Lee-Yang Zeros of Periodic and Quasiperiodic Anisotropic XY Chains in a Transverse Field

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The partition function zeros of the anisotropic XY chain in a complex transverse field are studied analytically and numerically. It is found that the partition function zeros of the periodic and quasiperiodic quantum Ising chain lie on the circle at zero temperature and the radius equal to the values of the critical field. For the periodic and quasiperiodic anisotropic XY chains, the closed curves are split to two or three closed curves as the anisotropic parameter γ decreases at a given ratio of two kinds of exchange interactions. For the isotropic XX case, the partition function zeros lie on the straight segments which are parallel to the real axis and the segments move towards the real axis as the temperature goes to zero.

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In 1952, Yang and Lee [1] proposed the famous method to analyze the equilibrium phase transition by studying the partition function zeros (PFZs) in the complex fugacity plane in the thermodynamical limit. Lee and Yang [2] proved the circle theorem, which states that the PFZs of an Ising ferromagnet lie on a unit circle in the complex fugacity plane. Afterward, the method of PFZs has been extensively applied to the Potts model [3,4], the 1D Blume-Capel model [5], continue systems [6], the ferromagnetic Ising model on the quasiperiodic systems [7] and the Sierpinski gasket [8], the antiferromagnetic Ising model [9], first-order phase transition [10], nonequilibrium phase transitions [11,12], self-organized criticality [13], and the Urn model [14]. The thermodynamical phase transitions of quantum systems, for example, the Heisenberg spin chain [15], the Hubbard model [16], and an ideal Bose gas in an external magnetic field [17], etc., are studied by the same method.

Recently, there has been a great deal of interest in studying the quantum phase transitions (QPTs) [18]. Different from the thermodynamical phase transition, the QPTs are associated with the changes of the ground state. Therefore, how to extend the method of PFZs to study the QPT is an interesting problem. Zou and Wang [19] studied the PFZs of the uniform quantum Ising and anisotropic XY chains in a transverse field and found that the zeros lie on the circles and ellipses in the complex field plane. The zero at the positive real axis corresponds to the QPT point of the system at zero temperature. However, to our knowledge, a detailed study of QPTs by using the method of PFZs is still lacking.

On the other hand, experimental work on quasicrystals [20] and quasiperiodic superlattices [21] has inspired theoretical interest in quasiperiodic systems. Recently, the QPTs of quasiperiodic spin chains were studied extensively using transfer matrix, renormalization-group, and numerical methods [22,23]. It is found that there is only one QPT point in quasiperiodic and random quantum Ising chains in a transverse field. Their critical behavior can be classified by invoking a relative criterion suggested by Luck [23]. We studied the QPTs of periodic and quasiperiodic anisotropic XY chains in a transverse field and found that there is more than one QPT point on some parameter regions for periodic and quasiperiodic chains, and the number of phase transition points is dependent on the parameters and the structure of systems, which is quite different from those of the quantum Ising chain in a transverse field and the anisotropic XY chain without transverse field [24]. In this Letter, we study the distributions of the PFZs of periodic and quasiperiodic anisotropic XY chains in a *complex* transverse field and their relationship with the QPTs.

The Hamiltonian of the general anisotropic XY model in a transverse field is given by

$$H = -\frac{1}{2}\sum_{i=1}^{N}\left\{\frac{\lambda_i}{2}[(1+\gamma)\sigma_i^x\sigma_{i+1}^x + (1-\gamma)\sigma_i^y\sigma_{i+1}^y] + h\sigma_i^z\right\}. \quad (1)$$

Here λ_i is the nearest neighbor interaction, σ_i^α the αth Pauli matrix ($\alpha = x$, y, or z) on site i, N the number of sites, γ the degree of anisotropy, and h a transverse field. The quantum Ising chain in a transverse field and anisotropic XY chain correspond to $\gamma = 1$ and $h = 0$, respectively. If λ_i depends on the position i, the system is a nonuniform chain. In our discussion, the λ_i takes two values according to periodic and quasiperiodic sequences.

