

Exact zeros of the partition function for a continuum system with double Gaussian peaks

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We calculate the exact zeros of the partition function for a continuum system where the probability distribution for the order parameter is given by two asymmetric Gaussian peaks. When the positions of the two peaks coincide, the two separate loci of the zeros that used to give a first-order transition touch each other, with the density of zeros vanishing at the contact point on the positive real axis. Instead of the second-order transition of the Ehrenfest classification as one might naively expect, one finds a critical behavior in this limit.

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I. INTRODUCTION

It has been a central theme since the discovery of statistical mechanics to understand how the analytic partition function for a finite-size system acquires a singularity in the thermodynamic limit if the system undergoes a phase transition [1]. The Lee-Yang theory [2] has partly furnished the answer to this quest. They proposed a scenario where the zeros of the partition function form a line and cut across the real axis. They showed that the discontinuity in the first-order derivative of the partition function is proportional to the angular density of zeros, using an analogy with two-dimensional electrostatics. Then they proved this scenario for Ising-like discrete systems under very general conditions. They could show that the zeros were distributed on a unit circle in this case.

There have been many attempts to generalize the Lee-Yang circle theorem ever since. Fisher [3] initiated a study of zeros of the partition function in the complex temperature plane and extensive studies of this topic followed [4–12]. In these works the authors considered continuous phase transitions or critical points.

The conceptual basis of the Lee-Yang circle theorem was finally clarified in Ref. [13] by considering the first-order transition of a system with more general continuous degrees of freedom, with a doubly peaked probability distribution for the order parameter. Since the Ising-like models considered by Lee and Yang would be described by two symmetric Gaussian peaks in the thermodynamic limit, this result provides a simple conceptual basis for the Lee-Yang unit circle theorem. Furthermore, it is a generalization since general asymmetric configurations were considered, whose zeros form a curve that is not a unit circle in general.

One interesting problem to consider is what happens when the positions of the two Gaussian peaks coincide. Since this is the limit where the latent heat l vanishes, one might naively expect that the system would exhibit a second-

order transition of the Ehrenfest classification [14], where there is a finite discontinuity in specific heat but no latent heat (Fig. 1).

However, when we consider the exact zeros of the partition function for the system with two Gaussian peaks, we find there is a branch of zeros other than the one described in Ref. [13]. For $l \neq 0$, this branch can be neglected, since for generic systems the Gaussian approximation breaks down at this point due to the contributions from the higher order cumulants. However, for $l=0$ this is no longer true and we have to take this branch into account. Because of this, the system exhibits a critical behavior instead of the second-order transition.

II. LOCUS AND DENSITY OF ZEROS

We consider a canonical partition function of a continuum system, which can be written as in Ref. [13],

$$\mathcal{M}(t) \equiv Z(\beta)/Z(\beta_0) = \int_{-\infty}^{\infty} e^{tx} f(x) dx, \quad (2.1)$$

where the probability density function is given by

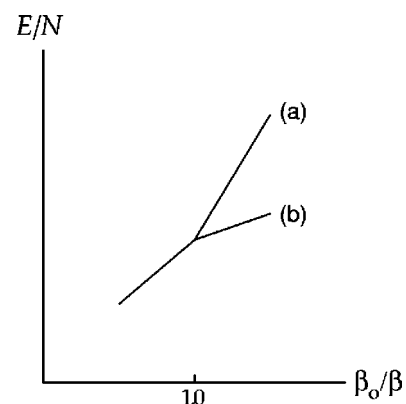


FIG. 1. The energy density as a function of the reduced temperature at the second-order transition. The branch (a) is for $\Delta c > 0$ and (b) is for $\Delta c < 0$.

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$$f(x) = \Omega(x/\beta_0) e^{-x/\beta_0} \int_{-\infty}^{\infty} \Omega(x/\beta_0) e^{-x/\beta_0} dx, \quad (2.2)$$

$t = 1 - \beta/\beta_0$, $x = \beta_0 E$, $\Omega(E)$ is the density of states at energy E , and β_0 is the inverse of the transition temperature we are interested in. When one is interested in a field driven phase transition, one may replace the energy E by the magnetization M and the inverse temperature β by the magnetic field H in the case of magnetic systems, and so on. We investigate the locus of zeros on the plane of complex temperature $z = r e^{i\theta} \equiv e^t$.

