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HOW TO CALCULATE THE ELASTIC SCATTERING MATRIX IN TWO-DIMENSIONAL QUANTUM FIELD THEORIES BY NUMERICAL SIMULATION

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A method to calculate the elastic scattering amplitude at low energies in two-dimensional quantum field theories is proposed and tested in a numerical simulation of the O(3) non-linear σ-model on a simple square lattice. We also compute the isospin current form factor in this model and compare our results with the known exact expressions for the S-matrix and the form factor in the continuum limit. As a technical improvement, we introduce a two-cluster simulation algorithm which leads to significantly reduced statistical errors in the calculation of four-point correlation functions.

1. Introduction

In the past few years, numerical simulations of (euclidean) quantum field theories have become a widely used and highly successful technique to determine their fundamental properties in various regions of the parameter space. In most cases, the quantities calculated are the particle mass spectrum and bulk quantities, such as specific heats, internal energies and fermion condensates. For partly technical and partly physical reasons, it is much harder to also determine coupling constants and the elastic scattering matrix, i.e. quantities that are derived from three- and four-point correlation functions. Thus, as far as we know, the ϕ^4-theory is actually the only four-dimensional field theory where one has succeeded to compute the scattering lengths associated with the scattering of the fundamental particles [1, 2].

The most important result obtained in this paper is the practical demonstration that the scattering phase shifts at low momenta can be calculated in a rather direct

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and comparatively simple manner in two-dimensional quantum field theories. The basic idea (which has already been sketched in an earlier publication [6]) is to compute the energy spectrum in the two-particle sector in a sufficiently large but finite periodic box. For any observed level with zero total momentum, definite internal quantum numbers and energy W, the corresponding scattering phase shift $\delta(k)$ at momentum k in the center-of-mass frame is then given by

$$e^{2i\delta(k)} = e^{-ikL}. \tag{1.1}$$

Here, L denotes the box size and k is related to W through

$$W = 2\sqrt{m^2 + k^2}\,, \tag{1.2}$$

m being the mass of the scattered particles (which we have assumed to be identical for simplicity). Thus, if W and m have been accurately determined in a numerical simulation, the momentum k can be extracted from eq. (1.2) and the scattering phase at this momentum is then given by eq. (1.1). Note that for any fixed value of L, one obtains the scattering phase at a discrete set of momenta k according to the measured spectrum of energy values W. If desired, a whole range of momenta k can be covered by varying L at fixed m.

As we shall discuss in greater detail later on, the fundamental relation (1.1) is only valid when scaling violations and polarization effects can be neglected, i.e. only when one is sufficiently close to the continuum limit and when the box size L is so large that virtual particle exchanges "around the world" are strongly suppressed. Physically speaking, what is required is that the Compton wave length m^{-1} of the particles should be several lattice spacings at least; in particular, the relativistic energy-momentum dispersion should be accurately valid for small momenta. Furthermore, the box size L should be significantly larger than the interaction range so that when two particles are contained in the box, they will have some space to propagate freely before they feel the presence of each other.

It is quite clear from these remarks that the procedure outlined above will require large lattices to be simulated at large correlation lengths and thus the calculation may turn out to be impractical for a given model due to critical slowing down of the commonly used simulation algorithms. To test the method we have therefore decided to consider the O(3) non-linear σ-model where a highly efficient algorithm (the "one-cluster update algorithm") has recently been found [8–11]. There seems to be no critical slowing down for this algorithm and thus we are able to obtain interesting results with about 240 hours of single processor CPU time on a CRAY-XMP.

Of course, there is also an independent interest to study this particular model, because here an exact formula for the scattering matrix in the continuum limit has been proposed many years ago by Zamolodchikov and Zamolodchikov [15] on the

basis of the existence of higher conservation laws plus some (weak) qualitative assumptions, and thus we have a good opportunity now to check to what extent the lattice model is able to reproduce these expressions. If we find agreement, not only our method and the exact S-matrix would be confirmed, but one would also obtain additional evidence that the continuum limit of the lattice model exists in the expected way, a commonly made assumption which has recently been critically discussed in a series of papers by Patrascioiu et al. [24–27].

There is actually another, more easily accessible quantity which can be used to obtain a similar consistency test of the lattice O(3) σ-model. This is the form factor $G(k)$ of the isospin current $j_\mu^{ab}(x)$ defined through

$$\langle p, c | j_\mu^{ab}(0) | q, d \rangle = -i(p_\mu + q_\mu)(\delta^{ac}\delta^{bd} - \delta^{ad}\delta^{bc})G(k), \tag{1.3}$$

where $|p, c\rangle$ denotes the one-particle state with momentum p and isospin label c, and k is given by

$$k = \tfrac{1}{2}\sqrt{-(p-q)^2} \geqslant 0. \tag{1.4}$$

Starting from the known S-matrix, an exact formula for the form factor has been derived by Karowski and Weisz [21], and thus we have decided to also compute this quantity at low momenta, which is, in principle, a much simpler task than the calculation of the scattering matrix.

The organization of our paper is as follows. We first summarize the known exact results on the scattering matrix and the form factor in the O(3) non-linear σ-model (sect. 2). The lattice version of the model is introduced in sect. 3 and the simulation algorithm that we have used is briefly discussed. In particular, a modification of the cluster algorithm is described here which is particularly effective for the calculation of the four-point correlation function of the fundamental spin field. In sect. 4 we explain how to compute the current form factor $G(k)$ and discuss our results for this quantity. We then proceed to the calculation of the scattering matrix according to the technique outlined above (sect. 5). This section also includes a discussion of the proof and limitations of the fundamental eq. (1.1). The paper ends with a few concluding remarks in sect. 6.

2. Exact results on the O(n) model

In this section we summarize what is known about the scattering matrix and the current form factor in the continuum limit of the O(n) non-linear σ-model in $1 + 1$ dimensions [15–23]. Apart from introducing our notations, this discussion gives us the opportunity to list the critical assumptions that have to be made to be able to derive the exact S-matrix and thus some feeling will result as to how credible this formula is.

2.1. NOTATIONS AND BASIC PROPERTIES

On a classical level, the O(n) model describes an n-component spin field*

$$s^a(z), \quad a = 1, \ldots, n, \quad x = (x^0, x^1) \in \mathbb{R}^2 \tag{2.1}$$

of unit length, viz.

$$s(x) \cdot s(x) = 1. \tag{2.2}$$

The classical action is

$$S = \frac{n}{2f} \int \mathrm{d}^2 x \, \partial_\mu s(x) \cdot \partial^\mu s(x), \tag{2.3}$$

where $f > 0$ denotes the coupling constant. The conserved current associated with the obvious O(n) symmetry (the "isospin" symmetry) of the action reads

$$j_\mu^{ab}(x) = \frac{n}{f} \left[s^a(x) \partial_\mu s^b(x) - s^b(x) \partial_\mu s^a(x) \right]. \tag{2.4}$$

There are many more symmetries in this model, which we shall briefly refer to later on.

It is well known that the scale invariance of the classical theory is broken after quantization by the conformal anomaly, and thus it is commonly believed that a mass gap develops. More specifically, one has reason to expect that the particle spectrum in the quantized model consists of an O(n) vector of particles of mass m and that the ground state $|0\rangle$ is O(n) invariant. Thus, there are one-particle states

$$|p, a\rangle, \quad a = 1, \ldots, n, \tag{2.5}$$

labelled by a momentum

$$p = (p^0, p^1), \qquad p^0 = \sqrt{m^2 + (p^1)^2} > 0, \tag{2.6}$$

and an isospin index a. The normalization and phase of these states may be chosen such that

$$\langle p, a | q, b \rangle = \delta^{ab} 2p^0 2\pi \delta(p^1 - q^1), \tag{2.7}$$

$$\langle 0 | s^a(x) | p, b \rangle = \delta^{ab} \sqrt{Z} \, \mathrm{e}^{-ipx}, \tag{2.8}$$

where $Z > 0$ is some constant that depends on how the regularization and

* Greek indices $\mu, \nu, \ldots$ run from 0 to 1 and Latin indices $a, b \ldots$ from 1 to n. Repeated indices are summed over. The space-time metric is taken to be $g_{\mu\nu} = \mathrm{diag}(1, -1)$, and the associated scalar product reads $xy = g_{\mu\nu} x^\mu y^\nu = x^\mu y_\mu$. Partial derivatives are abbreviated by $\partial_\mu = g_{\mu\nu} \partial^\nu = \partial / \partial x^\mu$.

renormalization of the theory has been performed. Instead of the momentum p, many authors use the rapidity variable

$$\eta = \ln(p^0 + p^1)/m\,, \tag{2.9}$$

$$p^0 = m\cosh\eta\,, \qquad p^1 = m\sinh\eta\,. \tag{2.10}$$

Accordingly, we shall also write $|\eta, a\rangle$ for the one-particle states and the normalization (2.7) then reads

$$\langle \eta, a|\chi, b\rangle = \delta^{ab} 4\pi\delta(\eta - \chi)\,. \tag{2.11}$$

As already mentioned above, the O(n) symmetry is expected to be unbroken in the quantized theory. The charge

$$J^{ab} = \int \mathrm{d}x^1\, j_0^{ab}(x) \tag{2.12}$$

thus annihilates the vacuum state $|0\rangle$ and we may choose the normalization of the isospin current in such a way that

$$J^{ab}|\eta, c\rangle = i(\ \delta^{ac}|\eta, b\rangle - \ \delta^{bc}|\eta, a\rangle)\,. \tag{2.13}$$

(On a formal level, eq. (2.13) is implied by the definition (2.4) and the canonical quantization rules; in what follows we just fix the normalization of the current by imposing (2.13).)

