Basis vector importance sampling for Hamiltonian lattice spectrum calculations

1985 J. Phys. A: Math. Gen. 18 1765

(http://iopscience.iop.org/0305-4470/18/10/029)

J. Phys. A: Math. Gen. **18** (1985) 1765-1779. Printed in Great Britain

Basis vector importance sampling for Hamiltonian lattice spectrum calculations

András Patkós† and Pál Ruján‡§

† Department of Atomic Physics, Eötvös University, H-1088 Budapest, Puskin u 5-7, Hungary

‡ Institut für Festkörperforschung der KFA Jülich GmbH, D-5170 Jülich, West Germany

Received 31 August 1984, in final form 7 December 1984

Abstract. Different numerical methods for accurate calculation of low-lying eigenvalues of lattice Hamiltonians are proposed and critically compared. A dynamical procedure, called basis vector importance sampling, is shown to select the relevant subspace of the Hilbert space very effectively. This method is used to compute the mass gap of O(2) symmetric quantum chains up to a length of nine sites. Kosterlitz-Thouless type freezing transitions of $Z(p)$ symmetric chains are also studied via the spectrum of quantum kinks.

1. Introduction

Finite lattice techniques are essential tools for exploring field theories. The numerical solution of the transfer operator in finite strips was used in the context of the so-called 'phenomenological scaling theory' (Nightingale 1976), which is recognised as one of the most reliable methods for extracting critical properties in various statistical mechanical systems (for a review see Barber (1983)). In the Hamiltonian formalism low-lying eigenvalues of finite two- and three-dimensional models have been computed for both spin and gauge systems (Roomany and Wyld 1980, 1981, Hamer and Barber 1981a, b, c, Irving and Thomas 1982, Hamer and Irving 1983, Irving *et al* 1983).

This paper deals with spectrum calculations in the Hamiltonian formalism. The general structure of the H operator is

$$\hat{H} = \hat{K} - x\hat{V}, \tag{1.1}$$

where $\hat{K}$ is the kinetic energy, $\hat{V}$ is the potential energy and x plays the role of the coupling (or inverse temperature). The evaluation of the mass gap in models of type (1.1) has been performed using mainly two different methods. Hamer (1979) put forward a simple but efficient method which consists of computing all matrix elements of $\hat{H}$ in the finite subspace generated by the action of $\hat{V}^n$ $(n \leqslant n_{\max})$ on the $x = 0$ ground state. The resulting matrix has a typical dimensionality of $(1\text{-}3) \times 10^4$ and is diagonalised by standard routines. The other method, proposed by Roomany *et al* (1980) is the Lánczos algorithm (see Wilkinson 1964). The starting vector ψ_0 for this procedure is chosen generally to be the $x = 0$ ground state and the auxiliary vectors

§ Permanent address: Institute for Theoretical Physics, Eötvös University, H-1088 Budapest, Puskin u 5-7, Hungary.

0305-4470/85/101765+15$02.25

are stored through their components in the strong coupling basis (eigenbasis of the operator $\hat{K}$). The former method has faster convergence while the latter requires smaller storage. A proposal which has both advantages was made recently by Alberty *et al* (1984).

In field theory one attempts to solve the eigenvalue problem in the vicinity of the critical point. In asymptotically free theories one has to work in the deep weak coupling region. There the dimensionality of the subspace spanned in the strong coupling basis necessary to reach a prescribed accuracy becomes horribly large.

The central idea of the present investigation is to closely follow the shape of the ground-state vector by appropriately selecting the relevant subspace from the full Hilbert space. This means that in a given basis (usually the strong coupling, $x = 0$ basis) one retains only those axes whose overlap with the eigenvector is sufficiently large. We call this principle basis vector importance sampling (BVIS). This terminology has been borrowed from the Green function Monte Carlo method (Ceperley and Kalos 1979), where a similar idea was introduced in order to make the stochastic evaluation of the ground-state energy more efficient.

In § 2 the BVIS principle is implemented using a variational technique. Starting with an optimised trial vector one first calculates its components in the strong coupling basis. A finite Hilbert subspace is then selected according to the chosen trial vector by neglecting those directions where its components are smaller than a given bound. The Lánczos iteration proceeds in this *fixed* subspace. In this way one obtains significant storage savings. In § 3 the BVIS is built into the algorithm of Alberty *et al* (1984). This version is very flexible and allows for a continuous tailor-made choice of the Hilbert subspace following the 'figure' of the actual eigenvector. The O(2) invariant quantum ring with nearest-neighbour interactions serves as an illustration for these two sections.

A complete description of our data for the O(2) chains follows in § 4. The new data (relative to chains solved earlier with the conventional Lánczos technique) come from chains of length $N = 8$ and 9. They allow a more accurate location of the critical point and parametrisation of the singularity in the correlation length. Up to size $N = 8$ we could avoid the use of any artificial truncation of the Hilbert space (like the angular momentum cut-off $|L|_{\max} = 3$ applied by Roomany and Wyld (1980)). The BVIS procedure is self-correcting, truncating the Hilbert space automatically in dimensions $\sim 10^4$ for $N \leqslant 8$. The data are analysed using finite size scaling and convergence improving techniques. Instead of the Roomany-Wyld approximant to the β function we propose to construct directly the finite scale change coupling renormalisation function $\Delta g(g)$.