Now consider the case of interest in this paper, when $f(x)$ is given by a summation of two Gaussian peaks up to normalization,

$$f(x) = \frac{1}{\sqrt{2\pi}\sigma_1} \exp\left(-\frac{(x-\mu_1)^2}{2\sigma_1^2}\right) + a \frac{1}{\sqrt{2\pi}\sigma_2} \exp\left(-\frac{(x-\mu_2)^2}{2\sigma_2^2}\right). \quad (2.3)$$

These two peaks represent two different phases of the system. When $\mu_1 \neq \mu_2$ the system undergoes a first-order transition. Let us denote two Gaussian functions by $f_1(x)$ and $f_2(x)$. Since we can relabel f_1 and f_2 , and redefine a , we may assume $m \equiv (\mu_2 - \mu_1)/2 > 0$ without loss of generality. We then have

$$\begin{aligned} \mathcal{M}(t) &= \int_{-\infty}^{\infty} e^{tx} [f_1(x) + a f_2(x)] dx \\ &= \exp(\psi_1) + \exp(\psi_2), \end{aligned} \quad (2.4)$$

where

$$\begin{aligned} \exp[\psi_1(t)] &\equiv \int e^{tx} f_1(x) dx, \\ \exp[\psi_2(t)] &\equiv \int e^{tx} a f_2(x) dx. \end{aligned} \quad (2.5)$$

From the expressions above, one can easily see that the locations of zeros are given by the solutions to the following equation as in Ref. [13]:

$$\psi_2(t_k) - \psi_1(t_k) = 2iI_k \equiv i(2k+1)\pi, \quad (2.6)$$

where k runs through all the integers. For the double Gaussian distribution the equation above can be rewritten as

$$iI_k = \frac{1}{2} \ln a + m(t_k) + \frac{\tilde{\sigma}^2}{2} (t_k)^2, \quad (2.7)$$

where $\tilde{\sigma}^2 = (\sigma_2^2 - \sigma_1^2)/2$. This equation is quadratic and easily solved. The solutions are

$$\begin{aligned} t_k^\pm &= -\frac{m}{\tilde{\sigma}^2} \pm \frac{\sqrt{2}}{|\tilde{\sigma}|} \sqrt{iI_k - \frac{1}{2} \ln a + m^2/2\tilde{\sigma}^2} \\ &= -\frac{m}{\tilde{\sigma}^2} \pm \frac{|I_k|}{|\lambda_k \tilde{\sigma}|} \pm i \operatorname{sgn}(I_k) \left| \frac{\lambda_k}{\tilde{\sigma}} \right|, \end{aligned} \quad (2.8)$$

where

$$\lambda_k \equiv \left[\sqrt{\left(\frac{m^2}{2\tilde{\sigma}^2} - \frac{\ln a}{2}\right)^2 + I_k^2} - \left(\frac{m^2}{2\tilde{\sigma}^2} - \frac{\ln a}{2}\right) \right]^{1/2}. \quad (2.9)$$

Note that there are two branches of solutions. One passes through the transition point $t=0$ in the thermodynamic limit and the other does not, so the latter was implicitly discarded in Ref. [13]. As we will see, the second branch closes in toward $t=0$ as we take the limit $l \rightarrow 0$.

Now we redefine the variables

$$\begin{aligned} m &= \frac{Nl}{2}, \\ I_k &= \frac{N y_k}{2}, \\ \tilde{\sigma}^2 &= \frac{N \Delta c}{2}, \end{aligned} \quad (2.10)$$

and consider the thermodynamic limit $N \rightarrow \infty$. We then get

$$\begin{aligned} \ln(r_k) &\equiv \operatorname{Re}(t_k) = -\frac{m}{\tilde{\sigma}^2} \pm \frac{|I_k|}{|\tilde{\sigma} \lambda_k|} \\ &= -\frac{l}{\Delta c} \pm \frac{|y_k|}{\sqrt{\sqrt{(l^2/2)^2 + y_k^2 (\Delta c)^2} - l^2/2}}, \\ \theta_k &\equiv \operatorname{Im}(t_k) = \pm \operatorname{sgn}(I_k) \left| \frac{\lambda_k}{\tilde{\sigma}} \right| \\ &= \pm \operatorname{sgn}(y_k) \left[\sqrt{\frac{1}{4} \left(\frac{l}{\Delta c}\right)^4 + \frac{y_k^2}{(\Delta c)^2}} - \frac{l^2}{2(\Delta c)^2} \right]^{1/2}. \end{aligned} \quad (2.11)$$

