SIMULATION OF STATISTICAL SYSTEMS WITH NOT NECESSARILY REAL AND POSITIVE PROBABILITIES*

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A new method to determine expectation values of observables in statistical systems with not necessarily real and positive probabilities is proposed. It is tested in a numerical study of the two-dimensional O(3)-symmetric nonlinear σ-model with Symanzik's one-loop improved lattice action. This model is simulated as a polymer system with field dependent activities which can be made positive definite or indefinite by adjusting additive constants of the action. For a system with indefinite activities the new proposal is found to work. It is also verified that local observables are not affected by far-away polymers with indefinite activities when the system has no long-range order.

1. Introduction

Numerical integration by means of Monte Carlo sampling techniques is only possible when the integration measure is positive. This is the case for euclidean lattice theories of bosonic fields ϕ with real action or hamiltonian $\mathscr{H}(\phi)$. The evaluation of path integrals $Z^{-1}\int\mathscr{D}\phi\,\mathscr{O}(\phi)e^{-\mathscr{H}(\phi)}$ can be done numerically by importance sampling of field configurations which are distributed according to the probability measure $d\mu(\phi) = Z^{-1}\mathscr{D}\phi\,e^{-\mathscr{H}(\phi)}$.

However, there are also models of physical interest with partition functions that are not integrals (or sums) over a positive density. (We shall call a density a probability density even when it is not positive definite.) Theories with indefinite probability densities are not amenable to a straightforward numerical simulation.

As an example of a possible indefinite statistical system we consider a polymer system [1–4] which is defined as follows. Given a set Λ (for instance a lattice) of sites x, one declares certain finite non-empty subsets P of Λ to be polymers. A notion of compatibility is specified, such that no polymer is compatible with itself, and a real or complex activity $A(\text{P})$ is assigned to each polymer P. The partition

function of the polymer system is

$$Z = \sum_{\mathcal{Y}} \prod_{P \in \mathcal{Y}} A(P),$$ (1.1)

where summation is over sets $\mathcal{Y}$ of compatible polymers, including $\mathcal{Y} = \varnothing$ which contributes 1. (An empty product is understood to be 1.) Later on when we consider a lattice field theory as a polymer system, the activities will be field dependent and there will be an additional integration over the field configurations on the r.h.s. of eq. (1.1). The polymer system is called indefinite when not all $A(P) > 0$. It was pointed out in ref. [5] that polymer representations can be useful in the context of Monte Carlo simulations when one deals with hamiltonians with small but nonlocal correction terms. Later, a breakthrough in computational efficiency for standard local models was achieved when very efficient cluster algorithms for models exhibiting an $O(N)$ symmetry were developed which practically eliminate critical slowing down [6]. All these cluster algorithms exploit a polymer representation of the partition function. Also, recently Montvay [7] referred to the fact that there exists a polymer representation of the euclidean fermion determinant which may be relevant for the design of new fermion algorithms. However, the non-positivity of the probability density is an obstacle. A satisfactory solution of the "negative activities" problem is also a prerequisite for the implementation of a proposal [1] to perform simulations for continuum systems without imposing a UV cutoff.

A first idea how to simulate an indefinite statistical system is to use absolute values for transition probabilities in a Monte Carlo process and to include the phase factors in observables. However, this way has generally proven to be impractical. Let us illustrate this with an example. We consider a trivial monomer system which is a special case of a polymer system. Only subsets $\{x\}$ of Λ consisting of a single site are polymers (monomers), they are mutually compatible and all of them have the same complex activity $A(\{x\}) = Me^{i\omega}$, $0 < M < 1$, $-\pi < \omega \le \pi$, $\omega \ne 0$. The partition function is $Z = \sum_{Y \subseteq \Lambda}(Me^{i\omega})^{|Y|} = (1 + Me^{i\omega})^{|\Lambda|}$ and the expectation value of an observable $\mathcal{O}(Y)$ is defined by $\langle \mathcal{O} \rangle = Z^{-1}\sum_{Y \subseteq \Lambda}\mathcal{O}(Y)(Me^{i\omega})^{|Y|}$. With the indefinite monomer system one can associate a "positive" system with partition function Z_+ and expectation values $\langle \cdot \rangle_+$, where $Me^{i\omega}$ is replaced by M. Defining $\sigma(Y) = e^{i\omega|Y|}$, we have the equality $\langle \mathcal{O} \rangle = \langle \mathcal{O}\sigma \rangle_+ / \langle \sigma \rangle_+$. In principle both the numerator and the denominator can be determined by a well-defined Monte Carlo process, but $|\langle \sigma \rangle_+| = |Z/Z_+| = \exp(-|\Lambda|[\ln(1 + M) - \frac{1}{2}\ln(1 + 2M\cos\omega + M^2)])$ goes to zero exponentially with the volume $|\Lambda|$. An accurate numerical determination of such very small numbers is not possible. The variance of $\mathcal{O}$ determined straightforwardly by this Monte Carlo method increases exponentially with $|\Lambda|$. Therefore one has to look for a method which is better suited. One may hope to replace the volume $|\Lambda|$ by an effective volume which is determined by the correlation length.