2.2. ELASTIC SCATTERING MATRIX

Consider now an elastic scattering process where two particles with initial momenta p, q and isospin labels a, b scatter and end up in the final state described by the momenta p', q' and isospin labels a', b'. Due to Bose symmetry, it suffices to discuss the case where the corresponding rapidities satisfy

$$\eta > \chi\,, \qquad \eta' > \chi'\,. \tag{2.14}$$

The associated scattering matrix element then reads

$$\langle \eta', a'; \chi', b' \text{ out}|\eta, a; \chi, b \text{ in}\rangle = (4\pi)^2\delta(\eta' - \eta)\delta(\chi' - \chi)S(\theta)_{a'b',ab}\,, \tag{2.15}$$

where $\theta = \eta - \chi$ and the matrix $S(\theta)$ can be decomposed according to

$$S(\theta)_{a'b',ab} = \delta^{a'b'}\delta^{ab}\sigma_1(\theta) + \delta^{a'a}\delta^{b'b}\sigma_2(\theta) + \delta^{a'b}\delta^{b'a}\sigma_3(\theta)\,. \tag{2.16}$$

In what follows we list a number of properties which the invariant amplitudes

$\sigma_k(\theta)$ are expected to have, and these almost fix their analytic form, as has first been remarked by Zamolodchikov and Zamolodchikov [15].

The most crucial set of relations satisfied by the σ_k's are the "factorization equations", viz.

$$\sigma_1 = -\frac{2\pi i}{i\pi - \theta} \cdot \frac{\sigma_2}{n-2}, \quad \sigma_3 = -\frac{2\pi i}{\theta} \cdot \frac{\sigma_2}{n-2}. \qquad (2.17), (2.18)$$

These relations follow directly from the higher non-local conservation laws, whose existence has been established making only weak structural assumptions [16–19]. A further consequence of the conservation laws (which is also implied by the higher *local* conserved currents [20]) is the absence of particle production. Thus, elastic unitarity holds for arbitrary energies, and, using the factorization equations, one concludes that

$$|\sigma_2|^2 = \frac{\theta^2}{\theta^2 + \lambda^2}, \quad \lambda = 2\pi/(n-2), \qquad (2.19)$$

for all $\theta > 0$.

From eq. (2.16) it is apparent that $\sigma_2(\theta)$ is a forward elastic scattering amplitude. On very general grounds (basically the Wightman axioms), it can therefore be analytically continued into the strip $0 \leqslant \mathrm{Im}\,\theta \leqslant \pi$ and, due to eq. (2.19), $\sigma_2(\theta)$ then extends to a meromorphic function in the whole complex plane. Furthermore, crossing symmetry and reality imply

$$\sigma_2(i\pi - \theta) = \sigma_2(\theta), \qquad \sigma_2(\theta)^* = \sigma_2(-\theta^*), \qquad (2.20), (2.21)$$

and the unitarity relation (2.19) may be rewritten in the form

$$\sigma_2(\theta)\sigma_2(-\theta) = \frac{\theta^2}{\theta^2 + \lambda^2}, \qquad (2.22)$$

which is valid for arbitrary complex θ.

The point now is that eqs. (2.20)–(2.22) almost determine $\sigma_2(\theta)$. In fact, if we add the constraint that $\sigma_2(\theta)$ is bounded by a power of $\cosh\theta$ for large $\mathrm{Re}\,\theta$ (which is reasonable because of asymptotic freedom) the most general solution is

$$\sigma_2(\theta) = f(\theta)Q(\theta)Q(i\pi - \theta), \qquad (2.23)$$

where $Q(\theta)$ is defined by

$$Q(\theta) = \frac{\Gamma(\Delta - i\theta/2\pi)\Gamma(\frac{1}{2} - i\theta/2\pi)}{\Gamma(\frac{1}{2} + \Delta - i\theta/2\pi)\Gamma(-i\theta/2\pi)}, \quad \Delta = 1/(n-2), \qquad (2.24)$$

and $f(\theta)$ is a so-called CDD factor, viz.

$$f(\theta) = \pm \prod_{k=1}^{K} \frac{\sinh\theta + iz_k}{\sinh\theta - iz_k} . \tag{2.25}$$

The constants z_k that enter here are arbitrary, except that they should either be real or come in complex conjugate pairs.

In our opinion, the presence of this CDD factor is the main ambiguity that remains and there is actually no very strong argument known today that would fix it. However, it has been remarked that the choice $f(\theta) = 1$ is minimal in the sense that $\sigma_2(\theta)$ then has no zeros in the physical sheet besides at $\theta = 0$ (while there are additional zeros for all other choices), and this particular solution was therefore proposed to be the scattering matrix of the O(n) model [15]. Further evidence for $f(\theta) = 1$ was later obtained by working out the scattering matrix to order $1/n^2$ in the large n expansion [23]. For these reasons, we shall in what follows refer to the solution with no CDD factor as the exact scattering matrix of the O(n) model.

Later on in the numerical work, we shall be mainly interested to calculate the scattering phase shifts $\delta_I(k)$ for a definite isospin $I = 0, 1, 2$. These are obtained from the scattering matrix $S(\theta)$ by going to isospin eigenstates, i.e. we decompose $S(\theta)$ according to

$$S(\theta)_{a'b',ab} = \sum_{I=0}^{2} s_I(\theta) P_I(a'b'|ab) , \tag{2.26}$$

where the isospin projectors are given by

$$P_0(a'b'|ab) = \frac{1}{n}\delta^{a'b'}\delta^{ab} , \tag{2.27}$$

$$P_1(a'b'|ab) = \frac{1}{2}(\delta^{a'a}\delta^{b'b} - \delta^{a'b}\delta^{b'a}) , \tag{2.28}$$

$$P_2(a'b'|ab) = \frac{1}{2}(\delta^{a'a}\delta^{b'b} + \delta^{a'b}\delta^{b'a}) - \frac{1}{n}\delta^{a'b'}\delta^{ab} . \tag{2.29}$$

For physical values of θ, unitarity implies $|s_I(\theta)|^2 = 1$ so that, following standard conventions, we can define the scattering phases through

$$e^{2i\delta_I(k)} = s_I(\theta) , \qquad k = m \sinh \tfrac{1}{2}\theta \tag{2.30}$$

(in the centre-of-mass frame, $k = p^1$ is the absolute value of the momentum of the incoming particles).

From the exact expressions (2.23) and (2.24) for σ_2, the other amplitudes σ_1 and σ_3 can be determined through the factorization equations and hence an exact formula for the scattering phases is obtained. In the case of the O(3) model, the resulting expressions assume the intriguingly simple form

$$e^{2i\delta_0(k)} = \frac{\theta + 2i\pi}{\theta - 2i\pi}, \tag{2.31}$$

$$e^{2i\delta_1(k)} = \frac{\theta + 2i\pi}{\theta - 2i\pi} \cdot \frac{\theta - i\pi}{\theta + i\pi}, \tag{2.32}$$

$$e^{2i\delta_2(k)} = \frac{\theta - i\pi}{\theta + i\pi}, \tag{2.33}$$

(see fig. 1). Note that $\delta_I(k)$ is only slowly (logarithmically) going to zero for $k \to \infty$ in accordance with asymptotic freedom.

We would like to mention at this point that in a weakly coupled linear σ-model, the phase shifts at low energies have the same qualitative behaviour as in the non-linear model, except that $\delta_0(k)$ starts at $-\pi/2$ and then monotonically increases towards zero for $k \to \infty$, i.e. $\delta_0(k)$ has a similar shape as $\delta_2(k)$. When the (renormalized) quartic coupling in the model is increased to its maximal value, corresponding to the non-linear model, the phase shift develops a zero and, at some intermediate coupling, its value at $k = 0$ jumps from $-\pi/2$ to $+\pi/2$ (this can be verified explicitly in the large n limit). Thus, the fact that $\delta_0(k)$ behaves as shown in fig. 1 is indicative of the truly nonperturbative nature of the non-linear σ-model in two dimensions.

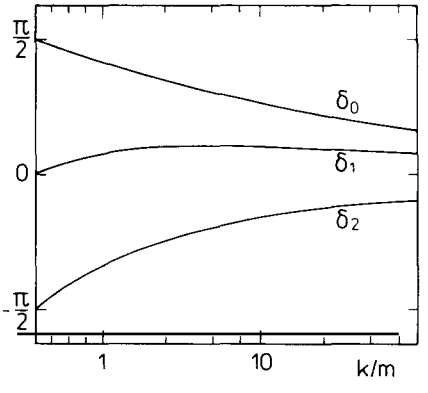

Fig. 1. Scattering phase shifts in the O(3) non-linear σ-model (eqs. (2.31)–(2.33)). The scale on the abscissa is linear for $k/m \leqslant 1$ and logarithmic for $k/m \geqslant 1$.

