Yang-Lee and Fisher zeros generalized on some far-from-equilibrium systems.

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A generalization of the Yang-Lee and Fisher zeros on far-from-equilibrium systems coupled with two thermal baths is proposed. The Yang-Lee zeros were obtained for minimal models which exhibit complicated behavior in the context of the partition function zeros and provide an analytical treatment. This type of models may be considered as a simplest one and analogous to Ising model for equilibrium. The obtained distributions of generalized Yang-Lee zeros show nontrivial behavior for these simple models.

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More than five decades ago Yang and Lee proposed an approach to clarify how singularities of the thermodynamic functions appears within the canonical ensemble \(^{[1]}\). They considered liquid-gas transition and wrote down partition function in grand-canonical description as a polynomial with respect to fugacity. The main idea was an analysis of the fugacity in complex plane. Complex roots of this polynomial with respect to fugacity cross the real positive semi-axis in the singularity points in the thermodynamic limit and single out the points of the phase transition. Further, these roots in the complex fugacity plane are called Yang-Lee zeros. After Yang and Lee pioneer work many papers are devoted to this description of the phase transitions.

The approach of Yang-Lee zeros was used to describe spin system where complex fugacity in grand-canonical ensemble was replaced by the complex value of \(e^{-\beta h}\) with \(h\) as a magnetic field. It was shown that the density of the Yang-Lee zeros is in a close relation with the critical exponents describing the phase transition and may be used as a measure of the strength of the transition. Besides the Yang-Lee zeros so-called Fisher zeros were invented in complex temperature plane \(^{[2]}\). Their properties are more dependent on the particular system. For the historical details and useful references on Yang-Lee and Fisher zeros see review \(^{[3]}\). Here we describe only some general aspects.

It was shown by Binek \(^{[4]}\) et al. that the Yang-Lee zeros are not fully and only a theoretical concept. They proposed an experimental way to measure the Yang-Lee edge singularity exponents from the isothermal magnetization data in 2D Ising ferromagnet.

In summary, the partition function zeros are rather well investigated in case of the systems in equilibrium and provides us a clue in understanding of the phase transitions. One can measure some quantities which are directly related to the partition function zeros and get some experimental evidence. The question is how generalize an approach of Yang-Lee zeros to nonequilibrium systems and when such a possibility exists.

A standard approach to describe the behavior of the nonequilibrium system is to derive master equation and determine the rates of the processes in it. After a long time, the system may settle in a nonequilibrium steady-state. The exact meaning of the “long time” depends on the rates of processes in it. According to initial state and values of the parameters describing the system there may be different steady states and the transition from one of them into one another may be considered as an analogy to equilibrium phase transition. The one possibility to generalize the partition function approach is a consideration of the nonequilibrium models which allow the transfer matrix description. As it is proposed by Arndt \(^{[5]}\) some nonequilibrium models which are useful for the description of the driven diffusive systems, traffic flow, biological transport and other processes give us a possibility to invent the partition function and its zeros. In these models we can express the stationary probability distribution as a trace over some algebra elements, formulate the concept of partition zeros and show the direct relation between steady-state transition and the distribution of the partition function zeros. However, it is possible to derive the distribution of the Yang-Lee zeros without having the exact expression for the partition function. One can consider the zeros of a steady-state normalization factor in the complex plane of the transition rates \(^{[6]}\).

In this work one another possibility to generalize the the partition function zeros is proposed. Let us consider thermodynamics of two temperature systems with different time-scales and Hamiltonian \(H(\sigma, s)\) depending on fast variables \(\sigma\) coupled with thermal bath at temperature \(T_\sigma\) and slow variables \(s\) coupled with bath at temperature \(T_s\). The system may be considered as a minimal model having easily controlled nonequilibrium properties \(^{[7]}\). The one of the real examples may be NMR/ESR physics, where one of the baths is realized by weak dipole interactions and the second one is a lattice temperature \(^{[8]}\).

In such a system one can expect that after some long time system settles in a nonequilibrium steady-state with heat currents between the baths. This state is called steady adiabatic \(^{[9]}\). Although the stationary distribution is far from Gibbsian, one can derive the Gibbs like corresponding stationary distribution. As it is shown in \(^{[10]}\) this type of nonequilibrium systems has complicated and unusual behavior from equilibrium point of view. There may be
nonequilibrium phase transitions with no equilibrium counterpart. Also, it is possible for latent heat to be negative in presence of conflicting interactions \[10\]. We expect that the properly generalized partition function zeros may violate some usual equilibrium statements too.

According to \[10\] and taking into account a huge difference of rates between fast and slow variables one can write down the conditional probability

$$\begin{align*}
P(\sigma|s) &= \frac{1}{Z(s)} e^{-\beta H(\sigma,s)},
Z(s) &= \text{Tr} e^{-\beta H(\sigma,s)}.
\end{align*}$$

Here we assume that on the times relevant to \(\sigma\), \(s\) does not change and the conditional probability Eq. (1) is Gibbsian.

