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Lee–Yang zeros in the scaling region of a two-dimensional quasiperiodic Ising model

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Abstract. Quasiperiodic, planar Ising models with ferromagnetic nearest-neighbour interactions should show the same universal critical behaviour as the classical Ising model on the square lattice. We use the eightfold symmetric Ammann–Beenker tiling to investigate this and employ the distribution of the Lee–Yang and the temperature zeros of the partition function in the complex plane. Our results support, as expected, the existence of an Onsager-type phase transition, i.e. a second-order transition with critical exponents $\alpha = 0$, $\beta = \frac{1}{8}$ and $\delta = 15$.

1. Introduction

The Ising model is among the best understood models of statistical mechanics. Nevertheless, despite Onsager's spectacular solution of the field-free Ising model on the two-dimensional (2D) square lattice, exact solutions on other graphs are very rare and, especially if they are aperiodic, restricted to very special cases, see [4, 12] and references therein. Consequently, one needs other methods for an approach to the critical behaviour of the Ising model on quasiperiodic tilings. One such technique can be developed from what was proposed in 1952 by Lee and Yang [17, 22]. They investigated the zeros of the partition function in the complex field variable or fugacity of the system. Later, also the zeros in the temperature variable were studied by Fisher [11], which is why these zeros are sometimes also called Fisher zeros. Both, the field and the temperature zeros, provide valuable information not only about the phase diagram of the system but also about its characteristic critical behaviour, see [13] for an overview.

The temperature zeros have been studied extensively for the Potts model on hierarchical graphs [10, 14, 15]. The main reason was that, for these models, they can be calculated exactly and show an interesting feature: their distribution forms fractal patterns known as Julia sets, whereas in the periodic case they are expected to lie on simple curves (or at least to fill simple regions). For one-dimensional (1D) quasiperiodic structures, however, self-similar distributions of the magnetic field zeros can be observed. Due to the Lee–Yang circle theorem they still lie on the unit circle, but only fill a fractal subset of it in the quasiperiodic case [6, 19]. A similar phenomenon is well known for the spectra of quasiperiodic Hamiltonians [5] and theoretically understood by means of the gap-labelling theorem for quasiperiodic Hamilton operators [9]. As we will see, this theoretically quite interesting property of 1D quasiperiodic Ising models is usually not present in two dimensions.

The subject of this contribution is the phase transition of 2D quasiperiodic Ising models, which, from the physical point of view, is certainly much more interesting. We show that the location and the properties of the Lee–Yang zeros contain important information that enables us to confirm the scaling picture for a quasiperiodic Ising model and to provide an independent method for the determination of the critical exponents of its phase transition. It will turn out that the critical behaviour of this model cannot be distinguished from that of a periodic one, as expected from [18].

Since the use of partition function zeros and their distribution might look slightly unusual for this task, let us add some remarks in favour of it. First, it is a straightforward method to extract a rather complete picture in one go, namely nature and position of the phase transition as well as critical exponents. Secondly, the actual numerical estimates are not as bad as one might expect, although we admit that for each single quantity better methods exist (some of which will be mentioned). Finally, for the rather specific case of quasicrystals of high symmetry, the combination with the corner transfer matrix technique enables the calculation of partition sums for sufficiently large patches.

Let us also add that the following discussion is meant to illustrate this concept and to convince the reader of its usefulness. All calculations and results shown were obtained with an average modern workstation—we did not hunt for the maximum accuracy possible.

2. The partition function

Let us consider an Ising model on a finite graph with classical spins $\sigma_i = \pm 1$ on each site $i = 1, \ldots, N$. Restricting ourselves to nearest-neighbour interactions with equal strength J and homogeneous magnetic field H, the partition function simply reads:

$$Z_N = \sum_{\sigma_1,\ldots,\sigma_N=\pm 1} \exp\bigg(-\beta J \sum_{\langle ij\rangle} (\sigma_i\sigma_j - 1) - \beta H \sum_i (\sigma_i - 1)\bigg) \qquad (1)$$

