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The Application of the Yang–Lee Theory to Study a Phase Transition in a Non-Equilibrium System

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We study a phase transition in a non-equilibrium model first introduced in ref. 5, using the Yang–Lee description of equilibrium phase transitions in terms of both canonical and grand canonical partition function zeros. The model consists of two different classes of particles hopping in opposite directions on a ring. On the complex plane of the diffusion rate we find two regions of analyticity for the canonical partition function of this model which can be identified by two different phases. The exact expressions for both distribution of the canonical partition function zeros and their density are obtained in the thermodynamic limit. The fact that the model undergoes a second-order phase transition at the critical point is confirmed. We have also obtained the grand canonical partition function zeros of our model numerically. The similarities between the phase transition in this model and the Bose–Einstein condensation has also been studied.

KEY WORDS: Matrix Product Ansatz; Asymmetric Exclusion Process; Yang–Lee theory.

1. INTRODUCTION

One of the most important activities in the field of equilibrium statistical physics is the study of the phase transitions; nevertheless, there is a general framework for the statistical description of the equilibrium systems and also different approaches for studying their equilibrium phase transitions. One of these theories was proposed by Yang and Lee in 1952.[3] The Yang–Lee theory of equilibrium phase transitions is based on the zeros of the partition function. It is known that the zeros of the grand canonical partition function of finite systems $Z(z)$ (in which z is fugacity) are

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generally complex or negative if real. In the thermodynamic limit roots might move down (or up) and touch the positive real axis. When this happens, a phase transition occurs because the system can have different behaviors for $z < z_0$ and $z > z_0$, where z_0 is the value of the root on the real axis. For example the pressure $P = k_B T \lim_{V\to\infty}((1/V)\log Z)$ will be non-analytic and the density $\rho = (\partial/\partial \log z)(P/k_B T)$ will be discontinuous at the transition point which predict a first-order phase transition. Similarly, one can investigate the zeros of the canonical partition function as a function of complex-temperature and find the same transition points.[4] By calculating the line of zeros and also their density in the thermodynamic limit one can find the transition point and also the order of transition exactly.

Recently much attention has been focused on one-dimensional out of equilibrium systems because of their interesting properties such as first-order phase transitions and spontaneous symmetry breaking.[1,2] However, in contrast to the equilibrium systems many powerful concepts are missing in this context. For example, the applicability of the Yang–Lee theory to the non-equilibrium systems such as one-dimensional driven diffusive models is a quite non-trivial question and yet without answer. People have tried to apply the Yang–Lee theory to describe phase transitions in these models.[6,7] It seems that one can define similar quantities such as a grand canonical partition function and then apply this theory to the out of equilibrium systems without any problem. In this paper we will apply the Yang–Lee theory to an exactly solvable one-dimensional non-equilibrium model and investigate its phase transitions. This model has already been solved in our previous work and exact results are available.[5] Here we are going to compare our previous results with those obtained from application of the Yang–Lee theory; however, we should mention some of the differences between our work in this paper and what other people have done so far. In ref. 6 the author studies a particle-conserving driven diffusive model consists of two different classes of particles with finite densities[8] [2] and applies the Yang–Lee theory to it. He aimed to locate a phase transition induced by varying the density of particles. By introducing a grand canonical partition function as a function of a fugacity-like quantity a first-order phase transition is located by studying the numerically obtained zeros of this function. In another paper[7] the authors investigate the phase transitions in the asymmetric simple exclusion process (ASEP) with open boundaries[10,11] by studying the zeros of the partition function of the model. In their approach the boundary rates were generalized to the complex plane. They obtained the distribution of zeros near the transition point and also

[2] This model is known as AHR model in related literature.

their density near the real axis using the similarities with electrostatic theory. They could also calculate the line of zeros analytically.

