Detecting the Lee-Yang zeros of a high-spin system by the evolution of probe spin

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received 8 October 2018; accepted in final form 21 December 2018
published online 29 January 2019

PACS 05.30.-d – Quantum statistical mechanics
PACS 03.65.Yz – Decoherence; open systems; quantum statistical methods
PACS 02.20.Uw – Quantum groups

Abstract – Recently in the paper by Peng X. et al., Phys. Rev. Lett., 114 (2015) 010601, the experimental observation of the Lee-Yang zeros of an Ising-type spin-(1/2) bath, by measuring the coherence of a probe spin, was reported. We generalize this problem to the case of an arbitrary high-spin bath. Namely, we consider the evolution of a probe arbitrary spin which interacts with a bath composed by \( N \) arbitrary spins. As a result, the connection between the observed values of the probe spin, such as magnetization and susceptibility, and the Lee-Yang zeros is found. We apply these results to some models, namely, a triangle spin cluster, the Ising model with a long-range interaction and the 1D Ising model with nearest-neighbor interaction. Also we propose the implementation of these models on real physical systems.

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Introduction. – Lee, Yang and Fisher in their works [1–3] discovered a new way of studying the thermodynamics properties of different systems [4] which is based on an analysis of the partition function zeros. Zeros of the partition function define the analytic properties of free energy and thus are used as a tool for studying the nature of phase transitions. Lee and Yang considered the general ferromagnetic Ising model with Hamiltonian

\[
H_b = -\sum_{i,j} J_{ij} s_i^z s_j^z - h \sum_i s_i^z ,
\]

where \( s_i^z \) is the \( z \) component of the spin-(1/2) operator, \( J_{ij} \geq 0 \) are the interaction couplings and \( h \) is the value of the magnetic field. Note that instead of the Ising model the isotropic Heisenberg model with interaction \( -\sum_{i,j} J_{ij} s_i s_j \) or some other interactions that commute with the total spin of the system can be used. The partition function of system (1) at temperature \( T \) can be expressed as an \( N \)-th polynomial of \( z \equiv \exp(-\beta h) \) as

\[
Z(\beta, h) = \text{Tr}[e^{-\beta H_b}] = e^{\beta N_h} \sum_{n=0}^{2N_h} p_n z^n ,
\]

where \( p_n \) is the partition function with zero magnetic field under the constraint that the total spin of the system has a projection \( Ns - n \), \( \beta = 1/T \) is the inverse temperature and \( s \) is the value of each spin in the bath which equals 1/2. Here, the Boltzmann constant is taken as unity. For specific \( z \) this partition function becomes zero. These \( z \) are called Lee-Yang zeros [2] and we denote them as \( z_n \) with \( n = 1, 2, \ldots, 2N_s \). They are located in the complex plane which corresponds to complex parameters of the Hamiltonian. So, in [2] Lee and Yang proved the theorem that the zeros of partition function of the ferromagnetic Ising model are lying on the unit circle in the complex plane \( z \). Therefore, we can write \( z_n = e^{i\theta_n} \). Then, the partition function (2) can be expressed as follows:

\[
Z(\beta, h) = p_0 e^{\beta N_h} \prod_{n=1}^{2N_h} (z - z_n) .
\]

In later works this theorem was generalized to the ferromagnetic Ising model of an arbitrary high spin [5–7] and other types of interaction [8–11] including the ferromagnetic anisotropic Heisenberg model [12]. However, for others many-body systems, the Lee-Yang zeros are not always distributed along the unit circle. Also, it is worth noting that the Lee-Yang zeros can be generalized as zeros of a partition function with respect to other physical parameters. For instance, Fisher considered the zeros of a partition function with a complex temperature [3].
The zeros of a partition function of different many-body systems such as spin systems (see, for example, [13–19] and references therein), Bose (see, for example, [20–24] and Fermi (see, for example, [25,26]) systems are studied in many papers. The difficulty in the direct experimental observation of these zeros relates to the impossibility of preparing a many-body system with complex parameters. However, in articles [14,27] this problem was solved. The authors for the first time made an experimental research on the detection of the density function of zeros on the Lee-Yang circles. This study is based on the analysis of isothermal magnetization of the Ising ferromagnet FeCl₂ in an axial magnetic field. In papers [15,16] it was suggested to measure the Lee-Yang zeros in the time domain. The relation of the Lee-Yang zeros of the Ising ferromagnet with the decoherence of the probe spin was obtained. So, direct experimental observation of Lee-Yang zeros on trimethylphosphite molecule was reported in [13]. The methods of the detection of dynamical Lee-Yang zeros was considered in [28]. In [23] the possibility of experimental observation of Lee-Yang zeros of an interacting Bose gas was proposed. The relation between zeros of two-time correlation function of probe spin and zeros of a partition function of a spin bath was found in [19]. This relation gives a new possibility for the experimental detection of Lee-Yang zeros.