The terms involving $\ln a$ are finite-size corrections and vanish in this limit. We solve the second equation of (2.11) in terms of y_k to get

$$y_k = \pm \theta_k l \sqrt{1 + \theta_k^2 \left(\frac{\Delta c}{l}\right)^2}. \quad (2.12)$$

We substitute Eq. (2.12) into the first equation of (2.11) to get the locus of zeros,

$$r_\pm = \exp\left[-\frac{l}{\Delta c} \pm \frac{l}{|\Delta c|} \sqrt{1 + \theta_k^2 \left(\frac{\Delta c}{l}\right)^2}\right]. \quad (2.13)$$

We can also obtain the angular density of zeros. By taking the formal derivative with respect to the integer k , we get

$$\begin{aligned} \left| \frac{d\theta_k}{dk} \right| &= \frac{1}{2 \left[\sqrt{\frac{1}{4} (l/\Delta c)^4 + y_k^2 / (\Delta c)^2} - l^2 / 2 (\Delta c)^2 \right]^{1/2}} \\ &\times \frac{2y_k \pi}{N(\Delta c)^2 \sqrt{\frac{1}{4} (l/\Delta c)^4 + y_k^2 / (\Delta c)^2}} \\ &= \frac{2\pi l \sqrt{1 + \theta^2 (\Delta c/l)^2}}{N[l^2 + 2(\Delta c)^2 \theta^2]}. \end{aligned} \quad (2.14)$$

Therefore, the angular densities of zeros g_{\pm} of the two branches are given by

$$2\pi g_{\pm}(\theta) \equiv \frac{2\pi}{N} \left| \frac{dk}{d\theta} \right| = l \frac{1 + 2(\Delta c/l)^2 \theta^2}{\sqrt{1 + (\Delta c/l)^2 \theta^2}}. \quad (2.15)$$

III. FIRST-ORDER TRANSITIONS

We will now consider both loci of zeros of the partition function at a first-order transition. Note that all the quantities above depend only on the ratio $l/\Delta c$ except for an overall factor of l in front of $g(\theta)$.¹ When $l/\Delta c \neq 0$, we get the first-order transition. This is the case considered in Ref. [13]. There only the loci of zeros near the transition point $t=0$ were treated carefully since these were the only things of interest. In fact, for generic systems we expect that the Gaussian approximation breaks down away from the transition point $t=0$ due to the higher order cumulants.

Let us elaborate on this point. The locus of zeros crosses the real axis at $t=0$ and $t=-2l/\Delta c$, indicating that there are two phase transitions. This can be easily understood. The probability density at arbitrary temperature is given by

$$\begin{aligned} e^{tx} \Omega(x) &= \frac{e^{tx} e^{-(x-x_1)^2/(2\sigma_1^2)}}{\sqrt{2\pi\sigma_1}} + \frac{e^{tx} e^{-(x-x_2)^2/(2\sigma_2^2)}}{\sqrt{2\pi\sigma_2}} \\ &= \frac{e^{-(x-x_1-\sigma_1^2 t)^2/(2\sigma_1^2) + x_1 t + \sigma_1^2 t^2/2}}{\sqrt{2\pi\sigma_1}} \\ &\quad + \frac{e^{-(x-x_2-\sigma_2^2 t)^2/(2\sigma_2^2) + x_2 t + \sigma_2^2 t^2/2}}{\sqrt{2\pi\sigma_2}}. \end{aligned} \quad (3.1)$$

We see that for nonzero t the positions of the peaks are shifted, and also the relative weights change. We see that the position of the peak for large σ_i gets shifted by a larger amount for given temperature change, consistent with the fact that it has larger specific heat. The weight of the peak 1 relative to the peak 2 is given by

¹When both l and Δc are zero these quantities are ill defined and we can no longer use the Gaussian approximation. One then has to take into account higher order cumulants.