The solvability of our model allows us calculate its canonical partition function exactly. This was done in our previous paper[(5)] and will be reviewed in the second section. Apart from numerical estimates for the zeros of the canonical partition function as a function of reaction rates, we have calculated the line of zeros and also their density (which determines the order of the phase transition) analytically using the equilibrium statistical physics toolbox. Having the exact analytical results we can discuss the possibility of phase transition and also obtain its order. Next we will define a grand canonical partition function and study its zeros in the complex-fugacity plane. The properties of this function reveal the similarities between the phase transition in our model and that of a Bose gas. In the last section we will summarize our results and generalize our approach to other non-equilibrium models.

2. THE MODEL

In ref. 5 we introduced a one-dimensional exclusion model consists of two different classes of particles (we call them positive and negative particles hereafter) which occupy the sites of a chain of length L with periodic boundary condition. Each site of the chain is either empty or occupied by a negative or by a positive particle. The positive (negative) particles hop to their immediate right (left) sites with unit rate provided that the target sites are empty. Adjacent particles with different charge type might exchange their positions with asymmetric rates 1 and q. Specifically, the interaction rules are

$$\begin{array}{llllll} + & 0 & \longrightarrow & 0 & + & \text{with the rate} \quad 1 \\ 0 & - & \longrightarrow & - & 0 & \text{with the rate} \quad 1 \\ + & - & \longrightarrow & - & + & \text{with the rate} \quad q \\ - & + & \longrightarrow & + & - & \text{with the rate} \quad 1. \end{array} \tag{1}$$

Assuming that there are M positive particles and only one negative particle on the chain[3] we showed that the steady state weights $P(\mathscr{C})$ of the model can be obtained exactly using a so-called Matrix Product formalism.[(11)] One can define the sum of these steady state weights as a quantity which

[3] In this case our model is a special case of AHR model[(8)] in which the number of the positive and negative particles on the ring are equal.

plays the role analogous to the canonical partition function in equilibrium statistical physics

$$Z = \sum_{\mathscr{C}} P(\mathscr{C}).$$

It turns out that Z has a closed form in terms of the transition rate q, the number of the positive particles M and the length of the chain L

$$Z_{L,M}(q) = \sum_{i=0}^{M} \frac{(q-3)(\frac{2}{q})^{i}+1}{q-2} C_{L-i-2}^{M-i} \tag{2}$$

in which $C_i^j = \frac{i!}{j!(i-j)!}$ is the binomial coefficient. In the thermodynamic limit

$$L, M \longrightarrow \infty \qquad \text{with} \quad \rho = \frac{M}{L} \quad \text{being fixed} \tag{3}$$

using the steepest decent method it can be shown that

$$\begin{aligned} &\text{for} \quad q < 2\rho \quad Z_{L,M}(q) \simeq \left(\frac{q-3}{q-2}\right) \frac{(\frac{2}{q})^{L-1}}{(\frac{2}{q}-1)^{L-M-1}} \\ &\text{for} \quad q > 2\rho \quad Z_{L,M}(q) \simeq (1-\rho)\left(1+\rho\,\frac{(q-2\rho)-(q-2)^2}{(q-2)(q-2\rho)}\right) C_L^M. \end{aligned} \tag{4}$$

The existence of two different phases is apparent. In the same reference we have shown that the density profile of the positive particles has an exponential behavior for $q < 2\rho$ with a correlation length $\xi = |\ln \frac{q_c}{q}|^{-1}$ which diverges as q approaches its critical value $q_c = 2\rho$, while it is an error function for $q > 2\rho$. This proves the existence of a second-order phase transition from a *power-law phase* to a *jammed phase*. Using the Matrix Product formalism one can also calculate the speed of the different species of particles on the ring in the thermodynamic limit. Both speeds are linearly increasing functions of q for $q \leqslant 2\rho$. However, for $q \geqslant 2\rho$ the speed of the positive particles is a constant equal to $1-\rho$ while the speed of the negative particle is a complicated increasing function of q. In the following section we will apply the Yang–Lee theory of equilibrium phase transitions to our model. As we will see, it will not only recover all the above mentioned results but also shed more light on the unknown aspects of our problem.

