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Perturbation series for the mass gap of the (1 + 1)-dimensional O(2)-model

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Abstract. The strong coupling mass gap series to 10th order in the dimensionless coupling is presented for the (1 + 1)-dimensional O(2)-model. The second logarithmic derivative of the Euler transformed series is examined using Padé techniques to yield the critical parameter estimates $\lambda_c \approx 0.89 + 0.02$ and $\sigma \approx 0.50 \pm 0.08$. These results are consistent with the model exhibiting a Kosterlitz-Thouless transition.

1. Introduction

The quantum Hamiltonian in which we are interested will be taken as

$$H = \sum_i L_i^2 - \lambda \sum_i (\Omega_i^+ \Omega_{i+1} + \Omega_i \Omega_{i+1}^+) = H_0 - \lambda V. \tag{1.1}$$

The normalised eigenstates of L_i are denoted by $|S_i\rangle$ and the energy scale is chosen so that

$$L_i^2 |S_i\rangle = S_i^2 |S_i\rangle \tag{1.2}$$

with S_i an integer. The scale of λ is chosen so that

$$\Omega_i^+ |S_i\rangle = |S_i + 1\rangle, \qquad \Omega_i |S_i\rangle = |S_i - 1\rangle. \tag{1.3a, b}$$

In addition, the eigenstates of H_0 are denoted by

$$|\boldsymbol{S}\rangle = |S_1, S_2, \ldots\rangle = \bigotimes_i |S_i\rangle. \tag{1.4}$$

The Hamiltonian (1.1) is the quantum Hamiltonian analogue in (1 + 1) dimensions of the two-dimensional planar rotor O(2)-model (Fradkin and Susskind 1978). Universality implies that the mass gap of (1.1) should vanish at a critical coupling λ_c as

$$G(\lambda) \approx A \exp(-k|\lambda - \lambda_c|^{-\sigma}) \tag{1.5}$$

with $\sigma = \frac{1}{2}$ (Kosterlitz 1974). Strong coupling mass gap series to 8th order in λ have been derived and analysed previously (Hamer *et al* 1979). The coupling constant x used there is related to λ by $x = 2\lambda$. The results of the mass gap series were later complemented by series expansions of the susceptibility (Hamer and Kogut 1979). While the results were not inconsistent with (1.5) and $\sigma = \frac{1}{2}$, they were far from

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conclusive. In this paper we add two more terms to the mass gap expansion. This addition considerably improves the quality of the estimates, lending much stronger support to the value $\sigma = \frac{1}{2}$.

2. Generation of series

The method used to generate the series is by now standard (Hamer *et al* 1979, Barber and Duxbury 1982). The required coefficients can be calculated by restricting the lattice to be a finite periodic chain of M sites and applying Rayleigh-Schrödinger perturbation theory. The state space of the unperturbed Hamiltonian H_0 can be broken up into sectors labelled by the eigenvalues of the translation operator (momentum) and ΣL_i. Since V is also translationally invariant and does not change the value of ΣS_i, these sectors do not mix in perturbation theory on a finite lattice. To compute the mass gap we require the perturbation expansion of the lowest lying state in the zero momentum sectors with $\Sigma S_i = 0$ and $\Sigma S_i = -1$, corresponding to the ground state and first excited state of H respectively.

For high-order expansions, involving large lattices, it is most efficient to divide the calculation into two stages.

(1) Construction of matrix representation of V in the basis formed by the eigenstates of H_0.

(2) Generation of the series.

The construction of the matrix of V is the same as for a standard finite lattice calculation (see e.g. Roomany *et al* 1980, Hamer and Barber 1981, Irving and Thomas 1982, Hamer 1983), except for several minor modifications. This matrix is sparse and can be stored sequentially in an appropriate data structure.

The series generation technique given a matrix representation of V has not been published in any detail previously. Since care in its computer implementation is critical to high-order calculations, we outline the method here.