where $\langle ij\rangle$ indicates the summation over all nearest-neighbour pairs in the lattice. We use the formulation of the Ising model as a Potts-2 model for convenience. An important observation is that this partition function is essentially a polynomial in the two variables $z = \exp(2\beta J)$ and $w = \exp(2\beta H)$, where we follow Itzykson [14] with this slightly unusual definition. This convention (where the ferromagnetic regime is $0 < \mathrm{Re}(z) < 1$) turns out to be more suitable numerically for non-vanishing magnetic fields, where the zero pattern is no longer invariant under $z \to 1/z$. The analytic structure of the partition function is completely determined by the distribution of its zeros. As proposed by Lee and Yang, their investigation in the complex plane provides an approximative approach to quite general, even quasiperiodic, Ising models. The work to be done essentially splits into two parts: first one has to exactly calculate the partition function for sufficiently large patches and, as the second step, the critical behaviour in the thermodynamic limit has to be extrapolated from their complex zeros.

As a generic example of a 2D Ising model, we have chosen the Ammann–Beenker tiling [3], with spins on the vertices interacting with each other via the edges of the tiling. One reason for this choice was that it has only one kind of edges, which suggests taking equal couplings for all bonds. This means that the quasiperiodic tiling simply defines the pairs of indices $\langle ij\rangle$ which appear as neighbours in the summation for the partition function in equation (1). The second and much more important reason for this choice was that its octagonal symmetry allows an efficient application of corner transfer matrices (CTMs) [8]. In this tiling, one can find arbitrarily large patches with perfect octagonal symmetry like in figure 1. This can easily be proved using the substitution rule in figure 2, but it also follows directly from the standard projection method for this tiling, see [7] for details. The general definition of CTMs is slightly technical [8], but the idea itself is very simple.

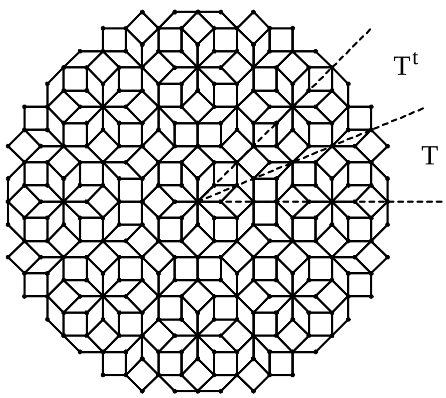

Figure 1. Octagonal patch of the Ammann–Beenker tiling and its decomposition into 16 sectors. Each one corresponds to a corner transfer matrix $\mathbf{T}$ or $\mathbf{T}^t$.

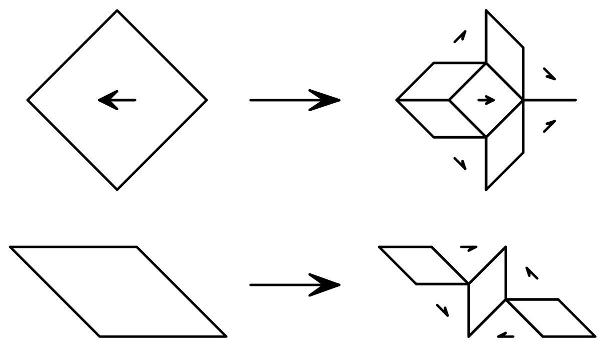

Figure 2. Inflation rule for the Ammann–Beenker tiling.

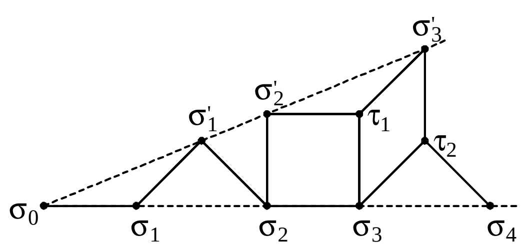

Figure 3. A small sector defining a $2^4 \times 2^3$ corner transfer matrix $\mathbf{T}_{\sigma_0}$.