3. THE PARTITION FUNCTION ZEROS

Let us study the phase transition of the our model using the Yang–Lee theory. We consider the zeros of the canonical partition function of the

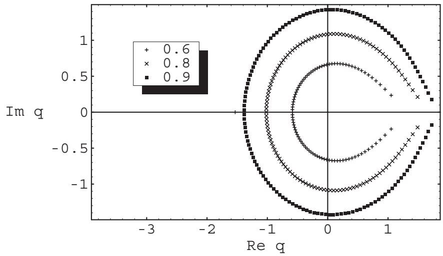

Fig. 1. The numerical estimates for the roots of $Z_{L,M}(q)$ in the complex-q plane for different values of density $\rho = 0.6, 0.8, 0.9$ and $L = 150$. It is seen that the roots accumulate to the positive real q axis at 1.2, 1.6, and 1.8 respectively.

model $Z_{L,M}(q)$ given by (2) in the complex-q plane at fixed L and M. In Fig. 1 we have plotted the numerical estimates of these zeros for a chain of length $L = 150$ and three different values of ρ. As can be seen the zeros accumulate slowly to the real q axis at a critical value $q_c = 2\rho$. As we will see later this accumulation takes place at an angle $\frac{\pi}{4}$ which is the reminiscent of a second-order phase transition.(4) In what follows we will try to find the line of the canonical partition function zeros and also their density near the positive real-q axis using the equilibrium statistical physics tools. We will see that the equilibrium-type calculations give the same results obtained from the numerical estimates.

It has been shown that the line of zeros can be obtained from(4)

$$\mathrm{Re}\, g_1 = \mathrm{Re}\, g_2. \tag{5}$$

In equilibrium statistical physics g is the extensive part of free energy and is generally a function of the temperature (here q) and the density of particles ρ. The indexes 1 and 2 show the values of the function g in the right and the left hand side of the critical point. Here we define this function as

$$g(q, \rho) = \lim_{L, M \to \infty} \frac{1}{L} \ln Z_{L,M}(q) \tag{6}$$

where $\lim \cdots$ is in fact the thermodynamic limit given by (3). Using the asymptotic behavior of $Z_{L,M}(q)$ given by (4) we can calculate $g(q, \rho)$ in each phase. After further calculations we obtain

$$\begin{aligned} &\text{for} \quad q < 2\rho \quad g(q, \rho) = \ln \frac{2}{q^{\rho}(2-q)^{1-\rho}} \\ &\text{for} \quad q > 2\rho \quad g(q, \rho) = \ln \frac{1}{\rho^{\rho}(1-\rho)^{1-\rho}}. \end{aligned} \tag{7}$$

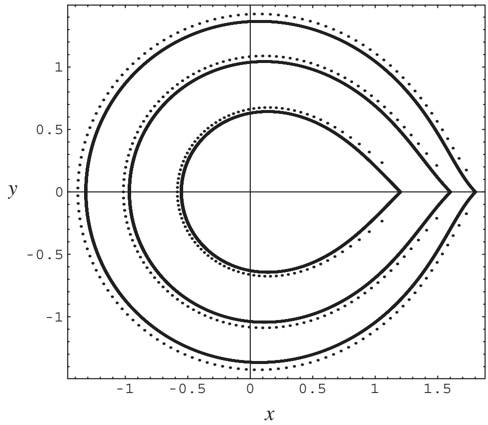

Fig. 2. Plot of the Eq. (8) (solid lines) for three values of density of the positive particles $\rho = 0.6$ (inner), $\rho = 0.8$ (center), and $\rho = 0.9$ (outer). They cross the positive x axis at $x = 2\rho$. The dotted lines belong to the numerical estimates of the canonical partition function zeros for the same values of densities and are taken from the Fig. 1.

