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# Properties of phase transitions of higher order*

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There is only limited experimental evidence for the existence in nature of phase transitions of Ehrenfest order greater than two. However, there is no physical reason for their non-existence, and such transitions certainly exist in a number of theoretical models in statistical physics and lattice field theory. Here, higher-order transitions are analysed through the medium of partition function zeros. Results concerning the distributions of zeros are derived as are scaling relations between some of the critical exponents.

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## 1. Introduction

In the original Ehrenfest scheme for their classification, the order of phase transitions was given as that of the lowest derivative of the Helmholtz free energy in which a discontinuity is manifest. While first-order solid-liquid-vapour transitions and second-order superconducting transitions, for example, fit into this scheme, there is only limited evidence for the existence in nature of transitions of strictly higher order (i.e., of order three or above). However, on the basis of experiment, recent claims have been made which support the existence of a fourth-order transition in a cubic superconductor [1] and a theoretical analysis of higher-order transitions was provided in [2].

There are many other well known transitions signaled by divergent rather than discontinuous behaviour of the appropriate free energy derivatives. By far the most common transitions of this type are second-order ones such those associated with symmetry breaking of the Higgs field in particle physics and ferromagnetic transitions in metals. The modern classification scheme includes these scenarios and the order of a transition is now generally taken to mean that of the lowest derivative of free energy in which any type of singular behaviour occurs.

Notwithstanding the dearth of experimental evidence, higher-order transitions (especially of order three) abound in theoretical models, such as pure spin models [3], spin models coupled to quantum gravity [4, 5] and lattice (as well as continuum) toy models of QCD [6]. In the notation of spin models, where $t = 1 - T/T_c$ is the reduced temperature ($T_c$ being the critical value of the temperature variable $T$) and $h = H/k_BT$ is the reduced external field ($H$ being the field strength), the critical point is often located at $(0,0)$. This may be the endpoint of a line of first-order transitions, in which case we assume that $t$ parameterises its arc length with $h$ in the orthogonal direction. We denote the free energy by $f(t,h)$ and its $n^{\rm th}$ derivatives by $f_t^{(n)}(t,h)$ and $f_h^{(n)}(t,h)$. If $t$ or $h$ vanishes, we simply drop it from the argument. For an $m^{\rm th}$-order transition $f_t^{(n)}(t)$ is continuous for $n \le m-1$ while $f_t^{(m)}(t)$ experiences either a disontinuity or is unbounded at $t = 0$. It is also possible that $f_h^{(n)}(t)$ is continuous for $n \le m'-1$ while $f_h^{(m')}(t)$ is singular. The specific heat, $C(t) = f_t^{(2)}(t)$, is thus continuous if $m > 2$ and the susceptibility, $\chi(t) = f_h^{(2)}(t)$, is continuous if $m' > 2$ (a situation not normally possible in a ferromagnet).

We distinguish between transitions characterised by a discontinuity in $f_t^{(m)}(t)$ and those characterised by divergences. In the latter case, allowing for the possibility that $m'$ is not necessarily the same as $m$, the scaling behaviour at the transition may be described by critical exponents:

$$f_t^{(m)}(t) \sim t^{-A} , \quad f_h^{(m')}(t) \sim t^{-G} , \quad f_h^{(1)}(t) \sim t^{\beta} , \quad f_h^{(1)}(h) \sim h^{1/\delta} . \tag{1.1}$$

In the second-order case ($m = m' = 2$), the exponents $A$ and $G$ become the usual critical exponents $\alpha$ and $\gamma$ associated with specific heat and susceptibility, respectively.

Here, some results concerning the properties of partition function zeros close to higher-order transitions are presented. The Fisher zeros of systems governed by a single thermal parameter are analysed in Sec. 2 where restrictions on their properties are outlined. The Lee-Yang zeros appropriate to the field variable are examined in Sec. 3 and a number of scaling relations are derived. These recover the higher-order relations of [2] in the case where $m' = m$ and, when $m = 2$, they recover the standard Rushbrooke and Griffiths scaling relations appropriate to second-order transitions where the specific heat and susceptibility are unbounded. Conclusions are presented in Sec. 4.