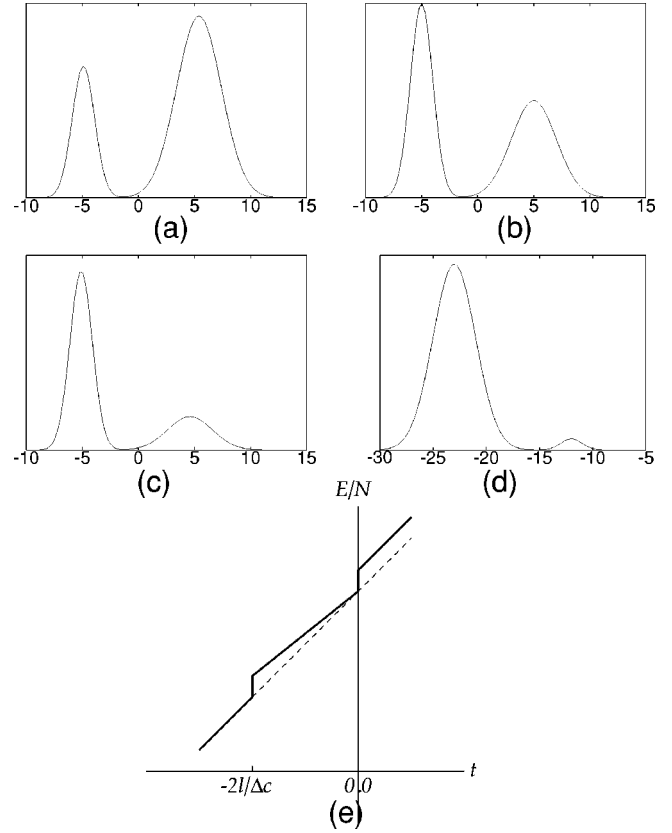


FIG. 2. Qualitative behavior of $e^{tx} \Omega(x)$ versus x , where we take $\mu_{1,2} = \pm 5$ in this example. (a) For $t > 0$ peak 2 dominates. (b) At $t = 0$ the weights of the two Gaussian peaks are equal by construction, meaning the areas under the curves are same. (c) As t decreases below 0, the weight of peak 1 becomes larger. The first-order transition has occurred with latent heat l and a discontinuity in the specific heat Δc . The positions of the peaks begin to be shifted to the left, with peak 2 moving faster. (d) For $t < -2l/\Delta c$, the weight of peak 2 becomes larger than that of 1 again. At this point peak 2 is at the left of peak 1, so this is another first-order transition, with latent heat l and a discontinuity in the specific heat $-\Delta c$. (e) Schematic diagram of energy versus reduced temperature for the system with double Gaussian peaks. Note that there are two first-order transitions with the same latent heat but opposite sign for the discontinuity in the specific heat. The transition at $t = -2l/\Delta c$ is discarded for generic systems.

$$w^1/w^2 \equiv \exp\left(\frac{(\sigma_1^2 - \sigma_2^2)}{2} t^2 + (x_1 - x_2)t\right). \quad (3.2)$$

By construction, at $t=0$, the weights of the two Gaussian peaks are equal. Assuming $\sigma_2 > \sigma_1$, we see that for $t > 0$ the peak labeled 2 dominates. When t becomes slightly negative, then the peak 1 dominates. Also, the positions of the Gaussian peaks are shifted to the left, but peak 2 moves faster. For $t < -(x_1 - x_2)/(\sigma_1^2 - \sigma_2^2)$ peak 2 goes to the left of peak 1. At $t = -2l/\Delta c$, the weight of peak 2 becomes equal to that of 1 again, and peak 2 is dominant for $t < -2l/\Delta c$. Therefore at this temperature there is another first-order transition with latent heat l and specific heat change $-\Delta c$. We can make similar arguments for $\sigma_1 > \sigma_2$. This process is depicted in Fig. 2.