By substituting (7) in (5) we find the following equation for the line of zeros in the complex-q plane

$$\left(\left(\frac{2-x}{1-\rho}\right)^2 + \left(\frac{y}{1-\rho}\right)^2\right)^{1-\rho} \left(\left(\frac{x}{\rho}\right)^2 + \left(\frac{y}{\rho}\right)^2\right)^{\rho} = 4. \tag{8}$$

in which $x \equiv \mathrm{Re}(q)$ and $y \equiv \mathrm{Im}(q)$. In Fig. 2 we have plotted both (8) and the numerical estimates of zeros given in the Fig. 1 for three values of ρ.

As can be seen the curves lie on the numerical estimates of the canonical partition function zeros. The small difference belongs to the fact that the numerical estimates have not been calculated in real thermodynamic limit. The curves also cross the positive x axis at $x_c = 2\rho$ which is the transition point as we had mentioned above. In the equilibrium Yang–Lee theory it is well known that the density of zeros on the real positive axis is zero at a second-order phase transition. In order to obtain the density of zeros μ in this region (on the positive real x axis and near the critical point) we use the following equation first introduced in ref. 4

$$2\pi\mu(s, \rho) = \frac{\partial}{\partial s} \mathrm{Im}(g_1 - g_2) \tag{9}$$

in which s is the arc length of the line of the zeros which is zero at the critical point and increases along with the line of zeros in the positive y direction. The values of g_1 and g_2 are given by (7). In order to calculate $\mu(s, \rho)$ first we find an equation for the line of zeros which is valid for small y's in the vicinity of the critical point $x_c = 2\rho$.

Using (8) it can be shown that this is actually a line

$$y = 2\rho - x \qquad \text{for} \quad |x - 2\rho| \ll 1, \quad 0 < y \ll 1. \tag{10}$$

The Eq. (10) confirms that the accumulation of zeros in the vicinity of the real-q axis takes place at angle $\frac{\pi}{4}$. Using (7), (9), and (10) we find for $\rho \neq 1$

$$2\pi\mu(y, \rho) = -\frac{\partial y}{\partial s}\frac{\partial}{\partial y} \operatorname{Im}\left(\ln \frac{2}{(x+iy)^{\rho}\,(2-x-iy)^{1-\rho}}\right) \propto \frac{y}{2\rho(1-\rho)}. \tag{11}$$

Therefore, as y approaches to zero the density of zeros becomes zero as we expect for a second-order phase transition. Comparing the numerical data given in Fig. 1 with the results obtained from the application of the equilibrium statistical physics tools shows good agreement between the two approaches; therefore, we it is reasonable to believe that the analytical approach presented here gives the exact result.

It is also interesting to look for the zeros of the grand canonical partition function of our model. In this case we can investigate the similarities between the phase transition in our model with that of a Bose gas. As opposed to the equilibrium statistical physics, the definition of a grand canonical ensemble for the steady state of a non-equilibrium system is not unique. We adopt the following definition first used in ref. 12

$$Z_L(q, z) = \sum_{M=0}^{L-1} z^M Z_{L,M}(q) \tag{12}$$

in which z is the fugacity of the positive particles and $Z_{L,M}(q)$ is given by (2).

It is seen that the grand canonical partition function (12) is a polynomial of degree $L-1$ in z so, in the complex-z plane it has $L-1$ zeros z_i and can be written as

$$Z_L(q, z) = \prod_{i=1}^{L-1} (z - z_i).$$

Using (2) one can easily calculate the grand canonical partition function (12) explicitly

$$Z_L(q,z) = \left(\frac{q-3}{q-2}\right)\left[\left(\frac{2z}{q}\right)^{L-1} + \frac{(1+z)^{L-1}}{(q-3)} + \frac{(\frac{2z}{q})^{L-1} - (1+z)^{L-1}}{(\frac{2z}{q}) - (1+z)}\right]. \quad (13)$$