In the present paper we find the relation between the Lee-Yang zeros of the ferromagnetic high-spin bath and observed values, such as magnetization, susceptibility and higher derivatives of magnetization, of the probe spin. In the third section we present our results for some models, namely, triangle spin cluster, Ising model with long-range interaction and 1D Ising model with nearest-neighbor interaction. Also we propose the experimental implementation of these considerations on real physical systems. Conclusions are presented in the last section.

Connection between the Lee-Yang zeros and observation values of probe spin. — We consider the system of N spins s described by a general Ising model with ferromagnetic interaction under a magnetic field $\mathbf{h}$. The Hamiltonian of this system has the form (1), where the spin operators correspond to the spins $s$ and their projections on some direction take the values $-s \leq m \leq s$. Using the Lee-Yang theorem for the case of an arbitrary high-spin bath [5–7] the partition function of this system at temperature $T$ can be expressed as an 2sN-th polynomial of $z \equiv \exp (-\beta h)$ as (3).

Let us assume that the spin bath defined by Hamiltonian $H_b$ (1) is in thermodynamic equilibrium. Then we use a probe spin $s_0$ coupled to the bath. The general Hamiltonian of the system takes the form

$$H = H_b + H_p + H_i,$$  

where $H_p = -h_0 s_0^z$ is the Hamiltonian of the probe spin which interacts with the magnetic field of the value $h_0$, and $H_i = \lambda s_0^z \sum_i s_i^z$ describes the interaction between the bath and the probe spins with the coupling constant $\lambda$. It is worth noting that the results which we obtain for the Ising interaction between the spins of a bath are valid for the case of isotropic Heisenberg interaction between these spins.

The evolution of system (4) can be represented as follows:

$$\rho(t) = e^{-iH_t \rho(0)} e^{iH_t} = e^{-iH_p t} e^{-iH_i t} \rho(0) e^{iH_i t} e^{iH_p t},$$  

where the initial state has the form

$$\rho(0) = |\Psi(0)\rangle \langle \Psi(0)| e^{-\beta H_b} / Z(\beta, h).$$

Here $|\psi(0)\rangle = \sum_{m=-s_0}^{s_0} a_m |m\rangle$ is the initial state of the probe spin, with normalization condition $\sum_{m=-s_0}^{s_0} |a_m|^2 = 1$, which is determined by the complex parameters $a_m$ and is spanned by the basis vectors $|m\rangle$. The basis vectors are the eigenstates of the $z$-components of spin operator with value $m$. We use the system of units where the Planck constant is $h = 1$. To obtain (5) we use the fact that $H_p$, $H_b$, and $H_i$ mutually commute, which allows us to get rid of $-iH_p t$ part of the evolution operator. The evolution of the system due to the interaction between the probe and bath spins can be expressed as follows:

$$e^{-iH_i} \rho(0) e^{iH_i} = \sum_{m,k=-s_0}^{s_0} a_m a_k^* e^{-i\lambda(m-k)t} \sum_i s_i^z \times Z(\beta, h) |m\rangle \langle k|.$$  

So, using the above results the evolution of the system (4) takes the form

$$\rho(t) = \sum_{m,k=-s_0}^{s_0} a_m a_k^* e^{i(h_0(m-k)t - i\lambda(m-k)t)} \sum_i s_i^z \times Z(\beta, h) |m\rangle \langle k|.$$  

We consider the evolution of the probe spin by averaging expression (6) over the states of the remaining system,

$$\rho_p(t) = \sum_{m,k=-s_0}^{s_0} a_m a_k^* \times e^{i(h_0(m-k)t - i\lambda(m-k)t)} Z(\beta, h) |m\rangle \langle k|,$$  

where we use the fact that $\text{Tr} [e^{-i\lambda(m-k)t} \sum_i s_i^z H_b] = Z(\beta, h - i\lambda(m-k)t) / Z(\beta, h)$. This expression contains the partition functions of the bath system with a complex magnetic fields $h - i\lambda(m-k)t / \beta$ for different values of $m-k$. Each of these functions vanishes when the time of evolution $t$ is such that $\exp (-\beta h + i\lambda(m-k)t)$ equals Lee-Yang zeros.