By use of the famous Jordan-Wigner transformation [25], the Hamiltonian can be written as

$$H = \sum_{i,j=1}^{N}\left[c_i^\dagger A_{ij}c_j + \frac{1}{2}(c_i^\dagger B_{ij}c_j^\dagger + \text{H.c.})\right], \quad (2)$$

where c_i and $c_i^\dagger$ are the anticommuting fermion operators. $A_{ij} = -\frac{1}{2}\lambda_i\delta_{j,i+1} - \frac{1}{2}\lambda_j\delta_{j,i-1} - h\delta_{ij}$, $B_{ij} = -\frac{1}{2}\lambda_i\gamma\delta_{j,i+1} + \frac{1}{2}\lambda_j\gamma\delta_{j,i-1}$; $A_{1N} = -\frac{1}{2}\lambda_N = A_{N1}$, $B_{1N} = \frac{1}{2}\lambda_N\gamma = -B_{N1}$. The quadratic Hamiltonian equation (2) can be diagonalized by Bogoliubov transformation,

$$\eta_k = \frac{1}{2}\sum_{i=1}^{N}[(\phi_{ki}+\psi_{ki})c_i + (\phi_{ki}-\psi_{ki})c_i^\dagger],$$
$$\eta_k^\dagger = \frac{1}{2}\sum_{i=1}^{N}[(\phi_{ki}+\psi_{ki})c_i^\dagger + (\phi_{ki}-\psi_{ki})c_i], \tag{3}$$

which yields $H = \sum_k \Lambda_k(\eta_k^\dagger \eta_k - \frac{1}{2})$. The eigenequation of excitation energy Λ_k is

$$\Lambda^2\psi_{k,i} = \tfrac{1}{4}(1-\gamma^2)\lambda_{i-1}\lambda_{i-2}\psi_{k,i-2} + \lambda_{i-1}h\psi_{k,i-1} + \tfrac{1}{4}[(1+\gamma)^2\lambda_{i-1}^2 + 4h^2 + (1-\gamma)^2\lambda_i^2]\psi_{k,i} + \lambda_i h\psi_{k,i+1} + \tfrac{1}{4}(1-\gamma^2)\lambda_i\lambda_{i+1}\psi_{k,i+2}. \tag{4}$$

Therefore, the partition function of the system is

$$Z = \mathrm{Tr}(e^{-\beta H}) = \prod_k \sum_{n_k} e^{-\beta\Lambda_k(n_k-1/2)} = \prod_k (e^{-\beta\Lambda_k}+1)e^{\beta\Lambda_k/2}, \tag{5}$$

where $n_k = \eta_k^\dagger\eta_k = 0, 1$ and $\beta = 1/k_BT$. The partition function zeros correspond to

$$\Lambda_k = i(2n+1)\pi k_BT \equiv it, \tag{6}$$

where n is an integer and t is an effective temperature.

Periodic and quasiperiodic quantum Ising chains.—In this case, $\gamma = 1$. The λ_i takes two values based on periodic or quasiperiodic sequences. First, we discuss the period case. For simplicity, we consider a period-two case, i.e. $\lambda_{2i} = \lambda$ and $\lambda_{2i+1} = \alpha\lambda$. We shall take $\lambda = 1$ without loss of generality. By assuming that $\psi_{2n} = Ae^{i2nk}$ and $\psi_{2n+1} = Be^{i(2n+1)k}$, we can obtain Λ_k analytically, which yields

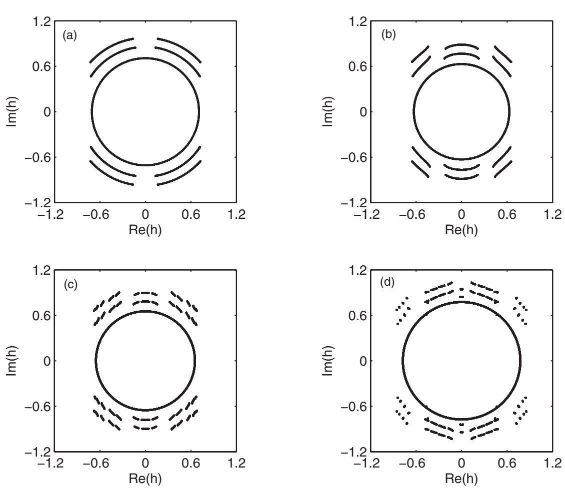

FIG. 1. The PFZs of four kinds of periodic and quasiperiodic quantum Ising chain in the complex h plane at effective temperature $t = 0$, 0.2, and 0.4 (from inside to outside), respectively. (a) Period-two, (b) period-three, (c) Fibonacci, and (d) general Fibonacci chains. $\alpha = 0.5$ and $N = 300$.