2.3. CURRENT FORM FACTOR

The current form factor is defined through eqs. (1.3) and (1.4) and the normalization condition (2.13). This implies, in particular, that

$$G(0) = 1. \tag{2.34}$$

For general values of k, an exact formula for the form factor has been derived by Karowski and Weisz [21]. The ideas involved in this derivation are similar to the ones that led to the exact scattering matrix. In particular, one relies on the analyticity, as implied by fundamental principles, the absence of particle production and the known form of the scattering phase shift in the isospin-1 channel. Their result is

$$G(k) = h(\theta)\exp\left\{-2\int_0^\infty \frac{\mathrm{d}t}{t}\,\frac{1-\mathrm{e}^{-2\Delta t}}{1+\mathrm{e}^{t}}\,\frac{\sin^2(\theta t/2\pi)}{\sinh t}\right\}, \tag{2.35}$$

where the rapidity variable θ is related to k through

$$k = m\sinh\tfrac{1}{2}\theta, \tag{2.36}$$

and $h(\theta)$ is some real polynomial in $\cosh\theta$ with $h(0) = 1$.

The polynomial $h(\theta)$ remains unspecified if only the general requirements of analyticity etc. are to be fulfilled, and in this respect $h(\theta)$ is similar to the CDD factor $f(\theta)$ which appears in the exact scattering matrix. However, because the O(n) model is asymptotically free, one would be very surprised if the form factor would increase to infinity at large momenta k. Thus, if we require that $G(k)$ remains bounded, it follows that $h(\theta) = 1$ and the form factor is then completely determined. In the case of the O(3) model, the integral (2.35) can be evaluated analytically and one ends up with

$$G(k) = \frac{\theta}{2\tanh\frac{1}{2}\theta}\cdot\frac{\pi^2}{\pi^2+\theta^2} \tag{2.37}$$

(a plot of the form factor will be shown later). We finally remark that an exact formula for the matrix elements of the current between in- and out-states with an arbitrary number of particles has recently been proposed by Kirillov and Smirnov [22].

3. Cluster simulation of the lattice O(3) model

In the following we define the lattice regularized non-linear σ-model and then briefly review the collective mode Monte Carlo method [8] that we employ for its

simulation. A new two-cluster (2C) variant of the basic algorithm is presented, that is particularly suitable for the calculation of the required four-point functions.

3.1. LATTICE FORMULATION

We use the lattice regularization as a standard tool to define a quantum field theory rigorously and independently of perturbation theory. The continuum limit for a large but finite physical volume is approached through a sequence of systems with a growing but finite number of degrees of freedom for which numerical simulation techniques are applicable. More precisely, we shall use euclidean square lattices Λ with $|\Lambda| = T \times L$ sites and periodic boundary conditions. The temporal extent T will always be kept very large compared to (inverse) physical energies, i.e. we work at zero temperature. The spin field $s^a(x)$ of sect. 2 is restricted to the sites of Λ, and ∂_μ is reinterpreted as the difference operator

$$\partial_\mu s^a(x) = s^a(x + \hat{\mu}) - s^a(x), \tag{3.1}$$

where $\hat{\mu}$ is the unit vector in the positive μ-direction*. The lattice version of eq. (2.3) then corresponds to the standard action for the O(n) non-linear σ-model,

$$S = -\beta \sum_{x\mu} s(x) \cdot s(x + \hat{\mu}), \quad \beta = n/f, \tag{3.2}$$

up to an irrelevant additive constant. Expectation values of arbitrary euclidean observable $A[s]$ are given by

$$\langle A \rangle = \frac{1}{Z} \int \prod_x \mathrm{d}\mu(s(x))\, \mathrm{e}^{-S} A[s], \tag{3.3}$$

where $\mathrm{d}\mu(s)$ denotes the O(n) invariant single spin distribution, normalized to 1, and the partition function Z is such that $\langle 1 \rangle = 1$. Finally, the euclidean O(n) current on the lattice is defined by

$$j_\mu^{ab}(x) = \beta \big[s^a(x)\, \partial_\mu s^b(x) - s^b(x)\, \partial_\mu s^a(x) \big]. \tag{3.4}$$

As we shall discuss later on, this current is conserved in the sense that it satisfies the exact Ward identities which are associated with the O(n) symmetry of the lattice theory.

* We use the symbol x both for continuum points and for lattice sites. Dimensionful quantities on the lattice will always be given in lattice units, i.e. the lattice spacing a is set equal to 1. In particular, a lattice site $x = (x^0, x^1)$ has integer coordinates. The operator ∂_μ means derivative or difference depending on the context.

3.2. COLLECTIVE MODE MONTE CARLO

The present study has become feasible due to the availability of new global Monte Carlo techniques, which, for all practical purposes, eliminate the problem of critical slowing down for O(n) symmetric spin models [8–12]. As originally suggested by Swendsen and Wang for discrete Potts spins [7], a bond percolation process is coupled with spin configurations in such a way, that certain global spin flips on whole percolation clusters furnish updates that respect detailed balance. For each such update step a random direction in spin space $r \in \mathbb{R}^n, r^2 = 1$, is chosen, and only the components $r \cdot s(x) = s_r(x)$ will be affected by this step. Bonds on links $(x, x + \hat{\mu})$ are activated with probabilities

$$p_r(s; x, \mu) = \begin{cases} 1 - \exp[-2\beta s_r(x) s_r(x+\hat{\mu})] & \text{if } s_r(x) s_r(x+\hat{\mu}) \geqslant 0, \\ 0 & \text{otherwise}. \end{cases} \tag{3.5}$$

For $n = 1$, eq. (3.5) coincides with the prescription of Swendsen and Wang [7] for the Ising model. In their algorithm all bonds on the lattice are conditionally activated with probability (3.5), and the resulting clusters c_i define a decomposition of the lattice

$$\Lambda = \bigcup_{i=1}^{\nu} \mathrm{c}_i . \tag{3.6}$$

The update is completed by flipping the spins on each cluster c_i with probability $\frac{1}{2}$. This generalizes to a valid algorithm for $n \geqslant 1$ [11, 12], if the sign-flips are carried out for s_r only,

$$s^a(x) \to s^a(x) - 2 s_r(x) r^a . \tag{3.7}$$

Further use of the information represented by the cluster geometry is made by introducing cluster-improved estimators [12]. For the fundamental two-point function the symmetry argument

$$\langle s^a(x) s^b(y) \rangle = \delta^{ab} f(x - y) \tag{3.8}$$

allows us to write

$$\langle s(x) \cdot s(y) \rangle = n \langle s_r(x) s_r(y) \rangle . \tag{3.9}$$

If we now average over the 2^ν states that a cluster update referring to r *could* choose with equal probability (of which only *one* is actually sampled), then we derive

$$\langle s(x) \cdot s(y) \rangle = n \left\langle s_r(x) s_r(y) \sum_{i=1}^{\nu} \theta_{\mathrm{c}_i}(x) \theta_{\mathrm{c}_i}(y) \right\rangle , \tag{3.10}$$

where θ_c is the characteristic function of cluster c. Taking into account eq. (3.5), we notice that $s_r(x)$ has only one sign on each cluster. Therefore we average over a positive quantity on the right-hand side of eq. (3.10). Technically, this is what leads to a reduced variance with the deeper reason being our averaging over a larger number of configurations. In numerical calculations we found that an exponential decay of the two-point function in the representation (3.10) is mainly caused by the cluster cutoff θ_c. This shows very clearly the linkage between the size of our update steps and the physically relevant scale. We think that this connection is crucial for the success of the algorithm.

In ref. [8] a single cluster (1C) variant of the many cluster Swendsen–Wang procedure just outlined has been introduced. Its elementary steps consist of picking a random site x_0 as a seed for a cluster and then growing a single cluster C connected to x_0. Again, the bond activation probability (3.5) is used here. When C is completed, all spins on C are flipped with (3.7). In comparing XY-model results [9, 12] we found the 1C algorithm superior to the already efficient many cluster method in decorrelating long-range observables. Similar conclusions have been drawn for the Ising model in refs. [13, 14]. The reason for these results presumably lies at least partly in the fact, that the random seed x_0 preferentially connects to large clusters. We shall exclusively use 1C-type updating in this work.