As an example, let us consider the small sector in figure 3. We can define a $2^4 \times 2^3$ matrix $\mathbf{T}_{\sigma_0}(\sigma_1, \sigma_2, \sigma_3, \sigma_4|\sigma_1', \sigma_2', \sigma_3')$ as the CTM of this sector. Its entries are the partition functions one obtains by summation over the interior spins τ_i for fixed values of the spins on the edges of the sector. Its indices depend on the values of these spins. The transposition $\mathbf{T}^t_{\sigma_0}$ of this rectangular matrix is equivalent to a sector with opposite direction. The multiplication of two CTMs simply corresponds to the combination of the two sectors and the summation of the new interior spins,

$$\mathbf{T}_{\sigma_0}\mathbf{T}^t_{\sigma_0}(\sigma_1, \sigma_2, \sigma_3, \sigma_4|\sigma_1', \sigma_2', \sigma_3', \sigma_4') = \sum_{\tau_1', \tau_2', \tau_3' = \pm 1} \mathbf{T}_{\sigma_0}(\sigma_1, \sigma_2, \sigma_3, \sigma_4|\tau_1', \tau_2', \tau_3') \times \mathbf{T}^t_{\sigma_0}(\tau_1', \tau_2', \tau_3'|\sigma_1', \sigma_2', \sigma_3', \sigma_4'). \quad (2)$$

Note that, for equation (2) to be correct, one has to give half weights to all bonds and magnetic fields on the edges of the sector. Doing this, equation (2) yields the CTM of the new larger sector.

Up to now, we have kept the centre spin σ_0 fixed. To obtain the full partition function one finally has to sum over its values. For an octagonal patch of the Ammann–Beenker tiling, it is simply given through the trace of the power of the CTM $\mathbf{T}$ for a single sector,

$$Z(z, w) = \sum_{\sigma_0 = \pm 1} \mathrm{tr}((\mathbf{T}_{\sigma_0} \mathbf{T}^t_{\sigma_0})^8). \tag{3}$$

This structure of the partition function allows the exact calculation of it, as a polynomial in z and w, for rather large patches. The major problem one encounters is that its coefficients get very large, roughly about 10^{50} for the largest patch with 249 spins we investigated, and the analysis of its zeros is quite sensitive to numerical errors. Practically, the large arbitrary precision numbers needed for the computation are the main factor increasing the computational time and so limiting the size of the patch we could handle numerically on a normal workstation.

3. Uniqueness and location of the critical point

As mentioned above, the partition function Z is a polynomial in two variables, the temperature z and magnetic field w. So, there are two complementary viewpoints. One is to keep the temperature fixed and look at the complex plane of the magnetic field variable. Let us begin with the other point of view, that of the zeros in the complex temperature plane z for fixed w. Although, in general, there is no simple theorem for the location of the zeros in this variable, for regular lattices there are empirically observed regularities. The zeros tend to accumulate to smooth arcs or at least their distribution in the vicinity of the critical point may be approximated by distributions on such curves. As, for a finite system, the partition function is a polynomial with all coefficients positive, the zeros cannot fall onto the real axis. But because of their connection to the free energy $F = -\frac{1}{\beta} \ln Z$, one encounters a phase transition where these zeros pinch the positive real axis in the thermodynamic limit.

The first and simplest application of this picture yields the existence and position of a phase transition point. In figure 4, the zeros of Z in the temperature plane (in zero magnetic field, i.e. $w = 1$) are shown for free and fixed boundary conditions (in the latter case, all outer spins of our octagonal patch were fixed to the same value, $+1$ say). Note that the zero pattern for free boundary conditions is invariant under $z \to 1/z$ (because the graph is bipartite), but the pattern for fixed boundary conditions is not. The distribution of the temperature zeros supports this picture of a unique phase transition (which is actually a critical point, see below) for our quasiperiodic model. In table 1, the values of the zeros closest to the ferromagnetic ($\mathrm{Re}(z) < 1$) critical point for patches with different sizes and boundary conditions are shown. Unfortunately, these numerical values depend significantly on the size and boundary conditions, but they still predict, in the ferromagnetic region, a unique critical point z^* in the range of $0.40 < z^* < 0.46$. To expand on this, a local circle fit for case (d) of table 1 gives $z^* \simeq 0.42(1)$ and $z^* \simeq 0.44(3)$ for free and fixed boundary conditions, respectively. A finite-size extrapolation from cases (a)–(d) then predicts the location to be $z^* \simeq 0.43(2)$. Although less accurate, this estimate is in good agreement with the value 0.434(8) extracted from [16] which was obtained by extensive Monte Carlo simulations.