We have also applied the method of § 3 to investigate the elementary kink excitations (walls or interfaces in the Hamiltonian limit) in $Z(p)$ symmetric models. This is a novel approach to the determination of critical characteristics of these systems. Our results were obtained by analysing the energy difference of the respective ground states with periodic and twisted rings. They compare favourably with critical points and indices from the dual investigations (Roomany and Wyld 1981). Here only preliminary data will be shown to illustrate the efficiency of BVIS, a full presentation of the kink spectrum will be published separately (Patkós and Ruján 1985). In both applications we have determined eigenvalues to the accuracy reported in earlier publications. Advantages of the proposed method are demonstrated, therefore, through the reduced dimensionality of the Hilbert space. The alternative view, which would use subspaces of maximal available dimensionality for finding eigenvalues of higher accuracy, has not yet been pursued in detail.

2. Lánczos iteration of variational ground-state vectors

A general Lánczos step consists of the following recursion

$$\hat{H}\psi_n = f_{n-1}\psi_{n-1} + g_n\psi_n + f_n\psi_{n+1} \tag{2.1}$$

($\psi_{-1} \equiv 0$, $(\psi_i, \psi_j) = \delta_{ij}$) which defines ψ_{n+1} using ψ_{n-1}, ψ_n iteratively. Usually one starts with ψ_0 chosen to be the $x = 0$ ground state of the O(2)-invariant Hamiltonian (Luther and Scalapino 1977):

$$\hat{H} = \sum_{i=1}^{N} L_i^2 - x \sum_{i=1}^{N} \cos(\phi_i - \phi_{i+1}), \qquad \phi_{N+1} \equiv \phi_1 \tag{2.2}$$

where $\phi_k \in [0, 2\pi]$ and $L_k = \mathrm{i}\,\partial/\partial\phi_k$. The ψ_k vectors are stored through their components in the L_i-eigenstate-basis

$$\psi_0 \equiv b_1 = (0, 0, 0, \ldots, 0), \qquad \psi_n = \sum_{l=1}^{\dim} a_l b_l \tag{2.3}$$

where $b_l (2 \leq l \leq \dim)$ are those basis vectors which arise in the nth successive application of $\hat{H}$ to b_1. They are added to the basis vector-list (BVL) in the order of their appearance. A code uniquely characterising the N angular momentum eigenvalues

$$b_l = (n_{l_1}, n_{l_2}, \ldots, n_{l_N}) \tag{2.4}$$

is stored in the computer memory. We used a translationally invariant basis. The application of H to any vector is written in this basis as follows

$$\hat{H}a[n_1 \ldots n_N] = \left(\sum_k n_k^2\right) a[n_1, \ldots, n_N] - \tfrac{1}{2}x \sum_k \{a[n_1, \ldots, n_k + 1, n_{k+1} - 1, \ldots, n_N] + a[n_1, \ldots, n_k - 1, n_{k+1} + 1, \ldots, n_N]\}. \tag{2.5}$$

The recursion was performed by storing $\Sigma_k n_k^2$ and using an auxiliary list containing all those b_l from which b_{l_α} can be reached through the potential in (2.5).

The dimensionality of the Hilbert space spanned in the above procedure is restricted by the finite fast-storage capability of the computer. However, the Lánczos iteration can be performed until this finite, fixed, Hilbert space is exhausted. The diagonalisation of the resulting tridiagonal matrix yields the eigenvalues of the Hamiltonian projected onto the maximal subspace.

The convergence of the Lánczos procedure in a fixed subspace is quite slow, as has been already pointed out by Hamer and Barber (1981c). A possible cure could be to use for ψ_0 a state having a bigger overlap with the $x \neq 0$ ground state.

Our suggestion is to start with the variationally optimised ansatz

$$\psi_0^{\mathrm{var}} = \exp\left(\alpha \sum_k \cos(\phi_k - \phi_{k+1})\right); \qquad \alpha = \alpha(x) \tag{2.6}$$

which has been extensively studied in infinite systems with both local and global symmetries (Greensite 1979, Horn and Karliner 1984). An elementary computation yields $\alpha(x)$ also for finite systems. $\alpha(x)$ was determined for the O(2) chain by minimalising the following eigenvalue estimate

$$\varepsilon_0 \leq \min_{\alpha}(\alpha - x) N \sum_n [I_{n+1}(2\alpha) + I_{n-1}(2\alpha)] I_n^{N-1}(2\alpha) \left(2\sum_n I_n^N(2\alpha)\right)^{-1}. \tag{2.7}$$

As above, ψ_0 was stored through its L_i-basis components, the reason being that the maximal Fourier component of (2.6) belongs again to

$$b_1 = (0, \ldots, 0).$$

At each updating of the basis the corresponding Fourier component of (2.6) is simultaneously computed. After exhausting the basis, the vector is normalised to unity on the subspace. The effect of implementing BVIS in the Lánczos iteration will be illustrated in table 1 for the ground-state eigenvalue of a five-site periodic chain in the weak coupling regime ($x = 2$). The entries in the subsequent rows of table 1 are estimates of the ground-state energy after the corresponding number of iterations. Comparing columns 1 and 2 we see that the variational ψ_0 leads to fast convergence down to 1% level of accuracy but a high accuracy solution needs the same number of iterations as without variational input. Nevertheless, this algorithm suggests a very powerful way of storage saving, which we call *basis vector importance sampling.* The main idea is to discard all those basis vectors for which the ratio $a_i^{\text{var}}/a_1^{\text{var}}$ is smaller than an arbitrarily prescribed r value. In practice $r = 10^{-3}$ was used. The extension of the Hilbert space can even stop before reaching the maximally allowed dimensionality if in the actual application of $\hat{V}$ the new vectors do not fulfil the selection criterion. The form of (2.6) ensures that this type of vector will not occur in the later steps either. A substantial reduction in the dimensionality of the Hilbert space sufficient to determine the lowest eigenvalues to six decimal places can be observed. This fact is demonstrated in the third column of table 1. However, the number of the necessary Lánczos iterations remains unchanged.