The fugacity of the positive particles in (12) has to be fixed by density of them

$$\rho(z) = \frac{z}{L}\frac{\partial}{\partial z}\ln Z_L(q,z). \quad (14)$$

Let us examine the zeros of the grand canonical partition function given by (13) in the complex-z plane. Since the grand canonical partition function is a real polynomial with positive coefficients (they are sum over probabilities) the zeros come in complex conjugate pairs and the real roots are negative. In Fig. 3 we have plotted the numerical estimates of the zeros of (13) in complex-z plane for three values of q. As long as $q < 2$ the roots lie on a vertical elliptic. It also appears that the zeros approach the real z axis at an angle $\frac{\pi}{2}$. It is a sign of a first-order phase transition. For $q > 2$ all of the roots have negative real parts; therefore, we do not expect any phase transition to take place. For $q = 2$, we should take the limit of (2) since it is undefined at this point. In the following we will investigate our model in order to see its similarities with the Bose–Einstein condensation. Using (13) one can calculate (14) in each phase in the thermodynamic limit explicitly. It turns out that

$$\rho(z) = \begin{cases} \frac{z}{z+1} & \text{for} \quad z < \frac{q}{2-q} \\ 1 & \text{for} \quad z > \frac{q}{2-q}. \end{cases} \quad (15)$$

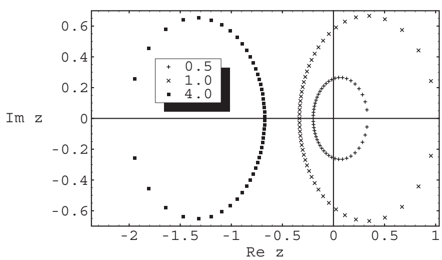

Fig. 3. Plot of the numerical estimates of the zeros of the grand canonical partition function (12) for $q = 0.5$, 1.0, and 4.0. The length of the chain is $L = 50$.

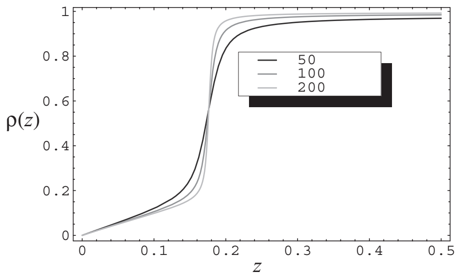

Fig. 4. Plot of the density of the positive particles (14) as a function of fugacity z for $L = 50$, 100, and 200 at $q = 0.3$. In the thermodynamic limit there is a finite discontinuity in the density of particles.

In Fig. 4 we have plotted (14) for different values of L. As can be seen the L dependence of the density suggests that in the thermodynamic limit, ρ increases with z and then at a specific point $z_0 = \frac{q}{2-q}$ it has a finite discontinuity. At this point, z does not fix the density anymore and the system undergoes a first-order phase transition.

The finite jump in the density is related to the finite density of roots of (13), $\mu(z)$, at the real z axis

$$\mu(z_0) = \frac{1-\rho(z_0)}{2\pi z_0}. \tag{16}$$

The critical fugacity z_0 can also be obtained by extrapolating the real part of the nearest root[4] to the real positive z axis for $L \to \infty$. In the Bose–Einstein condensation the density of the particles has such a behavior where the conservation of the number of particles is broken.[(13)] Another interesting quantity is the pressure which can be defined analogously to equilibrium physics

$$P(z) = \frac{1}{L} \ln Z_L(q, z). \tag{17}$$

However, P is not the physical pressure of the particles in the current context. The particles pressure in each phase in the thermodynamic limit can be calculated using (13)

$$P(z) = \begin{cases} \ln(1+z) & \text{for} \quad z < \frac{q}{2-q} \\ \ln(\frac{2z}{q}) & \text{for} \quad z > \frac{q}{2-q}. \end{cases} \tag{18}$$

[4] In fact there are two of them since the roots appear in complex conjugate pairs.