Let $|E\rangle$ be a (non-degenerate) eigenstate of H with energy E and define the expansions

$$|E\rangle = \sum_{r=0}^{\infty} \lambda^r |\psi_r\rangle, \tag{2.1}$$

$$E = \sum_{r=0}^{\infty} e_r \lambda^r. \tag{2.2}$$

Substituting these expressions into the eigenvalue equation for H and equating powers of λ in the usual way leads to

$$(H_0 - e_0)|\psi_r\rangle = V|\psi_{r-1}\rangle + \sum_{s=0}^{r-1} e_{r-s}|\psi_s\rangle. \tag{2.3}$$

Denoting the unperturbed energies of the basis states $|\boldsymbol{S}\rangle$ by

$$H_0|\boldsymbol{S}\rangle = E_0(\boldsymbol{S})|\boldsymbol{S}\rangle \tag{2.4}$$

and the components of the $|\psi_r\rangle$ in the $|\boldsymbol{S}\rangle$ basis by

$$\psi_r(\boldsymbol{S}) = \langle \boldsymbol{S}|\psi_r\rangle, \tag{2.5}$$

(2.3) becomes

$$\psi_r(\boldsymbol{S}) = \frac{\sum_{s=0}^{r-1} e_{r-s}\psi_s(\boldsymbol{S}) + \sum_{\boldsymbol{S}'} \langle \boldsymbol{S}|V|\boldsymbol{S}'\rangle \psi_{r-1}(\boldsymbol{S}')}{E_0(\boldsymbol{S}) - e_0}. \tag{2.6}$$

Now let

$$|\chi_m\rangle = \sum_{r=0}^{m} \lambda^r |\psi_r\rangle = |E\rangle + \lambda^{m+1}|\eta\rangle \tag{2.7}$$

be the perturbative wavefunction at order m. The energy estimate arising out of this wavefunction is

$$\xi_m = \frac{\langle \chi_m|H|\chi_m\rangle}{\langle \chi_m|\chi_m\rangle} = E + O(\lambda^{2m+2}), \tag{2.8}$$

so that knowledge of $|E\rangle$ to order m determines E to order $2m+1$. Thus, to obtain a perturbation expansion to order $2m+1$, one need only work in a set of basis states of order m or less. This means that it is not necessary to construct the entire finite lattice Hamiltonian in the matrix construction stage. Instead, it suffices to find only those matrix elements associated with the basis states of order $r \leqslant m$.

In view of the general form of (2.8) we now define

$$Q_m(\lambda) = \langle \chi_m|\chi_m\rangle = \sum_{s=0}^{2m} q_s^m \lambda^s, \tag{2.9}$$

$$P_m(\lambda) = \langle \chi_m|H|\chi_m\rangle = \sum_{s=0}^{2m+1} p_s^m \lambda^s. \tag{2.10}$$

It is then a straightforward exercise to show that the q_s^m and p_s^m satisfy

$$q_s^m = \begin{cases} q_s^{m-1}, & s = 0, \ldots, m-1, \\ q_s^{m-1} + 2\langle \psi_{s-m}|\psi_m\rangle, & s = m, \ldots, 2m-2, \\ 2\langle \psi_{s-m}|\psi_m\rangle, & s = 2m-1, \\ \langle \psi_m|\psi_m\rangle, & s = 2m, \end{cases} \tag{2.11}$$

$$p_s^m = \begin{cases} p_s^{m-1}, & s = 0, \ldots, m-1, \\ p_s^{m-1} + 2\langle \psi_0|H_0|\psi_m\rangle, & s = m, \\ p_s^{m-1} + 2\langle \psi_{s-m}|H_0|\psi_m\rangle - 2\langle \psi_{s-m-1}|V|\psi_m\rangle, & s = m+1, \ldots, 2m-1, \\ \langle \psi_m|H_0|\psi_m\rangle - 2\langle \psi_{m-1}|V|\psi_m\rangle, & s = 2m, \\ -\langle \psi_m|V|\psi_m\rangle, & s = 2m+1. \end{cases} \tag{2.12}$$

The initial conditions for these recurrence relations depend on the initial unperturbed eigenstate of H_0. For the ground state this is the (non-degenerate) state $|\psi_0\rangle = |0, 0, \ldots\rangle$ with $\Sigma S_i = 0$, while for the first excited state it suffices (see Hamer *et al* 1979) to consider the zero momentum superposition $|\psi_0\rangle = (1/\sqrt{M}) \sum_{i=1}^{M} \Omega_i |0, 0, \ldots\rangle$ of eigenstates of H_0 with $\Sigma S_i = -1$.