$$\Lambda_{k\pm}^2 = \tfrac{1}{2}[2h^2 + 1 + \alpha^2 \pm \sqrt{(1-\alpha^2)^2 + 4h^2(1+\alpha^2+2\alpha\cos(2k))}], \tag{7}$$

where $k = \frac{2\pi m}{N}$ ($m = -\frac{N}{2}+1, \ldots, \frac{N}{2}$) and N is the number of cells in the chain. The QPT point is determined by Λ_{k-}. Therefore, the PFZs in a complex field plane are

$$h^2 = \alpha\cos(2k) - t^2 \pm \sqrt{\alpha^2(\cos^2(2k)-1) - (1+\alpha^2+2\alpha\cos(2k))t^2}. \tag{8}$$

It is easy to check that the PFZs lie on a circle with radius equal to $\sqrt[4]{\alpha^2 + (1+\alpha^2)t^2 + t^4}$. In Fig. 1(a), we give the numerical results of PFZs of the period-two quantum Ising model in a complex h plane at zero temperature and two finite temperatures. It can be seen that the PFZs lie on the four arcs in a circle at finite temperature. At $T = 0$, the PFZs lie uniformly on a circle of radius $\alpha^{1/2}$. The circle cuts the positive real axis at the QPT point $h_c = \alpha^{1/2}$.

For the period-three case, $\lambda_{3i} = 1$ and $\lambda_{3i+1} = \lambda_{3i+2} = \alpha$. The numerical results of PFZs in the complex h plane at zero temperature and two finite temperatures are shown in Fig. 1(b). Generally, at finite temperature, the PFZs do not lie on a circle. But, at $T = 0$, the PFZs lie uniformly on the circle with radius $\alpha^{2/3}$.

For the quasiperiodic and aperiodic chains, it is well known [23] that the system has only one QPT point at $h_c^N = \prod_{i=1}^N \lambda_i$, where N is the length of the chain. The QPT of the aperiodic chain belongs to the universality class of a uniform quantum Ising chain and of a random quantum Ising chain for $\omega < 0$ and >0, respectively. $\omega = \ln|l_2|/\ln l_1$ ($l_{1,2}$ are the leading and next-to-leading eigenvalues of the substitute matrix) describes the fluctuations in the coupling.

As typical examples, we study the two-component Fibonacci and general Fibonacci chains. For the general Fibonacci chain, the λ_i takes two values $\lambda_A = \alpha$ and $\lambda_B = 1$ arranged in a general Fibonacci sequence. The general Fibonacci sequence S_∞ is constructed recursively as $S_{l+1} = \{S_l^n, S_{l-1}^m\}$, with $S_0 = \lambda_B$ and $S_1 = \lambda_A$. $n = m = 1$ corresponds to the usual Fibonacci sequence. Figures 1(c) and 1(d) plot the PFZs of the Fibonacci ($\omega = -1$) and general Fibonacci ($m = 3$, $n = 1$, $\omega \approx 0.3171$) chains at zero temperature and two finite temperatures. They are similar to those of the periodic cases. Although the QPTs of two quasiperiodic chains belong to two different universality classes, the distributions of PFZs at zero temperature are the same. It can be found that the PFZs lie uniformly on the circles of radius $(\prod_{i=1}^N \lambda_i)^{1/N}$ for all nonuniform quantum Ising chains at zero temperature.

Periodic and quasiperiodic anisotropic XY chains.—Different from the quantum Ising chain, the number of QPT points of the periodic and quasiperiodic anisotropic XY chains is more than one at some regions of parameter

[24]. This is due to the competition of periodicity and anisotropy. For example, a period-two chain corresponding to $\lambda_{2i} = 1$ and $\lambda_{2i+1} = \alpha$ has two quantum phase transitions for $\gamma < \gamma_c = \frac{1-\alpha}{1+\alpha}$. The quantum phase transition points are

$$h_c = \begin{cases} \frac{1}{2}\sqrt{(1+\alpha)^2 - (1-\alpha)^2\gamma^2} & \text{for } 0 < \alpha, \gamma < 1 \\ \frac{1}{2}\sqrt{(1-\alpha)^2 - (1+\alpha)^2\gamma^2} & \text{for } \gamma < \frac{1-\alpha}{1+\alpha}. \end{cases} \tag{9}$$

For the period-three chain, we take $\lambda_{3i} = 1$ and $\lambda_{3i+1} = \lambda_{3i+2} = \alpha$ as an example. The QPT points have been obtained numerically, which show similar results with that of the period-two chain. For a given α, there is a critical $\gamma_c(\alpha)$. When $\gamma < \gamma_c$, the system has three QPT points and one QPT point otherwise. The properties of the different phases in the period-two and -three cases are discussed in Ref. [24].

