Thermodynamic ζ functions for Ising models with long-range interactions

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The use of cycle expansions for spin systems with long-range interactions is explored numerically. It is found that the thermodynamic ζ function is an effective tool, both in practice and in principle, for the study of Ising models with power-law interactions. To deal with phase transitions the cycle expansion is factorized, and accurate phase-transition points for several power-law models are obtained, together with other thermodynamic quantities.

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I. INTRODUCTION

Thermodynamic ζ functions offer an alternative means for evaluating partition functions in statistical mechanics. They deal directly with the infinite system and make precise the intuitive notion of "relevant" configurations. The application of the ζ function to evaluate the partition function is not dependent on any special properties of statistical mechanics and can therefore be used wherever partition functions occur formally. This includes the computation of thermodynamic invariants in dynamical systems [1,2] and the evaluation of eigenenergies in quantum mechanics [3]. Here we investigate the behavior of ζ functions in the presence of a phase transition. Because phase transitions are better understood in the case of statistical mechanics, the formalism is developed in that language.

A thermodynamical ζ function can be thought of as a formal infinite product over the states of a system in the grand canonical ensemble. It was introduced by Ruelle [4] as a generalization of the generating function of Artin and Mazur [5] for counting periodic orbits in dynamical systems. Thus it originated as an alternative to the partition function, but not as a practical method for determining thermodynamic quantities. The difficulties with the infinite product were enumerated by Voros [6] in the context of quantum mechanics. The basic problem has to do with the irregular nature of the convergence of the thermodynamic ζ function, which mimics that of the Riemann ζ function, an infinite product involving the prime numbers [7]. The convergence problem was solved in the context of dynamical systems by Cvitanović and co-workers [2,8,9] by interpreting the various terms of the inverse of the ζ function. The inverse ζ function at first seems an unlikely object to study, as it becomes a diverging infinite product at the point of interest to thermodynamics. The realization of Cvitanović was that the infinite product of Ruelle can be analytically continued and the power series obtained is the sum of exponentially decreasing terms, and therefore computationally useful. The analytic continuation—called the cycle expansion—involves sums of weight associated with periodic orbits and can be interpreted in light of Bowen's shadowing theorem [10], where certain configurations are well approximated by "shadow" pseudoconfigurations.

Here we develop the ζ function formalism for spin systems and apply it to an Ising system with Coulomb interactions. The ζ function for a system at temperature $1/\beta$ and fugacity z is obtained from the exponential of a variant of the grand canonical partition function

$$\zeta(z,\beta)=\exp\left[\sum_{n\geq 1}\frac{z^n}{n}Z_n(\beta)\right]. \tag{1}$$

The formalism proves to have conceptual and computational advantages over alternative descriptions of models with long-range interactions.

The conceptual advantage of ζ functions is that they deal directly with an infinite system, making them better suited than transfer matrices for the study of systems with long-range interactions. They also offer a computational advantage over transfer matrices. To compute a thermodynamic quantity from a transfer matrix, its largest eigenvalue must be computed, with the size of the matrix being proportional to a power of the range of the interaction. In modern computers the amount of real memory limits the size of the matrices that can be handled. With the ζ function formalism the memory bottleneck is completely eliminated.

Direct solutions of spin systems with long-range interactions have been obtained by a variety of methods [11,12], but there is no unified treatment for all models. All solutions require at one point or another a resort to numerical schemes, and the ζ function formalism provides an unified approach to all long-range models and leads to an efficient numerical scheme.

The motivation for studying a one-dimensional Ising model with power-law interactions is threefold: it is a physically interesting model, as it is the basis for the solution of the Kondo problem, it is related to the behavior of orbits in Hamiltonian systems that are in the stochastic region but close to the periodic islands; and it is an example of a model with a phase transition. Polynomial interactions are also the most difficult to handle numerically.

In Sec. II we develop the basic formalism of ζ functions for spin systems. The emphasis will be on one-

dimensional long-range models, but the formalism is directly applicable to other spin systems in more than one dimension (see Mainieri [13]). In Sec. III the formalism is applied to the one-dimensional Ising model with Coulomb interaction. The free energy, the phase-transition temperature, and the heat capacity are obtained using the cycle expansion. The ζ-function methods are compared to transfer matrices away from the phase-transition point in Sec. III A and it is shown that even away from the transition point it is difficult to extract reliable numbers from the largest eigenvalue of the transfer matrix when the interaction is power law. In Sec. III H some of the results for other potentials are shown as further illustration of the method.

II. BASIC FORMALISM

We will derive the ζ function for a lattice system where each lattice site can have a finite number of states, as in the Ising model where the states are + and − or as in a lattice gas where the states are 0 and 1 (see also Ruelle [1] and Cvitanović [2]). In taking the thermodynamic limit we will consider the subsets Λ_n of the lattice consisting of the n sites from 0 to $n-1$, although different choices are possible. The Hamiltonian evaluated at a configuration σ that is restricted to the subset of sites Λ_n is denoted by $H_n(\sigma)$ and is usually the sum of pairwise interactions. The configuration σ is defined for the full infinite lattice, and not just Λ_n.

The partition function $Z_n(\beta)$ for the system restricted to the sublattice Λ_n at a temperature $1/\beta$ is given by summing over all the possible configurations C_n of the sublattice

$$Z_n(\beta)=\sum_{\sigma\in C_n} e^{-\beta H_n(\sigma)} , \tag{2}$$

with a fixed configuration for the rest of the lattice. The thermodynamics can be derived from the free energy f per site in the limit of large sublattices

$$\beta f(\beta)=-\lim_{n\to\infty}\frac{1}{|\Lambda_n|}\ln Z_n(\beta) . \tag{3}$$

Because in the limit $n\to\infty$ the quantity $n^{-1}\ln n$ is zero we can subtract this function from the logarithm of the partition function (3) and write the limit for the free energy as

$$\beta f(\beta)=-\lim_{n\to\infty}\frac{1}{|\Lambda_n|}\ln\frac{Z_n(\beta)}{n} . \tag{4}$$

We will now consider the generating function for the quantities $Z_n(\beta)/n$. Except for the factor $1/n$, this generating function is the grand partition function. We define

$$G(z,\beta)=\sum_{m\geq 1}\frac{z^m}{m}Z_m(\beta) , \tag{5}$$

where z is the formal parameter of the generating function. In general, when the thermodynamic limit exists and the choice of sublattices Λ_n has a vanishing surface-to-volume ratio (as is the case for segments) the partition function $Z_n(\beta)$ will grow exponentially as a function of n, that is,

$$Z_n(\beta)\to e^{-n\beta f(\beta)} \text{ as } n\to\infty . \tag{6}$$

We can then choose a value for z such that each term of the generating function G in (5) is of order 1 for large n. With this choice of z, which depends on β, the generating function will diverge. Because all the terms of the sum in the generating function are positive, one can show that there is a smallest z for which the generating function diverges,

$$z_0(\beta)=\inf\{z>0:\ 1/G(z,\beta)=0\} , \tag{7}$$

and that for all values of $|z|<z_0(\beta)$ the generating function (5) is an analytic function. The positivity of the terms tells us more: z_0 gives the asymptotic growth of the coefficients of the series; that is, there are two constants independent of n such that for large enough n,

$$A_1 z_0^{-n}\leq Z_n\leq A_2 z_0^{-n} . \tag{8}$$

By comparing this expression with the definition of the free energy per site (3) we conclude that the radius of convergence of the generating function, z_0, is related to the free energy by

$$\beta f(\beta)=\ln z_0 , \tag{9}$$

which connects the generating function to the thermodynamics of the system.