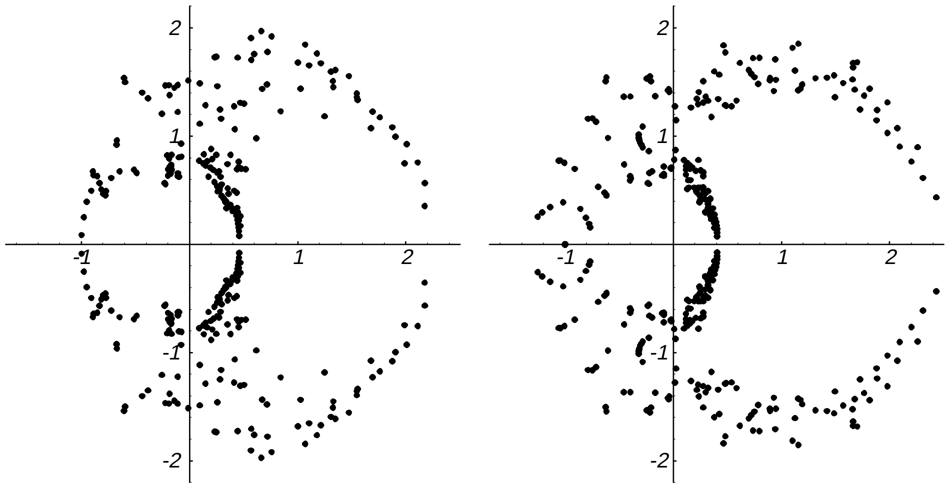

Figure 4. Zeros of the partition function Z in the temperature variable z, with fixed (left) and free (right) boundary conditions and vanishing magnetic field, for the patch with 249 spins.

Table 1. Partition function zeros located closest to the real axis, in the ferromagnetic region ($0 < \mathrm{Re}(z) < 1$), for vanishing magnetic field.

	N	Free boundary	Fixed boundary
(a)	73	$0.3602 \pm 0.1465\mathrm{i}$	$0.4935 \pm 0.1641\mathrm{i}$
(b)	121	$0.3785 \pm 0.1072\mathrm{i}$	$0.4714 \pm 0.1109\mathrm{i}$
(c)	185	$0.3941 \pm 0.0787\mathrm{i}$	$0.4639 \pm 0.0857\mathrm{i}$
(d)	249	$0.4048 \pm 0.0725\mathrm{i}$	$0.4592 \pm 0.0779\mathrm{i}$

4. Scaling behaviour near the critical point

More interesting than the location of the critical point are the universal scaling properties of our quasiperiodic model. There are two standard approaches in order to reproduce the scaling behaviour near the critical point. The first one uses the renormalization group properties of the model, see [14] for details. We have chosen the other one here, which relates the critical exponents directly with the distribution of zeros [1, 2], for details of this approach and complete results for the Ising model on the Ammann–Beenker tiling see [20]. In what follows, we will show that the Lee–Yang picture of the phase transition of our quasiperiodic Ising model is compatible with that of the Onsager universality class, as is to be expected from [18].

Let us start with the distribution of zeros in the complex temperature plane for the vanishing magnetic field. From the assumption that these zeros, at least near the critical point, lie on a simple curve, one can represent the singularity of the specific heat in terms of a Cauchy integral which also allows for a treatment by residue calculus. If φ is the slope of this curve near the critical point and α is the specific heat critical exponent, one finds [2, 20]

$$\tan[(2-\alpha)\varphi] = \frac{\cos(\pi\alpha) - A_-/A_+}{\sin(\pi\alpha)} \tag{4}$$

where $A_\pm$ are the amplitudes of the singularity of the specific heat. For the critical exponent

$\alpha = 0$ of the Onsager universality class this predicts: $A_+ = A_-$ and $\varphi = 90^\circ$. This is in good agreement with the observed distribution of zeros in figure 4, for a more detailed discussion and a magnified view, we refer to [20]. An unbiased estimate of φ by means of fitting a tangent to the zeros near the real axis would actually give $\varphi = 90^\circ$ with an uncertainty of less than 2°.

Some more work has to be done to explain the motion of the temperature zeros in a magnetic field, but the result is quite simple. The position of the Lee–Yang edge singularity implies that the trajectories of the temperature zeros as a function of the magnetic field in the scaling region enclose an angle of $\psi = \pi/2\beta\delta$ with the x-axis. In figure 5, the motion of the temperature zeros in a magnetic field is shown. The Onsager values $\beta = \frac{1}{8}$ and $\delta = 15$ imply an angle of precisely $\psi = 48^\circ$ and it shows up clearly in the trajectories of the zeros near the critical point. Here, precision is even better than before, and a least squares fit would result in $\psi = 48^\circ$ with an uncertainty of significantly less than 1°.