For the period-two case, the spectrum of excitation can be obtained [24] analytically from Eq. (4) by the same method as that for periodic quantum Ising chain, which yields

$$\Lambda_{k\pm}^2 = \tfrac{1}{2}[A \pm \sqrt{A^2 - 4B}], \tag{10}$$

with $A = \frac{1}{2}[4h^2 + (1+\gamma^2)(1+\alpha^2) + 2(1-\gamma^2)\alpha\cos(2k)]$ and $B = \{[(1-\gamma^2)/2]\alpha\cos(2k) + h^2\}^2 + \{[(1-\gamma^2)/4]\alpha \times \cos(2k) + (h^2/2)\}(1+\gamma^2)(1+\alpha^2) + \frac{1}{16}[(1-\gamma)^2 + \alpha^2(1+\gamma)^2][(1+\gamma)^2 + \alpha^2(1-\gamma)^2] - (2\alpha\cos(2k) + 1 + \alpha^2)h^2$.

In Fig. 2, we give the numerical results of PFZs of period-two and -three chains in the complex transverse field at zero and a finite temperature. From Fig. 2, we can see that, for finite temperature, the PFZs form some segments of a curve. At zero temperature, they form closed curves. For the period-two case [see Figs. 2(a) and 2(b)], and a given α, when $\gamma > \gamma_c$, the PFZs lie in a closed curve, which is deformed from the circle at $\gamma = 1$. The closed curve cuts the positive real axis at the QPT point. As γ decreases, the zeros closing to the imaginary axis tend to the original point. At γ_c, the deformed closed curve is split to two closed curves. The right closed curve cuts the positive real axis at two points which correspond to the two QPT points. The period-three case is similar to the period-two case. At $\gamma = 1$, the PFZs lie on a closed curve. The curve is deformed as γ decreases, and at $\gamma = \gamma_c$ the deformed closed curve splits *simultaneously* into three closed curves. The three curves cut the positive real axis at the three QPT points obtained by the transfer matrix method [24].

For the quasiperiodic chain, we give the results of the two-component Fibonacci chain at a different periodic approximant. At a given α, it is found [24] that the number of QPTs increases from 1 to F_l (for the lth approximant of a Fibonacci chain, and F_l is the lth Fibonacci number) as γ decreases. Figure 3 shows the numerical results of the distributions of the PFZs of one approximant ($F_l = 8$) of the Fibonacci chain at zero temperature and four different γ. It is clear to see that for γ close to 1, the PFZs lie on a closed curve and this curve splits into three curves as γ decreases. As γ decreases further, the three closed curves split to form several more closed curves. At γ tends to 0, the PFZs lie on the F_l closed curves (see Fig. 4 for three approximants of Fibonacci at $\gamma = 0.02$).

Isotropic XX chain.—It is well known that the QPT in the *XX* chain (i.e. $\gamma = 0$) is in a different universality class from that in the anisotropic *XY* chain. For the uniform *XX* chain with $\lambda_i = 1$, the critical field h_c is in the interval $[0, 1]$. The critical behavior in this model is described by the *conformal field theory* of a free massless boson in 1 + 1 dimensions with *central charge* $c = 1$, whereas the critical behavior of the anisotropic *XY* chain is described by the conformal field theory of a free massless fermion in 1 + 1 dimensions with the central charge $c = \frac{1}{2}$.

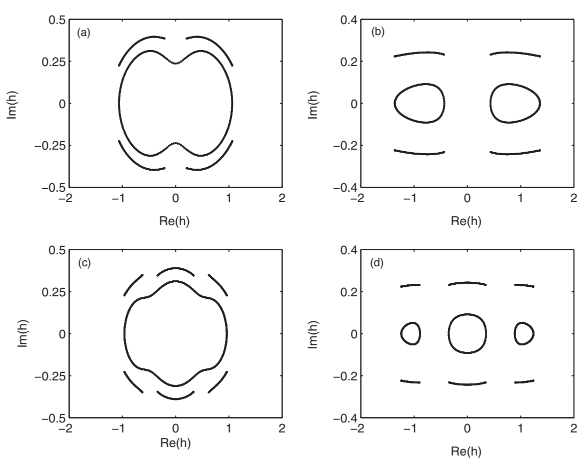

FIG. 2. The PFZs of the periodic anisotropic *XY* chain in the complex h plane at zero temperature and effective temperature $t = 0.05$ (from inside to outside). (a) Period-two, $\gamma = 0.4$. (b) Period-two, $\gamma = 0.1$. (c) Period-three, $\gamma = 0.4$. (d) Period-three, $\gamma = 0.1$. $\alpha = 0.5$ and $N = 300$.