We will now restrict ourselves to translation-invariant systems. This means that the interaction between sites is independent of the position of the site. This excludes systems that have position-dependent external magnetic field, for example, but includes the familiar case of the Ising model with a constant magnetic field.

To make explicit the translation-invariant nature of the system, the energy of a configuration can be written as the sum of an interaction Φ of one site with all the others of the lattice. If we do this for every site of the segment Λ_n there will be a double counting of the interactions between different sites. To avoid this we can consider either half of Φ or we can consider only the interactions to one side of the one-dimensional lattice. In what follows we will adopt the second choice and make Φ the one-sided interaction.

A few common choices for Φ are the nearest-neighbor Ising model with external magnetic field

$$\Phi(\sigma_a,\sigma_b)=-J\sigma_a\sigma_b+B\sigma_a , \tag{10}$$

or the Ising model with exponentially decaying interaction

$$\Phi(\sigma_1,\sigma_2,\ldots)=J\sum_{k>1}\sigma_1\sigma_k e^{-\alpha k} . \tag{11}$$

With the definition of Φ we can compute the energy H_n of a configuration σ when restricted to a segment Λ_n:

$$H_n(\sigma)=\sum_{0\leq k<n}\Phi(\sigma_k,\sigma_{k+1},\ldots) . \tag{12}$$

Notice that this expression is not the sum of the interac-

tion within Λ_n plus the interaction of the sites of Λ_n with the rest of the lattice, but it does give the correct energy per site in the thermodynamic limit. This unusual choice of H is convenient when periodic boundary conditions are used. Also, if Φ is a long-range interaction, the value of H_n depends not only on the values of the sites within Λ_n, but also on the value of the sites outside Λ_n.

When the interactions are short range the effects of the boundaries are irrelevant for determining the state of the system, but this may not be the case if the interactions are long range. With long-range interactions the boundaries must be specified in order to compute the energy of a configuration H_n, even when the system is restricted to a small box. We can evaluate the partition function (2) by adopting periodic boundary conditions. If there is only one phase to the system, or we are only interested in its high-temperature behavior, the boundary conditions adopted are irrelevant for the thermodynamics. But if there is more than one phase then which one is obtained in the thermodynamic limit is a function of the boundary adopted. In the case of periodic boundaries one usually obtains a simple average of each of the phases. In the case studied here the multiple-phase problem will be solved by isolating some of the configurations (see Sec. III F).

An alternative way to implement the periodic boundary conditions is to work on the infinite lattice and use only periodic configurations. For a configuration σ of the whole lattice we will indicate its period by $|\sigma|$. As the term $z^n\exp[-\beta H_n(\sigma)]$ appears frequently, we adopt the abbreviation t_σ for it. With this notation the partition function is

$$z^n Z_n = \sum_{\substack{\sigma \\ (|\sigma|=n)}} t_\sigma \ , \tag{13}$$

the z^n being there to compensate for the z factor in t_σ. The summation is over all configurations that have period equal to n, and this includes the "harmonic" and "out of phase" orbits. For example, the orbit $\cdots + - + - \cdots$ is counted as an orbit of period 2, 4, 6, etc.; and in each case is counted twice, once for the plus at site zero and once for the minus at site zero.

The generating function (5) is then

$$\begin{aligned} G(z,\beta) &= \sum_{n\geq 1} \frac{1}{n} \sum_{\substack{\sigma \\ (|\sigma|=n)}} t_\sigma \\ &= \sum_{\sigma\in\Omega} \frac{t_\sigma}{|\sigma|} \ , \end{aligned} \tag{14}$$

where the last sum is over all possible periodic configurations on the lattice, a set we indicated by Ω.

There are several properties of the Boltzmann factors that permit the simplification of the generating function. First, there is a relation between a harmonic orbit and its "fundamental." We define the maximum number of times a shorter pattern needs to be repeated to form the orbit's multiplicity, and indicate it by $m(\sigma)$. For example, the multiplicity of the harmonic orbit $\sigma^2=(++-++-)$ of period 6 is 2 as its fundamental $\sigma=(++-)$ has length 3. The relation between the weight of t_σ and the weight of t_{σ^n} is

$$\frac{t_{\sigma^n}}{|\sigma^n|} = \frac{(t_\sigma)^n}{n|\sigma|} \ . \tag{15}$$

Next, the Boltzmann factor for all orbits that differ by a phase is the same, for example, $t_{(++-+)}=t_{(-+++)}$. The number of times a given orbit occurs in the generating function (14) is $|\sigma|/m(\sigma)$.

We can rewrite the generating function as a sum over periodic orbits that *do not* differ by a phase, indicating the set by Ω', by multiplying each factor by the number of times it occurs in the sum:

$$G(z,\beta) = \sum_{\sigma\in\Omega'} \frac{t_\sigma}{|\sigma|}\frac{|\sigma|}{m(\sigma)} \ . \tag{16}$$

This sum can be grouped by the multiplicity of the orbits. If the set of all periodic configurations of multiplicity m that do not differ by a phase is Ω'_m, the generating function is

$$G = \sum_{\sigma\in\Omega'_1} t_\sigma + \tfrac{1}{2}\sum_{\sigma\in\Omega'_2} t_\sigma + \tfrac{1}{3}\sum_{\sigma\in\Omega'_3} t_\sigma + \cdots \ . \tag{17}$$

Recalling the relation between t_{σ^n} and t_σ we have

$$\begin{aligned} G &= \sum_{\sigma\in\Omega'_1} \left[t_{\sigma^1} + \frac{t_{\sigma^2}}{2} + \frac{t_{\sigma^3}}{3} + \cdots \right] \\ &= \sum_{\sigma\in\Omega'_1} \left[(t_\sigma)^1 + \frac{(t_\sigma)^2}{2} + \frac{(t_\sigma)^3}{3} + \cdots \right] \\ &= -\sum_{\sigma\in\Omega'_1} \ln(1-t_\sigma) \ , \end{aligned} \tag{18}$$

where we have summed the series. The sum now is reduced to the set of orbits that have multiplicity 1 and we denote this set by P, for prime orbits. We will take as definition of the ζ function the exponential of G,

$$\zeta(z,\beta) = e^{G(z,\beta)} = \prod_{\sigma\in P} (1-t_\sigma)^{-1} \ , \tag{19}$$

and by expanding the terms $(1-t_\sigma)^{-1}$ into power series we obtain the Euler product form of the Ruelle ζ function, but now for spin systems.