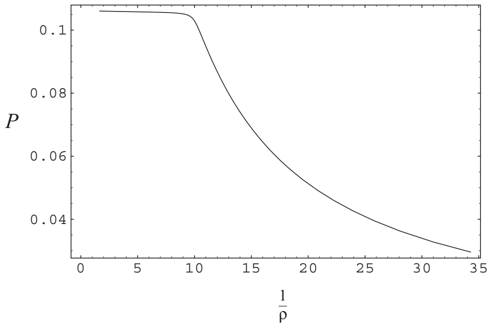

Fig. 5. The pressure P as a function of ρ^{-1} for $q = 0.2$ and $L = 15000$.

Now by using (15) and (18) it can easily be verified that in the power-law phase ($\rho < \frac{q}{2}$) the particles pressure P as a function of density has the form $P(\rho) = \ln(\frac{1}{1-\rho})$ while in the jammed phase ($\rho > \frac{q}{2}$), as can be seen from (15), the density-fugacity relation (14) breaks down and results in $\rho = 1$;[5] however, the particles pressure remains constant in this phase $P(\rho) = \ln(\frac{q}{2-q})$. In Fig. 5 we have plotted (17) as a function of the inverse of density of particles ρ^{-1} for $L = 15000$ and $q = 0.2$. The critical density in this case is $\rho = 0.1$. As can be seen for $\frac{1}{\rho} > 10$ the pressure decreases as the density gets smaller; however, for $\frac{1}{\rho} < 10$ it is nearly constant. This *isotherm* (here q instead of temperature T) is similar to the isotherm of the free Bose gas when the Bose–Einstein condensation takes place. One can also look at the compressibility κ which is defined as

$$\kappa = L\zeta^2 \tag{19}$$

in which

$$\zeta = \frac{\sqrt{\langle\rho^2\rangle - \langle\rho\rangle^2}}{\rho} \tag{20}$$

and the fluctuation of the density of the positive particles can be obtained using

$$\langle\rho^2\rangle - \langle\rho\rangle^2 = \frac{z}{L}\frac{\partial}{\partial z}\left(\frac{z}{L}\frac{\partial}{\partial z}\ln Z_L(q, z)\right). \tag{21}$$

Figure (6) shows ζ as a function of the chain length L for $\rho = 0.6$ and two values of q above and bellow of the transition point. The transition point in

[5] Physically, this is related to the existence of a shock in this phase.

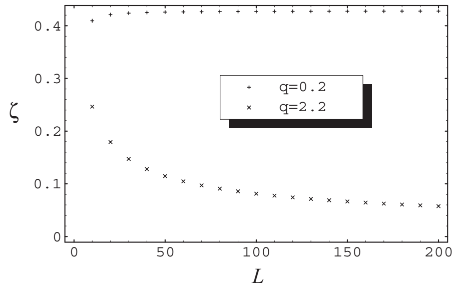

Fig. 6. Plot of (20) as a function of L for $\rho = 0.6$ and two values of q.

this case occurs at $q_c = 1.2$. It can be seen that ζ is a decreasing function of L in the power-law phase ($q > q_c$) while it is nearly constant in the jammed phase ($q < q_c$). Using (13) and (21) it can be verified that in the thermodynamic limit ζ drops down as $\frac{1}{\sqrt{L}}$ in the power-law phase while in the jammed phase it remains constant which gives a divergent compressibility.

4. CONCLUDING REMARKS

In this paper we have used the Yang–Lee description of equilibrium phase transitions in terms of the zeros of both canonical and grand canonical partition function to study a non-equilibrium phase transition in a driven diffusive system. By studying the canonical partition function zeros a second-order phase transition was predicted. This is in quite close agreement with our previous results in ref. 5. The line of zeros and also their density on the real axis near the transition point were obtained exactly. By introducing the grand canonical partition function of our model (12) the similarities between the phase transition in our model and the one seen in the equilibrium Bose gas were elegantly observed.