We also tested the moment method devised by Bessis and Villani (1975), which is equivalent in the unrestricted Hilbert space to the original Lánczos iteration. We performed the test in a truncated space spanned by the 'important' components of (2.6) with $r = 10^{-4}$. A systematic overshoot was observed when the order of the moments taken into account was increased, followed by a relaxation to the true ground-state eigenvalue. At $x = 2$, one has to calculate 17 moments for a five places accurate estimate

Table 1. Comparison of the Lánczos iteration scheme (second column) to variationally started iteration (third column) and to implemented basis vector importance sampling (fourth column). LI stands for Lánczos iteration and data represent ground-state energy values of five-site O(2) chain at $x = 2$.

Order of LI	Ordinary LI on SC ground state	Ordinary LI on var. ground state	LI with basis vector importance sampling
1	−2.316 62	−4.289 25	−4.289 25
2	−3.520 36	−4.338 15	−4.338 22
3	−4.156 29	−4.335 56	−4.356 02
4	−4.312 48	−4.363 30	−4.364 25
5	−4.352 94	−4.367 14	−4.368 14
6	−4.366 32	−4.369 04	−4.369 75
7	−4.369 52	−4.369 93	−4.370 43
8	−4.370 38	−4.370 38	−4.370 69
9	−4.370 64	−4.370 63	−4.370 77
12	−4.370 80	−4.370 80	−4.370 81
dim	1000	1000	609 ($r = 10^{-3}$)

and there is a 20 order of magnitude change in these quantities. This makes this algorithm sensitive to the accuracy of higher moments. Our experience disfavours it in comparison with the Lánczos iteration with basis vector importance sampling.

A variant of this idea will be carried over to § 3, where also the efficiency of the genuine Lánczos iteration will be improved by some additional simple modifications.

3. Lánczos iteration with continuous basis vector importance sampling

The concept of basis vector importance sampling introduced previously restricts the eigenvalue problem to the Hilbert subspace which fits the shape of the trial eigenvector. The variational state (2.6) is adequate in the strong coupling region and may be in the crossover region, but not in the weak coupling regime. It would be more convenient to work with an algorithm which finds the low-lying states iteratively, so that their evolution could be monitored at each iteration step. Then the basis vector importance sampling procedure might flexibly follow the shape of the eigenvector.

An algorithm to meet our goals might be a variant of the procedure proposed by Alberty *et al* (1984). Consider the series of Hilbert subspaces arising from subsequent applications of $\hat{V}$ to the starting $x=0$ ground-state vector:

$$\mathcal{H}_1 \subset \mathcal{H}_2 \subset \ldots \subset \mathcal{H}_m \subset \ldots$$
$$\mathcal{H}_m = \hat{V}(\mathcal{H}_{m-1}) \cup \mathcal{H}_{m-1}. \tag{3.1}$$

A sequence of 2×2 Lánczos iterations is used to find the best ground state $\psi_{0,(m)}$ and energy $\varepsilon_{0,(m)}$ in $\mathcal{H}_m$. The basis vector importance sampling is implemented by the following rule.

If $(\psi_{0,(m)}, b_l)$, $b_l \in \mathcal{H}_m$ is smaller than an arbitrarily fixed constant $\tilde{r}$, the action of $\hat{V}$ on b_l is cancelled when extending $\mathcal{H}_m$ to $\mathcal{H}_{m+1}$. One has to emphasise that b_l itself is never erased from the BV list if once it has been put on it. If at some later stage $(\psi_{0,(p)}, b_l)$ exceeds $\tilde{r}$ (we have used in our study $\tilde{r}=10^{-3}$–10^{-5}), the vectors $\{\hat{V}b_l\}$ are added to the base.

The actual series of Hilbert subspaces will be

$$\mathcal{H}_1 \equiv \mathcal{H}'_1 \subset \mathcal{H}'_2 \subset \ldots \mathcal{H}'_m \subset \ldots,$$
$$\mathcal{H}'_m = \hat{V}[\mathcal{H}'_{m-1}/\{b_1 : (\psi_{0,(m-1)}, b_l) < \tilde{r}\}] \cup \mathcal{H}'_{m-1}. \tag{3.2}$$

Our experience with the O(2) and $Z(p)$ invariant chains shows that the dimensionality of the subspaces sufficient to determine the lowest eigenvalues to six decimal places can be reduced considerably (we found a reduction factor of 2 to 4).

We have determined the ground-state and the first excited-state eigenvalues of O(2) invariant chains with nearest-neighbour interaction up to length 9. The gap state was found in the $J=1$ sector of the Hamiltonian, which is spanned by subsequent applications of $\hat{V}$ on

$$b_1^{(J=1)} = \frac{1}{\sqrt{N}} \sum_{\text{transl}} (0, \ldots, 0, 1, 0, \ldots, 0). \tag{3.3}$$

The longest chain considered by Roomany and Wyld (1980) contained seven sites. The Hilbert space there has been truncated putting $|J_{\max}|=3$ and they have dealt with a ~ 9000 dimensional subspace. For the same length and without applying any angular

momentum cut-off, we obtained (using $\tilde{r} = 10^{-3}$) an $O(10^{-5})$ accurate solution in dimensions less than 4000. Table 2 illustrates the variation of the effective dimensionality as a function of x for both the ground and the excited state.

Table 2. Effective dimensions of Hilbert subspaces when the parameter $r = 10^{-3}$ in the BVIS for the O(2) chain. No truncation is performed in J_{max}.

