k+1$ or $2k-1$, $2k$. Moves involving operators acting between pairs of sites are then made in the corresponding sub-sequences. The time needed to check for illegal operations is thus independent of the size of the system. Changes in the state vector $|\alpha\rangle$ are also made with the index sequence split. We now consider the different types of moves in detail.

(i) Moves changing the length of the sequence: starting with $p = 1$, an attempt is made to remove the operator $\binom{a}{b}_p$ if $a = 4$. Thereafter an attempt is made to insert an operator $\binom{4}{b'}_{p'}$, with $p' = p + 1 - n_r + n_i$, where n_r and n_i are the number of operators so far removed and inserted respectively. These steps are repeated a number, L, of times with $p \to p + 1$. L is chosen larger than the maximum length that the sequence will reach, so that each position is visited at least once in a series of moves. (After the last position has been visited we continue from $p = 1$ in the new sequence.) Half of the times the series of moves is made in the opposite direction, i.e. starting from $p = n$ and attempting the insertions in the direction of decreasing position numbers. There are $n + 1$ positions at which an operator can be inserted in a sequence of length n. Thus the above scheme gives the correct *a priori* frequency for attempting insertions and removals. We can then use the heat-bath acceptance probabilities

$$P[\text{insert 4-operator}] = \frac{N\beta}{n+1+N\beta}$$
$$P[\text{remove 4-operator}] = \frac{n}{n+N\beta} \tag{4.11}$$

which satisfy detailed balance if b' above is chosen with equal probabilities amongst

$1,\ldots,N$.

(ii) Moves changing the number of 3-operators: starting from $p = 1$ a change $\binom{a}{b}_p \to \binom{a'}{b'}_p$ is attempted with $a' = 3$ if $a = 4$ and vice versa. If $a = 1$ or $a = 2$ the state $|\alpha(p-1)\rangle$ is propagated with $\binom{a}{b}_p$, generating $|\alpha(p)\rangle$. The above steps are repeated with $p = 2,\ldots,n$. An attempted move $\binom{4}{b}_p \to \binom{3}{b'}_p$ results in zero weight for the new configuration if the site b' is doubly occupied in $|\alpha(p-1)\rangle$. Such an attempt is therefore rejected. For the allowed moves we use the Metropolis acceptance probabilities

$$P\left[\binom{3}{b} \to \binom{4}{b'}\right] = \min[1, 1/U]$$
$$P\left[\binom{4}{b} \to \binom{3}{b'}\right] = \min[1, U]\,. \tag{4.12}$$

(iii) Moves changing the number of 1- and 2-operators: the index sequence is first split into $N/2$ sub-sequences with each sub-sequence containing all 1-, 2- and 3-operators acting on a distinct pair of sites $i, i+1$, and the 4-operators $\binom{4}{i}$. Moves of the type $\binom{t}{i}\binom{t}{i} \leftrightarrow \binom{4}{i}\binom{4}{i}$ are then attempted within the sub-sequences. There are two ways of splitting the sequence; with the kth sub-sequence containing the operators at sites $2k-1, 2k$ (A) or $2k, 2k+1$ (B). In the updating process the two sites are labelled 1, 2 and the operators are renumbered so that all sub-sequences contain operators $\binom{t}{1}, \binom{t}{2}, \binom{t}{3}, \binom{3}{1}, \binom{3}{2}, \binom{4}{2}$, $t = 1, 2$, with the operators $\binom{t}{2}$ acting between sites 1, 2 and the operators $\binom{3}{i}$ acting on site i. The moves considered are then of the type $\binom{t}{2}\binom{t}{2} \leftrightarrow \binom{4}{2}\binom{4}{2}$. The positions of the operators in the original sequence are stored, so that the full sequence can be recombined after performing a number of moves in each sub-sequence. Figure 1 shows an example of an index sequence and the way it is split into sub-sequences. Now consider the actual updating of a sub-sequence. Let

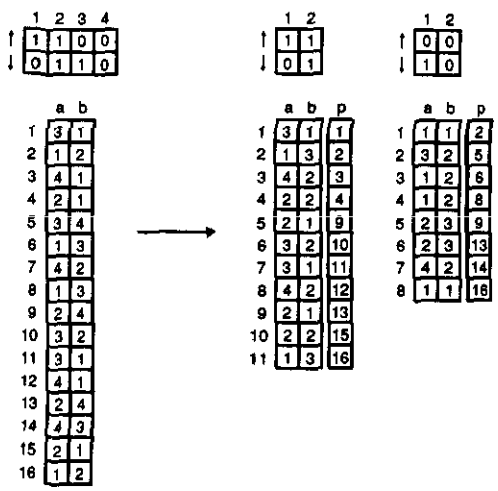

Figure 1. Example of a state and an index sequence for a 4-site system (left). To the right are the two renumbered sub-sequences obtained by splitting the sequence according to (A) in (iii), along with the corresponding two-site states. a and b refer to an operator $\binom{a}{b}$ and p in the sub-sequences is the position of the operator in the full sequence.