So, we can observe the Lee-Yang zeros of the bath system by exploration of the evolution of the probe system.

Examining the evolution of the probe spin under the action of the bath we can observe the Lee-Yang zeros of

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this bath. For this purpose, we calculate the mean value of the operator \((s_0^z)^{m-k}\) as a function of time,

\[
((s_0^z)^{m-k}) = \text{Tr}[\rho_{p}(t)(s_0^z)^{m-k}]
\]

where \(s_0^z = s_0^x + is_0^y\) is the ladder operator. Using representation (3) and taking \(h = h_0 = 0\) we can rewrite this expression as follows:

\[
((s_0^z)^{m-k}) = e^{i\lambda(m-k)t} \frac{\prod_{n=1}^{2N_0} e^{-i\lambda(m-k)t} - e^{i\theta_n}}{\prod_{n=1}^{2N_0} (1 - e^{i\theta_n})} \times \sum_{l=-s_0}^{s_0} a_l a_{l+m-k} \times \prod_{q=1}^{m-k} \sqrt{s_0(s_0+1) - (l + q - 1)(l + q)}, \tag{8}
\]

As we can see, for the specific Lee-Yang zero \(z_n\) the following condition \(-\lambda(m-k)t_n = \theta_n\) is satisfied. The values of \(t_n = -\theta_n/\lambda(m-k)\) which correspond to zeros of the expression (9) are related to the Lee-Yang zeros of the partition function of the bath. Also we can see that the greater \(m - k\) is the faster this expression vanishes. Therefore, to detect the zeros of the partition function of the bath it is enough to measure the mean value (9) for a particular value of \(m - k\). It is easy to verify that a similar connection (9) exists in the case of isotropic Heisenberg interaction between the spins of the bath.

The measurement of the mean value of \((s_0^z)^{m-k}\) as a function of time allows us to observe a Lee-Yang zeros. So, if \(m-k = 1\), then to observe the Lee-Yang zeros the \(x\) and \(y\) components of magnetization should be measured. If \(m-k = 2\), then the components of the magnetic susceptibility should be measured for the observation of the Lee-Yang zeros. For larger values of \(m - k\) it is necessary to measure the higher derivatives of magnetization for this purpose. However, as we mentioned earlier, to observe the Lee-Yang zeros of the partition function of the bath it is enough to measure the mean value (9) with a particular value of \(m - k\). Therefore, further we will present our results for \(m-k = 1\) \(((s_0^z) = (s_0^x) + i(s_0^y)\). The experimental techniques for the measurement of magnetization as a function of time is described in the supplementary materials of the paper in ref. [13]. Let us study this problem in detail in the case of different models of the bath.

**Models of bath and their application.** In this section we apply our results to some models. Namely, we examine the connection between the Lee-Yang zeros of the spins bath with different structures and observation values of the probe spin. Also we suggest the physical realization of these considerations.

**Triangle spin cluster.** First of all, let us study the triangle spin cluster which consists of two spins \(s_1\) and \(s_2\) as the bath and one spin \(s_0\) as the probe spin (see fig. 1). The interaction between bath spins is ferromagnetic and is described by the Ising Hamiltonian. Also the interaction between the spin bath and the probe spin is defined by Ising Hamiltonian. The Hamiltonian of the complete system has the form

\[
H = -J s_1^x s_2^x + \lambda s_0^z (s_1^z + s_2^z). \tag{10}
\]

The connection between the Lee-Yang zeros of the bath and the observable values of the probe spin is determined by eq. (8) with \(h = h_0 = 0\). Here the partition function of the two-spin bath in the external magnetic field \(h\) has the following form:

\[
Z(\beta, h) = \sum_{m_1 = -s_1}^{s_1} \sum_{m_2 = -s_2}^{s_2} e^{\beta J m_1 m_2} e^{\beta h (m_1 + m_2)}, \tag{11}
\]

where \(s_1, s_2\) are the values of each spin of the bath and \(m_1, m_2\) their projection on the z-axis, respectively.