The cluster estimator (3.10) can also be adapted to the 1C method [11]. We may imagine to perform the sum over clusters under the average stochastically. The probability $|c_i|/|\Lambda|$, with which the random seed falls into cluster c_i, has to be compensated for, giving

$$\langle s(x)\cdot s(y)\rangle = n\left\langle s_r(x)s_r(y)\frac{|\Lambda|}{|C|}\theta_C(x)\theta_C(y)\right\rangle^{1C}. \tag{3.11}$$

3.3. TWO CLUSTER ALGORITHM AND CLUSTER ESTIMATORS FOR FOUR-POINT FUNCTIONS

The physical observables that we focus on in this work lead us to consider a variety of four-point functions. The most general such object may be decomposed into isospin channels

$$\langle s^a(x)s^b(y)s^{a'}(x')s^{b'}(y')\rangle = \sum_{I=0}^{2} P_I(ab|a'b')f_I(x,y;x',y'), \tag{3.12}$$

with the isospin projectors (2.27)–(2.29). If we now introduce a pair of orthogonal

spin directions $r, u \in S^{n-1}$, $r \cdot u = 0$, it is trivial to contract and derive

$$\langle s_r(x) s_r(y) s_u(x') s_u(y') \rangle = \frac{1}{n}(f_0 - f_2), \tag{3.13}$$

$$\langle s_r(x) s_u(y) s_r(x') s_u(y') \rangle = \frac{1}{2}(f_1 + f_2), \tag{3.14}$$

$$\langle s_r(x) s_u(y) s_u(x') s_r(y') \rangle = \frac{1}{2}(f_1 - f_2). \tag{3.15}$$

All arguments of f_I are as in eq. (3.12) here. We insert these relations and find

$$P_0(ab|a'b')\langle s^a(x) s^b(y) s^{a'}(x') s^{b'}(y') \rangle$$

$$= n\langle s_r(x) s_r(y) s_u(x') s_u(y') \rangle + 2\langle s_{(r}(x) s_{u)}(y) s_{(r}(x') s_{u)}(y') \rangle, \tag{3.16}$$

$$P_1(ab|a'b')\langle s^a(x) s^b(y) s^{a'}(x') s^{b'}(y') \rangle$$

$$= n(n-1)\langle s_{[r}(x) s_{u]}(y) s_{[r}(x') s_{u]}(y') \rangle, \tag{3.17}$$

$$P_2(ab|a'b')\langle s^a(x) s^b(y) s^{a'}(x') s^{b'}(y') \rangle$$

$$= [n(n+1) - 2]\langle s_{(r}(x) s_{u)}(y) s_{(r}(x') s_{u)}(y') \rangle. \tag{3.18}$$

The bracketed subscripts denote (anti-) symmetrization,

$$s_{[r}(x) s_{u]}(y) = \tfrac{1}{2}[s_r(x) s_u(y) - s_u(x) s_r(y)], \tag{3.19}$$

$$s_{(r}(x) s_{u)}(y) = \tfrac{1}{2}[s_r(x) s_u(y) + s_u(x) s_r(y)]. \tag{3.20}$$

Eqs. (3.16)–(3.18) are the appropriate generalizations of (3.9) for the four-point function. It is now straightforward to construct cluster estimators by linking r, u with the update steps. To this end we pick them randomly with the measure

$$d\mu(r, u) = d^n r\, d^n u\, \delta(r^2 - 1)\delta(u^2 - 1)\delta(r \cdot u). \tag{3.21}$$

The proof of detailed balance given in ref. [11] – both for many cluster and for 1C-updating – now trivially generalizes to the case, where we perform such steps with both r and u. Note that, because of the orthogonality of r and u, the order in which we perform the r-update and the u-update is irrelevant. We are dealing with partial resamplings of independent degrees of freedom [12]. The 2C algorithm now corresponds to building clusters C_r and C_u independently.

By arguments entirely analogous to those leading to eq. (3.11) we construct cluster-improved versions of eqs. (3.16)–(3.18). They are obtained by substituting

$$s_r(x) \to \left(\frac{|A|}{|C|}\right)^{1/2} \theta_{C_r}(x) s_r(x) \tag{3.22}$$

and similarly for s_u and C_u. A positive estimator results for the $I = 2$ channel, and both tensor channels $I = 1, 2$ include cluster cutoffs: nonzero contributions can only occur if the groups of points x, y and x', y' are bridged simultaneously by C_r and C_u. As for the two-point function, we therefore expect a reduced variance in these cases while in the isoscalar case (eq. (3.16)) no comparable improvement is expected (cf. sect. 5.3).

4. Computation of the current form factor

In this section we present our numerical results for the current form factor. All simulations have been done for the O(3) model, and thus we set $n = 3$ in what follows (the generalization to arbitrary values of n is trivial). Furthermore, for the theoretical discussion we shall always assume that the time-like extent T of the lattice is infinite, while the space-like extent L is taken to be finite.

4.1. ONE-PARTICLE STATES ON THE LATTICE

The physical interpretation of the euclidean lattice theory is based on the transfer matrix construction (see e.g. ref. [28]). This construction involves a Hilbert space $\mathscr{H}$, the space of physical states, and the transfer matrix $\mathbb{T}$, which is a self-adjoint positive operator acting in $\mathscr{H}$. The hamilton operator $\mathbb{H}$ of the theory is related to the transfer matrix through $\mathbb{T} = \exp(-\mathbb{H})$ (recall that the lattice spacing has been set equal to one). As in the continuum we expect that the ground state $|0\rangle$ of $\mathbb{H}$ is non-degenerate. Without loss, we may choose the normalization of the transfer matrix such that the ground-state energy vanishes. Furthermore, the translations by any integer number of lattice spacings in the space direction and the isospin symmetry (which are represented by unitary operators in the space $\mathscr{H}$ of physical states) act trivially on $|0\rangle$.

The connection between the euclidean correlation functions of the spin field and the transfer matrix is expressed through

$$\langle s^{a_1}(x_1) \dots s^{a_k}(x_k) \rangle$$

$$= \langle 0 | \hat{s}^{a_1}(x_1^1) \mathbb{T}^{x_1^0 - x_2^0} \hat{s}^{a_2}(x_2^1) \mathbb{T}^{x_2^0 - x_3^0} \dots \hat{s}^{a_k}(x_k^1) | 0 \rangle , \tag{4.1}$$

where we have ordered the fields such that $x_1^0 \geqslant x_2^0 \geqslant \ldots \geqslant x_k^0$ and where $\hat{s}^a(x^1)$ denotes the spin field operator at time $x^0 = 0$.

One-particle states $|p, a\rangle$ also exist on a lattice, but as compared to the continuum case a number of complications occur. In particular, the momentum p^1 is restricted to the values

$$p^1 = \frac{2\pi\nu}{L}, \qquad \text{where } \nu \in \mathbb{Z}, \qquad -L/2 < \nu \leqslant L/2, \tag{4.2}$$

and the energy p^0 of these states is some function of p^1 and L, which is not a priori known. If we define the particle mass m to be the one-particle energy at $p^1 = 0$ and $L = \infty$, one may however expect that the relativistic energy-momentum relation (2.6) holds, provided $L \gg m^{-1} \gg 1$ and $p^1 \ll 1$. The first of these inequalities expresses that L must be much larger than the physical scale in the model so that finite-size effects are negligible. In fact, these are known to decrease exponentially with L and their contribution to the one-particle energy can be estimated [3, 4] to be of the order of a few per mille at most if

$$mL \geqslant 6. \tag{4.3}$$

In our simulations the observed deviations of the one-particle energy from the relativistic form are larger than these finite size corrections and they are thus essentially due to lattice effects, i.e. due to the presence of a finite ultraviolet cutoff (see table 1 for an example). On general grounds [29], these effects should decrease with approximately the square of the lattice spacing. The data listed in

TABLE 1
One-particle energy values p^0 as a function of the momentum p^1 on a lattice with $L = 128$ and $m^{-1} = 13.632(6)$.

ν	p^1/m	$p^0\Big/\sqrt{m^2 + (p^1)^2}$
1	0.6692(3)	0.9992(3)
2	1.3383(6)	0.9993(3)
3	2.0075(9)	0.9989(3)
4	2.677(1)	0.9979(4)
5	3.346(1)	0.9963(4)
6	4.015(2)	0.9947(5)
7	4.684(2)	0.9928(4)
8	5.353(2)	0.9904(4)

table 1 can in fact be represented rather well by

$$\frac{p^0}{\sqrt{m^2+(p^1)^2}} = 1 - 0.06 \times (p^1)^2, \tag{4.4}$$

and thus we conclude that the systematic errors in this part of our calculations are under control.

The normalization and phase of the lattice one-particle states may be chosen such that

$$\langle p, a | q, b \rangle = \delta^{ab} 2p^0 L \delta_{p^1 q^1}, \tag{4.5}$$

$$\langle 0 | \hat{s}^a(x^1) | p, b \rangle = \delta^{ab} \sqrt{Z(p)}\, \mathrm{e}^{ip^1 x^1}, \tag{4.6}$$

where the dependence of the wave-function renormalization factor $Z > 0$ on L has been suppressed. These conventions are such that one recovers the normalizations (2.7) and (2.8) in the (infinite volume) continuum limit of the model.

4.2. METHOD OF CALCULATION

The euclidean current (3.4) is proportional to the change of the lattice action (3.2) under an infinitesimal local O(3) rotation of the spin field, and since this operation is a symmetry of the a priori measure in the functional integral (3.3), one concludes (as in the continuum) that the current satisfies a set of Ward identities. In particular, we have

$$\begin{aligned}\left\langle \partial^*_\mu j^{ab}_\mu(x) s^c(y) s^d(z) \right\rangle &= \delta_{xy} \left\langle \left(\delta^{ac} s^b(y) - \delta^{bc} s^a(y)\right) s^d(x) \right\rangle \\ &\quad + \delta_{xz} \left\langle s^c(y) \left(\delta^{ad} s^b(z) - \delta^{bd} s^a(z)\right) \right\rangle, \end{aligned} \tag{4.7}$$

where ∂^*_μ is the backward lattice derivative (the adjoint of $-\partial_\mu$). As we shall see shortly, eq. (4.7) guarantees that the normalization condition (2.13) is fulfilled in the continuum limit. Furthermore, since there is only one local field of dimension less than or equal to 1 in this model which transforms like an anti-symmetric tensor under O(3), operator mixing by renormalization can be excluded and the lattice current is hence expected to converge to the continuum current, at least on the level of correlation functions smeared with suitable test functions.