The phase transition and its scaling behaviour also appear in the properties of the distribution of the magnetic field zeros. The rather general Lee–Yang circle theorem states that these zeros lie on the unit circle in the complex plane (this is always true in the thermodynamic limit but also for finite patches with free boundary conditions). Figure 6 shows these zeros for different temperatures z. For our 2D model, the distribution of the magnetic field zeros is remarkably regular. This is in contrast to 1D quasiperiodic Ising models where one observes a fractal distribution of the magnetic field zeros, as mentioned in the introduction. The only gap remaining is the physically important Lee–Yang gap in the distribution of the magnetic field zeros near $w = 1$ corresponding to zero magnetic field. Below the critical point, the magnetization of a ferromagnetic Ising model, which is continuous at high temperatures, becomes discontinuous at $H = 0$. This implies that the Lee–Yang gap in the distribution of the zeros for large z closes at the critical point.

The details of the magnetic field zeros also contain some information about the critical exponent δ. At the critical point, their distribution must reproduce the magnetization $m \sim H^{1/\delta}$. Again, expressing the magnetization as a Cauchy integral on the unit circle in the complex magnetic field variable, in order to reproduce this magnetization, the density of zeros has to be proportional to $\varphi^{1/\delta}$, where $\varphi = \ln(w)$ is the angle of w on the unit circle. Labelling the zeros consecutively with respect to this angle, this distribution yields

$$\varphi_j \propto j^{\delta/(\delta+1)} \Rightarrow j^{-\delta/(\delta+1)}\varphi_j = \text{constant} \qquad \text{for } T = T_c. \tag{5}$$

In figure 7(a), the values of the first nine zeros are plotted as a function of the temperature z. In figure 7(b), these zeros have been rescaled according to equation (5), with the Onsager value $\delta = 15$. As expected for an Onsager phase transition, the curves have a common intersection at the critical point $z \simeq 0.43$. Admittedly, as the rescaling value $\delta/(\delta + 1)$ depends just weekly on δ, this does not allow for an independent calculation of δ, but it is an important consistency check and shows that the scaling properties of our quasiperiodic model cannot be distinguished from the periodic case.

5. Conclusions

The partition function zeros for the Ising model on the Ammann–Beenker tiling do not lie on simple curves in the complex temperature plane. But the unique ferromagnetic phase transition of our quasiperiodic model clearly shows up where these zeros pinch the real axis, in agreement with detailed Monte Carlo simulations, compare with [16] and appendix B of [20] for details. The qualitative behaviour, for a closely related model, can be substantiated by a renormalization group approach [20, 21] which further supports Luck's conjectures.