Number of sites	State	Coupling (x)			
		1.6	1.8	2.0	2.2
7	ground	2491	2853	3191	3563
	excited	2553	2908	3345	3642
8	ground	6456	7591	8588	9604
	excited	6501	7603	8643	9715

It is evident, however, that the basis vector importance sampling is effective only in the range where the strong coupling basis is adequate. For the O(2) system its application greatly increases the efficiency because the phase transition occurs around $x = 2$. The maximal dimensionality was reached in the nine-site system (dim = 25 000), where besides $\tilde{r} = 10^{-3}$ we had to apply also an angular momentum cut-off. The storage required for the BV list was then around 8 MB and the CPU time needed for the calculation of one point was around 40 min in an IBM 3081 machine. The angular momentum cut-off was $J_{max} = 4$.

For the study of the weak coupling phase the use of the eigenbase of $\hat{V}$ is the appropriate choice. Following Elitzur *et al* (1979) we have considered the $Z(p)$ invariant Hamiltonian:

$$\hat{H}_p(x) = \sum_l \frac{1-\cos(2\pi/pL_l)}{1-\cos(2\pi/p)} - x\sum_l \cos\left(2\pi/p(n_l - n_{l+1})\right), \tag{3.4}$$

which in the $p \to \infty$ limit goes over into (2.2). The conjugate variables n_l and L_l fulfill the commutation relations $[n_i, L_j] = i(p/2\pi)\delta_{ij}$. We have investigated the dependence of the ground-state eigenvalue on the boundary conditions:

$$n_{N+1} = n_1 + l2\pi/p; \qquad l = 0, 1, \ldots, [p/2]. \tag{3.5}$$

The energy difference

$$m_l = \varepsilon_{0,l} - \varepsilon_{0,0} \tag{3.6}$$

defines the mass of a kink of strength l. In the disordered high-temperature phase $m_l = 0$ for all values of l. This corresponds to the introduction of interfaces in the transfer-matrix formalism (Nightingale and Schick 1982).

The twisted boundary conditions require

$$\psi_{0,l}(n_1 \ldots n_N) = \psi_{0,l}((n_N + l), n_1, \ldots, n_{N-1}). \tag{3.7}$$

We start the iteration from the $Z(p)$ and translationally invariant states:

$$\psi_{0,(0)}^{l=0} = \frac{1}{\sqrt{p}} \sum_{k=1}^{p} (k, \ldots, k), \qquad l = 0,$$

$$\psi_{0,(0)}^{l=1} = \frac{1}{\sqrt{pN}} \sum_{k=1}^{p} \{(k, \ldots, k) + ((k+1), k, \ldots, k) + \ldots ((k+1), \ldots, (k+1), k)\}, \qquad l = 1 \tag{3.8}$$

and so on for higher values of l; $(k+1)$ means $(k+1)$ mod p.

The analogue of recursion (2.5) reads as follows in the configuration representation (for simplicity the symmetrisation of the basis is not presented here):

$$\hat{H}a[n_1, \ldots, n_N] = \frac{1}{1-\cos(2\pi/p)} \sum_k \{a[n_1, \ldots, n_k+1, \ldots, n_N] + a[n_1, \ldots, n_k-1, \ldots, n_N]\} - \left(\sum_k \cos\frac{2\pi}{p}(n_k - n_{k+1})\right) a[n_1, \ldots, n_N]. \tag{3.9}$$

In order to find the eigenvalues of (3.4) one has to add to the spectrum of (3.9) the value $N/(1-\cos 2\pi/p)$.

We have evaluated the respective ground states of the periodic and twisted chains for $N = 2$-6 site lattices up to $p = 9$. The maximal dimensionality used for the six-site $Z(9)$ system was ~ 1500 in the translationally invariant basis. The neighbourhood of the critical point of this model could be described in a ~ 450 dimensional vector space in the case of the five-site chain instead of the full ~ 1300 dimensional space. Although the implementation of BVIS requires extra program steps, the reduction of the necessary subspace leads to a faster algorithm. For example, at $x = 9$, in the five-site $Z(9)$ system the ground-state eigenvalue required ~ 6 s CPU time on the IBM 3081, while the ordinary Lánczos algorithm needs ~ 13 s. We notice also that with the present algorithm much longer chains can be treated in the low-temperature critical region of $Z(p)$ models for $p \gtrsim 7$.

4. Finite size scaling analysis of the mass gap in the O(2) chain

We have determined the mass gap values for O(2) chains of length up to nine spins. One possibility of extrapolating these values to the $N = \infty$ limit is to use the finite size scaling assumption (Fisher 1971, Fisher and Barber 1972, Roomany and Wyld 1981):

$$M_g(x = x_c, N) \simeq A/N. \tag{4.1}$$

x_c is determined by measuring the power of N from the log-log plot as shown in figure 1 for three characteristic x values. Figure 1 clearly indicates that the Kosterlitz-Thouless transition point cannot be located accurately, although the existence of a critical line is suggested very convincingly by the values of the ratios

$$R_N(x) = NM_g(x, N)/(N-1)M_g(x, N-1) \tag{4.2}$$

displayed in table 3. Except for $N = 9$ the values are correct up to $O(10^{-6})$, at $N = 9$