For any momentum p^1 in the set (4.2), we define the Fourier transform $\tilde{s}^a(x^0, p^1)$ of the spin field through

$$\tilde{s}^a(x^0, p^1) = \sum_{x^1=1}^{L} \mathrm{e}^{-ip^1 x^1} s^a(x). \tag{4.8}$$

By inserting the spectral resolution of $\mathbb{T}$ in the representation (4.1) of the spin correlation function, it is then easy to show that the asymptotic relation

$$\langle \tilde{s}^a(x^0, p^1) s^b(0) \rangle \underset{x^0 \to \infty}{\sim} \delta^{ab} \frac{Z(p)}{2p^0} \mathrm{e}^{-p^0 x^0} \tag{4.9}$$

holds up to terms vanishing exponentially fast relative to the displayed term (here and below, p^0 denotes the one-particle energy at momentum p^1). Similarly, one may show that the limit

$$g(k, L) \overset{\text{def}}{=} -\frac{1}{2} \lim_{t \to \infty} \frac{\langle \tilde{s}^a(t+1, k) j_0^{ab}(0) \tilde{s}^b(-t, k) \rangle}{\langle \tilde{s}^c(2t+1, k) s^c(0) \rangle} \tag{4.10}$$

exists and, furthermore, that it is given by

$$g(k, L) = -\left\{ \frac{1}{12p^0} \langle p, a | \hat{j}_0^{ab}(0) | q, b \rangle \right\}_{p^1 = -q^1 = k} . \tag{4.11}$$

The current operator $\hat{j}_0^{ab}(x^1)$ occurring here is defined by

$$\hat{j}_0^{ab}(x^1) = \beta \left[\partial_0 \hat{s}^b(x^1) \hat{s}^a(x^1) - \partial_0 \hat{s}^a(x^1) \hat{s}^b(x^1) \right], \tag{4.12}$$

$$\partial_0 \hat{s}^a(x^1) = \mathrm{e}^{\mathbb{H}} \hat{s}^a(x^1) \mathrm{e}^{-\mathbb{H}} - \hat{s}^a(x^1) . \tag{4.13}$$

If we would consider the same ratio $g(k, L)$ of correlation functions in the infinite volume continuum limit, eq. (4.11) would hold again and $\hat{j}_0^{ab}(x^1)$ would be $-i$ times the current operator of subsect. 2.1 (the factor of $-i$ arises because we are here dealing with the euclidean current). Recalling eq. (1.3), we therefore expect that $g(k, L)$ converges to the current form factor $G(k)$ in the (large volume) continuum limit, and thus we have found a way to extract $G(k)$ from the euclidean two-point and four-point correlation functions of the lattice spin field $s^a(x)$, which are, in principle, calculable by numerical simulation. That this method of calculation also works in practice will be demonstrated in the following subsection.

As we have already mentioned above, the normalization of the lattice currents is such that the normalization condition (2.13) (or, equivalently, eq. (2.34)) is satisfied in the continuum limit. Indeed, it follows from the Ward identity (4.7) and Stokes' theorem on the lattice that

$$g(0, L) = 1 \tag{4.14}$$

for all values of the coupling β and all L, and hence in the continuum limit.

4.3. SIMULATION RESULTS

We have simulated three different lattices, labelled A, B, C, as specified in table 2. On the lattice C, the quoted value for the mass m is obtained by measuring the one-particle energy at zero momentum and subtracting an analytically determined finite size correction $\Delta m = 0.0019 \times m$ [3,4]. On the large lattices A and B, this correction would be negligible compared to the statistical error. The lattices A and B are about equally big in physical units, i.e. the difference between these two cases is essentially that the lattice spacing is doubled when going from A to B. By comparing the results obtained on these two lattices we can therefore estimate the size of the finite lattice spacing effects. The lattice C, on the other hand, is substantially smaller in physical units than A while the correlation length is about the same (in lattice units). Thus, a comparison between A and C will give us information on the size of the finite size effects.

For each lattice we have measured the correlation functions entering the definition (4.10) of the lattice form factor $g(k, L)$, where, of course, we averaged over time and space translations to improve our statistics. It then turned out that the ratio of these correlation functions converges to a constant at values of t around one correlation length $\xi = m^{-1}$. This constant is taken as our estimate for $g(k, L)$ (see table 3; the errors quoted there are statistical only). As a check we have verified that eq. (4.14) holds within errors.

TABLE 2
Basic lattice data.

lattice	β	$T \times L$	m^{-1}	mL
A	1.54	256×128	13.632(6)	9.390(4)
B	1.40	128×64	6.883(3)	9.298(4)
C	1.50	128×64	11.054(7)	5.790(4)

TABLE 3
Simulation results for the lattice form factor $g(k, L)$ at momentum $k = 2\pi\nu/L$, and comparison with the exact form factor $G(k)$ (eqs. (2.36) and (2.37)).

lattice	ν	k/m	$g(k, L)$	$G(k)$	$g(k, L)/G(k)$
A	1	0.6692(3)	0.975(2)	0.9727(1)	1.002(2)
	2	1.3383(6)	0.935(4)	0.9218(1)	1.014(4)
	3	2.0075(9)	0.891(7)	0.8745(1)	1.019(8)
B	1	0.6757(3)	0.982(1)	0.9723(1)	1.010(1)
	2	1.3515(6)	0.947(3)	0.9208(1)	1.028(3)
	3	2.0272(9)	0.921(3)	0.8732(1)	1.055(3)
C	1	1.0852(7)	0.959(3)	0.9414(1)	1.019(3)
	2	2.170(1)	0.903(6)	0.8643(1)	1.045(7)
	3	3.256(2)	0.874(7)	0.8072(1)	1.083(9)

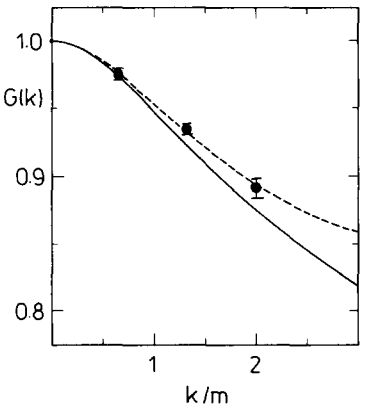

Fig. 2. Form factor $G(k)$ in the O(3) non-linear σ-model as a function of the momentum k. The solid line represents the exact formulae (2.36) and (2.37). The dashed line includes the lattice correction (4.15), as appropriate for the lattice A, and the data points are our result for this lattice (first block in table 3).

Our results show that the lattice form factor reproduces the exact form factor $G(k)$ quite well, especially in the case of the lattice A, where the systematic errors are expected to be minimal (see fig. 2). Still, almost all data points are off by a small, statistically significant amount, and it is the purpose of the following discussion to identify the possible origins of these discrepancies.

As shown in fig. 2, the data on the lattice A can be represented, within errors, by

$$g(k, L)/G(k) = 1 + k^2, \tag{4.15}$$

and this suggests that the observed deviation from the exact curve is a lattice effect which will disappear when we go closer to the continuum limit (recall that k is measured in lattice units in eq. (4.15)). This first impression is corroborated by comparing the results obtained on the lattice A with those obtained on the lattice B, where the lattice spacing (in physical units) is about twice as large as on A. At all values of k, the deviations from the exact form factor are much larger on B than on A, by factors of 5, 2 and 3 for $\nu = 1, 2, 3$. Theoretically, one would expect the errors to increase by a factor of 4 approximately [29] when going from A to B, and this is roughly what we find, although the fluctuations in the factors for different values of k indicate that our statistical errors do not allow for a more quantitative analysis of the effect.

Another possible source of systematic errors are the finite-volume effects. Their size can be estimated by comparing the lattice A with the lattice C which is about a factor 1.6 smaller than A (in physical units), while the lattice spacing is about the same. From table 3 and the interpolation (4.15), one infers that the size of this

effect is about 1–2% for $k \leqslant 2m$. Finite-size effects are decreasing exponentially with increasing mL and since they are already small on the lattice C, we expect that they are negligible compared to the statistical errors on the large lattices A and B.

To sum up, we believe that the systematic errors in our calculations are under control and conclude that within statistical errors, and accounting for the presence of small lattice effects as discussed above, there is complete agreement between "theory" and "experiment" in the momentum range $0 \leqslant k \leqslant 2m$.

5. Computation of the scattering phases

As explained in sect. 1, the numerical calculation of the scattering matrix is based on eq. (1.1), which relates the scattering phase $\delta_I(k)$ to the energy spectrum of two-particle states with isospin I in a finite volume with periodic boundary conditions. In this section we shall first discuss the derivation and physical interpretation of eq. (1.1). The problem of how to extract the two-particle energy spectrum from the (euclidean) four-point correlation function will be considered after that and, finally, the results of our numerical study of the O(3) model will be presented.

5.1. DERIVATION OF EQ. (1.1)

The basic relation (1.1) has a simple physical meaning which can already be understood in the following quantum mechanical model.