Given $|\psi_0\rangle$,

$$q_0^0 = \langle \psi_0|\psi_0\rangle = 1, \tag{2.13}$$

while the initial conditions on the p_s^m are obtained from $P_0(\lambda) = \langle \psi_0|H_0|\psi_0\rangle - \lambda\langle \psi_0|V|\psi_0\rangle$,

implying

$$p_0^0 = \langle\psi_0|H_0|\psi_0\rangle, \qquad p_0^1 = -\langle\psi_0|V|\psi_0\rangle. \tag{2.14a, b}$$

Finally, a little algebra (using the fact that $q_0^m = 1$ for all m) yields

$$e_{2m} = p_{2m}^m - \sum_{r=0}^{2m-1} e_r q_{2m-r}^m, \tag{2.15a}$$

$$e_{2m+1} = p_{2m+1}^m - \sum_{r=1}^{2m} e_r q_{2m+1-r}^m, \tag{2.15b}$$

for the perturbation coefficients.

The series generation algorithm can now be stated.

(1) Initialise a vector we shall refer to as $|\psi_{\text{current}}\rangle$, to the required eigenstate $|\psi_0\rangle$ of H_0. Set $m = 0$.

(2) Using (2.11), update the q_s^m. When $m = 0$, only the $s = 2m$ case of (2.11) is active.

(3) Using (2.12), begin the update of the p_s^m by first adding on the terms involving H_0. Computationally, this requires a linear scan through the previously generated $|\psi_r\rangle$, and a few inner products. This can be done concurrently with step (2). In the case $m = 0$ only the $s = 2m$ part of (2.12) (with $|\psi_{-1}\rangle = 0$) is operable.

(4) Multiply $|\psi_{\text{current}}\rangle$ by V to form a new $|\psi_{\text{current}}\rangle$, and use this vector to complete the update of the p_s^m. In the case $m = 0$ only the $s = 2m + 1$ part of (2.12) is operable.

(5) Using (2.15*a*, *b*) calculate e_{2m} and e_{2m+1} and exit if one has finished.

(6) Now update $|\psi_{\text{current}}\rangle$ to the next perturbative wavefunction coefficient $|\psi_{m+1}\rangle$ using (2.6).

(7) Set $m = m + 1$ and go to (2) above.

Several points contribute to the efficiency of this method. Firstly, the computation can be arranged so that the matrix elements and the $|\psi_r\rangle$ components are stored sequentially. Thus it is possible to efficiently implement this method with only one vector array resident in central memory. The rest of the information may even reside on tapes. Secondly, most of the inner products of the form $\langle\psi_r|\text{operator}|\psi_m\rangle$ can be calculated relatively quickly for $r < m$. In fact, the proliferation of basis states as the order increases results in *all* of the inner products for $r < m$ consuming about as much time as the $r = m$ inner product by itself. A similar comment applies to the multiplication of the $|\psi_r\rangle$ by V. Therefore, despite the initially formidable appearance of many inner products in (2.11) and (2.12), these equations do lend themselves to a fast, memory efficient algorithm. Thirdly, while it is necessary to find $V|\psi_m\rangle$ in order to calculate e_{2m} and e_{2m+1}, this does not require knowledge of states at order $m + 1$, since only terms of the form $\langle\psi_r|V|\psi_m\rangle$ ($r \leq m$) appear in (2.12). Therefore, one only needs to know the component of $V|\psi_m\rangle$ overlapping basis states of order m or less. This detail can be taken into account in the matrix construction stage by storing only those matrix elements of V (and H_0) associated with basis states of order $r \leq m$. Care must also be taken that the boundaries of the periodic lattice do not cause contributions to $\langle\psi_r|V|\psi_m\rangle$ which would not normally arise on an infinite lattice. For example, on a $2m$-site periodic lattice, consider the mth-order basis state $|1, -1, 1, -1, \ldots, 1, -1\rangle$. Acting with $\Omega_{2m+1}\Omega_{2m+2}^+ = \Omega_1\Omega_2^+$ results in a basis element of order $m - 1$. However, on an infinite lattice one would obtain a basis element of order $m + 1$, which would not overlap with $|\psi_{m-1}\rangle$. In the present case, a periodic lattice of size $2m + 1$ yields a mass gap expansion which agrees with the bulk to order $2m$.