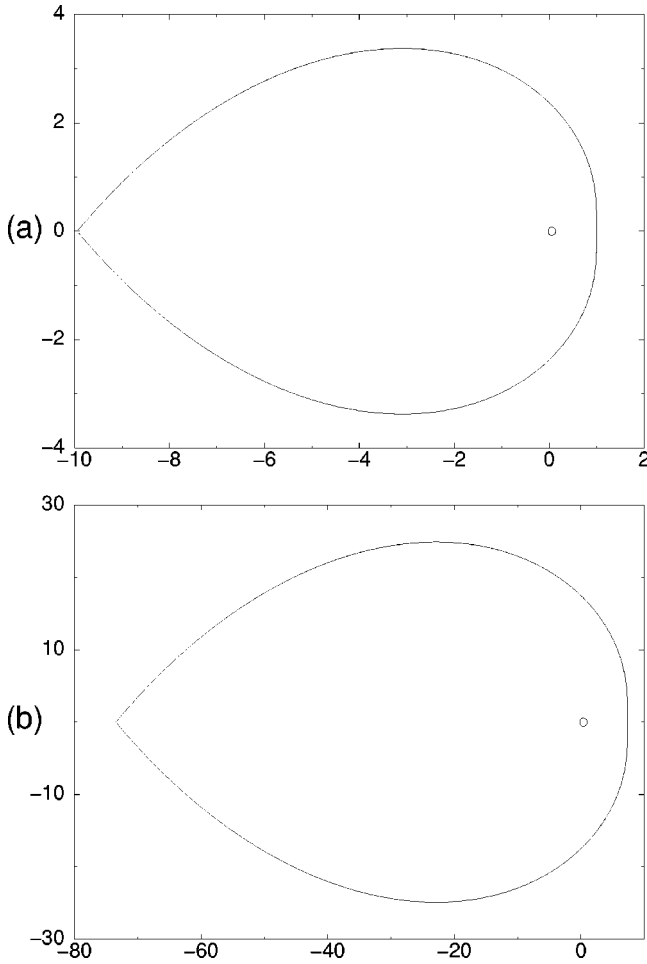


FIG. 3. (a) $\Delta c/l=1$. As $\Delta c/l \rightarrow 0$, the outer curve becomes a unit circle and the inner curve degenerates to the origin. (b) $\Delta c/l = -1$. As $\Delta c/l \rightarrow 0$, the inner curve becomes a unit circle and the outer curve goes away to infinity.

This mechanism works only if we trust that the Gaussian form given in Eq. (2.3) is exact. However, for a generic system, this is just a leading truncation of the cumulant expansion

$$\exp[-Nf(x)] = \exp\left[-N\left(f(x_0) + \frac{f''(x_0)}{2}(\Delta x)^2 + \frac{f'''(x_0)}{3!}(\Delta x)^3 + \dots\right)\right], \quad (3.3)$$

so the higher order cumulants can be ignored only when $\Delta x \ll O(1/\sqrt{N})$. But at the first-order transition at $t = -2l/\Delta c$, the system is dominated by the peaks which are located at distances of $O(1)$ from the positions of the peaks at $t=0$. Therefore the higher order cumulants will contribute, and we cannot trust the picture above. However, when $\Delta x \ll O(1/\sqrt{N})$, or when the higher order cumulants are extremely small for some reason, the transition at $t = -2l/\Delta c$ can no longer be neglected. In particular, in the limit $l \rightarrow 0$, the second branch touches the first branch, preventing the system from exhibiting the second-order transition.

The behaviors of the loci of zeros for various values of $\Delta c/l$ are depicted in Figs. 3–5 in the complex $z \equiv \exp(t)$