It is proposed in this paper to use a different equality between the expectation value $\langle \mathcal{O} \rangle$ of an observable $\mathcal{O}$ in a general polymer system and certain expectation values $\langle \cdot \rangle_+$ in the associated positive system. To start with let us consider a polymer system with real but not necessarily positive activities. We call a polymer P negative if $A(P) < 0$.

If we suppose that $\mathcal{O}$ is a real observable and denote the number of negative polymers in Λ by n, the proposed formula reads

$$\langle \mathcal{O} \rangle = \sum_{k \geq 0} (-1)^k \frac{\pi^{2k}}{(2k)!} \langle \mathcal{O}; \underbrace{n; \ldots; n}_{2k \text{ factors}} \rangle^c_+ , \tag{1.2}$$

where $\langle \cdot \rangle^c_+$ are connected expectation values in the polymer system with activities replaced by their absolute values. $\langle \mathcal{O}; n; \ldots; n \rangle^c_+$ is truncated as if all the $2k + 1$ entries ($\mathcal{O}$ plus $2k$ times n) are different; for instance $\langle \mathcal{O}; n; n \rangle^c_+ = \langle \mathcal{O} n^2 \rangle_+ - \langle \mathcal{O} \rangle_+ \langle n^2 \rangle_+ - 2\langle \mathcal{O} n \rangle_+ \langle n \rangle_+ + 2\langle \mathcal{O} \rangle_+ \langle n \rangle^2_+$ etc.

When the system has no long-range order one can hope that local observables are not affected by the presence of far-away negative polymers. This expectation can be supported by (1.2): Let us define the density of negative polymers at the lattice site x by $\varrho(x) = \sum'_{P \in \, / \, : x \in P} 1/|P|$, where the sum is restricted to polymers with negative activities and $|P|$ is the number of points in P. Then the number of negative polymers in Λ is

$$n = \sum_{x \in \Lambda} \varrho(x), \tag{1.3}$$

and because of the multilinearity of connected expectation values we get

$$\langle \mathcal{O}; \underbrace{n; \ldots; n}_{2k \text{ factors}} \rangle^c_+ = \sum_{x_1} \ldots \sum_{x_{2k}} \langle \mathcal{O}; \varrho(x_1); \ldots; \varrho(x_{2k}) \rangle^c_+ . \tag{1.4}$$

In the absence of long-range order in the positive system, the truncated correlation functions on the r.h.s. of eq. (1.4) will decrease exponentially with the distance* $\text{dist}(x_j, \text{supp} \, \mathcal{O})$. Therefore, when $\mathcal{O}$ is a local observable it should be allowed to restrict any of the $2k$ summations on the r.h.s. of eq. (1.4) to sites x_i which have a distance from supp $\mathcal{O}$ that is less than a certain maximum distance; the latter will be determined by the correlation length. By this truncation of the sums, n is replaced by the number $n(V)$ of negative polymers which are included in a neighbourhood V of extent of the order of the correlation length about the support of $\mathcal{O}$. Thus

$$\langle \mathcal{O}; \underbrace{n(V); \ldots; n(V)}_{k \text{ factors}} \rangle^c_+ \simeq \langle \mathcal{O}; \underbrace{n; \ldots; n}_{k \text{ factors}} \rangle^c_+ \equiv \langle \mathcal{O}; \underbrace{n(\Lambda); \ldots; n(\Lambda)}_{k \text{ factors}} \rangle^c_+ \tag{1.5}$$

* The support of $\mathcal{O}$ (supp $\mathcal{O}$) is the smallest subset Y of Λ such that $\mathcal{O}(X) = 0$ if $X \not\subseteq Y$.

should be valid for all V which are greater than a certain minimal effective neighbourhood of supp $\mathcal{O}$ for all $k \geqslant 1$ and any given Λ. Then the error of $\langle \mathcal{O} \rangle$ does not increase with $|\Lambda|$, but can be bounded by a function of the effective neighbourhood.

Eq. (1.2) is proved in sect. 2. There we consider a general lattice field theory as a polymer system with field dependent activities, and the generalization of eq. (1.2) for systems with complex activities is derived. For real observables in real systems we find a supplementary equation which can be used for a consistency check.

An investigation to examine the numerical usefuless of eq. (1.2) is presented in sect. 3 where we turn to two questions. The first one is: At which order can the expansion on the r.h.s. of eq. (1.2) be truncated? The use of eq. (1.2) is only convenient when a few terms suffice to reach convergence, because the numerical determination of truncated expectation values is an intricate task. The second question concerns the validity of eq. (1.5) for a local observable in the absence of long-range order.

These questions were addressed in a numerical simulation of the two-dimensional O(3)-symmetric nonlinear σ-model with Symanzik's one-loop improved lattice action [8,9] as a polymer system. The energy $1 - \phi(x)\phi(x + \hat{\mu})$ of next-neighbour interaction was examined. The field of the nonlinear σ-model takes its values in a compact space. This fact permits to add field independent terms to the action so that all activities are non-negative. Thus, one is able to determine the true value on the l.h.s. of eq. (1.2) by standard methods also, and this can be compared with the results of the expansion on the r.h.s. obtained from a simulation of an indefinite system. It will be found that the first three terms on the r.h.s. of eq. (1.2) are sufficient for numerical convergence, and the unimportance of far-away polymers for local observables can be ascertained.