Let us consider the obtained results on a real physical system of manganese ferrite \((\text{MnFe}_2\text{O}_4)\) [29–31]. The manganese ferrite contains two ions of \(\text{Fe}^{3+}\) as a bath spin and one ion of \(\text{Mn}^{2+}\) as a probe spin. Each ion has spin \((5/2)\). The interaction between the spins has the exchange nature and described by isotropic Heisenberg model. The exchange integrals of this system are calculated in papers [32–34]. Similarly as in paper [13], the interaction between spins can be simulated by the Ising model (10).

Indeed, calculating the partition function at high temperatures (or small \(\beta\)) the Heisenberg model can be approximated by the Ising model. Figure 2 shows the Lee-Yang zeros of a two-spin bath composed of \(5/2\) spins and the mean value of the \(s_0^z\) operator of the probe spin-(5/2) for different temperatures. Here and further in the article we take the eigenstate of \(s_0^z\) with the highest eigenvalue as an initial state of the probe spin. This state can be easily prepared in the experiment. Due to the corresponding form
Fig. 2: Correspondence between the Lee-Yang zeros of the partition function (11) of the bath composed by two spin-(5/2) and the mean value of the $s_0^i$ operator (8) with $h = h_0 = 0$ of the probe spin-(5/2) as a function of time. The results are presented for different temperatures: (a) $T = \infty$, (b) $T = 32J$, (c) $T = 8J$ and (d) $T = J$.

of the initial state and the fact that $h = h_0 = 0$ we obtain that $\langle s_0^0 \rangle$ vanishes and $\langle s_0^+ \rangle = \langle s_0^- \rangle$. Therefore, in fig. 2 and in further cases we have the time dependence of the $\langle s_0^i \rangle$ operator. Also, it is worth noting that similar structure and properties have the following ferrites: ZnFe$_2$O$_4$, CoFe$_2$O$_4$, NiFe$_2$O$_4$, where Zn$^{2+}$, Co$^{2+}$, Ni$^{2+}$ play the role of the probe spins, respectively.

**Ising model with long-range interaction.** In this subsection we consider the bath with long-range Ising-type interaction. We assume that the interaction couplings between each pair of spins are the same and equal to $J_{ij} = J/N$. Then the partition function takes the form (2), where

$$ p_n = e^{\frac{\beta J}{N}(Ns-n)^2} \times \frac{1}{2\pi} \int_0^{2\pi} e^{-i\phi(Ns-n)} \left( \sum_{m_1 = -s}^s e^{-m_1^2 \frac{2\beta J}{N}} \cos(m_1 \phi) \right)^N d\phi. $$

Here $m_1$ is the projection of the spin on the $z$-axis. So, for this case the mean value of the probe spin ladder operator is described by eq. (8) without external magnetic field, where the partition function (2) has $p_n$ defined by eq. (12). The effective spin system with long-range interaction can be easily prepared using trapped ions [35–37] or ultracold atoms [38–41].

We express the results of this subsection on the five-spin cluster (fig. 3), where the bath is composed of four spins $s$ which form a tetrahedron and interact between themselves due to ferromagnetic Ising-type interaction. The interaction with the probe spin $s_0$ is also described by the Ising model. Such a structure has the methane molecule with $^{13}$C. The molecule CH$_4$ consists of four atoms of $^1$H and one atom of $^{13}$C. Each of them has nuclear spin-(1/2).

Here $m_1$ is the projection of the spin on the $z$-axis.