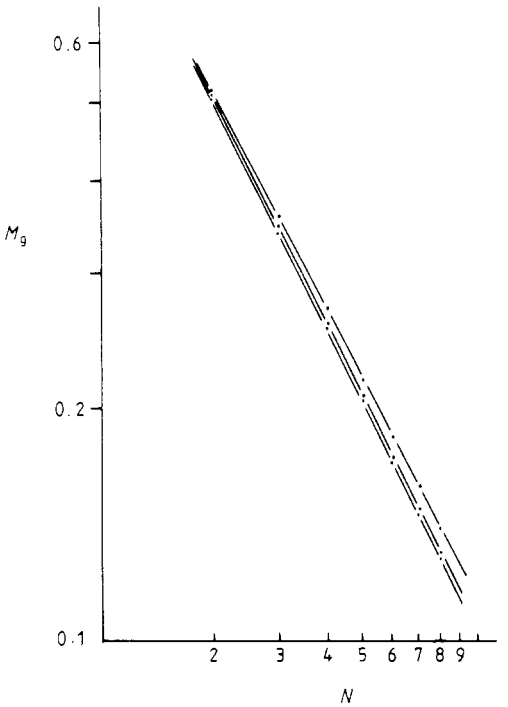

Figure 1. Log-log plot of the mass gap $M_g(x, N)$ against N for $x=1.6$, 2.0 and 2.3 in the O(2) model. The slope varies from $\simeq 0.95$ to 1.02, respectively.

Table 3. $R_N = NM_g(x, N)/(N-1)M_g(x, N-1)$ ratios for the O(2) chain. Note that for $x > 1.7$ the results for nine sites are biased by the $J_{max}=4$ truncation. $R_N(x) = NM_N(x)/(N-1)M_{N-1}(x)$.

N \ x	1.5	1.6	1.7	1.8	1.9	2.0	2.1	2.2	2.3
4	1.0203	1.0147	1.0106	1.0105	1.0054	1.0037	1.0026	1.0017	1.0011
5	1.0161	1.0112	1.0077	1.0052	1.0034	1.0023	1.0014	1.009	1.0005
6	1.0136	1.0090	1.0060	1.0039	1.0023	1.0015	1.0009	1.0005	1.0002
7	1.0117	1.0076	1.0048	1.0031	1.0021	1.0009	1.0005	1.0004	
8	1.0103	1.0067	1.0042	1.0025	1.0018	1.0010	1.0005	1.0004	
9	1.0096	1.0059	1.0037	1.0033	1.0022	1.0034	1.0032	1.0030	

the angular momentum cut-off $|J_{max}|=4$ has biased the data for $x \gtrsim 1.7$ towards the strong coupling values.

In order to obtain more accurate results both for x_c and the scaling law, more sophisticated extrapolation techniques to speed up the convergence were invoked. We used sets of data $N=1, 2, 5, 8$; $N=1, 2, 4, 8$, etc in a modified self-consistent Romberg-type algorithm (Beleznay 1984). The main idea is to fit the mass gap to an asymptotic expansion of the form

$$M_g(x, N) = M_g^{(0)}(x, N) \simeq \sum_{l=1}^{3} A_l N^{-\alpha l}. \tag{4.3}$$

By subsequent elimination of A_1, A_2 and A_3 in the final step one extrapolates the mass gap to zero. The intermediate estimates can be ordered into the following scheme $((N_iM)^{(l)} \equiv N_iM_g^{(l)}(x, N_i))$:

$$
\begin{array}{llll}
(N_1M)^{(0)} & & & \\
(N_2M)^{(0)} & (N_2M)^{(1)} & & \\
\vdots & \vdots & \ddots & \\
(N_kM)^{(0)} & (N_kM)^{(1)} & \ldots\ (N_kM)^{(k-2)} & (N_kM)^{(k-1)}.
\end{array}
$$

The index α is determined by requiring that the difference $N_kM_g^{(k-2)}(x, N_k) - N_{k-1}M_g^{(k-2)}(x, N_{k-1})$ is minimal. Then the errors of our data are taken into account and the error of α established. Recalculating the sequence with α *fixed* within this bound, one obtains a new error estimate for the extrapolated gap values which should be consistent with the error due to the finite precision of the data. This extrapolation procedure seems to give better results than the Van den Broeck-Schwartz (1979) procedure (Beleznay 1984). Figure 2 contains values of the extrapolated gap obtained through this procedure for different sets of data. The transition point seems clearly to be at $x_c = 2.00 \pm 0.05$ both from the $\alpha(x_c) = 1$ condition, and also from the error analysis when α is fixed to be equal to unity. The error of the extrapolated mass gap is then minimal around $x = x_c$. Note that $M_g^{\text{extra}} = 0$ is also within error bars for $x > x_c$.

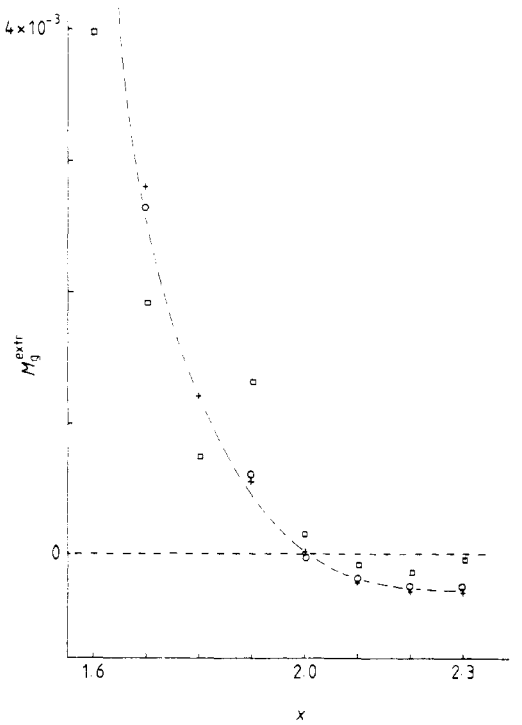

Figure 2. Extrapolated mass gap values of O(2) chains using a modified self-consistent Romberg algorithm. Crosses are results extrapolated from $N = 1, 2, 4, 8$ while circles and squares correspond to $N = 1, 2, 5, 8$ and $N = 2, 4, 6, 8$ respectively.