Unfortunately, the determination of the fourth-order terms $\langle \mathcal{O}; n(V); n(V); n(V); n(V) \rangle_+^c$ with small error bars is very time-consuming with any of the methods tested yet. (These are explained in sect. 3.) But the connected expectation values needed for the expansion (1.2) have a special form and this raises hope that improved estimators for them will be found in the future.

2. Expansion formula connecting expectation values with truncated ones in a positive system

2.1. DERIVATION OF THE EXPANSION FORMULA

Let us consider a general polymer representation of a lattice theory of fields ϕ (matter or/and gauge fields) with partition function [5]

$$Z = \sum_{\gamma} \int_{\phi} e^{-\mathcal{H}_{\gamma}(\phi)} \prod_{P \in \gamma} A(P, \phi) .$$

(2.1)

As in eq. (1.1), $\Sigma_{/}$ is a summation over collections of compatible polymers and $\int_{\phi}$ denotes the integration over field configurations. The action $\mathcal{H}_0(\phi)$ shall be real. The polymer activities $A(P,\phi)$ are field dependent and we allow them to be complex:

$$A(P,\phi) = e^{i\omega(P,\phi)}|A(P,\phi)|,$$ (2.2)

with real phases $\omega(P,\phi)$, restricted conveniently to the interval

$$-\pi < \omega(P,\phi) \le \pi$$ (2.3)

for all polymers P and all field configurations ϕ.

The sum of the phases of the polymer activities of a state $(\phi, \mathcal{X})$ will be denoted by

$$\Omega(\phi,\mathcal{X}) = \sum_{P \in /} \omega(P,\phi).$$ (2.4)

To derive (1.2) one defines an interpolating partition function $Z(t)$ and interpolating expectation values of observables $\langle \mathcal{O} \rangle_t$ which depend on a parameter t by

$$Z(t) = \sum_{/} \int_{\phi} e^{-\mathcal{H}_0(\phi)} \prod_{P \in /} \left[e^{i\omega(P,\phi)t}|A(P,\phi)| \right]$$ (2.5)

and

$$\langle \mathcal{O} \rangle_t = \frac{1}{Z(t)} \sum_{/} \int_{\phi} \mathcal{O}(\phi,\mathcal{X}) e^{-\mathcal{H}_0(\phi)} \prod_{P \in /} \left[e^{i\omega(P,\phi)t}|A(P,\phi)| \right].$$ (2.6)

They have the property that $Z(t = 1)$ is the desired partition function (2.1) and $\langle \mathcal{O} \rangle_{t=1} \equiv \langle \mathcal{O} \rangle$ are the expectation values we are interested in. The partition function $Z(t = 0) \equiv Z_+$ is that of a positive polymer system which can be treated numerically, and expectation values $\langle \mathcal{O} \rangle_{t=0} \equiv \langle \mathcal{O} \rangle_+$ can be determined by standard Monte Carlo methods. To arrive at the expansion formula we perform a Taylor expansion of $\langle \mathcal{O} \rangle_t$ as a function of t about zero and fix $t = 1$. Recalling the definition of truncated expectation values by means of a generating functional,

$$\langle \mathcal{O}_1; \ldots; \mathcal{O}_n \rangle^c = \frac{\partial^n}{\partial h_1 \ldots \partial h_n} \ln\left\langle \exp\left(\sum_{i=1}^{n} h_i \mathcal{O}_i \right) \right\rangle \Bigg|_{h=0}$$ (2.7)

and noticing that

$$\langle \mathcal{O} \rangle_t = \frac{\partial}{\partial s} \ln\left\langle \exp(s\mathcal{O} + it\Omega) \right\rangle_+ \Big|_{s=0}$$ (2.8)

one obtains

$$\langle \mathscr{E} \rangle = \sum_{k \geqslant 0} \frac{i^k}{k!} \langle \mathscr{E}; \underbrace{\Omega; \ldots; \Omega}_{k \text{ factors}} \rangle_+^c .$$ (2.9)

2.2. SPECIAL CASE OF REAL PROBABILITIES

If the activities $A(P, \phi)$ of all polymers P are real for all field configurations ϕ, the phases $\omega(P, \phi)$ are either 0 or π. In this case only polymers with negative activities contribute to (2.4), their contribution is always π. Thus, denoting the total number of negative polymers in a set $\mathscr{X}$ for given field configuration ϕ by $n(\phi, \mathscr{X})$, we have $\Omega(\phi, \mathscr{X}) = \pi n(\phi, \mathscr{X})$ and (2.9) reads

$$\langle \mathscr{E} \rangle = \sum_{k \geqslant 0} \frac{(i\pi)^k}{k!} \langle \mathscr{E}; \underbrace{n; \ldots; n}_{k \text{ factors}} \rangle_+^c .$$ (2.10)

If $\mathscr{E}(\phi, \mathscr{X})$ is real, eq. (2.10) splits into two equations. The one for the real part is (1.2), and as a supplementary equation we have for the imaginary part

$$0 = \sum_{k \geqslant 0} (-1)^k \frac{\pi^{2k+1}}{(2k+1)!} \langle \mathscr{E}; \underbrace{n; \ldots; n}_{2k+1 \text{ factors}} \rangle_+^c .$$ (2.11)