Consider two spinless bosons moving on a line. The Schrödinger wave function $\psi(x, y)$ of this system depends on the positions $x, y \in \mathbb{R}$ of the particles and has to be symmetric under an interchange of x and y. Thus, if we restrict ourselves to states with vanishing total momentum, we have

$$\psi(x, y) = f(x - y) \tag{5.1}$$

where

$$f(z) = f(-z) .$$

The stationary Schrödinger equation (in infinite volume) then reduces to

$$\left\{ -\frac{1}{m} \frac{\mathrm{d}^2}{\mathrm{d}z^2} + V(|z|) \right\} f(z) = E f(z) , \tag{5.2}$$

where $V(|z|)$ is some interaction potential, which will be assumed to be short ranged.

Since we require $f(z)$ to be symmetric, the differential equation (5.2) has actually only one admissable linearly independent solution, denoted by $f_E(z)$, for

any energy value E. In particular, for

$$E = k^2/m, \quad k \geqslant 0, \tag{5.3}$$

$f_E(z)$ is a stationary scattering solution, which can be normalized such that

$$f_E(z) \underset{|z|\to\infty}{=} \cos(k|z| + \delta(k)), \tag{5.4}$$

where $\delta(k)$ is the scattering phase.

If the particles are now enclosed in a periodic box of size L (a circle, in other words), the corresponding wave function $\psi(x, y)$ and hence the reduced wave function $f(z)$ is periodic with period L. The stationary Schrödinger equation remains the same as before (eq. (5.2)) except that the potential is replaced by

$$V_L(|z|) = \sum_{\nu=-\infty}^{\infty} V(|z + \nu L|) \tag{5.5}$$

to take into account interactions "around the world". A solution to this equation for some energy $E \geqslant 0$ can be interpreted as a stationary scattering state, where the particles are running around the circle in opposite directions.

For $|z| \leqslant L/2$ and if L is much larger than the interaction range, the additional interactions "around the world" are negligible and the solution $f_E(z)$ to the Schrödinger equation is therefore the same as for $L = \infty$. The requirement of periodicity then implies

$$f_E'(-L/2) = f_E'(L/2) = 0 \tag{5.6}$$

and, recalling eq. (5.4), one concludes that

$$kL + 2\delta(k) = 0 \pmod{2\pi}, \tag{5.7}$$

which is equivalent to eq. (1.1). For any given interaction potential V and box size L, eq. (1.1) has a discrete set of solutions k_ν, $\nu = 0, 1, 2, \ldots$, and this then yields the possible finite volume energy values $E_\nu = k_\nu^2/m$. In other words, eq. (1.1) is a quantization condition.

The physical meaning of eq. (1.1) becomes more transparent by looking at fig. 3, where the solution $f_E(z)$ of the Schrödinger equation is drawn for the free case (wave a) and a typical interacting case (wave b). In both cases the momentum k is equal to $2\pi\nu/L$ with $\nu = 8$. Thus, in the non-interacting case, eq. (1.1) is satisfied and the wave smoothly connects to itself when the points $z = \pm L/2$ are identified. This is in general not so in the presence of interactions, because these distort the wave in the interaction region around $z = 0$ in such a way that the asymptotic free waves near $z = \pm L/2$ (where the interactions are negligible) are phase shifted

relative to each other by $2\delta(k)$. In fig. 3, this phase shift is half a wavelength, and the wave therefore does not smoothly connect to itself at $z = \pm L/2$ in this case. However, it is obvious from the picture that periodicity of the wave can be achieved either by increasing L by half a wavelength or by increasing k by some amount until eq. (1.1) is satisfied. In other words, eq. (1.1) just says that the kinematical phase shift (equal to kL), which one picks up when translating a free wave of momentum k by the distance L, and the phase shift, which results from the scattering of the particles, must compensate each other (modulo 2π) to guarantee the periodicity of the wave.

In view of this simple physical meaning of the fundamental relation (1.1), it should be quite plausible now that it is also valid in quantum field theory. Indeed, the interpretation of the scattering phase shift is the same as above and the phase by which a free-particle state transforms under translations over a distance L is again kL, where k denotes the momentum of the particle. The only place where a change occurs is in the energy–momentum relation, where eq. (1.2) should be used instead of eq. (5.3).

Eq. (1.1) can actually be derived in the framework of the Feynman diagram expansion which was set up in sect. 3 of ref. [6] to establish certain asymptotic formulas for the finite-volume energy spectrum in four-dimensional quantum field theories. It is not our aim to present this proof in full detail here, but for the interested reader we briefly describe the key steps involved.

The crucial observation is that in quantum field theory an equation can be derived, which plays almost exactly the role the Schrödinger equation (5.2) did in the non-relativistic case. For a simple one-component scalar field theory, such as the ϕ^4-theory, this equation reads

$$-\frac{1}{m}f''(z) + \frac{1}{2}\int \mathrm{d}z' U_E(z,z') f(z') = E f(z), \tag{5.8}$$

where $U_E(z,z')$ is the Fourier transform of the modified Bethe–Salpeter kernel $\hat{U}_E(k,k')$ introduced in ref. [6]. E is a parameter, which is related to the true

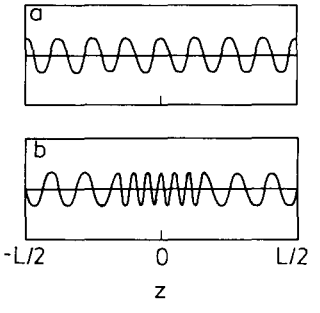

Fig. 3. Plot of the solution $f_E(z)$ of the Schrödinger equation (5.2) for $k = 16\pi/L$. Wave a is for the non-interacting case ($V = 0$), while wave b is what one expects for a short range attractive potential.

energy W of the two-particle state described by f through

$$W = 2\sqrt{m^2 + mE} \ . \tag{5.9}$$

In the elastic region $0 \leqslant E < 3m$, the "potential" $U_E(z, z')$ is an analytic function of E and a rapidly decaying C^∞-function of z and z'. By the Fredholm theory, eq. (5.8) therefore has in general a unique solution $f_E(z)$, and this solution can be shown to have the asymptotic behaviour (5.4), where $\delta(k)$ is the true scattering phase shift (this can be proved, for example, by expanding $f_E(z)$ in a Born series and comparing with the corresponding expansion of the four-point vertex function established in ref. [6]).

For finite L, the two-particle energy spectrum below the four-particle threshold is also determined by the wave equation (5.8), where $U_E(z, z')$ is to be replaced by its periodic extension and the integration over z' is from $-L/2$ to $L/2$. Actually, as discussed in more detail in ref. [6], this is only true up to polarization effects which vanish more rapidly than any power of L^{-1} for $L \to \infty$. If we neglect these corrections, the discussion now proceeds in exactly the same way as in the non-relativistic case, and one finds that the spectrum of two-particle energy levels is determined by eqs. (1.1) and (1.2) as anticipated.

From the above, one expects that eq. (1.1) holds in any two-dimensional quantum field theory with only massive particles provided the following conditions are satisfied:

(1) The finite-volume two-particle states considered have quantum numbers and energies such that mixing with other many particle states are impossible. For example, in the non-linear σ-model at zero total momentum, fixed isospin I and positive isospin parity, all states below the four-particle threshold $W = 4m$ are two-particle states, and mixing with other states can be excluded. For $W > 4m$, multi-particle states interfere and it is, in fact, no longer clear that one means by a two-particle energy eigenstate in this case.

(2) L must be much larger than the interaction range so that the wave function $f_E(z)$ is accurately given by the free wave (5.4) when z is near $\pm L/2$.

(3) L must also be sufficiently large to suppress the polarization effects mentioned above. These arise from virtual particles going "around the world" and decay rapidly with increasing mL. We therefore expect them to be small as soon as (2) is satisfied.

(4) If the theory is formulated on a euclidean lattice, there will be further corrections to eqs. (1.1) and (1.2), which vanish like a power of the lattice spacing.

5.2. NUMERICAL CALCULATION OF THE TWO-PARTICLE ENERGY SPECTRUM

We now proceed to discuss the problem of how to extract the two-particle energy spectrum from the (euclidean) four-point correlation functions of a given

lattice quantum field theory. This is not entirely trivial, because we are not only interested in the lowest level and because the level spacing is small for large L.

Consider for simplicity a lattice theory of a single scalar field $\phi(x)$, such as the ϕ^4-theory, and suppose $\phi \to -\phi$ is an unbroken symmetry of the system and that the particle spectrum consists of a single massive particle, which has odd parity under this symmetry. In the sector with even parity, zero total momentum and energy $0 < W < 4m$, all energy eigenstates are two-particle states, and it is the energies of these states that we are interested in.