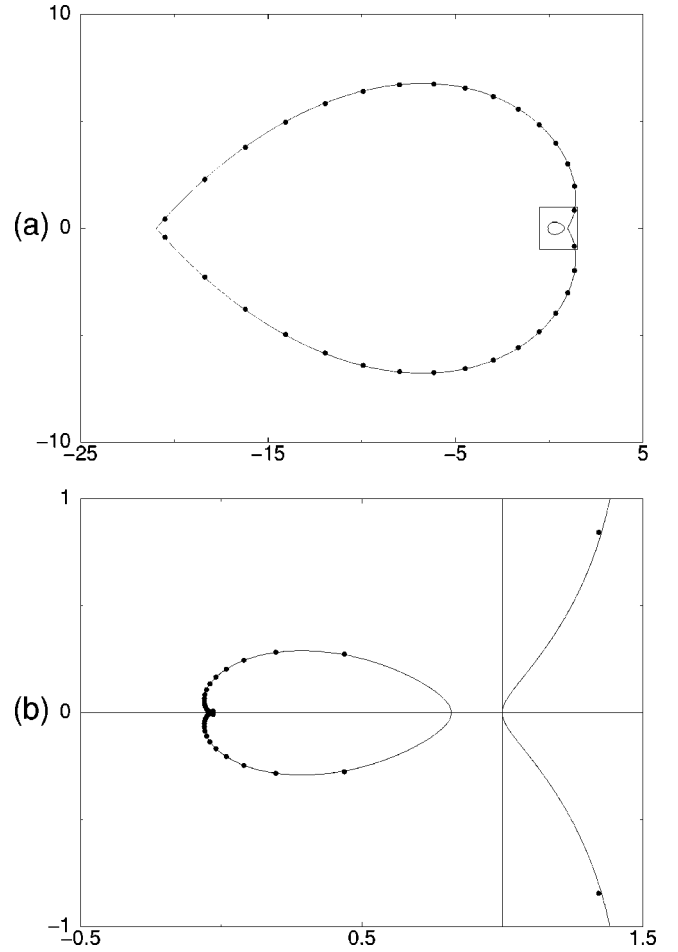


FIG. 4. (a) $\tilde{\sigma}^2/m = \Delta c/l = 10$. The zeros for finite N are also plotted as dots, for $2\tilde{\sigma}^2 = N\Delta c = 10$ and $a = 1.0$. The dots deviate from the curve if $a \neq 1.0$. (b) Magnification of the box in (a). The horizontal line indicates the real axis, and the vertical line is given by $\text{Re}(z) = 1$. Note that the outer curve passes through the point $z = 1.0$, and the angles between both loci and the real axis are 90° .

plane. t_+ is the outer curve and t_- is the inner curve. Only the zeros in the first Riemann sheet are shown. When $\Delta c/l > 0 (< 0)$, t_+ (t_-) passes through $t=0$, and becomes a unit circle as one approaches the symmetric limit $\Delta c/l \rightarrow 0$. This is consistent with Lee-Yang's unit circle theorem. The other branch $t_-(t_+)$ degenerates to the origin (goes to infinity). The loci intersect the real axis orthogonally as long as $l \neq 0$.

IV. $l \rightarrow 0$ LIMIT AND THE CRITICAL BEHAVIOR

The limit $l/\Delta c = 0$ may be considered as the opposite limit from the symmetric case $\Delta c/l = 0$. Now the two loci t_\pm , which were separate when $l \neq 0$, touch each other at $\theta = 0$ and form a single curve (Fig. 6). Their loci are given by

$$r_\pm = \exp(\pm|\theta|). \quad (4.1)$$

The density of zeros is

$$2\pi g(\theta) = 2\pi[g_+(\theta) + g_-(\theta)] = 4\Delta c|\theta|. \quad (4.2)$$

Note that $g(\theta)$ is zero at $\theta=0$, consistent with the fact that the first derivative of the partition function has no discontinuity.