2.3. LOCAL OBSERVABLES

To examine the validity of (1.5) we shall consider neighbourhoods V of the support of a local observable $\mathscr{E}$ which are centred about supp $\mathscr{E}$. A particular example will be quoted in sect. 3. Let us define the density $\varrho(x, \phi, \mathscr{X})$ of negative polymers at the lattice site x by

$$\varrho(x, \phi, \mathscr{X}) = \sum_{P \in \mathscr{X}: x \in P} \Theta(-A(P, \phi)) \frac{1}{|P|} .$$ (2.12)

Here Θ denotes the step function, as usual, and $|P|$ is the number of points in the polymer P. The total number of negative polymers in Λ is

$$n(\phi, \mathscr{X}) = \sum_{x \in \Lambda} \varrho(x, \phi, \mathscr{X}) .$$ (2.13)

The number $n(V)$ of negative polymers which are included in a neighbourhood V

that is used in eq. (1.5) is defined by

$$n(\mathrm{V})(\phi, \mathscr{X}) = \sum_{x \in \mathrm{V}} \varrho(x, \phi, \mathscr{X}). \tag{2.14}$$

When there are also polymers with complex activities, one has to replace $\Theta(-A(\mathrm{P}, \phi))$ in eq. (2.12) by $\omega(\mathrm{P}, \phi)$ and $\pi n(\mathrm{V})(\phi, \mathscr{X})$ has to be replaced by $\Omega(\mathrm{V})(\phi, \mathscr{X}) = \sum_{x \in \mathrm{V}} \varrho(x, \phi, \mathscr{X})$, where the modified definition of ϱ is used.

2.4. A TRIVIAL EXAMPLE

Before we turn to the numerical examination of eq. (2.10) let us investigate an analytically soluble model and see how the expansion formula works in this case. Consider the trivial monomer system which was cited in sect. 1. For simplicity we inspect an extensive quantity U. Its value in subset Y is proportional to $|\mathrm{Y}|$: $U(\mathrm{Y}) = u|\mathrm{Y}|$. When u is a real or complex number we have

$$\langle U \rangle = uM \frac{\partial}{\partial M} \ln Z = u|\Lambda| \frac{Me^{i\omega}}{1 + Me^{i\omega}}.$$

The connected expectation values of U and the phase Ω are

$$\langle U; \underbrace{\Omega; \ldots; \Omega}_{k \text{ factors}} \rangle_{+}^{\mathrm{c}} = u|\Lambda|\omega^{k} \frac{\partial^{k+1}}{\partial h^{k+1}} \ln(1 + Me^{h}) \Big|_{h=0}.$$

Since M is less than 1 we can Taylor expand the logarithm, obtaining

$$\langle U; \underbrace{\Omega; \ldots; \Omega}_{k \text{ factors}} \rangle_{+}^{\mathrm{c}} = u|\Lambda|\omega^{k} \sum_{l \geqslant 1} (-1)^{l-1} M^{l} l^{k},$$

and with eq. (2.9) we arrive at

$$\langle U \rangle = u|\Lambda| \sum_{k \geqslant 0} \sum_{l \geqslant 1} \frac{(i\omega l)^{k}}{k!} (-1)^{l-1} M^{l},$$

which is the correct result.

Finally, consider the worst case for the expansion which arises when $|\langle U \rangle_{+} - \langle U \rangle|$ = maximal. This happens when $\omega = \pi$. With the approximation $M \ll 1$ (where $\langle \sigma \rangle_{+} = e^{-2M|\Lambda|}$), we have $\langle U \rangle_{+} = u|\Lambda|M = -\langle U \rangle$ and eq. (2.9) reads $\langle U \rangle = u|\Lambda| \sum_{k \geqslant 0} (i^{k}/k!)\pi^{k} M = u|\Lambda|Me^{i\pi}$. Thus, to achieve an accuracy of 0.2% for the expectation value of the extensive quantity U in this example, the series (2.9) can be truncated at the tenth order. This result is not so bad, because the leading term has to be changed by -100%.

To conclude this section the author remarks that absolute convergence of eq. (2.9) can be proved when the activities are field independent and when two non-identical polymers are compatible. In this case the radius of convergence of the Taylor expansion of $\langle \mathcal{C} \rangle_t$ about zero is

$$\min_P \frac{1}{|\omega(P)|} \sqrt{\pi^2 + (\ln|A(P)|)^2} .$$

(It is the modulus of that root of $Z(t)$ which is closest to the origin.)

3. Numerical examination of the expansion formula

3.1. SIMULATION OF AN INDEFINITE POLYMER SYSTEM

The numerical use of the expansion formula (2.10) was examined in a simulation of the two-dimensional O(3)-symmetric nonlinear σ-model with Symanzik's one-loop improved lattice action [8,9] as a polymer system. The improved action is summarized in appendix A. There the reader also finds how one arrives at the polymer representation of the model. The way in which the polymer system was made indefinite is also explained in appendix A. For details concerning the possibilities of Monte Carlo updating procedures for polymer systems, the reader is referred to refs. [5, 10].