Let us now define the two-particle fields

$$\mathcal{O}_j(x^0) = \sum_{x^1, y^1} e^{ip^1(x^1 - y^1)} \phi(x^0, x^1) \phi(x^0, y^1), \tag{5.10}$$

where $p^1 = (j-1)2\pi/L$ and $j = 1, \ldots, r$ (r will be fixed below). From the above, one expects the two-particle states to contribute to the spectral decomposition of the correlation function

$$C_{ij}(t) = \langle \mathcal{O}_i(t)^* \mathcal{O}_j(0) \rangle - \langle \mathcal{O}_i(t)^* \rangle \langle \mathcal{O}_j(0) \rangle . \tag{5.11}$$

The general form of this decomposition is, for $t \geqslant 0$,

$$C_{ij}(t) = \sum_{\alpha=1}^{\infty} v_i^{\alpha *} v_j^{\alpha} e^{-tW_\alpha}, \tag{5.12}$$

$$v_j^{\alpha} = \langle \alpha | \mathcal{O}_j(0) | 0 \rangle, \qquad \mathbb{H} |\alpha\rangle = W_\alpha |\alpha\rangle, \tag{5.13}$$

where α labels the even parity energy eigenstates $|\alpha\rangle$ with $W_\alpha > 0$. Furthermore, the labelling may be chosen such that the two-particle levels come first, i.e. such that $W_1 \leqslant W_2 \leqslant \ldots \leqslant W_A < 4m$ and $W_\alpha \geqslant 4m$ for $\alpha > A$ (the number A of pure two-particle states is approximately equal to $mL/3$ and is thus much smaller than L close to the continuum limit).

In a numerical simulation, the correlation matrix $C(t)$ can be expected to be computable for some range of t, and the basic technical problem then is to extract the levels W_α from $C(t)$. From eqs. (1.1) and (1.2), it is clear that degeneracies in the two-particle spectrum occur only accidentally and we shall therefore assume for simplicity that $W_1 < W_2 < \ldots < W_A$ and that the r-component vectors v^α, $\alpha = 1, \ldots, A$, are linearly independent. This requires, in particular, that the number r of two-particle operators considered is greater or equal to A. In practice r will not be chosen much greater than A because the statistical errors in the correlation functions in general increase with growing momenta. In any case, r should be less than or equal to $L/2$ to guarantee that the fields $\mathcal{O}_j$ are linearly independent.

An important mathematical result now is

Lemma. For every $t \geqslant 0$, let $\lambda_\alpha(t)$ be the eigenvalues of the correlation matrix $C(t)$ ordered such that $\lambda_1 \geqslant \lambda_2 \geqslant \ldots \geqslant \lambda_r$. Then, for all $\alpha = 1, \ldots, A$ we have

$$\lambda_\alpha(t) \underset{t\to\infty}{=} c_\alpha \mathrm{e}^{-tW_\alpha}\left[1 + \mathrm{O}(\mathrm{e}^{-t\Delta W_\alpha})\right], \tag{5.14}$$

where $c_\alpha > 0$ and ΔW_α is the distance of W_α from the other spectral values W_β.

The proof of this technical lemma is simple but somewhat lengthy and it is therefore deferred to appendix A. In principle, the lemma provides a basis for the calculation of the two-particle energy spectrum given the correlation matrix $C(t)$. However, $C(t)$ cannot usually be determined very accurately at large t so that it may not be possible to guarantee that the error term in eq. (5.14) is negligible.

A method which we expect to be superior to a straightforward application of the lemma starts from the generalized eigenvalue problem

$$C(t)\psi = \lambda(t, t_0)C(t_0)\psi, \tag{5.15}$$

where t_0 is fixed and small ($t_0 = 0$ for example). This problem is well posed if $C(t_0)$ is non-singular, which is certainly the case, because the euclidean fields $\mathcal{O}_j(t)$, $j = 1, \ldots, r$, are linearly independent. Thus, there are r independent solutions to eq. (5.15), and it is not difficult to show that the corresponding eigenvalues $\lambda_\alpha(t, t_0)$, $\alpha = 1, \ldots, A$, again satisfy eq. (5.14). However, the amplitudes c_α and the coefficients of the subleading exponentials are different. More precisely, one expects that $c_\alpha \simeq \mathrm{e}^{t_0 W_\alpha}$ and that the other coefficients are suppressed so that the leading term in eq. (5.14) dominates already at moderately large values of t.

To see this, first note that the spectral sum (5.12) is absolutely convergent even for $t = 0$. Thus, by appropriate selection of the states $|\alpha\rangle$ with $\alpha = A + 1, \ldots, r$, the truncated correlation matrix

$$C^0_{ij}(t) = \sum_{\alpha=1}^{r} v_i^{\alpha *} v_j^{\alpha} \mathrm{e}^{-tW_\alpha} \tag{5.16}$$

can be expected to approximate $C(t)$ rather well. In particular, $C^0(t_0)$ will be non-singular and one may show immediately that the spectrum of eigenvalues $\lambda^0_\alpha(t, t_0)$ of the associated modified eigenvalue problem is *exactly* given by

$$\lambda^0_\alpha(t, t_0) = \mathrm{e}^{-(t-t_0)W_\alpha} \qquad \text{for all } \alpha = 1, \ldots, r. \tag{5.17}$$

Now we write $C = C^0 + C^1$ and treat C^1 as a perturbation. At least the larger eigenvalues (the two-particle levels, in particular) should not be strongly affected by this perturbation, and they are thus approximately equal $\lambda^0_\alpha(t, t_0)$, i.e. the higher exponential corrections are suppressed as asserted above.

To sum up, what we propose is to calculate the eigenvalues $\lambda_\alpha(t, t_0)$ of $C(t_0)^{-1/2}C(t)C(t_0)^{-1/2}$ and to extract W_α by

$$W_\alpha = \ln\left(\frac{\lambda_\alpha(t, t_0)}{\lambda_\alpha(t+1, t_0)}\right), \tag{5.18}$$

where t is taken as large as possible and t_0 is small (although this would be theoretically desirable, it is our experience that t_0 cannot be chosen large, because the inversion of $C(t_0)$ then becomes numerically unstable and the statistical errors run out of control). Of course, an energy value W_α determined in this way will only be accepted if the right-hand side of eq. (5.18) is stable within errors in the range of t where it is evaluated. In addition one can check for the stability with respect to changes of t_0 and, finally, one can compute the amplitude c_α to see whether indeed it is close to $\mathrm{e}^{t_0 W_\alpha}$.

5.3. RESULTS FOR THE O(3) NON-LINEAR σ-MODEL

The scheme proposed above can be readily applied to the lattice O(3) spin model introduced in sects. 3 and 4. The appropriate two-particle field is

$$\mathcal{O}_j^{ab}(x^0) = \sum_{x^1, y^1} \mathrm{e}^{ip^1(x^1-y^1)} s^a(x^0, x^1) s^b(x^0 y^1), \tag{5.19}$$

and the associated correlation functions with only isospin I intermediate states are defined by

$$C_{ij}^I(t) = P_I(ab|cd)\left\langle \left[\mathcal{O}_i^{ab}(t)^* - \delta_{I0}\mathcal{O}_i^{ab}(t+1)^*\right]\mathcal{O}_j^{cd}(0)\right\rangle. \tag{5.20}$$

The subtraction for $I = 0$ in this formula is made to cancel the vacuum contribution in the spectral representation of $C^I(t)$, which looks as in eqs. (5.12) and (5.13) except that a factor $1 - \delta_{I0}\,\mathrm{e}^{-W_\alpha}$ must be included in the definition of v^α. Note that due to bose symmetry C_{ij}^1 vanishes if $i = 1$ or $j = 1$, and these indices are hence restricted to values greater or equal to 2 for $I = 1$ in what follows. The theoretical analysis presented in the preceding subsection thus applies to all correlation functions $C^I(t)$ in the same way, but the subtraction needed for $I = 0$ goes along with a loss of numerical significance and this eventually leads to substantially larger statistical errors in the final result for $I = 0$ as compared to the other cases*.

Using the cluster algorithm described in sect. 3, we have computed the correlation functions $C^I(t)$ on the lattices A, B, C (cf. table 2). On the lattice A, the

* A related reason for the lower quality of our $I = 0$ data is that with the measured correlations saturating to nonzero constants at large t, the cluster variance reduction is less powerful.

TABLE 4
Simulation results for the two-particle energies W and the associated scattering phase shifts $\delta_I(k)$ as determined through eqs. (1.1) and (1.2).

lattice	I	W/m	k/m	$\delta_I(k)$
A	0	2.14(1)	0.38(1)	1.36(7)
	0	2.94(1)	1.077(7)	1.22(3)
	1	2.372(2)	0.638(2)	0.15(1)
	1	3.264(3)	1.290(2)	0.23(1)
	2	2.086(2)	0.296(4)	−1.39(2)
	2	2.681(3)	0.893(2)	−1.05(1)
	2	3.639(4)	1.520(2)	−0.85(1)
B	0	2.12(1)	0.35(2)	1.51(7)
	0	2.97(3)	1.10(2)	1.2(1)
	1	2.381(3)	0.646(3)	0.14(1)
	1	3.299(4)	1.312(3)	0.18(1)
	2	2.086(2)	0.296(4)	−1.38(2)
	2	2.683(3)	0.894(2)	−1.02(1)
	2	3.649(5)	1.526(3)	−0.81(2)
C	0	2.34(1)	0.61(1)	1.38(3)
	1	2.851(5)	1.016(4)	0.20(1)
	2	2.180(3)	0.434(4)	−1.26(1)
	2	3.411(5)	1.382(3)	−0.86(1)

number r of independent momenta used in (5.19) and (5.20), and thus the rank of C^I, was 5, 8 and 9 for $I = 0$, 1 and 2 respectively. An increase of these numbers up to a factor of 2 did not affect our results. For $t_0 = 0, 1$, the ratio of eigenvalues $\lambda_0(t, t_0)$ on the r.h.s. of eq. (5.18) turned out to converge rapidly to a constant as t increases and W_α could be determined at $t \simeq 1.5W_\alpha^{-1}$ for $I = 0$ and $t \simeq 2W_\alpha^{-1}$ in the other cases. Within statistical errors, no dependence on t_0 was observed and $c_\alpha = \mathrm{e}^{t_0 W_\alpha}$ was satisfied to an accuracy better than 10% (for $I = 0$) and 3% (for $I = 1, 2$).