In a recent paper Luck (1984) has presented a detailed discussion of the different types of corrections to finite size scaling laws of type (4.1). Some corrections are due to the reparametrisation of temperature in terms of nonlinear scaling fields (Privman and Fisher 1983), others are due to irrelevant operators. The main correction originates from corrections to scaling and is governed by the leading correction exponent (Derrida and de Seze 1982):

$$NM_g(x_c, N) \simeq A_0 + \sum_l B_l N^{-l\omega}. \tag{4.4}$$

Applying the Romberg scheme to eliminate B_1, B_2 and B_3, A_0 was calculated up to O $(N^{-4\omega})$ accuracy. At $x_c = 2$ the value of A_0 was 1.045(1) for $\omega = 0.95$. This indicates that the O(2) chain does not obey the relationship (Derrida and de Seze 1982)

$$A_0 = \pi\eta \tag{4.5}$$

found in other models and resulting from the conformal invariance near a critical point in two dimensions (Cardy 1984).

A second possibility for extrapolation is to consider (1.1) as the discretisation of some continuous field theory on a finite length (L) ring. Then the requirement of the invariance of the physical mass when the number of sites is changed by a factor λ is expressed as

$$gNM_g(x, N) = g'N'M_g(x', N'), \qquad \lambda = N'/N, \qquad x = 2/g^2. \tag{4.6}$$

This allows one to deduce the function $\Delta g_\lambda(g) = g' - g$, which becomes zero at the critical point. In figure 3 we display gNM_g for different N's as a function of g. It is clear that for $g \leqslant 1$, the curves are almost identical. We have calculated Δg for $\lambda = \frac{8}{7}$ and $\lambda = \frac{8}{4}$ in the region $x \in [1.7\text{-}1.95]$ and using Lagrange's interpolating polynomials we have extrapolated them to zero. In this way we have obtained for the critical coupling the following estimates:

$$\lambda = 2, \qquad g_{KT} = 0.983 \qquad (x_{KT} = 2.07),$$
$$\lambda = \tfrac{8}{7}, \qquad g_{KT} = 0.998 \qquad (x_{KT} = 2.01).$$

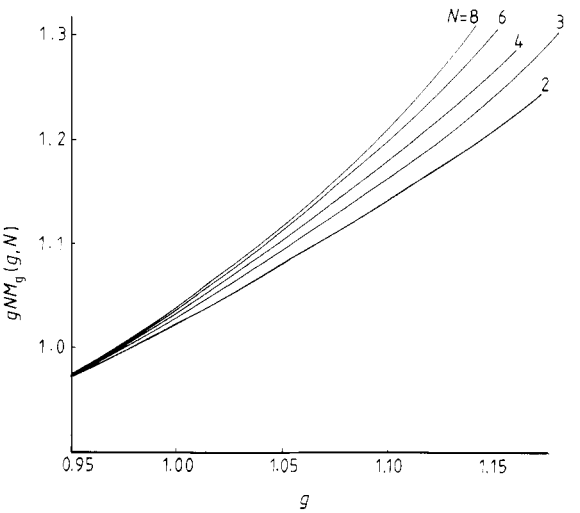

Figure 3. The physical mass gap gNM_g in O(2) chains.

Next one can test the Kosterlitz-Thouless scaling as characterised by the β function (Hamer and Kogut 1979, Hamer and Barber 1981): $\beta(g) = (g - g_{KT})^{1+\sigma}$.

Assuming this behaviour (without correction) in the above region and integrating the definition of $\beta(g)$

$$\beta(g) = a\,\partial g/\partial a$$

$$\int_{a_1}^{a_2} \frac{da}{a} = \int_{g(a_1)}^{g(a_2)} \frac{dg}{\beta(g)}$$

one arrives at

$$\ln \lambda = -\frac{1}{\sigma}\left(\frac{1}{(g_2 - g_{KT})^{\sigma}} - \frac{1}{(g_1 - g_{KT})^{\sigma}}\right) \tag{4.7}$$

and $\Delta g(g_1) = g_2 - g_1$. From figure 3 we see that $\Delta g \ll |g_1 - g_{KT}|$, therefore (4.7) can be linearised in Δg. Putting into this simplified form the value of g_{KT} found above, one gets

$$\lambda = 2\text{:}\quad \sigma = 0.54$$

$$\lambda = \tfrac{8}{7}\text{:}\quad \sigma = 0.45 \tag{4.8}$$

which agrees fairly well with $\sigma = \frac{1}{2}$ predicted by Kosterlitz (1974).

If the finite lattice effects really were minor, then the $\lambda = 2 = \frac{8}{4}$ and $\lambda = \frac{6}{3}$ results should coincide. Unfortunately, they are significantly different, which means that longer chains are necessary to reach the true asymptotics.

5. Kink mass calculation in $Z(p)$-symmetric chains

In this section we present some preliminary results concerning the calculation of the kink mass spectrum in $Z(p)$ models. As explained in § 3 kinks are non-perturbative low-temperature weak coupling excitations corresponding to interface-type objects in the Euclidean formulation. Kinks are imposed into the quantum chain through appropriate twisted boundary conditions. In field theoretical terms kinks are lattice counterparts of solitons (which are real, observable, particles) while the Euclidean vortex excitations are instantons (pseudo particles travelling in imaginary time). In the Hamiltonian limit the Kosterlitz-Thouless transition can be related to the condensation of kinks (Patkós and Ruján 1979).