The conjecture that negative polymers affect a local observable $\mathcal{C}$ only when they are contained in a neighbourhood V about supp $\mathcal{C}$ that is of order of the correlation length ξ was investigated. The examined local observable is the energy of next neighbour interaction $\mathcal{C} = 1 - \phi(x)\phi(x + \hat{\mu})$. In order to have a ξ that is not too large, β was chosen to be 0.8 which corresponds to $\xi = 2.29 \pm 0.04$ in the system with positive semidefinite activities [10]. Λ was fixed to be a 12^2 lattice with periodic boundary conditions. In a simulation of the polymer system with positive semidefinite activities the true expectation value of the link energy was determined to be $\langle 1 - \phi(x)\phi(x + \hat{\mu}) \rangle = 0.5053 \pm 0.0005$. For the indefinite polymer system the ratio of its partition function Z to Z_+ was measured in a preliminary run of 200 000 sweeps with the result $Z/Z_+ \equiv \langle \sigma \rangle_+ \equiv \langle (-1)^n \rangle_+ = 0.0011 \pm 0.0029$. Thus, the naive method to use the equality $\langle \mathcal{C} \rangle = \langle \mathcal{C}\sigma \rangle_+ / \langle \sigma \rangle_+$ is completely impractical for the determination of expectation values in the present situation.

To investigate the dependence of $\langle \mathcal{C}; n(V); \dots; n(V) \rangle^c_+$ on V, neighbourhoods of supp $\mathcal{C}$ of two kinds were considered. The first kind consists of the union of all lattice sites which have a distance of at most m lattice spacings from x or $x + \hat{\mu}$ in the "taxi-driver" or "Manhattan" norm, $m = 0, 1, \dots$ The second kind of considered V's are rectangles of sidelength $2l \times (2l - 1)$, $l = 1, 2, \dots$, centred about x and $x + \hat{\mu}$. The connected expectation values $\langle \mathcal{C}; n(V); \dots; n(V) \rangle^c_+$ were examined for 10 different neighbourhoods V, namely those for $m = 0, \dots, 5$ and for

$l = 1, \ldots, 5$ ($m = 0$ and $l = 1$ both correspond to $V = \{x, x + \hat{\mu}\} = \mathrm{supp}\, \mathscr{E}$). These V's have a volume $|V|$ of 2, 8, 18, 32, 50, 72 and 2, 12, 30, 56, 90 lattice sites respectively.

The author tried to determine truncated expectation values by three different methods. Two less successful attempts are reported in sect. 4. In this section results are quoted which were obtained by simulating a single system and by measuring $\mathscr{E} n(V)^k$, $k = 0, \ldots, 6$, and $n(V)^k$, $k = 1, \ldots, 6$, to determine $\langle \mathscr{E}; n(V); \ldots; n(V) \rangle_+^c$ with $k \leqslant 6$ factors $n(V)$ conventionally. A sample of 5 Msweeps($= 5 \times 10^6$ sweeps) with measurements after every sweep was accumulated. The CPU time needed with a FORTRAN 77 programme amounted to 17.7 h per Msweep on a Siemens 7882 computer. (Two thirds of this computer time are required for updating ϕ and $\mathscr{X}$, and one third is used up for measurements.) The gathered data indicate that the connected correlation functions $\langle \mathscr{E}; n(V); \ldots; n(V) \rangle_+^c$ become indeed independent of V for larger neighbourhoods, and that the expansion (1.2) has already converged (numerically) when only the three leading terms are taken into account. To corroborate this with small error bars (which increase with $|V|$) further measurements were performed for $|V| \geqslant 32$ and $k \leqslant 4$ with an additional statistics of 21.5 Msweeps. The computer time needed for this is
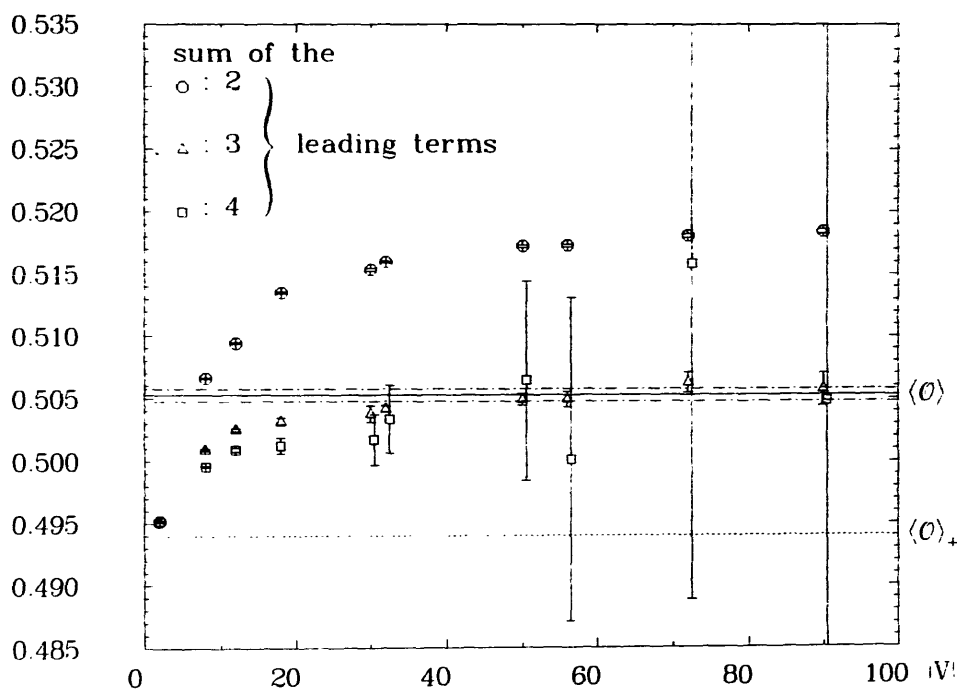