l denote the length of the sub-sequence. One of the operators $\binom{a}{2}_p$, $a = 1, 2, 4$, is chosen at random, where p now is a position in the sub-sequence, $p \in \{1, \ldots, l\}$. If $a = 4$ let $a' = 1, 2$ with equal probabilities. If $a = 1$ or $a = 2$ let $a' = 4$. Since there are two ways of choosing a' if $a = 4$, compared to only one otherwise, the change is cancelled with probability 0.5 in the latter case. The *a priori* probabilities of attempting moves are then equal in both directions at this point. Define t such that $t = a'$ if $a = 4$ and $t = a$ otherwise. Consider a change $\binom{a}{2}_p \binom{a}{2}_{p'} \rightarrow \binom{a'}{2}_p \binom{a'}{2}_{p'}$. This change will result in a forbidden operation if the sub-sequence contains an operator $\binom{t}{1}_{p''}$ or $\binom{t}{3}_{p''}$ with $p < p'' < p'$ (the position variables p are periodic with period l). We therefore search the sub-sequence in the forward direction, starting from the chosen $p + 1$. The numbers N_a, $N_{a'}$ of operators $\binom{a}{2}$ and $\binom{a'}{2}$ encountered are stored, along with the positions p_i of the operators $\binom{a}{2}$. The search is terminated when an operator $\binom{t}{1}$ or $\binom{t}{3}$ is encountered. A position p_i, $i = 1, \ldots, N_a$, is then chosen at random and a change $\binom{a}{2}_p \binom{a}{2}_{p_i} \rightarrow \binom{a'}{2}_p \binom{a'}{2}_{p_i}$ is attempted. As the weights for the new and the old configurations are the same if the new configuration is an allowed one, only an acceptance probability need be constructed in order to make the number of moves attempted equal in both directions. With the above procedure of choosing the operators to be exchanged, we can use

$$P\left[\binom{a}{2}\binom{a}{2} \rightarrow \binom{a'}{2}\binom{a'}{2}\right] = \frac{N_a}{N_a + N_{a'}}. \tag{4.13}$$

If the change is accepted the states $|\alpha(k)\rangle_{12} = |n_{1,\uparrow}(k), n_{2,\uparrow}(k)\rangle \otimes |n_{1,\downarrow}(k), n_{2,\downarrow}(k)\rangle$, $k = p, \ldots, p_i - 1$, are checked for forbidden doubly occupied sites, and the move rejected if such states are found. To allow for a speedy check, all the states $|\alpha(i)\rangle_{12}, i = 0, \ldots, l - 1$, are stored, and updated in the case where a move is accepted.

(iv) Moves changing the winding number: thinking of the operators $\binom{1}{b}$ and $\binom{2}{b}$ as creating links between the sites b and $b + 1$, changing the winding number by one corresponds to adding or removing a ring of N links. This can be achieved as follows. A set of $N/2$ operators $R_1 = \{\binom{t}{b_1}_{p_1}, \binom{t}{b_2}_{p_2}, \ldots, \binom{t}{b_{N/2}}_{p_{N/2}}\}$, $t = 1, 2$, is replaced by a set $R_2 = \{\binom{t}{c_1}_{p_1}, \binom{t}{c_2}_{p_2}, \ldots, \binom{t}{c_{N/2}}_{p_{N/2}}\}$, with the bs and the cs constituting the set $\{1, \ldots, N\}$. First choosing $t = 1, 2$ at random, the set R_1 is formed by searching the sequence for operators $\binom{t}{b}$, starting from a randomly chosen position. If some $\binom{t}{b}$ is encountered more than once before a set of $N/2$ distinct operators have been found, the move is cancelled. Otherwise the set R_1 is replaced by R_2 and the state $|\alpha\rangle$ is propagated by the new sequence to check for forbidden operations. If the new sequence is allowed, the move is always accepted. Since the possibility of a non-zero winding number is a result of the boundary conditions chosen these kinds of moves are needed only for small systems, unless one wants to calculate a quantity which is a function of the winding number.