Here we consider $Z(p)$-symmetric Hamiltonians of the form

$$H_\lambda = \sum_l \cos\frac{2\pi}{p} L_l - \lambda \sum_l \cos\frac{2\pi}{p}(n_l - n_{l+1}), \tag{5.1}$$

which are self-dual, that is

$$H_\lambda = \lambda H_{1/\lambda}. \tag{5.2}$$

The parametrisation (5.1) is related to (3.4) by

$$x = \lambda[1 - \cos(2\pi/p)]^{-1}. \tag{5.3}$$

We use the BVIS to investigate the three-phase structure of these models ($p \geqslant 5$) (Elitzur *et al* 1979, Horn *et al* 1979). The physical mechanism underlying the two phase transitions was analysed by Einhorn *et al* (1980). They have shown that for $\lambda_{KT} < 1$

a Kosterlitz-Thouless transition occurs between the paramagnetic, disordered phase and a massless phase as indicated by the exponential divergence of the correlation length. At the low-temperature $\lambda_{c_2} = 1/\lambda_{KT}$ transition point a p-fold symmetric magnetic phase transforms into the massless phase. Note that the self-duality relation (5.2) implies similar critical behaviour only for ground-state properties and correlations invariant under both $Z(p)$ and translational symmetry transformations, but not for mass gap type properties. It is thus of interest to characterise the low-temperature phase transition using the behaviour of the elementary (twist-1) kink-mass. We present here only results for the $Z(9)$ model, where the presence of the middle massless phase is well established. According to Roomany and Wyld (1981) the KT transition occurs at $x \simeq 2$, and hence $x_{c_2} \simeq 9.2$. It is clear that an accurate diagonalisation using the L basis requires very large subspaces, and in this basis the application of BVIS is useless.

In our calculation we used the configuration basis and the recursion (3.9). The energy difference of the ground states with periodic and twist-1 boundary conditions was determined for $N = 3$–6 long chains and is presented in table 4. We have also compared the ground-state energy of periodic chains with the O(2) chains of the same length. We have found that in this respect the $Z(9)$ model ground-state energy differs by $\sim 2\%$ from that of the O(2) system and as expected on the basis of the correlation inequalities the $Z(p)$ eigenvalues approach the $p \to \infty$ O(2) values from below.

A similar analysis to the one presented in § 4 was performed on the data of table 4. A simple look at the ratios (figure 4)

$$R_{\text{kink}} = NM_k(x, N)/(N-1)M_k(x, N-1) \tag{5.4}$$

already makes evident that the kink mass vanishes exponentially, as for a Kosterlitz-Thouless transition. Our data give

$$x_c(\tfrac{4}{3}) = 9.387, \qquad x_c(\tfrac{5}{4}) = 9.247, \qquad x_c(\tfrac{6}{5}) = 9.218 \tag{5.5}$$

which is in very good agreement with the dual value of 9.135 (Roomany and Wyld 1981).

For the illustration of the effectiveness of the BVIS in $Z(9)$ chains we add that for $N = 6$ periodic systems the ground-state energies were found from a ~ 1400 dimensional subspace (close to the critical point), while the full Hilbert space is $\sim 10^4$ dimensional.

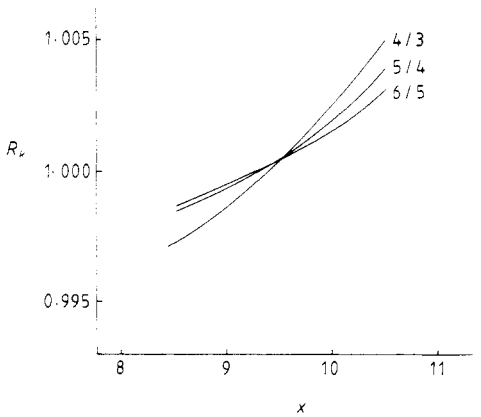

Figure 4. Kink-mass ratios (equation (5.4)) for $Z(9)$ chains. $N'/N = \frac{4}{3}, \frac{5}{4}$, and $\frac{6}{5}$, respectively, in the order of decreasing slope.

Table 4. Ground-state energy (first row) and $NM_k(x, N)$ kink-mass (second row) values for the $Z(9)$ chain at low temperatures.

x \ N	3	4	5	6
8.5	−18.987 63	−24.965 584	−31.008 35	−37.081 940
	1.852 419	1.847 264	1.844 52	1.842 078
9.0	−20.312 455	−26.722 898	−33.199 875	−39.708 528
	1.982 733	1.980 08	1.978 91	1.977 768
9.2	−20.844 296	−27.428 482	−34.079 861	−40.763 221
	2.035 725	2.034 352	2.034 130	2.034 060
9.4	−21.377 186	−28.135 536	−34.961 733	−41.820 230
	2.068 9221	2.089 316	2.09 065	2.090 784
10.0	−22.981 905	−30.265 162	−37.618 146	−45.004 366
	2.252 916	2.258 672	2.263 315	2.266 770
10.5	−24.325 766	−32.049 084	−39.843 634	−47.672 121
	2.393 202	2.405 292	2.414 474	2.422 014

6. Conclusions

The main obstacle blocking progress in numerical solutions of lattice regularised field theoretic Hamiltonians is the necessity of exceedingly large subspaces in order to obtain high accuracy eigenvalues. The basis vector importance sampling has the virtue of slowing down the explosive increase of the dimension when one moves away from the strong (weak) coupling regime, but of course cannot remedy the lack of a more appropriate basis. Our calculations were partly inspired from and have some implications on Green functions Monte Carlo type methods for the stochastic diagonalisation of such Hamiltonians. For example, we now know that for nine-site O(2) chains around $x = 2$ a five digit accurate ground-state energy can be obtained only from a subspace with a dimensionality around 25 000, *even* if variational importance sampling is used. This implies much larger populations and longer runs than the ones performed up to date.