Fig. 1. Dependence of the sum of the two, the three and the four leading terms of the expansion (1.2) for $\mathscr{E} = 1 - \phi(x)\phi(x + \hat{\mu})$ upon the volume $|V|$ of the neighbourhood V of $\mathrm{supp}\,\mathscr{E}$ when negative polymers are only considered if they are contained within V. The dotted line indicates the leading term $\langle \mathscr{E} \rangle_+$. The solid line and the surrounding dashed-dotted lines mark the true value $\langle \mathscr{E} \rangle$ and its error. The abscissae of the boxes are slightly displaced for clarity where their error bars intersect other terms. Recall that neighbourhoods of different shapes are used.
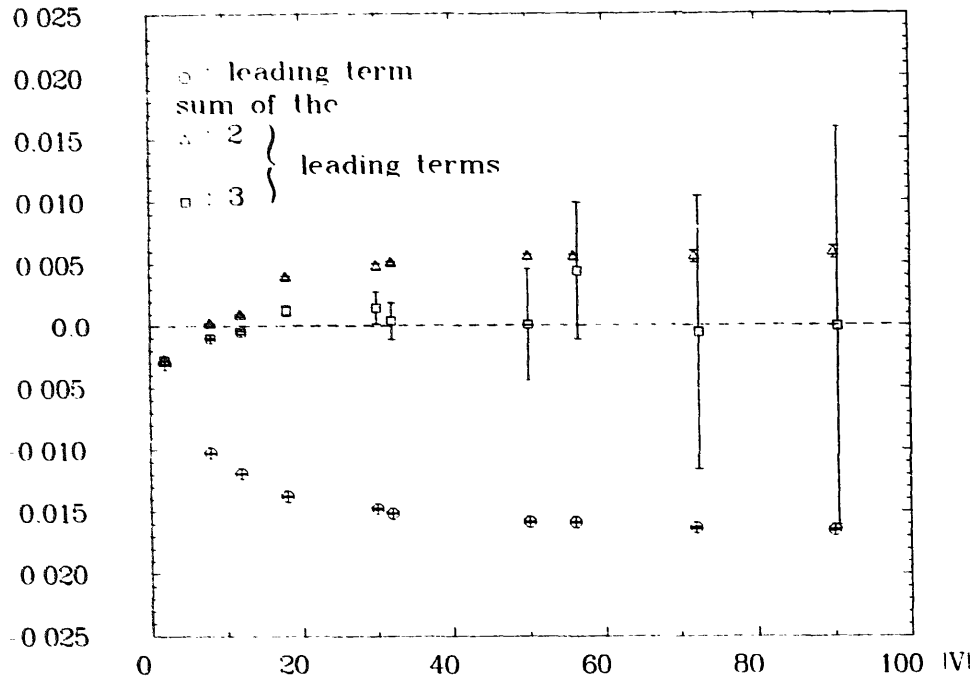
Fig. 2. Dependence of the leading term and the sum of the two and three leading terms of the expansion (2.11) for $\ell = 1 - \phi(x)\phi(x + \hat{\mu})$ upon the volume $|V|$ of the neighbourhood V of supp ℓ when negative polymers are only considered if they are contained within V. The abscissae of the boxes are slightly displaced for clarity where their error bars intersect other terms. Recall that neighbourhoods of different shapes are used.

15.1 h per Msweep on the machine mentioned above. (The Siemens 7882 is about a factor of 4 slower than the IBM 3090 with scalar code.)

Diagrams representing the dependence of the expansion (2.10) for $\ell = 1 - \phi(x)\phi(x + \hat{\mu})$ on the volume $|V|$, when replacing n by $n(V)$, are displayed in figs. 1 and 2. Fig. 1 shows the expansion (1.2) of the real part. The solid line and the surrounding dashed-dotted lines mark the true value $\langle \ell \rangle$ and its error. The dotted line indicates the leading term of the r.h.s. of eq. (1.2) which is $\langle 1 - \phi(x)\phi (x + \hat{\mu})\rangle_+ = 0.49401 \pm 0.00002$. Circles, triangles and squares are the results of the expansion with the two, three and four leading terms added up respectively. The results are consistent with independence on the neighbourhood V when the extent of V exceeds approximately the order of the correlation length. They also show that it is sufficient to take only the three leading terms into consideration.

In fig. 2 the expansion (2.11) of the imaginary part of (2.10) is plotted. The leading term is represented by circles, triangles and squares indicate the sum of the two and three leading terms respectively. As for the real part, the results are also in agreement with independence of $\langle \ell; n(V); \ldots; n(V)\rangle^c_+$ (with an odd number of factors $n(V)$) on V when $|V|^{1/2} \geq O(\xi)$, and this, too, confirms the unimportance of far-away negative polymers for local observables. To guide the eye the dashed line in fig. 2 marks zero. The sum of the three leading terms for large $|V|$ is consistent with vanishing.