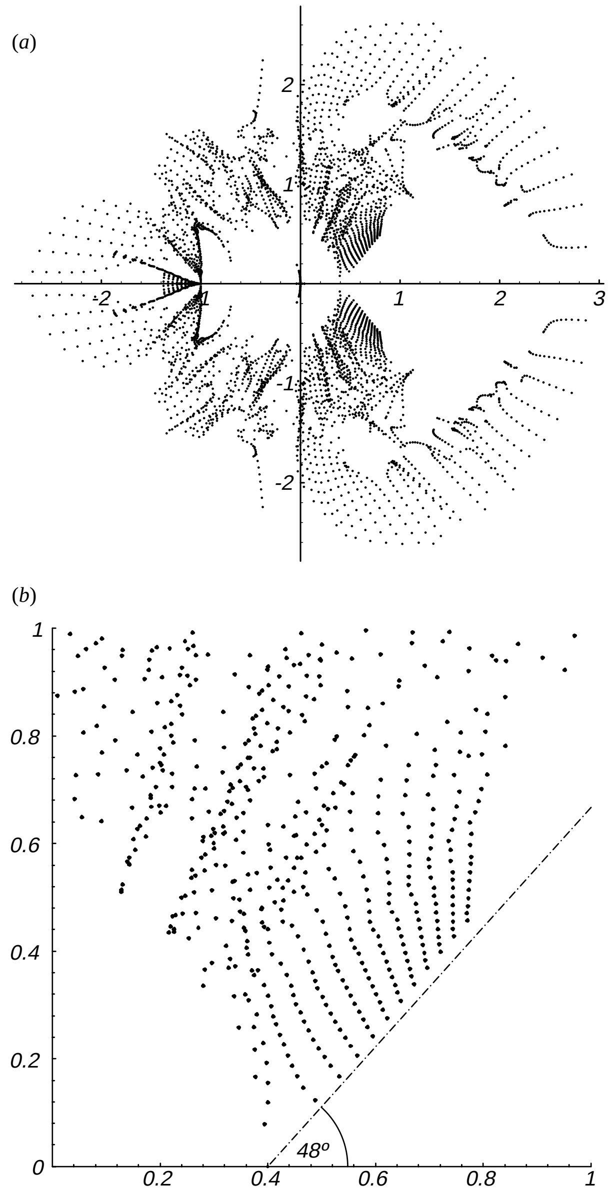

Figure 5. (*a*) Motion of the temperature (z) zeros in a magnetic field. H runs from 0 to 1.5 by equal steps. (*b*) An enlargement of the ferromagnetic region.

In contrast to the 1D quasiperiodic Ising model, we did not observe any apparent gap structure for the magnetic field zeros, except the physically important Lee–Yang gap. By means of the corner transfer matrix technique it was possible to investigate the scaling of the Lee–Yang zeros. The properties of the temperature as well as the magnetic field zeros in the scaling region of the ferromagnetic phase transition turned out to be in fair agreement with the critical exponents of the Onsager universality class. Our results presented here, together with those of the renormalization approach mentioned above, therefore support the

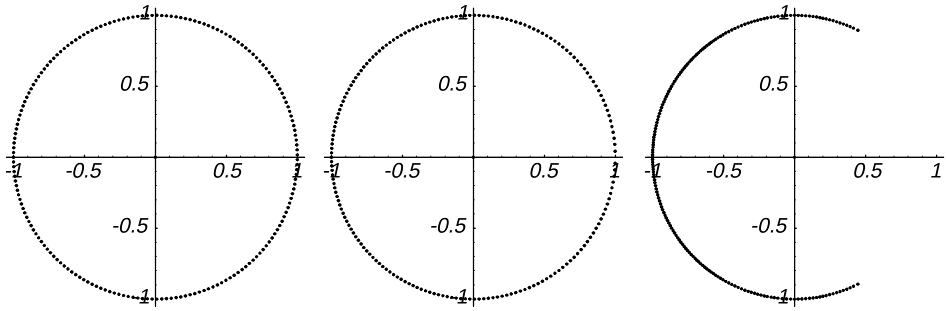

Figure 6. Distribution of the magnetic field (w) zeros for different temperatures (z), from the left: above, at and below the critical point.

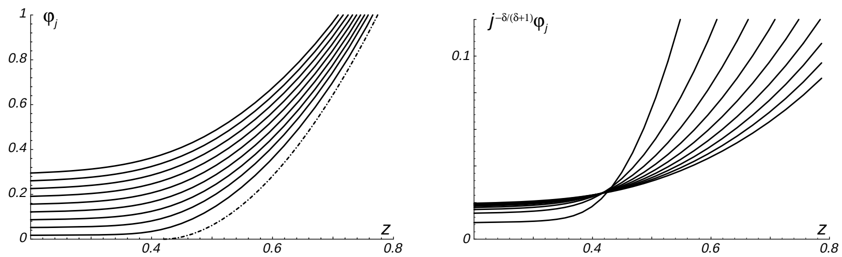

Figure 7. (a) The phases $\varphi = \arg(w)$ of the first nine zeros as a function of the temperature (z). The chain curve indicates the expected behaviour of the Lee–Yang gap $\theta_c \propto (z - z^*)^{\beta\delta}$. ($b$) The scaling of these zeros for the Onsager value $\delta = 15$. Rescaled by $j^{-\delta/(\delta+1)}$, the curves have a common intersection at the critical point $z^* \simeq 0.43$.

common belief (compare with [18] for details) that the universal critical behaviour of a 2D quasiperiodic Ising model cannot be distinguished from that of the periodic case.

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