The inverse of ζ can be expanded as a power series of z (on which the weights depend)

$$\zeta^{-1} = 1 - c_1 z^1 - c_2 z^2 - c_3 z^3 - \cdots \ , \tag{20}$$

which is the Cvitanović cycle expansion [2] of the Ruelle ζ function. The smallest root in absolute value of this function will always be real, as is stated in a theorem of Ruelle [1].

III. LONG-RANGE ISING MODEL

In this section we will apply the methods that have been developed to the one-dimensional Ising model with long-range interactions. As an example we will use the model with an interaction falling off as the square of the

distance, but the techniques are applicable to other long-range interactions as shown in Sec. III H. The one-dimensional inverse square problem has attracted attention because of its connection with the Kondo problem and because of the inverse square interaction being the borderline case for one-dimensional models having phase transitions.

The Kondo problem consists of the determination of the behavior of electrons in a metal with magnetic impurities. At low temperatures the spin of the electron couples to the spin of the impurities governing the electronic properties of the metal. Yuval and Anderson [14,15] and Anderson, Yuval, and Hamann [16] were able to show that the Kondo problem is equivalent to the study of a one-dimensional Ising model with a combination of nearest-neighbor and inverse-square interactions.

There is an heuristic argument, probably due to Landau and Lifshitz [17], about the occurrence of phase transitions as a function of the rate of decay of the interaction, for models with Hamiltonians of the form

$$H(\sigma)=-\tfrac{1}{2}\sum_{i,j} J(|i-j|)\sigma_i\sigma_j \tag{21}$$

with $J(x)=x^{-s}$. Landau argued that for interactions that fall off faster than the x^{-2} there would be no phase transitions, and that for interaction that fall off slower than x^{-2} there would be a phase transition. His argument left undecided the borderline case $J(x)=x^{-2}$. Later Thouless [18] heuristically argued that the borderline case of inverse square would also have a phase transition with a discontinuity of the magnetization at the critical point.

The conjectures of Landau were proven correct by Ruelle [19], who showed that there is no phase transition in one dimension for $s>2$, and by Dyson [20], who showed that there is a phase transition in one dimension for $s<2$. Simon and Sokal [21] have proven results similar to Ruelle's by following the essence of Landau's arguments. None of these methods was sufficient to settle the x^{-2} case. The possibility of a phase transition in the inverse-square case was studied using the renormalization group by Anderson and Yuval [22] and proven to exist by rigorous methods by Fröhlich and Spencer [23]. The conjectures of Thouless were shown to hold (although for different reasons) by the work of Aizenman *et al.* [24].

The proofs for the existence of the phase transition for the inverse-square model are all indirect: the existence of the phase transition is established by showing that there is spontaneous magnetization for low enough temperatures, and not by explicitly solving the model. This makes it difficult to use the proof to develop methods for evaluating thermodynamic quantities, and only general techniques are applicable. For most models the thermodynamic average of an observable can be evaluated away from a phase-transition point by the use of series expansions, transfer matrices, or Monte Carlo methods. Most numerical methods truncate the interaction J at some finite range, substituting for it the interaction

$$J_T(x)=\begin{cases} J(x) & \text{if } |x|\le r\ , \\ 0 & \text{if } |x|>r\ . \end{cases} \tag{22}$$

The quantity r is the range of J_T. This is a good approximation if the interaction falls off exponentially or faster, but not if the interaction is power law.

A. Transfer-matrix methods

The general approach to using a transfer-matrix method for solving a one-dimensional model with long-range interactions consists of truncating the interaction at some finite range and exactly solving the truncated model. By solving the model with ever increasing truncation lengths, it may be possible to extrapolate the thermodynamic average of interest (for example, the free energy).

The formalism of transfer matrices is simplified if we adopt periodic boundary conditions. As the models may have infinite range interactions, periodic boundary conditions are implemented by repeating a segment of sites Λ_n to cover the entire line. This is equivalent to assuming that the model is a segment Λ_n with n sites numbered $0,\ldots,n-1$, and that all sites calculations are done mod$n$.

The interaction cannot depend on the site nor on the relative orientation for the development of the transfer-matrix approach, and we have indicated this by making the interaction between two spins depend only on the absolute value of their distance on the lattice, as in (21). Also the interaction must have a range r smaller than the size n of the system. The problem is then to compute the partition function $Z_n(\beta)$ at a temperature $1/\beta$ in the thermodynamic limit of $n\to\infty$. The partition function is given by considering all possible configurations Ω_n in the lattice Λ_n:

$$Z_n(\beta)=\sum_{\sigma\in\Omega_n} e^{-\beta H(\sigma)}\ . \tag{23}$$

We will use the interaction Φ that depends on as many sites as there are in the lattice Λ_n, the "one-sided" interaction

$$\Phi(\sigma)=\Phi(\sigma_1,\sigma_2,\ldots,\sigma_n)=\sum_{1<j\le n} J(|1-j|)\sigma_1\sigma_j\ , \tag{24}$$

as it gives the contribution to the Hamiltonian of one site with all the spins to its right. As we are restricting ourselves to the truncated interaction of range r, there is no need to consider more than $r+1$ spins in the argument of Φ, that is, one can take $n=r+1$ in its definition. With this interaction function we define a matrix T that relates two configurations $\sigma=(\sigma_1,\ldots,\sigma_r)$ and $\omega=(\omega_1,\ldots,\omega_r)$ of r spins

$$T_{\sigma\omega}(\beta)=\delta_{\sigma_2\omega_1}\delta_{\sigma_3\omega_2}\cdots\delta_{\sigma_r\omega_{r-1}}e^{\beta\Phi(\sigma_1,\ldots,\sigma_r,\omega_r)}\ . \tag{25}$$

With this choice of T the partition function can be written as

$$Z_n(\beta)=\mathrm{tr}T^n(\beta)\ , \tag{26}$$

as can be seen from substituting the definitions of T and the trace in (26) and comparing the result with the definition of the partition function (23).

To evaluate the right-hand side of (26) one has to sum

the eigenvalues of T to the power n. In the thermodynamic limit one will have that the free energy f is given by the largest eigenvalue of T as in

$$\beta f(\beta) = -\ln\lambda_{\max} . \tag{27}$$

As T is a positive matrix it has an isolated largest eigenvalue, which can be obtained by the mapping

$$|v\rangle \rightarrow \frac{1}{\langle v|T|v\rangle} T|v\rangle , \tag{28}$$

between vectors, and its repeated application. It can be shown that for almost all vectors, the repeated application of this mapping will converge to the vector $|\lambda_{\max}\rangle$ associated with the largest eigenvalue $\lambda_{\max}$.