All error bars were determined by means of a binning procedure with large bin sizes. The error bars for the fourth contribution to (1.2) and the third contribution to (2.11) are very large for larger V. In spite of this, an argument can be given that the result has converged numerically when only the six leading terms of (2.10) are considered. The order of magnitude of the individual terms can be estimated from their value at $|V| = 18$ where they can be accurately determined. Using this estimate one concludes that the fourth contribution to (1.2) will be no larger than the error bars of the sum of the three leading contributions for $|V| \geq 56$.

3.2. OTHER METHODS FOR THE DETERMINATION OF TRUNCATED EXPECTATION VALUES

The conventional method to determine truncated expectation values with small error bars is very time-consuming. The author can report on two attempts to reduce statistical noise. Both of them, however, were not successful.

The first attempt relies on a representation of connected correlation functions, which we shall call the "multiplication trick" (MT). It generalizes the well-known "doubling trick" for connected two-point functions. Originally the MT was used to prove some correlation inequalities in ferromagnetic spin systems [11]. The author's attention to the MT was called by the work of Pinn [12], who used the MT in another context a few years ago.

Any connected r-point correlation function can be expressed as a simple correlation function of modified observables in a suitably chosen auxiliary system. This auxiliary system consists of r non-interacting copies of the original system. To apply the MT to the present problem of determining the truncated expectation values in (2.10), take the union of $k + 1$ identical copies of the polymer system and label quantities which refer to the jth copy $[j = 0, 1, \ldots, k]$ by an index (j). When one defines observables $\tilde{\mathcal{O}}$ and $\tilde{n}(V)$ which refer to the $(k + 1)$-fold system by the following linear combinations of observables in the individual systems:

$$\tilde{\mathcal{O}} = \sum_{j=0}^{k} \lambda^j \mathcal{O}^{(j)}, \qquad \tilde{n}(V) = \sum_{j=0}^{k} \lambda^j n^{(j)}(V), \tag{3.1}$$

where $\lambda = e^{2\pi i/(k+1)}$, then

$$\langle \mathcal{O}; \underbrace{n(V); \ldots; n(V)}_{k \text{ factors}} \rangle^c_+ = \frac{1}{k+1} \langle\langle \tilde{\mathcal{O}} \tilde{n}(V)^k \rangle\rangle_+. \tag{3.2}$$

Here $\langle\langle \cdot \rangle\rangle_+$ denotes the expectation value in the $(k + 1)$-fold positive polymer system.

The numerical implementation of the MT is obvious. To determine the r.h.s. of eq. (3.2) one simulates (at least) $k + 1$ non-interacting copies of the polymer system simultaneously, and estimators for (3.1) are computed appropriately. (Evi-

dently, a disadvantage when using the MT is a $(k + 1)$-fold demand for computer store.) The reason why the MT was expected to yield reduced errors for truncated expectation values, is the following. To get estimators for $\bar{\mathscr{E}}$ and $\bar{n}(V)$, eq. (3.1) tells us only to add up measured quantities from $k + 1$ non-interacting systems accordingly. But, because of translational invariance, we can consider independently $|\Lambda|$ sites in each system as the reference site of a local observable. Also, when one simulates $s > k + 1$ systems and estimators for (3.1) have to be computed, one has $\binom{s}{k+1}$ possibilities to choose the necessary $k + 1$ systems. Furthermore, quantities of different systems do not have to date from the same sweep. Altogether there are numerous possibilities to extract estimators for the r.h.s. of eq. (3.2).

However, CPU time has to be taken into consideration when one judges the efficiency of a Monte Carlo method. By testing various possibilities of averaging, the MT was found to be inferior to the conventional method of determining truncated expectation values. The inferiority of the MT is about a factor of 2 in computer time for the second term of the expansion (1.2) and a factor up to 30 for the third term, increasing with $|V|$.

Finally, for the second attempt to get truncated expectation values with reduced error bars, a generalized version of Wolff's cluster algorithm [13] – which was suitably modified for the polymer representation (2.1) – was implemented. Use was made of the estimators for $\mathscr{E} = 1 - \phi(x)\phi(x + \hat{\mu})$ in the cluster representation [14]. However, a test run showed that these estimators do not yield a reduced error for $\langle \mathscr{E}; n(V); \ldots; n(V) \rangle^c_+$.

After finishing the present article ref. [15] was published were it is reported that Wolff's estimator for the two-point function does not work well for short distances. Perhaps the implementation of Niedermayer's proposal – generalized for the polymer representation – might also improve the estimators for the truncated expectation values which are relevant for this paper.

4. Summary

It was demonstrated that a proper numerical treatment of an indefinite polymer system by means of the expansion formula presented in this paper is practical in principle. An additional very nice result is the verification that local observables are not affected by far-away polymers with indefinite activities when the system has no long-range order. This means that in case of a polymer system with real activities the expansion formula can be used with n – the total number of negative polymers in the lattice – replaced by $n(V)$, where V is an effective neighbourhood about the support of the local observable, and $n(V)$ is the number of negative polymers which are included herein. (In case of a polymer system with complex activities the phases of activities only have to be summed over the polymers in V.)

V is of extent of the order of the correlation length. From the numerical point of view this fact is welcome, because statistical noise is increasing with $|V|$. To improve the numerical efficiency of the expansion formula, it is desirable to find estimators which yield reduced errors for the necessary truncated expectation values in the future.