The most interesting field theoretical models have to be examined deep in the weak coupling region, where the configurational basis is the most appropriate one. Its definition implies the discretisation of the field variables, preferably by defining also the discrete version on a group manifold. Our $Z(p)$ example demonstrates the effectiveness of the BVIS principle in such situations, too. Discrete subgroups of the physically interesting Lie groups have been used with some success in Lagrangian Monte Carlo investigations. We believe that a similar approach to Hamiltonian non-Abelian theories would be extremely interesting.

New results of the present paper support the Kosterlitz-Thouless predictions for the O(2) phase transition. However, even the use of the new data is not sufficient to remove the uncertainty in the critical parameters when different convergence improving methods are applied. Our results also indicate that the fluctuations do not obey conformal symmetry near the KT transition. This may be related to problems of degeneracy of conformal operators in the O(2) model (Fateev, private communication).

A preliminary study of the low-temperature transition in $Z(p)$ models using the kink as order parameter shows that the kink mass vanishes exponentially ($p = 9$)

around $x = 9.2$. The full description of the massless phase of $Z(p)$ models ($p \geq 5$) in terms of kinks of different strength support the picture of a continuous kink condensation (Patkós and Ruján 1979) and will be published elsewhere (Patkós and Ruján 1984).

Acknowledgments

We are indebted to F Beleznay and Anna Hasenfratz for helpful discussions and suggestions. PR is grateful to the Institut für Festkörperforschung der KFA Jülich for hospitality and the possibility of using the KFA computer facilities. We also would like to thank the referee for a very careful reading of the original manuscript.

Note added. After completing our paper we received a paper by Dagotto and Moreo (1985) in which a 2×2 Lánczos iteration is applied to variational ansätze of the type discussed in § 2. The free parameters are varied after a fixed number of iterations are performed.

References

Alberty J, Greensite J P and Patkós A 1984 *Phys. Lett.* **138B** 405
Barber M N 1983 *Phase Transitions and Critical Phenomena* vol 8, eds C Domb and J Lebowitz (London: Academic)
Beleznay F 1984 to be published
Bessis D and Villani M 1975 *J. Math. Phys.* **16** 462
Blöte H W J and Nightingale M P 1982 *Physica* **112A** 405
Cardy J L 1984 *J. Phys. A: Math. Gen.* **17** L385
Ceperley D M and Kalos M H 1979 in *Monte Carlo Methods in Statistical Physics* ed K Binder (Berlin: Springer)
Derrida B and de Seze L 1982 *J. Physique* **43** 470
Dagotto E and Moreo A 1985 *Phys. Rev.* D **31** 865
Einhorn M B, Savit S and Rabinovici E 1980 *Nucl. Phys.* B **170** (FS1) 16
Elitzur S, Pearson R B and Shigemitsu J 1979 *Phys. Rev.* D **19** 3698
Fisher M E 1971 *Critical Phenomena, Proc. E. Fermi Int. School of Physics* vol 51, ed M S Green (New York: Academic)
Fisher M E and Barber M N 1972 *Phys. Rev. Lett.* **28** 1516
Greensite J P 1979 *Nucl. Phys.* B **158** 469
Hamer C J 1979 *Phys. Lett.* **82B** 75
Hamer C J and Kogut J B 1979 *Phys. Rev.* B **20** 3859
Hamer C J and Barber M N 1981a *J. Phys. A: Math. Gen.* **14** 259
—— 1981b *J. Phys. A: Math. Gen.* **14** 241
—— 1981c *J. Phys. A: Math. Gen.* **14** 2009
Hamer C J and Irving A C 1983 *Nucl. Phys.* B **225** (FS9) 289
Horn D and Karliner M 1984 *Nucl. Phys.* B **235** (FS11) 148
Irving A C and Thomas A 1982 *Nucl. Phys.* B **200** (FS2) 424
Irving A C, Owens J F and Hamer C J 1983 *Phys. Rev.* D **28** 2059
Kosterlitz J M 1974 *J. Phys. C: Solid State Phys.* **7** 1046
Luck J M 1982 *J. Phys. A: Math. Gen.* **15** L169
—— 1984 *Saclay preprint SPh-T/84/52*
Luther A and Scalapino D J 1977 *Phys. Rev.* B **16** 1153
Nightingale M P 1976 *Physica* A **83** 561
Nightingale M P and Schick M 1982 *J. Phys. A: Math. Gen.* **15** L39
Patkós A and Ruján P 1979 *Phys. Lett.* **73A** 1
—— 1985 *Phys. Lett.* **152B** 346
Privman V and Fisher M E 1983 *J. Phys. A: Math. Gen.* **16** L295

Roomany H H and Wyld H W 1980 *Phys. Rev.* D **21** 3341
—— 1981 *Phys. Rev.* B **23** 1357
Roomany H H, Wyld H W and Holloway L E 1980 *Phys. Rev.* D **21** 1357
Van den Broeck J M and Schwartz L W 1979 *SIAM J. Math. Anal.* **10** 658
Wilkinson J M 1964 *The Algebraic Eigenvalue Problem* (Oxford: Clarendon)