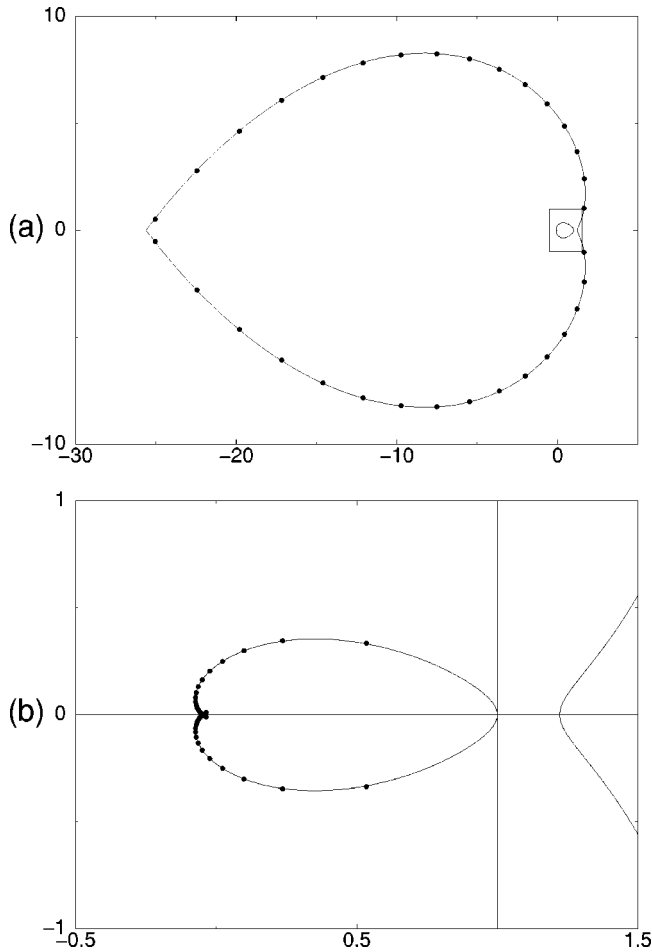


FIG. 5. (a) $\Delta c/l = -10$. The dots indicate zeros for $2\tilde{\sigma}^2 = N\Delta c = -10$ and $a = 1.0$. (b) Magnification of the box in (a). It is the inner curve that passes through $z = 1.0$ in this case.

nuity. The loci intersect the real axis at angles of 45° , and the intermediate region dominated by peak 1 with the smaller specific heat, which used to separate two domains dominated by peak 2 with the larger specific heat, touches the real axis at just one point. Therefore the system is dominated by peak 2 for $t \neq 0$, and peak 1 has same weight as peak 2 only at $t = 0$, when their positions coincide. The qualitative behaviors of the two peaks for $t > 0$ and $t < 0$ are the same as the ones depicted in Figs. 2(a) and 2(d).

Therefore the system is exhibiting a critical behavior where it is just on the verge of making a phase transition. However, in contrast to many familiar examples of critical behavior, the specific heat near $t = 0$ remains finite instead of blowing up. At this stage it is not yet clear whether there is

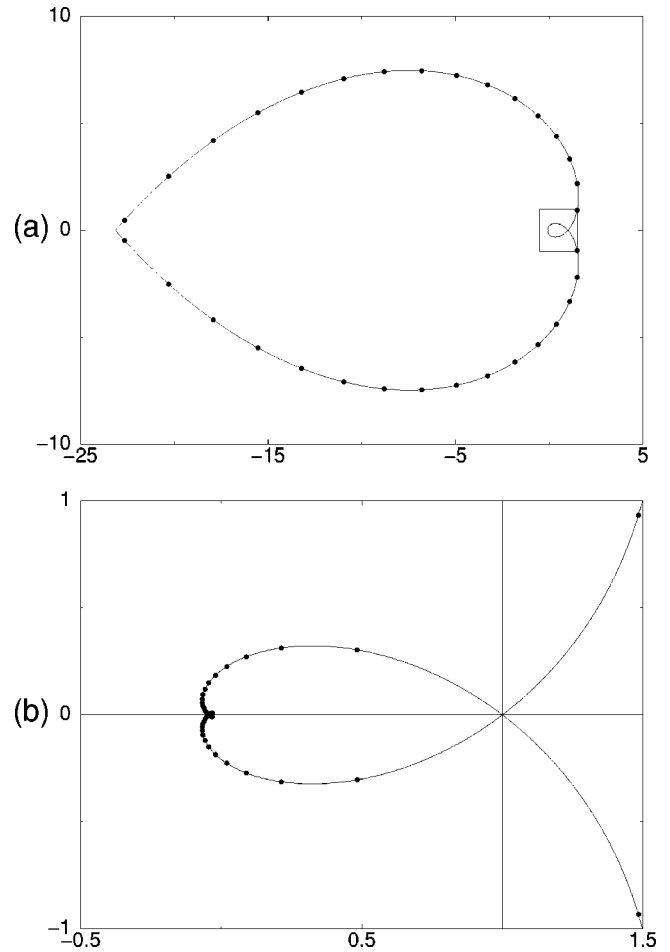


FIG. 6. (a) $l = 0$. The zeros for $N|\Delta c| = 10$ are plotted, with the same notation as before. (b) Magnification of the box in (a). Note that the two loci are now joined to form a single curve, which intersects the real axis at $z = 1.0$ at the angle of 45° . Both $\Delta c > 0$ (Fig. 4) and $\Delta c < 0$ (Fig. 5) approach this limit as $l \rightarrow 0$.

an example of a discrete system whose critical behavior at the thermodynamic limit can be described by this model.

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