Appendix A

O(3)-SYMMETRIC TWO-DIMENSIONAL NONLINEAR σ-MODEL WITH SYMANZIK'S ONE-LOOP IMPROVED LATTICE ACTION AS A POLYMER SYSTEM

Symanzik's one-loop improved lattice action for the $O(N)$-symmetric two-dimensional nonlinear σ-model in the absence of an external source is [9]

$$\mathcal{H}_{imp}(\phi) = \mathcal{H}_0(\phi) + \sum_{i=1}^{4}\sum_{P_i}\mathcal{H}_1(P_i,\phi),\qquad(A.1)$$

where $\mathcal{H}_0(\phi)$ contains next-neighbour interactions*

$$\mathcal{H}_0(\phi) = -\left(\tfrac{4}{3}\beta - 16c_5^1 - 8c_6^1 - 8c_8^1\right)\sum_{x\in\Lambda}\sum_{\mu=1}^{2}\phi(x)\phi(x+\hat{\mu})\qquad(A.2a)$$

and $\mathcal{H}_1(P_i,\phi)$ are the following nonlocal interactions, i.e. interactions with a range of more than one lattice spacing:

$$\mathcal{H}_1(P_1,\phi) = \left(\tfrac{1}{12}\beta - 2c_5^1 - 2c_6^1\right)\left[\phi(x)\phi(x+2\hat{\mu}) + a_1\right],\qquad(A.2b)$$

for $P_1 \in \{\{x,y\}|y = x + 2\hat{\mu}, \mu = 1,2\}$,

$$\mathcal{H}_1(P_2,\phi) = -4c_5^1\left[\phi(x)\phi(x+\hat{\mu}+\hat{\nu}) + a_2\right],\qquad(A.2c)$$

for $P_2 \in \{\{x,y\}|y = x + \hat{\mu} + \hat{\nu}, \mu = \pm1, \nu = 2\}$,

$$\mathcal{H}_1(P_3,\phi) = -c_8^1\left((\phi(x)[\phi(x+\hat{\mu}) + \phi(x-\hat{\mu})])^2 + a_3\right),\qquad(A.2d)$$

* $\hat{\mu}$ denotes a vector of length of the lattice spacing in the μ-direction.

for $P_3 \in \{\{x, y, z\} | y = x + \hat{\mu}, \ z = x - \hat{\mu}, \ \mu = 1, 2\}$,

$$\mathscr{H}_1(P_4, \phi) = -\tfrac{1}{16}c_9^1\Bigg(\Big\{\big([\phi(x + \hat{\mu}) - \phi(x - \hat{\mu})]^2\big)^2 + \big([\phi(x + \hat{\nu}) - \phi(x - \hat{\nu})]^2\big)^2$$

$$+ 2([\phi(x + \hat{\mu}) - \phi(x - \hat{\mu})][\phi(x + \hat{\nu}) - \phi(x - \hat{\nu})])^2\Big\} + a_4\Bigg),$$

(A.2e)

for $P_4 \in \{\{x_1, x_2, x_3, x_4\} | \ \exists x : x_1 = x + \hat{\mu}, \ x_2 = x - \hat{\mu}, \ x_3 = x + \hat{\nu}, \ x_4 = x - \hat{\nu}, \ \mu = 1, \ \nu = 2\}$.

The one-loop improvement coefficients c_i^1 are adopted from ref. [9]. They are: $c_5^1 = -0.0245659$, $c_6^1 = -0.0032718$, $c_8^1 = -0.0087486$, $c_9^1 = +0.0194364$. The real parameters a_1, a_2, a_3 and a_4 are introduced by the author. Their aim is explained below.

The partition function $Z = \int_\phi e^{-\mathscr{H}_{imp}(\phi)}$ is converted to the polymer representation (2.1) by declaring the sets P_1, P_2, P_3 and P_4 to be polymers with activities $A(P_i, \phi) = (e^{-\mathscr{H}_i(P_i, \phi)} - 1)$, and two polymers are compatible when they are not identical. (Details can be found in ref. [10].) For the nonlinear σ-model $\int_\phi$ means integration over all possible field configurations, subject to the restriction $\phi(x)^2 = 1$ for all $x \in \Lambda$.

The parameters $a_1, \ldots, a_4$ fix the maxima and minima of the activities. However, expectation values of observables remain unchanged under variations of these parameters, because the only effect when changing $a_1, \ldots, a_4$ is to multiply the partition function by a field-independent positive constant. A polymer system with positive semidefinite probability density is obtained by fixing $a_1 = a_2 = -1$, $a_3 = -4$, $a_4 = 0$. To get an indefinite polymer system, the activities of the polymers P_1, P_2 and P_3 were kept positive semidefinite, while a_4 was fixed to -32.622 which means that the polymers P_4 can become negative with $\max_\phi A(P_4, \phi) = -\min_\phi A(P_4, \phi) = 0.039$.

The probabilities for $P_1, P_2, P_3, P_4 \in \mathscr{X}$ in the system with positive semidefinite activities are 8.68%, 6.14%, 2.27%, 1.04% respectively [10]. Those for $P_1, P_2, P_3, P_4 \in \mathscr{X}$ in the indefinite system are 8.42%, 5.98%, 2.24%, 2.87% respectively. The conditional probability for $A(P_4, \phi) < 0$ when $P_4 \in \mathscr{X}$ in the indefinite system is 99.5%. The absolute error is less than 0.02% for any of the probabilities mentioned.

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