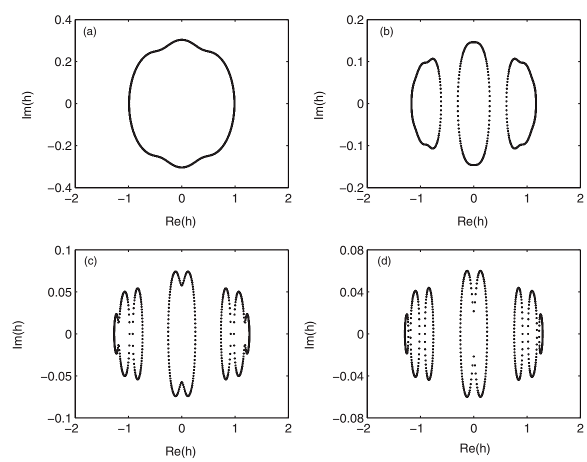

FIG. 3. The PFZs of the Fibonacci anisotropic *XY* chain in the complex h plane for $F_l = 8$ at zero temperature. (a) $\gamma = 0.4$, (b) $\gamma = 0.2$, (c) $\gamma = 0.11$, and (d) $\gamma = 0.09$. $\alpha = 0.5$ and $N = 300$.

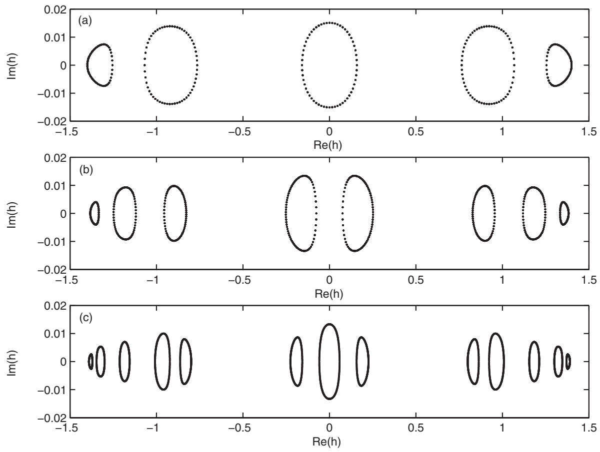

FIG. 4. The PFZs of the Fibonacci anisotropic XY chain in the complex h plane for $\gamma = 0.02$ at zero temperature. (a) $F_l = 5$, (b) $F_l = 8$, (c) $F_l = 13$. $\alpha = 0.5$ and $N = 300$.

For the uniform XX chain, the matrix $\mathbf{B}$ in Eq. (2) is zero and the Hamiltonian can be diagonalized easily, which yields $\Lambda_k = h + \cos(k)$, and the partition function zeros are

$$h = -\cos(k) + i(2n + 1)\pi k_B T, \tag{11}$$

which are parallel segments in the complex h plane. At zero temperature, the PFZs lie in the segment at the real axis from -1 to 1. For the periodic and quasiperiodic XX chains, the distributions of the PFZs in the complex h plane are similar. The distribution of the XX chain in a complex external field is quite different from those of the anisotropic XY chain.

In summary, the partition function zeros of the anisotropic XY chain in a complex transverse field are studied analytically and numerically. It is found that the PFZs of the periodic and quasiperiodic quantum Ising chain lie on the circle and the radius goes to the values of the critical field at zero temperature. For the periodic and quasiperiodic anisotropic XY chains, the closed curves are split into two or three closed curves as the anisotropic parameter γ decreases from 1 (quantum Ising case) to 0 (isotropic XX case) at a given ratio of two kinds of exchange interactions. This is due to the competition of the periodicity and anisotropy. At zero temperature, the closed curves cut the positive real axis at the QPT points. For the isotropic XX case, the situation is quite different. The partition function zeros lie on the parallel segments which are parallel to the real axis and the segments move to the real axis as the temperature goes to zero. Therefore, similar to the classic spin model, the analysis of PFZs in a complex field can provide a useful method to study the QPT of the general kind of solvable quantum spin models.

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