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**Table 1:** Impact angles (in the upper half-plane) permitted at a discontinuous phase transition of order $m$.

| $m$ | Permitted values of impact angle, $\phi$ | | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | | | | | | | | | $\frac{\pi}{2}$ | | | | | | | | |
| 2 | | | | | $\frac{\pi}{4}$ | | | | | | | | $\frac{3\pi}{4}$ | | | | |
| 3 | | | | $\frac{\pi}{6}$ | | | | | $\frac{\pi}{2}$ | | | | | $\frac{5\pi}{6}$ | | | |
| 4 | | | $\frac{\pi}{8}$ | | | | $\frac{3\pi}{8}$ | | | | $\frac{5\pi}{8}$ | | | | $\frac{7\pi}{8}$ | | |
| 5 | | $\frac{\pi}{10}$ | | | | $\frac{3\pi}{10}$ | | | $\frac{\pi}{2}$ | | | $\frac{7\pi}{10}$ | | | | $\frac{9\pi}{10}$ | |
| 6 | $\frac{\pi}{12}$ | | | | $\frac{\pi}{4}$ | | | $\frac{5\pi}{12}$ | | $\frac{7\pi}{12}$ | | | $\frac{3\pi}{4}$ | | | | $\frac{11\pi}{12}$ |

## 2. Fisher zeros

In the situation where the locus of Fisher zeros is linear and can be parameterized near the transition point in the upper half-plane by $t(r) = r\exp(i\phi(r))$ – the locus in the lower half-plane given by it complex conjugate – the (reduced) free energy and its derivatives are

$$f(t) = 2\mathrm{Re}\int_0^R \ln(t-t(r))g(r)dr \;, \qquad f_t^{(n)}(t) = 2(-1)^{n-1}(n-1)!\mathrm{Re}\int_0^R \frac{g(r)}{(t-t(r))^n}dr \;, \tag{2.1}$$

where $R$ is a suitable cutoff.

The difference in the free energy on either side of the transition can be expanded as $f(t > 0) - f(t<0) = \sum_{n=1}^{\infty} c_n t^n$. For a discontinuous transition, $c_n = 0$ for $n < m$, while $c_m \neq 0$ and the discontinuity in the $m^{\rm th}$ derivative of the free energy is $\Delta f^{(m)} = m! c_m$. Matching the real parts of the free energies across the singular line gives $\sum_{n=m}^{\infty} c_n r^n \cos n\phi(r) = 0$, so that the impact angle is

$$\lim_{r\to 0}\phi(r) \equiv \phi = \frac{(2l+1)\pi}{2m} \qquad \text{for} \quad l = 0,\ldots,m-1 \;. \tag{2.2}$$

The formula (2.2) gives a very direct way to read off the order of a transition. A list of permitted impact angles in the upper half-plane for discontinuous transitions of various orders is given in Table 1. It is clear that while vertical impact is allowed at any discontinuous transition of odd order, an impact angle of $\pi/6$, for example is only allowed at a transition of order 3 or 9 or 15, etc. On the other hand, a discontinuous second-order transition with impact angle $\pi/2$ is, for example, not permitted here. These observations are in accord with various results for first-, second- and third-order transitions in [7], [8] and [4, 5] which are associated with impact angles $\pi/2$ (corresponding to $l = 0$), $\pi/4$ ($l = 0$) and $\pi/2$ ($l = 1$), respectively. The question as to the mechanism by which the system selects its $l$-value is open.

Assuming analytic behaviour for the density of zeros, it is straightforward to show that the necessary and sufficient condition to generate an $m^{\rm th}$-order discontinous transition is

$$g(r) = g_0 r^{m-1} \;, \tag{2.3}$$

where $g_0$ is a constant. Inserting this into (2.1), and using (2.2), one finds

$$\Delta f^{(m)} = 2\pi g_0 (m-1)! \sin m\phi = (-1)^l (m-1)! 2\pi g_0 \ , \tag{2.4}$$

which generalizes a well known result in the $m = 1$ case [7].