This algorithm can be used to efficiently compute the eigenvector (which is an approximation to the Gibbs state of the system) and from it obtain the eigenvalue. The difficulty in implementing the algorithm in a computer is that the matrix T needs to be stored in the memory of the computer as its product with the vector $|v\rangle$ is evaluated. For a general matrix of size m by m, one needs to store m^2 terms. In general, an interaction of range r requires that a 2^r by 2^r matrix be used. A computer with eight megabytes of memory, using single-precision (four bytes) numbers, could store the matrix for a range r up to 10. There are more efficient numerical schemes for obtaining the largest eigenvalue of a matrix, such as Lanczos's method [25], that do not require storing the full matrix for all iterations, but only a few columns of it. In the sense of efficiency of storage, the choice of the transfer matrix we have made is optimum, as it is duo-diagonal, requiring a storage of only 2^{r+1} terms, which is less than what Lanczos's algorithm requires. This allows the use interactions with ranges up to 20 in a 8-megabyte machine.

Memory constraints are the bottleneck for exact transfer-matrix calculations, and not processing time. A typical workstation in 1990 (a Sun Sparcstation) can compute the largest eigenvalue of the $r=20$ case to machine precision in 20 min. Speed increases of the order of 200 can be expected with the use of a supercomputer.

The rate of convergence of the method used is linear: one gains a constant number of "digits" per iteration. The rate of convergence, or how many digits one gains, is dictated by the ratio of the second largest eigenvalue to the largest eigenvalue. These only become comparable near a phase-transition point, and one should expect fast convergence away from it. For temperatures away from a transition point typically 50 iteration are sufficient to attain machine accuracy for the eigenvalue.

In Fig. 1 we have the plot of the free energy for an Ising model with the long-range interaction

$$J(x) = e^{-2x} , \tag{29}$$

and computed from a transfer matrix. Notice that there is no need to extrapolate, as the values obtained are accurate to machine precision. A few values for $\beta=0.5$ are given in Table I.

The same does not happen if instead we use a power-law interaction. In Fig. 2 we have the values of the free energy for the interaction

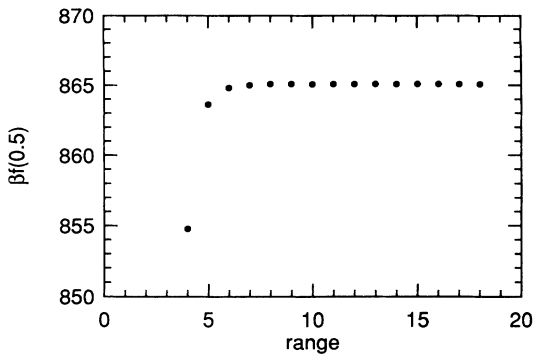

FIG. 1. Points represent the convergence of the free energy for the one-dimensional Ising model with exponential interactions, as in Eq. (29), as the size of the matrix is increased. For clarity, only the last three digits of the free energy are indicated, the origin of the plot being 0.732 850. The points rapidly converge to a limit.

$$J(x) = x^{-2} . \tag{30}$$

This interaction leads to a model with a phase transition for β around 1, and in Fig. 2 the free energy has been computed for the larger temperature of $\beta=0.5$. The slowness of the convergence can be appreciated if we try to extrapolate the result for the infinite range of the interaction. The extrapolated value is indicated by a dotted line in the plot. Notice that the large distance between the actual points and the extrapolated values diminishes one's confidence on the extrapolated value.

As a test of the extrapolation procedure, and on the absence of any error bounds on the procedure, we have used several different procedures to do the extrapolation. We have used a modified Euler method, and the Levin T and U transforms (see the review by Guttmann in Domb and Lebowitz [26]). The results are indicated in Table II, and tend to agree with one another.

The slow convergence is not due to the existence of a phase transition in the model, but just a reflection of the longer range of the interaction, and we have studied the model with the inverse fifth-power interaction. In Fig. 3 we have compared the gain in precision of the plotted points as the range is increased. The precision Δ is indi-

TABLE I. The free energy, computed from a transfer matrix, for the system with exponential interaction for $\beta=0.5$. It reaches machine precision with a short truncation of the potential.

Range	$\beta f(0.5)$
4	0.732 854 740 737 943 3
6	0.732 864 823 174 496 5
8	0.732 865 007 715 138 1
10	0.732 865 011 095 032 8
12	0.732 865 011 156 939 0
14	0.732 865 011 158 070 9
16	0.732 865 011 158 098 2
18	0.732 865 011 158 072 3

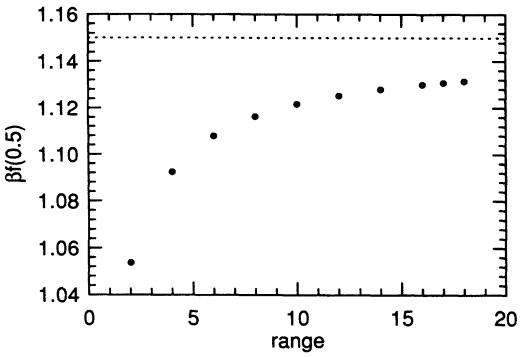

FIG. 2. Free energy for the Ising model, but now with power-law interactions. Notice that there is a large distance between the last computed point and the limit indicated by the dotted line.

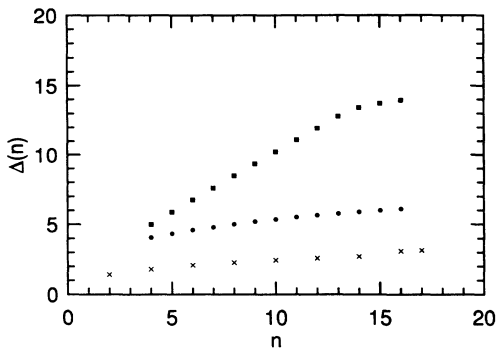

FIG. 3. Rate at which digits are gained as a function of the range n in the computations of the free energy for different interactions with transfer matrices. Squares are for the e^{-2x} interactions, circles for x^{-5}, and crosses for x^{-2}.

cated by the number of unchanged digits:

$$\Delta(n)=\log_{10}[f_n(0.5)-f_{n-1}(0.5)] . \tag{31}$$

B. Cycle expansions

The long-range Ising model with x^{-2} interaction and Hamiltonian

$$H_n(\sigma)=-\sum_{\substack{i(\in\Lambda_n)\\ j(>i)}}\frac{\delta_{\sigma_i,\sigma_j}}{|i-j|^2} \tag{32}$$

is known to have a phase transition for a temperature β_c in the range from 1 to 2. Anderson and Yuval [22] have estimated that $\beta_c=1.23\pm0.06$ by a renormalization-group calculation. (They apparently invented the renormalization group independently of Wilson for this calculation.) In this section we will use the ζ-function formalism to compute some of the properties of this model. As we have seen in the transfer-matrix approach, even away from the phase-transition point it is difficult to obtain good estimates for the thermodynamic averages.

To develop the cycle expansion for the long-range Ising model, we need to determine the Boltzmann factors t_σ associated with each prime periodic configuration σ. This is done in two steps. First we determine the interaction function of one site with the rest of the system, and second we determine the Boltzmann factor by considering translations of the periodic configuration.