(v) State changes: for a given index sequence all allowed states $|\alpha\rangle$ result in configurations of equal weights. Thus state changes made with equal probabilities in both directions should always be accepted if they do not cause forbidden operations. This can be rapidly checked for when the index sequence is split into sub-sequences. Note that the state $|\alpha\rangle$ can change also as a result of the moves (iii) above.

A complete updating cycle (an MC step) consists of the following steps.

A sequence of L length-changing moves (i) are made.

All positions in the sequence are up-dated in moves of type (ii).

The sequence is split into sub-sequences according to (A) in (iii) and a number of the moves described in (iii) are made in each sub-sequence. The number of moves attempted is chosen proportional to the number of 1- 2- and 4-operators in the sub-sequence and so that the total number of moves attempted in each MC step is constant. The total number of moves attempted is chosen such that on average approximately 30–50% of the involved operators are exchanged in one MC step.

A number, of the order of N, of state changes are performed.

The full sequence is recombined and split again according to (B) in (iii). Moves are attempted as above.

A number, of the order of N, of state changes are performed.

The full sequence is recombined.

A number of winding number moves are attempted if the system is small.

The time needed for an MC step scales linearly with the size of the system if the number of winding number moves attempted is taken to be independent of the system size. In practice the acceptance ratio for these moves approaches zero rapidly when the system size increases, and there is no point in considering them at all for large systems. As the average length of the sequence is determined by (3.8), the simulation time scales roughly linearly with the inverse temperature. The memory requirements are very small, since the full intermediate states $|\alpha(p)\rangle$, $p \neq 0$, need not be stored.

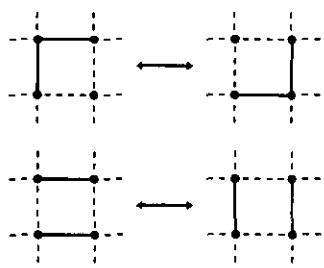

Figure 2. Graphical representation of local loop moves needed in the case of a two-dimensional square lattice. The links represent operators $\binom{t}{b}$, $t = 1, 2$.

To generalize the scheme described here for higher-dimensional systems, additional moves involving local loops of 1- and 2-operators must be included (see figure 2 for an example). Moves changing the winding number in higher dimensions can be made along the lines of (iv) above, but with the sequence split into a number of sub-sequences containing only the operators necessary to determine whether a move results in forbidden operations. For boson systems on bipartite lattices and non-frustrated spin systems the weight $W(\alpha, S_n)$ can generally be made positive-definite in any number of dimensions. For fermion systems in higher dimensions this is not possible; an index sequence corresponding to an operator product which permutes an odd number of particles results in a negative phase. The nature of the sign problem is similar in the world-line method, where it also always appears for fermions in more than one dimension [11]. In contrast, in the determinant method it can be avoided in some important cases, e.g. the half-filled Hubbard model [12]. In cases where it cannot be eliminated, the sign problem in the determinant method is typically much

less severe than in methods relying on a direct representation of the fermion degrees of freedom [14, 16]. Due to the sign problem the simulation scheme presented here is likely to be useful for fermions in one dimension only.

5. Results

In this section results of test runs on the 1D Hubbard model are presented. Comparisons with exact results are made for small systems. In order to investigate the potential of the simulation scheme, 32-site systems at various band-fillings were studied at a fairly low temperature. Results for structure factors and static susceptibilities are presented.

Defining

$$\begin{aligned}\rho_{\mathrm{S}}(q,\tau) &= \sum_k \mathrm{e}^{\mathrm{i}kq}[n_{k\uparrow}(\tau) - n_{k\downarrow}(\tau)] \\ \rho_{\mathrm{D}}(q,\tau) &= \sum_k \mathrm{e}^{\mathrm{i}kq}[n_{k\uparrow}(\tau) + n_{k\downarrow}(\tau) - \rho]\end{aligned} \tag{5.1}$$

where ρ is the particle density, the spin- and charge-density structure factors are

$$S_{\mathrm{S,D}}(q) = \frac{1}{N}\langle \rho_{\mathrm{S,D}}(q,0)\rho_{\mathrm{S,D}}(-q,0)\rangle \tag{5.2}$$

and the static susceptibilities are

$$\chi_{\mathrm{S,D}}(q) = \frac{1}{N}\int_0^\beta \mathrm{d}\tau \langle \rho_{\mathrm{S,D}}(q,\tau)\rho_{\mathrm{S,D}}(-q,0)\rangle\,. \tag{5.3}$$

The simulation runs are divided into a number of bins (≈ 10). (5.2) and (5.3) are measured in position space using formulae of the type (3.4) and (3.16) and the Fourier transforms are calculated for each bin. The final averages and errors are calculated using the binned data. In sums of the type (3.4) only partial sums with the summation variable $p = 0, 4N, 8N, \ldots$ are used, in order not to spend time measuring almost identical states. The time required for the measurements then scales as N^2.