We next consider an $m^{\text{th}}$-order diverging transition characterised by (1.1). To achieve the appropriate divergence for $f_t^{(m)}(t)$ it is necessary that

$$g(r) = g_0 r^{m-1-A} \ . \tag{2.5}$$

Putting this into (2.1), one finds that $f_t^{(n)}(t)$ is continuous for $n < m$, while

$$f_t^{(m)}(t) = -2g_0 |t|^{-A} \Gamma(m-A)\Gamma(A) \times \begin{cases} \cos{(m-A)\phi} & \text{if } t < 0 \\ \cos{((m-A)\phi + A\pi)} & \text{if } t > 0 \ . \end{cases} \tag{2.6}$$

This general relationship between critical amplitudes and impact angles recovers results derived in [9] in the $m = 2$ case. If $A = 0$ it turns out that $f^{(m)}(t)$ becomes logarithmically divergent and

$$f_t^{(m)}(t) = 2g_0 (m-1)! \cos{(m\phi)} \times \begin{cases} \ln |t| & \text{if } t < 0 \\ (\ln |t| + \pi \sin{(m\phi)}) & \text{if } t > 0 \ . \end{cases} \tag{2.7}$$

When $m = 2$ this recovers known behaviour in the second-order case [9] and the discontinuity across the transition is consistent with (2.4).

A quite natural origin for finite-size scaling (which is alternatively and traditionally viewed as a hypothesis) was offered in [10] by matching the integrated density of zeros on a finite lattice to its infinite-volume counterpart. Here, from (2.3) and (2.5), this quantity is $G(r) \sim r^{m-A}$ (where $A = 0$ in the case of a discontinuous transition). For a finite system of linear extent $L$, the integrated density at the $j^{\text{th}}$ zero is $G_L(|t_j|) = (2j-1)/2L^d$ [10, 11], and equating this to $G(|t_j|)$ leads to the scaling behaviour

$$|t_j| \sim L^{-\frac{d}{m-A}} \ . \tag{2.8}$$

In the unbounded case, assuming hyperscaling ($m - A = 2 - \alpha = \nu d$), this recovers the standard form $|t_j| \sim L^{-1/\nu}$ for Fisher zeros. In the discontinuous case, where $A = 0$, (2.8) yields

$$\nu = \frac{m}{d} \ , \tag{2.9}$$

which is a generalization of the usual formal identification of $\nu$ with $1/d$, applicable at a first-order transition. Support for this identification comes from the third-order ($m = 3$) discontinuous transition present in the $d = 3$ spherical model [12] as well as in the Ising model on planar random graphs if the Hausdorff dimension is used for $d$ [4].

## 3. Lee-Yang zeros

While the Fisher-zero analysis concerns only even exponents, mixed exponents are encountered in the Lee-Yang case, where both field and thermal variables enter. Scaling relations between such exponents were derived in [2] in the theoretical case where $m' = m$. These are

$$(m-1)A + m\beta + G = m(m-1) \ , \quad G = \beta\left((m-1)\delta - 1\right) \ . \tag{3.1}$$



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If $m = 2$, these become the standard Rushbrooke and Griffiths scaling laws, respectively:

$$\alpha + 2\beta + \gamma = 2\,, \quad \gamma = \beta(\delta - 1)\,. \tag{3.2}$$

Now, the free energy in the presence of an external field is

$$f(t,h) = 2\mathrm{Re}\int_{r_{\mathrm{YL}}(t)}^{R} \ln\left(h - h(r,t)\right) g(r,t)\,dr\,, \tag{3.3}$$

where $r_{\mathrm{YL}}(t)$ is the Yang-Lee edge and the locus of zeros is $h(r,t) = r\exp\left(i\phi(r,t)\right)$. The $n^{\mathrm{th}}$ field derivative is

$$f_h^{(n)}(t) = \frac{(-1)^{n-1}2(n-1)!}{r_{\mathrm{YL}}(t)^{n-1}}\mathrm{Re}\int_1^{\frac{R}{r_{\mathrm{YL}}}} \frac{g(xr_{\mathrm{YL}},t)}{(h/r_{\mathrm{YL}} - xe^{i\phi})^n}dx\,, \tag{3.4}$$