The interaction function Φ of one site with all the other sites to its right is read from the Hamiltonian to be

$$\Phi(\sigma_1,\sigma_2,\ldots)=\sum_{j\geq 2}\frac{\delta_{\sigma_1,\sigma_j}}{(j-1)^2} . \tag{33}$$

TABLE II. Three different methods were used to extrapolate the sequence of points for the power-law interaction: the modified Euler method and Levin's U and V transforms.

Method	Limit
Euler	1.146 92
Levin U	1.147 28
Levin V	1.147 26

This interaction requires the knowledge of an infinite number of sites and in general has to be approximated by truncation, but in the case of the ζ-function cycle expansions the configuration is periodic and the value of Φ for it can be exactly determined. For example, if we need to determine the value of Φ for the configuration 010101. . ., which has prime period 2, we write

$$\begin{aligned}\Phi(0,1,0,1,\ldots)&=\frac{\delta_{\sigma_1\sigma_2}}{(2-1)^2}+\frac{\delta_{\sigma_1\sigma_3}}{(3-1)^2}+\frac{\delta_{\sigma_1\sigma_4}}{(4-1)^2}+\cdots ,\\ &=\frac{1}{2^2}+\frac{1}{4^2}+\frac{1}{6^2}+\cdots ,\\ &=\frac{1}{2^2}\zeta_R(2)=\frac{\pi^2}{24} .\end{aligned} \tag{34}$$

That is, the value of $\Phi(0,1,0,1,\ldots)$ can be expressed in terms of the Riemann ζ function

$$\zeta_R(s)=\sum_{n\geq 1}\frac{1}{n^s} . \tag{35}$$

The same can be done for orbits of longer period, but now the values need to be expressed in terms of the Lerch transcendental function, defined as

$$\Phi_L(z,s,a)=\sum_{k\geq 0}\frac{z^k}{(k+a)^s} , \tag{36}$$

with the restriction that if a term of the sum has $k+a$ equal to zero, it is not included in the sum. In general, if $(\sigma_1,\sigma_2,\ldots,\sigma_p)$ is a periodic configuration of period p, then from the definition of the interaction we can conclude that

$$\begin{aligned}&\Phi(\sigma_1,\sigma_2,\ldots,\sigma_p,\sigma_1,\ldots)\\ &=\sum_{2\leq k\leq p}\delta_{\sigma_1,\sigma_k}\sum_{n\geq 0}\frac{1}{(k-1+np)^2}\\ &=\sum_{2\leq k\leq p}\frac{\delta_{\sigma_1,\sigma_k}}{p^2}\sum_{n\geq 0}\frac{1}{[n+(k-1)/p]^2}\\ &=\sum_{2\leq k\leq p}\frac{\delta_{\sigma_1,\sigma_k}}{p^2}\phi_L(1,2,(k-1)/p) .\end{aligned} \tag{37}$$

As we only consider periodic configurations we will often denote the interaction function $\Phi(\sigma_1,\sigma_2,\ldots,\sigma_p,\sigma_1,\ldots)$ by $\Phi(\sigma_1,\sigma_2,\ldots,\sigma_p)$, leaving it implicit that the prime period indicated as an argument is to be repeated indefinitely to obtain the complete argument. The determination of the numerical value of the Lerch transcendental function does not require the evaluation and estimation of the limit of its defining series, as there are efficient algorithms for evaluating the function.

Once the interaction function can be computed for any periodic configuration, we can evaluate its Boltzmann factor

$$t_\sigma = z^{|\sigma|}\exp\left[\beta \sum_{1\le i\le|\sigma|} \Phi(\sigma_i,\sigma_{i+1},\ldots,\sigma_{i+|\sigma|-1})\right] . \tag{38}$$

The summation rotates the periodic configurations so that every spin is once the first argument of the interaction Φ. For β equal to 1, we would have for the configuration (001) the Boltzmann factor

$$t_{(001)} = z^3 e^{\Phi(0,0,1)+\Phi(0,1,0)+\Phi(1,0,0)} = z^3 e^{2.01} . \tag{39}$$

The first few cycles for $\beta=1$ are listed in Table III, from which the values for any β can be computed by appropriate powers. Given the Boltzmann factors we can compute the cycle expansion:

$$\zeta^{-1}(z,\beta) = 1-(t_0+t_1)-(t_{01}-t_0t_1) -(t_{001}+t_{011}-t_0t_{01}-t_1t_{01})-\cdots , \tag{40}$$

where we have grouped terms in the powers of z that are implicit in the t_σ. In practice the cycle expansion is obtained from the Euler product of the ζ function

$$\zeta^{-1}(z,\beta) = \prod_\sigma (1-t_\sigma) , \tag{41}$$

where the factors are multiplied one by one, and only terms up to the largest period considered are kept. If we have the Boltzmann factors up to period m then all the powers up to z^m are kept in the cycle expansion.

To compute the cycle expansion from the product of n factors for periods up to p requires less than pn multiplications, and less than pn additions. An order-of-magnitude estimate of the total number of operations required when there are q states per site can be done by estimating the total number of factors as q^{p+1} and by bounding the number of floating-point operations by $2pq^{p+1}$. In an actual program the cycle expansion needs to be evaluated once for each value of β considered, but the Boltzmann factors need only be computed once. For the same precision in the result, the cycle expansion requires less computer time than the extraction of the largest eigenvalue from a transfer matrix.

TABLE III. The first few cycles for the power-law interaction. The spin-flip symmetric cycles are not listed.

Cycle	Weight
t_0	$e^{1.644\,93}$
t_{01}	$e^{0.822\,47}$
t_{001}	$e^{2.010\,47}$
t_{0001}	$e^{3.495\,48}$
t_{0011}	$e^{2.878\,63}$
t_{00001}	$e^{5.066\,40}$
t_{00011}	$e^{4.193\,47}$
t_{00101}	$e^{2.781\,05}$

C. Smallest-root determination

The thermodynamic properties are determined from the smallest root of the cycle expansion set to zero. A truncation of the cycle expansion to order z^2 furnishes a quadratic equation that can be solved to obtain a first guess to the root, which can then be refined by Newton's iterative root-finding algorithm. We routinely determine all the roots, real and complex, to determine if the smallest root is a multiple or single root, and if it is isolated in the complex plane.