The approach that we used in this paper can also be applied to other models. In a similar model consists of a group of first class particles hopping behind a slow (or a second class) particle on a closed chain of length L, with the following interaction rules

$$\begin{array}{lllll} 1 & 0 & \longrightarrow & 0 & 1 & \text{with the rate} & 1 \\ 2 & 0 & \longrightarrow & 0 & 2 & \text{with the rate} & \alpha. \end{array} \tag{22}$$

It is shown that by choosing the right reaction rates the probability distribution for the stationary state can be mapped to the one obtained for an ideal Bose gas.[9] The thermodynamic limit of the canonical partition function of this model is obtained in ref. 9

$$\begin{aligned} &\text{for} \quad \alpha < 1-\rho \quad Z_{L,M}(\alpha) \simeq \frac{(1-\alpha)^{1-M}}{(\alpha)^{L-M}} \\ &\text{for} \quad \alpha > 1-\rho \quad Z_{L,M}(\alpha) \simeq \frac{\alpha\rho^2}{\rho+\alpha-1} C_L^M \end{aligned} \tag{23}$$

in which $\rho = \frac{M}{L}$ is the density of the first class particles. Now using (5) and (6) we find the line of zeros in complex-α plane

$$\left(\left(\frac{1-x}{\rho}\right)^2 + \left(\frac{y}{\rho}\right)^2\right)^\rho \left(\left(\frac{x}{1-\rho}\right)^2 + \left(\frac{y}{1-\rho}\right)^2\right)^{1-\rho} = 1 \tag{24}$$

where $x \equiv \mathrm{Re}(\alpha)$ and $y \equiv \mathrm{Im}(\alpha)$. This function crosses the real positive α axis at $\alpha_c = 1-\rho$ at an angle $\frac{\pi}{4}$. It can be seen that the thermodynamic limit of the canonical partition function of our model (4) is quite similar to (23). Using (5) one can also obtain the line of zeros for the ASEP with open boundaries exactly.

For this model with two parameters α and β as injection and extraction rates of particles, the line of zeros in the complex-α plane (and β being fixed) is

$$(-x^2+x+y^2)^2+(y-2xy)^2 = J^2 \tag{25}$$

in which we have defined $x \equiv \mathrm{Re}(\alpha)$, $y \equiv \mathrm{Im}(\alpha)$ and the current of particles is

$$J = \begin{cases} \frac{1}{4} & \text{if} \quad \beta \geqslant \frac{1}{2} \\ \beta(1-\beta) & \text{if} \quad \beta \leqslant \frac{1}{2}. \end{cases}$$

The investigation of (25) confirms the existence of two phase transitions in the system. In Fig. 7 we have plotted the line of zeros (25) for two values of β. It can be seen that (25) gives exactly the same results obtained in ref. 7 from the numerical estimates of the canonical partition function zeros. In ref. 7 the line of zeros is stated to be $|\alpha(1-\alpha)| = J$. By putting $\alpha = x+iy$ one finds (25) for the line of zeros.

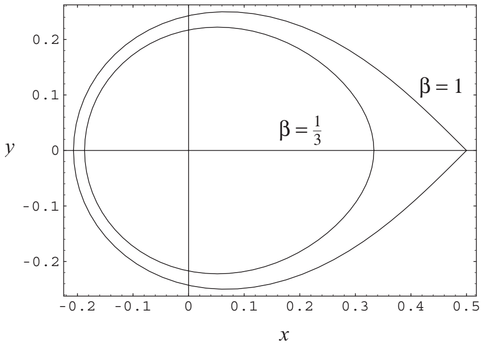

Fig. 7. Plot of the Eq. (25) for $\beta = \frac{1}{3}$ and $\beta = 1$.

Apart from the above mentioned models one can show that our approach can be applied to many other non-equilibrium systems like those introduced in ref. 14. Work in this direction is in progress.[15]

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