In tables 1 and 2 some simulation results for a 4-site ring at half-filling and an 8-site ring at quarter-filling are compared with data obtained by exact diagonalization of the Hamiltonian. In both cases $U = 4$. The simulations consisted of 2×10^6 and 10^6 MC steps for $N = 4$ and 8 respectively. Measurements were made every fifth MC step. The results agree within statistical errors. The potential energy can be calculated in two ways; using (3.7) or the number of doubly occupied sites. This provides for a good check on the simulations, as does calculating the expectation value of the operators $H_{4,i}$, which should be equal to one.

Table 1. Monte Carlo and exact results for the energy and density of doubly occupied sites and the spin- and charge-density structure factors and susceptibilities at the wavenumber $q = \pi$. The system is a 4-site ring at half-filling and inverse temperature $\beta = 8$.

Operator	MC	Exact
$-E$	0.6794(6)	0.68013
d	0.1194(1)	0.11936
$S_S(\pi)$	1.835(2)	1.83395
$\chi_S(\pi)$	2.94(2)	2.91680
$S_D(\pi)$	0.4405(3)	0.44040
$\chi_D(\pi)$	0.1671(4)	0.16756

Table 2. Monte Carlo and exact results for the spin-density structure factor as a function of the wavenumber. The system is a quarter-filled 8-site ring at inverse temperature $\beta = 8$.

q	MC	Exact
$\pi/4$	0.308(2)	0.30803
$\pi/2$	0.693(2)	0.69344
$3\pi/4$	0.5708(4)	0.57132
π	0.5526(4)	0.55254

We now discuss simulations carried out on 32-site rings at the inverse temperature $\beta = 8$ and band fillings $\frac{1}{4}, \frac{3}{8}$ and $\frac{1}{2}$ ($\rho = \frac{1}{2}, \frac{3}{4}, 1$). The simulations consisted of 1–1.5 x 10^6 MC steps with measurements made every fifth MC step. No winding number moves were made. The acceptance rates for the moves (i) and (ii) above are around 30%. For the moves of type (iii) the acceptance rate is of the order of 5–10%, depending of the band filling. Very few state changes are accepted at this low temperature. The simulations were carried out on a VAX 6000-510 and on an IBM Powerstation 530. The CPU time needed for 1000 MC steps, including the measurements, was approximately 1 minute on both machines.

As numerical studies of this system have been carried out before [17, 18], here we only briefly comment on the results. For a non-interacting system $\chi_S(2P_F)$ and

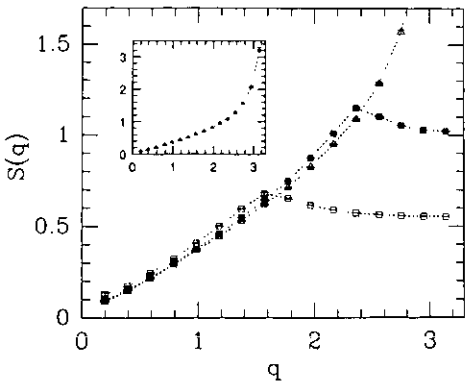

Figure 3. Spin-density structure factors for $\rho = \frac{1}{2}$ (open squares), $\rho = \frac{3}{4}$ (full squares), and $\rho = 1$ (triangles). The inset shows the complete $\rho = 1$ data. The lines connecting the points are only intended to guide the eye.

$\chi_D(2P_F)$ diverge logarithmically as $T \to 0$. P_F is the Fermi momentum of the system. In the limit of $U \to \infty$ the χ_D divergence is shifted to $q = 4P_F$ and $\chi_S(2P_F)$ diverges like $1/T^{1/2}$ away from half-filling [19,20]. At half-filling the model for $U \to \infty$ is equivalent to the Heisenberg model with $\chi(\pi) \sim 1/T$ and a logarithmically divergent $S_S(\pi)$. The interesting question is the $2P_F$ and $4P_F$ responses and structure factors for intermediate values of U [17]. All results presented here are for $U = 4$. Figures 3 and 4 show the spin structure and static susceptibility. There are clear $2P_F$ peaks in the susceptibility at all fillings. The charge-density structure factors (figure 5) do not have much structure. They are slowly increasing functions of q. An interesting feature is the structure factor up to wave vector $\approx \pi/2$, which is almost identical for $\rho = \frac{1}{2}$ and $\frac{3}{4}$, but considerably lower for $\rho = 1$. The charge-density susceptibility (figure 6) shows clear peaks at $2P_F$ and $4P_F$ for $\rho = \frac{1}{2}$. The peak at $4P_F$ is known to vanish as the temperature is further lowered. [17] For $\rho = \frac{3}{4}$ there is a clear peak at $4P_F$ and signs of a weaker peak at $2P_F$. The $\rho = 1$ response is a slowly increasing function of q.