The cycle expansion for $\beta=0.5$ for terms up to z^4 is

$$1-4.552\,22z+3.671\,99z^2+1.402\,71z^3+1.361\,35z^4 . \tag{42}$$

For calculations the ζ function is computed for periods up to 12. To estimate the quality of the root obtained from the cycle expansion, the root is also computed from cycle expansions of shorter periods and a plot is made of how the root is converging. Let N be the largest period in a given cycle expansion

$$\zeta^{-1}(z,\beta) = 1-\sum_{1\le k\le N} c_k z^k \tag{43}$$

and call $z^{(N)}(\beta)$ the smallest root of $\zeta^{-1}=0$. In Fig. 4 we have plotted the successive free energies obtained from these roots. The points of the plot are a sequence of numbers and one would like to know the root of the cycle expansion when all the cycles are considered, which corresponds to determining the limit of the sequence of numbers as $N\to\infty$. To accomplish this we can use one of the many sequence extrapolation methods. We have chosen to use the Levin U and V transforms and also a modified

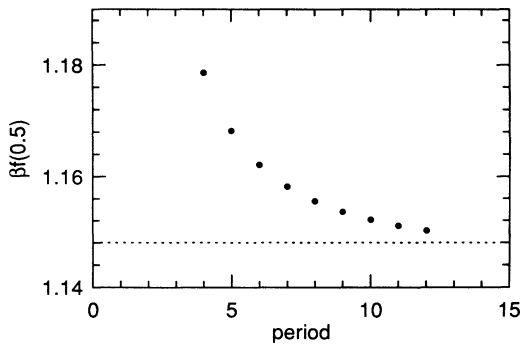

FIG. 4. Dots represent the value of the free energy as obtained from the ζ function by increasing the number of cycles considered. The scale of this figure is more detailed than that of Fig. 2. The dotted line is the numerical limit of the sequence of free energies.

Euler method. The Levin transforms have proven successful in handling statistical-mechanical models, and they are well tailored to estimate the partial sums of the Riemann ζ function. The Euler method is different from the Levin methods and it is used as a check. The distance of the last point of the plot ($n=12$) we take as an estimate of the order of magnitude of the error in the free energy. Even though the limit from the cycle expansion and the limit from the transfer matrix are close, the cycle-expansion points are closer to their limit than the transfer-matrix points are. We view this as a sign of the higher precision of the cycle expansion. These results take a few seconds of workstation time to obtain (as only of the order 2^{12} operations are required) and are to be compared to the transfer-matrix calculations, which reached the limits of the memory of the workstation after 20 min of computation without attaining the same accuracy (see also the discussion in Sec. III A).

One can intuitively understand why the cycle expansion should be more precise. The cycle expansion approximates the model by considering an infinite subset of all the configurations and does not introduce abrupt truncations of the interaction. Recall that the cycle expansion was obtained after summing up an infinite subset of configurations. Also, because the periodic configurations can be extended to cover an infinite chain, there is no need to truncate the interaction as in the transfer-matrix case.

D. Tail resummation

We can further improve the values obtained by observing that the coefficients of the cycle expansion, the curvatures, are growing (the name curvature was given by Cvitanović in Ref. [2]). The rate at which the coefficients are growing is an indication of the type of singularity that the cycle expansion may have. In Fig. 5 we have plotted the curvatures c_n of (43) as a function of n. Their growth rate can be well approximated by an exponential, and we shall assume this for the numerical calculations. Away from the phase-transition point this is a good approximation.

By assuming that the rate of growth of the curvatures is exponential we are implicitly assuming that the point of nonanalyticity is a pole. We can then remove the pole from the cycle expansion, therefore increasing the radius of convergence and improving the quality of the zero obtained. Notice that unless the root is at the point of nonanalyticity the residue of the pole does not affect the value of the zero. Assume, for example, that we have a pole at z_p; then the function

$$\zeta_p^{-1}(z,\beta)=A(\beta)(z-z_p)^s\zeta^{-1}(z,\beta)$$
$$=A(\beta)\prod_\sigma(1-t_\sigma)(z-z_p)^s \tag{44}$$

will in general have a larger radius of convergence than ζ^{-1} and have the smallest zero at the same point. Even if we do not locate the pole precisely, we can still remove most of its effects from the cycle expansion, therefore locating the smallest root with a higher accuracy.

Adding the term $(z-z_p)^s$ to the cycle expansion can be done by determining the slope of the points in Fig. 5 and assuming the form

$$c_n=Ae^{\alpha n} \tag{45}$$

for the curvatures beyond a certain N, that is,

$$\zeta^{-1}(\zeta,\beta)=1-\sum_{1\le n<N}c_nz^n-\frac{c_Nz^N}{1-e^\alpha z}\ , \tag{46}$$

indicating that the pole is at $z_p=e^{-\alpha}$. Assuming this we can again repeat the calculation for the free energy as a function of the truncation of the new cycle expansion of ζ_p^{-1}. The results are in Fig. 6, where we have kept the line that indicates the limit obtained for the cycle expansion without the resummation of the tail terms. The points are now closer to the previously estimated limit, and also to the limit one obtains from the Levin U extrapolation of the new sequence.

In general the quality of the results obtained are a function of the number of terms kept in the cycle expansion and upon assuming the correct form for the behavior of the points of nonanalyticity. We have been assuming that there is one nearby point of nonanalyticity that determines the radius of convergence and that it is well isolated from the other points of nonanalyticity that may exist. The radius of convergence has been assumed to be determined by the existence of a pole, as is the case for exponentially decaying interactions (see Ruelle [1]).

The lack of oscillations in the sign of the curvatures c_n

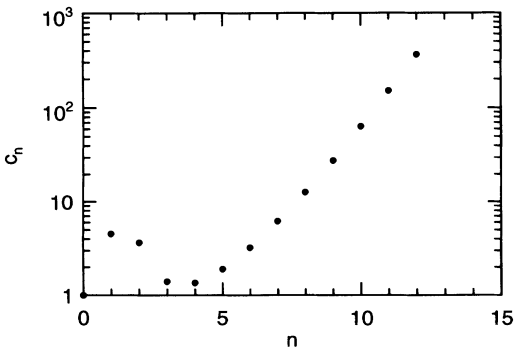

FIG. 5. Logarithm of the curvatures of the ζ function.

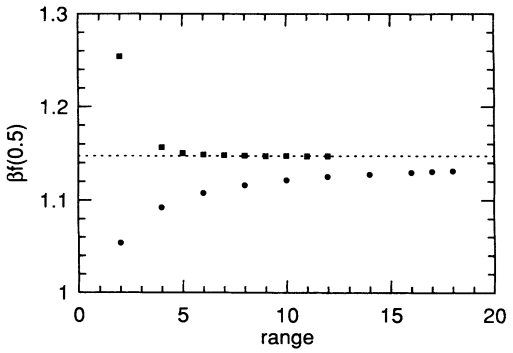

FIG. 6. Free energy obtained as the number of cycles increases, but now with tail resummation. Squares are the ζ-function calculation and circles the transfer matrix.

is an indication that only one singularity is relevant in the region of z and β considered. The form of the nonanalyticity is difficult to determine numerically, even if we assume it to be a pole. To obtain the order of the pole requires many terms of the series to be determined.

At first we may expect that the essential singularity that exists in the inverse-square model (see Anderson and Yuval [22]) manifests itself in the cycle expansion. But the essential singularity is of the free energy when expanded as a function of the inverse temperature β, and not of the parameter z.

In determining the derivatives of the cycle expansion, we will simpify the resummation by observing that there is a simple dependence on the resummed coefficient and the (inverse) temperature β, the term e^{α} in Eq. (46). The plot in Fig. 7 is the value of e^{α} for different temperatures, and from the plot we can see that the term can be assumed to be varying linearly with β. We will assume that the resummation can be expressed by a term of the form

$$\frac{c_N z^N}{1-(A+B\beta)z} \tag{47}$$

and use it in the cycle expansion.