The next step is to derive \(P(s)\). This may be done by averaging the force \(\partial_s H(\sigma,s)\) acting on \(s\) over the distribution \(P(\sigma|s)\)

$$\begin{align*}
P(s) &= \frac{1}{Z} \int Z(s/s) \text{Tr} \{\sigma\} e^{-\beta H(\sigma,s)},
Z &= \text{Tr} \{\sigma\} e^{-\beta H(\sigma,s)}
\end{align*}$$

where \(F(s) = -T_s \ln Z(s)\) is the conditional free energy and the common probability is \(P(\sigma,s) = P(s)P(\sigma|s)\).

It is possible to obtain the steady state distribution by minimizing the free energy

$$\begin{align*}
F &= -T_s \ln Z.
\end{align*}$$

Eq. (3) shows the way to define the partition function zeros. It may be done like the equilibrium one, after replacing the equilibrium partition function by \(Z\) in common equilibrium description. As it is in equilibrium, one may suppose that there is a possibility of the far-from-equilibrium phase transition between steady states in thermodynamic limit \[10\], when the probability distribution is quasi-Gibbsian \[2\] (as it is for Gibbsian). The example of phase transition is demonstrated in \[10\]. However, this simple example is still mathematically rather complicated. The motivation of usefulness of the partition function zeros and their application for the indication of the phase transition points in case of the quasi-Gibbsian distribution is the same as it is in equilibrium. The main purpose of this work is not to solve complicated models demonstrating phase transitions and rather difficult for exact solution. Our aim is to investigate the properties of the partition function zeros for the models providing analytical solution and compare the results with equilibrium analogs.

Let us discuss the simplest models which may be treated analytically and define the partition function zeros on those examples. As such simple systems one can take the one-dimensional Ising model with nearest-neighbor interactions and couplings or magnetic fields as fast variables

$$\begin{align*}
H &= -\sum_{i=1}^{N} J_i s_i s_{i+1} - \sum_{i=1}^{N} h_i s_i.
\end{align*}$$

For the simplicity, let the couplings \(J_i\) are the fast variables and take values \(\pm 1\). In that case one may write down for \(Z(s)\) the following expression

$$\begin{align*}
Z(s) &= \text{Tr} \{J\} e^{-\frac{1}{T_J} H} = 2^N \prod_i \cosh\left(\frac{s_i s_{i+1}}{T_J}\right) e^{\frac{s_i s_{i+1}}{T_J}},
\end{align*}$$

where \(T_J\) is a temperature of the thermal bath coupled to fast variables. From Eq. (5) we get for \(Z\)

$$\begin{align*}
Z &= \text{Tr} \{s\} Z(s)\frac{T_J}{T_J} = \text{Tr} V^N,
\end{align*}$$

where the transfer-matrix

$$\begin{align*}
V &= \left[2 \cosh\left(\frac{s_i s_{i+1}}{T_J}\right)\right] \frac{T_J}{T_J} e^{\frac{s_i s_{i+1}}{2T_J}}
\end{align*}$$

is introduced. Here we assume the periodic boundary conditions and that the system consists of \(N\) spins. The transfer-matrix \(V\) is symmetric and one can write \(Z\) with respect to eigenvalues of \(V\), as it is done in equilibrium case for one-dimensional models

$$\begin{align*}
Z &= \lambda_1^N + \lambda_2^N.
\end{align*}$$

The condition \(Z = 0\) leads to

$$\begin{align*}
\lambda_2 &= \lambda_1 e^{i\varphi}, \varphi = \frac{(2k+1)\pi}{N}, k = 0, ..., N - 1.
\end{align*}$$
One of the examples of this procedure and its more detailed description in equilibrium case may be found in [11].

As a generalization of the equilibrium Yang-Lee zeros one can consider solution of Eq. (9) with respect to $\mu = e^{\frac{\varphi}{T_h}}$. However, the model with fast random couplings is too trivial. After taking into account symmetry of the function $\cosh$ and some simple algebra one gets the set of the Yang-Lee zeros as $\mu = \pm 1$. A similar set of values $\mu = (\pm i)^{Th/T_s}$ would be obtained if we generalize Yang-Lee zeros as $\mu = e^{\frac{i\varphi}{T_s}}$.