The results of our numerical study are listed in table 4 along with the scattering phase shifts $\delta_I(k)$ calculated according to eqs. (1.1) and (1.2). The table includes all levels below the four-particle threshold.

We finally compare our numerical data with the exact expressions (2.31)–(2.33) for the scattering phases. As can be seen from figs. 4 and 5, the data closely follow the analytic curves. Within statistical errors, there is no discrepancy between the data from the lattices A and C, i.e. we do not observe any systematic effects of the type expected when the conditions (2) and (3) listed at the end of subsect. 5.1 would be violated.

Although barely significant, the data for $I = 1, 2$ from lattice B are systematically farther away from the exact curves than those from A, and this could very well be a lattice effect, especially so since the deviation is monotonically increasing with k. It would actually be surprising if no such effect would have been observed, because

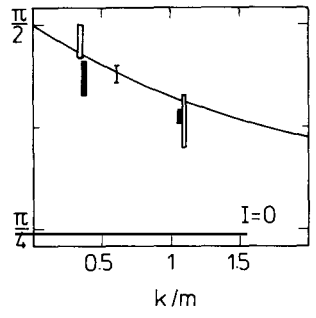

Fig. 4. Scattering phase shift $\delta_I(k)$ for isospin $I=0$ versus momentum k in the O(3) non-linear σ-model. The curve represents the exact expression (2.31), and the numerical data (table 4) are plotted in the form of vertical bars (full bars refer to the lattice A, open bars to B and the I-shaped symbols to C).

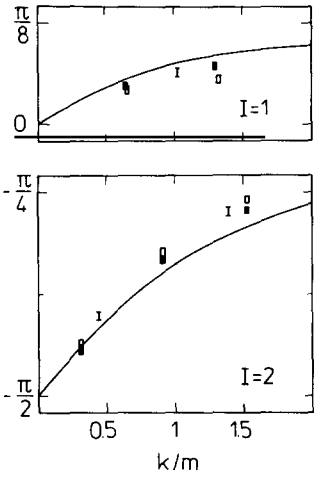

Fig. 5. Same as fig. 4 but for $I=1,2$. The curves represent the exact expressions (2.32) and (2.33).

W_α is as large as 0.5 (in lattice units) for the highest level on B. Thus, the small discrepancies between the data from our largest lattice and the exact curves are probably due to scaling violations. We again conclude that, within errors, there is complete agreement between "theory" and "experiment".

6. Conclusions

In this paper we have shown that following the method outlined in sect. 1, the elastic scattering matrix in two-dimensional (massive) quantum field theories can be accurately determined by numerical simulation. The only prerequisite needed is an efficient simulation algorithm which allows one to do calculations close to the continuum limit on lattices with a linear size much larger than the fundamental correlation length.

Our results for the current form factor and the scattering phase shifts in the O(3) non-linear σ-model agree with the known exact expressions for these quantities in the continuum limit up to some small deviations, which we believe are mainly due to scaling violations, i.e. to the fact that the lattice spacing (in physical units) is not sufficiently small. Little doubt remains, therefore, that the lattice non-linear σ-model approaches the continuum limit in the conventionally expected way even though asymptotic scaling apparently sets in only rather slowly [10, 11].

The generalization of our method to higher dimensions is unfortunately not straightforward, because the relation between the finite-volume energy spectrum and the elastic scattering matrix is much more complicated [5,6]. The difficulty arises from the fact that for a given two-particle energy W, there is an infinite set of scattering states, labelled by angular momentum quantum numbers. The finite-volume energy eigenstates are certain superpositions of these which must be chosen such that the periodic boundary conditions are satisfied. This leads to a complicated implicit eigenvalue equation, which, as far as we know, has only been solved for the lowest levels and at large L, where an expansion in powers of $1/L$ is possible [5,6]. In particular, a relation between the energy of the lowest two-particle state and the scattering length in the channel considered is obtained, and this result has already been applied successfully in a recent simulation of the ϕ^4 theory in four dimensions [1,2].

Appendix A

We here prove the lemma stated in subsect. 5.2. To this end, first consider the case of an $r \times r$ matrix $M_{ij}(t)$ of the form

$$M_{ij}(t) = \sum_{\alpha=1}^{r} u_i^{\alpha *} u_j^{\alpha} \, \mathrm{e}^{-tE_\alpha}, \tag{A.1}$$

where the matrix u_j^{α} is non-singular and $E_1 < E_2 < \ldots < E_r$. The claim is that the eigenvalues $\mu_\alpha(t)$ of this matrix, ordered such that $\mu_1 \geqslant \mu_2 \geqslant \ldots \geqslant \mu_r$, satisfy

$$\mu_\alpha(t) = b_\alpha \, \mathrm{e}^{-tE_\alpha}\left[1 + \mathrm{O}(\mathrm{e}^{-t\Delta E_\alpha})\right] \tag{A.2}$$

with $b_\alpha > 0$ and

$$\Delta E_\alpha = \min_{\beta \neq \alpha} |E_\alpha - E_\beta| \,. \tag{A.3}$$

The proof of this statement proceeds by induction on the rank r of the matrix $M(t)$. For $r = 1$, it holds trivially. Now suppose eq. (A.2) is true for all matrices of the specified type with rank $r = R$ and let $M(t)$ be such a matrix with $r = R + 1$. We then decompose $M(t)$ according to

$$M(t) = M^0(t) + M^1(t) \,, \tag{A.4}$$

$$M_{ij}^0(t) = \sum_{\alpha=1}^{R} u_i^{\alpha *} u_j^{\alpha} \, \mathrm{e}^{-tE_\alpha}, \tag{A.5}$$

$$M_{ij}^1(t) = u_i^{r *} u_j^{r} \, \mathrm{e}^{-tE_r} \,. \tag{A.6}$$

By performing a unitary transformation, we may arrange that $u_r^\alpha = 0$ for all $\alpha = 1, \ldots, R$, so that $M^0(t)$ is a matrix with zeros in the last line and column. Thus, by the induction hypothesis, the eigenvalues $\mu_\alpha^0(t)$ of $M^0(t)$ are given by

$$\mu_\alpha^0(t) = b_\alpha^0 \, \mathrm{e}^{-tE_\alpha}\left[1 + \mathrm{O}(\mathrm{e}^{-t\Delta E_\alpha})\right] \qquad \text{for } \alpha = 1, \ldots, r-1, \tag{A.7}$$

$$\mu_r^0(t) = 0, \tag{A.8}$$

where $b_\alpha^0 > 0$. In the basis chosen, the eigenvector associated with the zero eigenvalue is $\psi_j = \delta_{rj}$. It follows from eqs. (A.7) and (A.8) that

$$\|M^1(t)\| < \min_{\alpha \neq \beta} |\mu_\alpha^0(t) - \mu_\beta^0(t)| \tag{A.9}$$

for sufficiently large t. The matrix $M^1(t)$ is hence an analytic perturbation of $M^0(t)$, i.e. the Rayleigh–Schrödinger perturbation expansion of the eigenvalues $\mu_\alpha(t)$ of $M(t)$ in powers of $M^1(t)$ is absolutely convergent. To first order, we have

$$\mu_\alpha(t) = \mu_\alpha^0(t) + \mathrm{O}(\mathrm{e}^{-tE_r}) \qquad \text{for } \alpha < r, \tag{A.10}$$

$$\mu_r(t) = |u_r^r|^2 \, \mathrm{e}^{-tE_r}, \tag{A.11}$$

and the higher orders are easily seen to give corrections of order $\mathrm{e}^{-t\Delta E_r}$. Thus, the eigenvalues $\mu_\alpha(t)$ satisfy eq. (A.2) as asserted (that $b_r = |u_r^r|^2$ is not zero follows from the fact that u_j^α is a non-singular matrix and from our choice of basis).

The proof of the lemma is now straightforward. We first write

$$C(t) = M(t) + N(t), \tag{A.12}$$

$$M_{ij}(t) = \sum_{\alpha=1}^{A} v_i^{\alpha *} v_j^\alpha \, \mathrm{e}^{-tW_\alpha}, \tag{A.13}$$

$$N_{ij}(t) = \sum_{\alpha=A+1}^{\infty} v_i^{\alpha *} v_j^\alpha \, \mathrm{e}^{-tW_\alpha}. \tag{A.14}$$

By a constant unitary transformation, $M(t)$ can be brought to a form where all matrix elements vanish except those in the upper left $A \times A$ square. This submatrix is of the type considered above (with $r = A$), and we therefore conclude that the first A eigenvalues of M are given by eq. (5.14) for large t while the remaining eigenvalues vanish.

As in the case of the matrices M^0 and M^1, this implies that $N(t)$ is an analytic perturbation of $M(t)$ for sufficiently large t, and the lemma now follows from the perturbation expansion of the eigenvalues $\lambda_\alpha(t)$ in powers of $N(t)$.

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