E. Determination of β_c

Up to this point we have assumed that the calculations were performed at temperatures above the phase-transition point, but no method has been given for determining the phase-transition point. The phase transition occurs at the point where the largest eigenvalue becomes degenerate, so we shall look for this point numerically.

Once we perform the tail resummation for the ζ function the smallest root is simple. As the temperature is lowered the second smallest root approaches the smallest and at the critical point they fuse into a single double root. Both of the roots are within the radius of convergence of the ζ function and are therefore part of the spectrum of the transfer operator, or better, approximations to the two smallest eigenvalues of the Ruelle-Araki operator (see Ruelle [27]). In Fig. 8 we have plotted the ζ function at a temperature above the phase transition and at the point where the two smallest roots meet.

By using a root-finding method to locate the point when the two smallest roots are equal (or the first derivative equal to zero, but this is more expensive in computer time) the phase-transition point can be determined to be $\beta_c = 1.1803$, with the last digit being numerically correct within the procedure adopted. If the same calculation is repeated, but now keeping only cycles up to period 10, the result is 1.1816. The value of β_c is within the value estimated by Anderson and Yuval of $\beta = c\,1.23 \pm 0.06$.

To estimate the error in the critical temperature we notice that at $\beta = 1.17$ the tail resummation technique breaks down as one of the tail coefficients changes sign. We will then conservatively estimate the error to be the difference between the occurrence of the sign change and the double root, that is, $\beta_c = 1.18 \pm 0.01$. This number is higher than previous numerical estimates (see Bhattacharjee [28]), but within the uncertainty of the renormalization-group estimate of Anderson and Yuval [22].

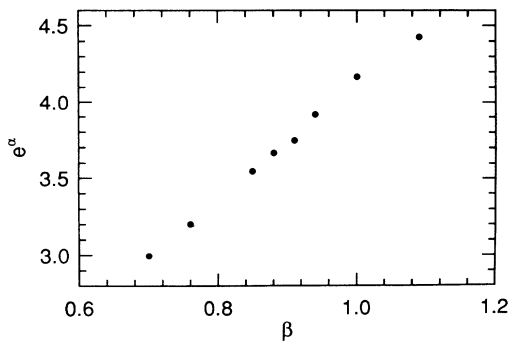

FIG. 7. Growth of factor e^{α} as a function of the inverse temperature β.

F. Factorization of the cycle expansion

There is a phase transition in this model that is a reflection of the spin-flip symmetry of the Hamiltonian.

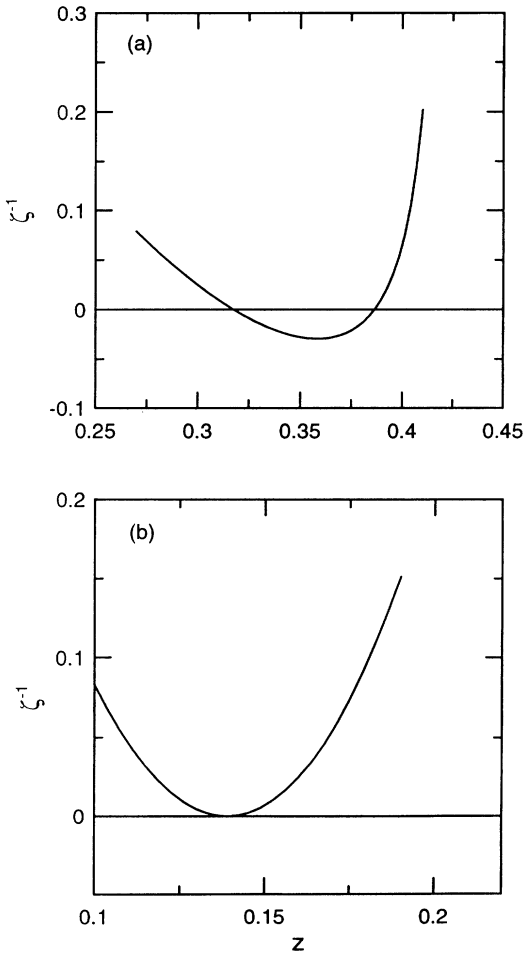

FIG. 8. (a) Plot of the cycle expansion with tail resummation for β equal to 0.5. (b) The cycle expansion, but now for β_c. Notice that the scales are not the same in both plots.

For low temperatures both phases coexist for the choice of periodic boundary conditions, which leads to a double root in the cycle expansion, degrading the quality of the numerical calculations for low temperatures. To eliminate this problem, we will factorize the ζ function so as to eliminate the spin-flip symmetry. This can be done by noticing that there are two types of configurations with respect to the value of the Boltzmann factor: the self-dual configurations that remain unchanged under spin flip, and those that do not. Those that are not self-dual contribute two identical factors to the product form of the cycle expansion, and those that are self-dual have an even number of spin sites and can be factored into the product of two terms.

The factorization then corresponds to keeping only one of the two terms that are not self-dual, and the "square root" of the self-dual configurations. That is, in the factorized cycle expansion substitute

$$\begin{aligned}&(1-z^{|\sigma|}t_\sigma)^2\to(1-z^{|\sigma|}t_\sigma)\ ,\\&(1-z^{|\sigma|}t_\sigma)\to(1-z^{|\sigma|/2}t_\sigma^{1/2})\ ,\end{aligned}\tag{48}$$

where in the last case the configuration σ is self dual. When the phase transition is a reflection of a symmetry of the system, this procedure can be justified by directly block diagonalizing the transfer matrix, see Mainieri [13] and Cvitanović and Eckhardt [30].

The factorized cycle expansion can again be resummed, and the results further improved, although the factorized cycle expansion without the resummation has an accuracy in the large-β regime comparable to the resummed cycle expansion in the small-β regime. The reason for this is that the cycle expansion for small β has a double root as the smallest zero that gets split when the expansion is resummed. In the case of the factored cycle expansion one does no have a double root, but the monotonic growth of the coefficients takes longer to set in. Any calculation in this model must trade the accuracy of the tail resummation for the gain in accuracy due to factorization.

In Fig. 9 we have plotted the free energy for the system using both methods: nonfactorized for small β and factorized for large β, and the smoothness of the plot is an indication of the consistency of the results. The arrow in the plot indicates the point where the methods were switched. It is also the phase-transition point and the point where the curves from the two methods cross.

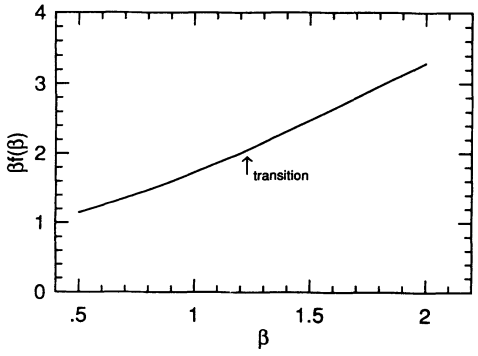

FIG. 9. Free energy obtained above and below the critical point. The curve is smooth in spite of the fact that two different methods were used above and below the critical point.