In case of fast magnetic fields $h_i = \pm \hbar$ the corresponding transfer-matrix is

$$V = \left[2 \cosh\left(\frac{h(s_i + s_{i+1})}{2T_h}\right)\right]^\frac{T_h}{Th} e^{\frac{s_is_{i+1}}{Th}}.$$

It is easy to obtain for the eigenvalues of Eq. (10) the following expression

$$\lambda_{1,2} = \left[2 \cosh\left(\frac{h}{T_h}\right)\right]^\frac{T_h}{Th} e^{\frac{h}{T_s}} \pm 2 e^{\frac{h}{T_s}} e^{-\frac{h}{T_s}}.$$

Here the natural and most simplest choice of the generalized Yang-Lee zeros is solution of Eq. (9) with respect to $\mu = e^{\frac{\varphi}{T_h}}$. For both $e^{\frac{\varphi}{T_h}}$ and $e^{-\frac{\varphi}{T_h}}$ the general assumption is a complex magnetic field and the corresponding temperature is chosen according to details of model. It is easy to obtain the second type of the Yang-Lee zeros if the first one is known and vice versa.

Denoting by $\mu = e^{\frac{\varphi}{T_h}}$ and $a = 2 e^{\frac{h}{T_s}} e^{-\frac{h}{T_s}}$ we obtain

$$\left[(\mu + \mu^{-1})\right]^\frac{T_h}{Th} e^{\frac{h}{T_s}} + a = \left[(\mu + \mu^{-1})\right]^\frac{T_h}{Th} e^{\frac{h}{T_s}} - a e^{i\varphi}.$$

Using condition on $\varphi$ one can derive a finite set of independent equations corresponding to all possible values of $\varphi$. These equations for generalized Yang-Lee zeros are transcendental in general. One can consider a simple choice of rational ratio $\frac{T_h}{T_s}$ or for more simplicity we assume it to be a natural number. It is possible for the natural ratio $\frac{T_h}{T_s}$ to solve the set of equations numerically for even a large numbers of $N \approx 10^5$. The obtained distribution may be considered as to be close to the thermodynamic limit. However, the fast magnetic fields model has an obvious analytical solution in thermodynamic limit. Near the thermodynamic limit one can treat $\varphi$ as a continuous parameter, running over the interval $(0, 2\pi)$ due to relation $N \to \infty$. One can derive from Eq. (12) the following relation

$$\left[(\mu + \mu^{-1})\right]^\frac{T_h}{Th} = 2 e^{\frac{h}{T_s}} - 2 e^{\frac{h}{T_s}} + 1.$$

As an example, if the ratio is $\frac{T_h}{T_s} = 2$ one gets two simple quadratic equations and the corresponding solutions are

$$\mu_{1,2,3,4} = \pm e \pm \sqrt{c^2 - 4}.$$

where $c = 2 e^{-\frac{h}{T_s}} \sqrt{\frac{e^{2\frac{h}{T_s}} + 1}{e^{2\frac{h}{T_s}} - 1}}$. The corresponding distribution is represented in Fig. 1. Four solutions of Eq. (13) form a complicated picture. This behavior is rather different from equilibrium one, when for a simple Ising-type model one gets partition function zeros lying on a unit circle. Also, it is easy to detect from Eq. (14) that for $\varphi \to 0$ the both four solutions are $\mu_{1,2,3,4} \to \infty$. In equilibrium case the usual condition on Yang-Lee edge singularity points is $\varphi = 0$ (see for examples [11, 12]). The second step one can do is to consider model with fast variables $\gamma_i = \pm \gamma$, slow variables $s_i = \pm 1$ and Hamiltonian as

$$H = - \sum_{i=1}^{N} \gamma_i s_i s_{i+1} - \sum_{i=1}^{N-1} \gamma_i s_i.$$

The corresponding transfer-matrix is

$$V = \left[2 \cosh\left(\frac{\gamma s_i s_{i+1}}{T_\gamma}\right) + \frac{\gamma (s_i + s_{i+1})}{T_\gamma} \right]^\frac{T_h}{T_\gamma}.$$

It is straightforward to define the generalized Yang-Lee zeros for this model, as partition function zeros with respect to $\mu = e^{\frac{i\varphi}{T_\gamma}}$. After writing down characteristic equation for transfer-matrix and obtaining the eigenvalues it is simple to get the Yang-Lee zeros due to Eq. (9). After some numerical calculation within Mathematica we obtained a highly
nontrivial distribution for such a simple model (see Fig. 2). The behavior of the zeros (Fig. 2) also violates the circle theorem.

In order to generalize the Fisher zeros one can introduce two types of the Fisher zeros according to two temperatures. In equilibrium limit, when the ratio $T_s/T_h$ is equal to one those two types of the Fisher zeros coincide. Simple algebra shows that the same pointless set we obtain for the Fisher zeros in case of fast couplings. For the model with fast magnetic fields one need to solve more complicated equations compared with those for Yang-Lee zeros.

Summarizing, the basic approach to generalize the partition function zeros for non-equilibrium systems coupled to two thermal baths is proposed. The described zeros show nontrivial behavior and need to more complete investigation. This approach of the generalized partition function zeros may be used to analyze phase transitions by numerical and analytical methods as it is done in equilibrium case. As author supposes, it is interesting to discuss the properties of nonequilibrium Yang-Lee and Fisher zeros in more details and for more complicated systems.

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