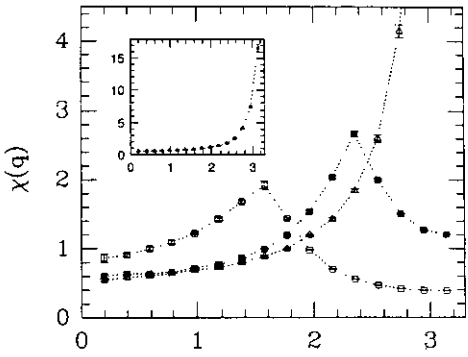

Figure 4. Spin-density susceptibilities for $\rho = \frac{1}{2}$ (open squares), $\rho = \frac{3}{4}$ (full squares), and $\rho = 1$ (triangles). The inset shows the complete $\rho = 1$ data.

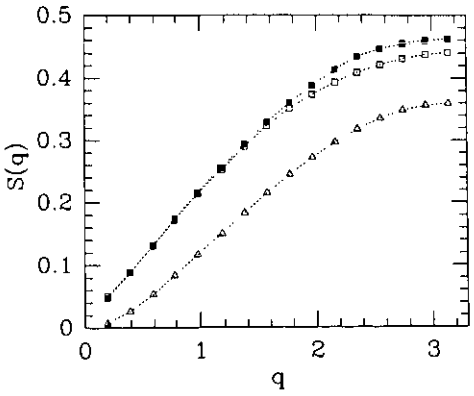

Figure 5. Charge-density structure factors for $\rho = \frac{1}{2}$ (open squares), $\rho = \frac{3}{4}$ (full squares), and $\rho = 1$ (triangles). Statistical errors are smaller than the symbols.

To illustrate the fact that only a limited range of powers of the Hamiltonian contributes significantly to the partition function, a histogram of the distribution of lengths of the index sequence in the simulation with $\rho = 1$ is displayed in figure 7.

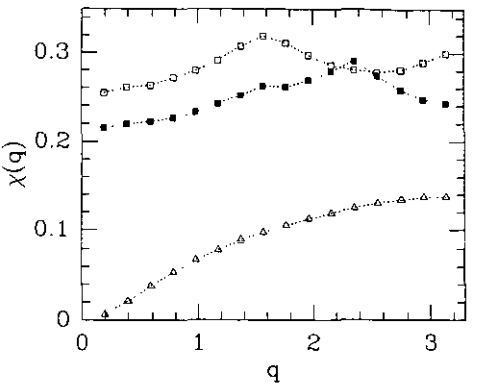

Figure 6. Charge-density susceptibilities for $\rho = \frac{1}{2}$ (open squares), $\rho = \frac{3}{4}$ (full squares), and $\rho = 1$ (triangles). Statistical errors are smaller than the symbols.

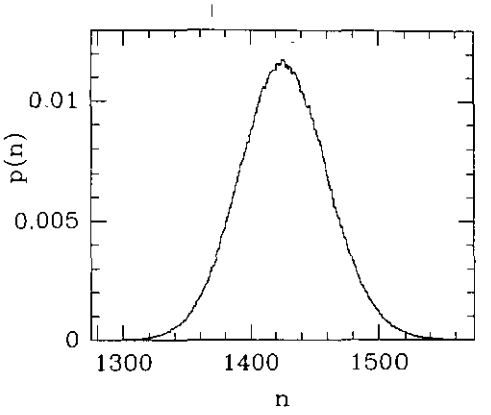

Figure 7. Distribution of the lengths of the index sequences for $\rho = 1$.

In conclusion, a generalization of Handscomb's quantum Monte Carlo scheme has been applied to the one-dimensional Hubbard model. Simulations of 32-site systems at a fairly low temperature have been carried out. The accuracy of the results achieved, using modest computer resources, indicate that simulations of large systems using this method are feasible. The scheme is easily generalized for application to other fermion models in one dimension as well as to spin systems and boson systems on bipartite lattices.

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