G. Derivatives of the free energy

Given that we can estimate the free energy accurately, we can now proceed to determine the other thermodynamic quantities. These can be obtained from the derivatives of the cycle expansion. For example, let us say we want to develop an expansion for the derivative of the free energy, the energy u

$$u(\beta)=-\frac{d(\beta f)}{d\beta}\ .\tag{49}$$

We have to determine the derivative of the free energy, which in turn is computed from the smallest root of the cycle expansion $z_0(\beta)$,

$$u(\beta)=-\frac{1}{z_0(\beta)}\frac{dz_0}{d\beta}\ .\tag{50}$$

As we do not have an explicit expression for the smallest root, the derivative must be determined implicitly in terms of the defining equation $\zeta^{-1}=0$. The derivative of z_0 as a function of β is computed from the total derivative with respect to β of the equation $\zeta^{-1}=0$ from which we get that

$$\frac{dz_0}{d\beta}=-\frac{\partial_\beta\zeta^{-1}}{\partial_z\zeta^{-1}}\ .\tag{51}$$

The derivatives are evaluated at a given β and for z equal to the smallest root at that temperature. Given the derivative we can compute the energy u.

To determine the heat capacity $c(\beta)$ at inverse temperature β we need the second derivative of the free energy, as

$$c(\beta)=\beta^2\frac{d^2p}{d\beta^2}=\beta^2\left[-\frac{1}{z_0^2}\left[\frac{dz_0}{d\beta}\right]^2+\frac{1}{z_0}\frac{d^2z_0}{d\beta^2}\right]\ .\tag{52}$$

To evaluate this second derivative we need the first and second derivatives of the smallest root. Again by implicit differentiation we get that

$$\frac{d^2z_0}{d\beta^2}=\frac{-\partial_{\beta\beta}\zeta^{-1}(\partial_z\zeta^{-1})^2+2\partial_\beta\zeta^{-1}\partial_{z\beta}\zeta^{-1}-(\partial_\beta\zeta^{-1})^2\partial_{zz}\zeta^{-1}}{(\partial_z\zeta^{-1})^3}\ .\tag{53}$$

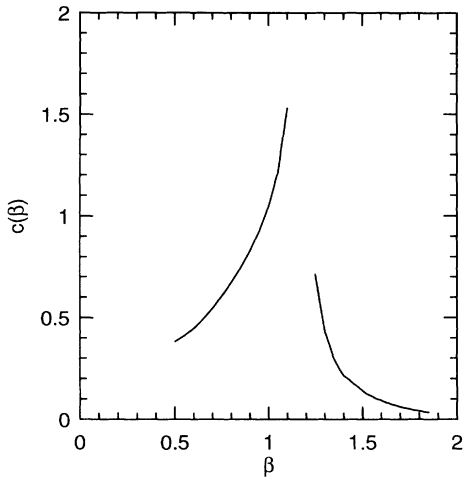

FIG. 10. Heat capacity curve obtained from the ζ function. The curve is continuous and the missing part corresponds to the region where the tail resummation fails.

We only need to compute derivatives in z and β of the cycle expansion and evaluate the resulting series at the root for a given β. These new series can again be resummed just as we did for the cycle expansion.

The results of these calculations are indicated in the plot in Fig. 10. Notice that the plot of the heat capacity is not symmetric, as was the plot obtained from Monte Carlo calculations for the same model [28]. The plot for the heat capacity actually goes to higher values as we approach the phase-transition point, but those points represent variation in β that are smaller than the ± 0.01 error in the transition point.

H. Other potentials

The methods described in the previous section are not limited to the inverse-square interaction, and can be applied to any translation-invariant interaction. This would include other types of power-law interactions, mixtures of long- and short-range interactions, and modulated interactions. In many of these cases there may be no explicit formulas to obtain the interaction energy of one site with the rest of the infinite configuration, but as the form of the potential is known it is simple to develop efficient numerical schemes to extrapolate partial sums with machine precision accuracy. (This can be done by summing the series using the Euler-Maclaurin summation formula.)

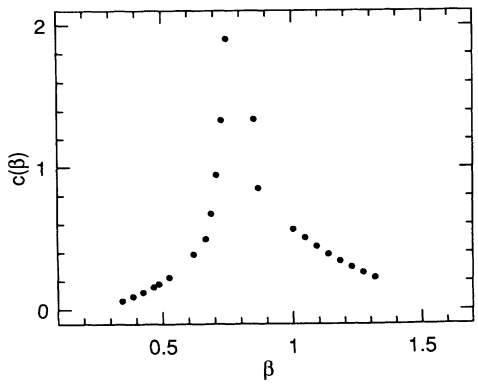

FIG. 11. Heat capacity as a function of the inverse temperature β for the $x^{-7/4}$ interaction.

TABLE IV. The critical inverse temperatures for the Ising model with power-law interaction of the form x^s, with s the exponent. The error on all values is of ± 0.01.

Exponent	β_c
$\frac{3}{2}$	0.46
$\frac{7}{4}$	0.775
$\frac{15}{8}$	0.95
2	1.18

As a form of example, in Fig. 11 we have plotted the heat capacity curve for the interaction $x^{-7/4}$. The methods for obtaining the curve are identical to those used in the inverse-square case. Also as an example we have listed in Table IV the critical points for several different interactions that are known to have phase transitions.

IV. CONCLUSION

ζ-function methods converge faster than transfer-matrix methods when dealing with long-range potentials, and as fast as transfer matrices when dealing with short-range potentials. In both case ζ functions are a better numerical scheme, as they require a fixed amount of computer memory, the bottleneck of transfer-matrix calculations, and the same amount of computer time. The improvement comes from *not* neglecting the interactions beyond a certain range.

The ζ-function method had not been used previously to compute thermodynamic quantities when there was more than one phase present. It has been remarked that ζ functions can only be used in the "hyperbolic phase" [9]. But, as we saw in Sec. III F, with the factorization of the ζ function it is possible to compute thermodynamic averages, even if there is a phase transition in the system. A consequence of factorizing the ζ function to deal with the states at low temperatures is that the transition point can be accurately computed by matching the behavior at low and high temperatures. In this way the critical points for the long-range Ising models were determined with higher accuracy than had been previously done, and the results show that the transition point is at higher temperatures than previous numerical estimates.

Given that ζ functions can successfully deal with phase transitions, one is now in a position to apply them to the problem that motivated this work: dynamical systems with marginal stability points. This is the case for mode locking or for Hamiltonian systems [31–34]. The problem there is that the marginal stability points give rise to thermodynamics with phase transitions and it becomes difficult to apply the usual techniques of $f(\alpha)$ curves [35], and previous methods [9] using ζ functions presuppose that the phase transition is of first order.

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