3. Results

An 11-site periodic lattice was used to derive a 10th-order mass gap expansion for the bulk. The matrix construction in the ground state sector (zero momentum, $\Sigma_i S_i = 0$) involved 5155 basis states. Of these 4066 were of 5th order. On a CDC CYBER 72, the matrix construction step took 148 seconds CPU time. Generation of the 11th-order ground state series from the matrix took 15 seconds on the same machine. The matrix elements were stored on tape and the $|\psi_r\rangle$ kept on disc. Only one working array was resident in central memory. The first excited state calculation (in the zero momentum, $\Sigma_i S_i = -1$ sector) involved 28 004 basis states. Again, most of these (21 204) were 5th-order states. The matrix construction took 808 seconds while the generation of an 11th-order perturbation expansion took only 93 seconds.

The resulting mass gap series agrees with the bulk to 10th order in λ and is given by

$$G(\lambda) = 1 - 2\lambda + 0.5\lambda^2 + 0.25\lambda^3 + 0.230\,2083\cdot\lambda^4 + 0.192\,065\,972\cdot\lambda^5 + 0.014\,473\,5794\lambda^6 + 0.089\,062\,2894\lambda^7 - 0.044\,807\,1196\lambda^8 + 0.035\,998\,7647\lambda^9 - 0.081\,801\,7597\lambda^{10}. \tag{3.1}$$

Our analysis of this series closely parallels that of Hamer *et al* (1979). The first logarithmic derivative of this series can be interpreted as the inverse β function of the model. This β function can be fitted with Padé approximants which turn out to be concave upward. This suggests an algebraic zero in the β function, a conjecture which is further supported by a ratio test on the coefficients of the logarithmic derivative series. Following the continuation of this analysis (Hamer and Kogut 1979) we Euler transform (3.1) to the variable $Z = \lambda/(\lambda + \alpha)$ and then take the second logarithmic derivative of the resulting series. In view of the ansatz (1.5), the first simple pole on the real axis should lie at $Z_c = \lambda_c/(\lambda_c + \alpha)$ while the residue of this pole should be $-1-\sigma$. Several Padé tables were constructed from the transformed series for a variety of values of α. The choice $\alpha = 1.5$ gave rise to the estimates for λ_c and σ shown in table 1. Other values of α yielded similar results; however, the choice of $\alpha = 1.5$ led to a Padé table free of spurious behaviour of the off-diagonal approximants. From table 1 we estimate

$$\lambda_c \approx 0.89 \pm 0.02, \qquad \sigma \approx 0.50 \pm 0.08,$$

which are considerable improvements on the 8th-order results. Moreover, a ratio test applied to the first logarithmic derivative of the Euler transformed series leads to very similar results, as was the case for the 8th-order series (Hamer and Kogut 1979). Ferer (1985) has recently analysed our extended series by his q-fit method (Ferer and Velgakis 1983), yielding a similar estimate of σ.

Table 1. Padé table of estimates λ_c and σ (bracketed figures).

N	$[N-1/N]$	$[N/N]$	$[N+1/N]$
1	0.9335 (0.642)	0.8866 (0.518)	0.9244 (0.641)
2	0.9089 (0.581)	0.9058 (0.507)	0.8776 (0.425)
3	0.9104 (0.584)	0.8802 (0.444)	0.8764 (0.420)
4	0.8885 (0.501)	0.8923 (0.529)	

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