Finally, let us consider the bath which consists of $N$ spins described by the 1D ferromagnetic Ising model with nearest-neighbor interaction $J$ and which has the form of a ring. The probe spin is placed in the center of this ring and interacts with each spin of the bath (see fig. 5). Then, in this case the partition function takes the form

$$ Z(\beta, h) = \sum_{m_1, m_2, \ldots, m_N = -s} e^{\beta J \sum_{i=1}^N m_i m_{i+1} + \beta h \sum_{i=1}^N m_i}, $$

where $m_i$ is the projection value of the $i$-th spin on the $z$-axis.
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Fig. 4: The connection between the Lee-Yang zeros of the partition function (2) with $p_n$ defined by eq. (12) and the mean value of the $s^x_n$ operator of the probe spin-(1/2) (8) with $h = h_0 = 0$ for the four-spin-(1/2) bath. The results are presented for different temperatures: (a) $T = \infty$, (b) $T = 8J$, (c) $T = J/2$ and (d) $T = J/16$.

Fig. 5: Ring consisting of ten spins $s_i$ (black circles) as the bath and the probe spin $s_0$ (gray circle). The interaction between the bath spins is described by the 1D ferromagnetic Ising model with nearest-neighbor interaction and the interaction of the probe spin with all the spins of the bath is defined by the Ising model.

Fig. 6: The connection between the Lee-Yang zeros of a ten-spins-1 Ising ferromagnet with the nearest-neighbor interaction and the mean value of the $s^x_0$ operator of the probe spin-(1/2) (8) with partition function (13). The results are presented for different temperatures: (a) $T = \infty$, (b) $T = 8J$, (c) $T = 2J$ and (d) $T = J/4$.

The effective spin ring with nearest-neighbor interaction can be prepared on trapped ions [35–37] or ultracold atoms [38–41]. In the paper in ref. [43] the method for simulation of the ground state of a spin ring with cavity-assisted neutral atoms was presented. Here we consider the example where the bath consists of ten spins 1 which interact with the probe spin-(1/2). The exact solution of the 1D Ising model for a spin-1 system can be obtained through the transfer matrix method (see, for example, [44]). The results for different temperatures are shown in fig. 6.

Conclusions. – We considered the evolution of the probe spin of an arbitrary value $s_0$ under the influence of a bath composed by $N$ arbitrary spins. The spin bath is defined by a general Ising model or isotropic Heisenberg model with a ferromagnetic interaction and at the initial moment of time it is in thermodynamic equilibrium. The interaction between the probe spin and each
spin of the bath is defined by the Ising model. We found the relation between the observed values of the probe spin and the partition function of the bath with complex magnetic field (8). We showed that vanishing of these values corresponds to the Lee-Yang zeros of the bath partition function. Thus, measuring the mean values of the probe spin as a function of time, such as magnetization or susceptibility, we can detect the Lee-Yang zeros of the bath. This fact allowed us to obtain the connection between the moments of time when the mean values of the probe spin vanish, and the Lee-Yang zeros of the bath.

We examined the connection between the measured values of the probe spin and the Lee-Yang zeros of the bath for some models. Namely, we considered the triangle spin cluster, where the bath consists of two spins s, and the third spin s0 is a probe. The interaction between all the spins was described by the Ising Hamiltonian (10). So, we obtained the correspondence between the magnetization of the probe spin and the Lee-Yang zeros of the bath in the case of s = s0 = 5/2 (fig. 2). We proposed to apply these results to the physical system of manganese ferrite (MnFe2O4), where the bath and probe spin consist of two ions of Fe3+ and ion of Mn2+, respectively. Also the obtained results can be applied to the following ferrites: ZnFe2O4, CoFe2O4, NiFe2O4, where the role of the probe spins play ions of Zn2+, Co2+, Ni2+, respectively. Finally, we studied the connection between the Lee-Yang zeros of the long-range Ising bath and 1D Ising bath with nearest-neighbor interaction, and mean values of probe spin, respectively. In the case of the long-range Ising model we considered the implementation of the obtained results on the nuclear spins of tetrahedron molecules such as CH4, SiH4, GeH4 and SnH4 (fig. 4). In the case of the 1D Ising bath the connection between the Lee-Yang zeros and the magnetization of the probe spin was obtained for a ten-spin ring bath prepared on trapped ions or ultracold atoms (fig. 6).

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The authors thank Dr. TARAS VERKHOLYAK and Prof. ANDRJU ROVENCZ for useful comments. This work was supported in part by Project FF-30F (No. 0116U001539) from the Ministry of Education and Science of Ukraine and by the State Fund for Fundamental Research under the project F76.

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