having used $r = xr_{\mathrm{YL}}(t)$. We assume that $r_{\mathrm{YL}}(t)$ is small near $t = 0$ so that $R/r_{\mathrm{YL}}(t) \to \infty$ and, when $n = m'$ and $h = 0$, compare with the limiting scaling behaviour in (1.1) to find

$$g(r,t) = t^{-G} r_{\mathrm{YL}}(t)^{m'-1}\Phi\left(\frac{r}{r_{\mathrm{YL}}(t)}\right)\,, \tag{3.5}$$

for some function $\Phi$ [13]. Using $n = 1$ in (3.4) gives, for the magnetization,

$$f_h^{(1)}(t,h) = 2t^{-G}r_{\mathrm{YL}}(t)^{m'-1}\mathrm{Re}\int_1^{\infty}\frac{\Phi(x)}{\frac{h}{r_{\mathrm{YL}}(t)} - xe^{i\phi}}dx \equiv t^{-G}r_{\mathrm{YL}}(t)^{m'-1}\Psi_\phi\left(\frac{h}{r_{\mathrm{YL}}(t)}\right)\,. \tag{3.6}$$

Comparison with (1.1) now gives $\Psi(h/r_{\mathrm{YL}}(t)) \sim \left(h/r_{\mathrm{YL(t)}}\right)^{1/\delta}$. Eq. (3.6) must become $t$-independent for small $t$ and, under these circumstances, the behaviour of the Yang-Lee edge is

$$r_{\mathrm{YL}}(t) \sim t^{\frac{G\delta}{(m'-1)\delta-1}}\,. \tag{3.7}$$

When $m' = 2$ and $G = \gamma$, this recovers second-order behaviour. Inserting (3.7) into (3.6), and comparing the $h \to 0$ limit of the resulting expression to (1.1), yields the scaling relation

$$\beta = \frac{G}{(m'-1)\delta - 1}\,. \tag{3.8}$$

When $m' = m$, this recovers the Griffiths-type scaling relation (3.1), derived in [2].

From (3.5) and (3.7), the integrated density of zeros is $G(r,t) = t^{G(\delta+1)/((m'-1)\delta-1)}F\left(r/r_{\mathrm{YL}}(t)\right)$ in which $F(x) = \int_1^x \Phi(x')dx'$, enabling (3.3) to be written as

$$f(t,h) = 2\mathrm{Re}\int_{r_{\mathrm{YL}}(t)}^{R}\frac{G(r,t)dr}{he^{-i\phi} - r} = t^{G\frac{\delta+1}{(m'-1)\delta-1}}\mathscr{F}_\phi\left(\frac{h}{r_{\mathrm{YL}}(t)}\right)\,, \tag{3.9}$$

for sufficiently small $t$ and where $\mathscr{F}_\phi(w) = 2\mathrm{Re}\int_1^\infty F(x)/(we^{-i\phi} - x)dx$. Its $m^{\mathrm{th}}$ temperature derivative at zero-field is therefore $f_t^{(m)}(t) \sim t^{G(\delta+1)/((m'-1)\delta-1)-m}$, an expression which, compared with (1.1), yields the scaling relation

$$A = m - G\frac{\delta+1}{(m'-1)\delta-1}\,. \tag{3.10}$$

In the case $m' = m$, (3.8) and (3.10) recover all four scaling relations derived in [2], and, in the second-order case ($m = 2$), they recover the standard Rushbrooke and Griffiths scaling laws (3.2).

## 4. Conclusions

The self-consistency of scaling at higher-order transitions has been examined using partition function zeros. While strong constraints on the linear locii (impact angles) of Fisher zeros associated with discontinuous $m^{\rm th}$-order transitions have been established, the mechanism whereby the system selects from $m$ possible locii is an open question and merits further study. For a transition characterised by an unbounded $m^{\rm th}$ moment, the impact angle is intimately linked with amplitude ratios. In both cases, analysis of the impact angle may provide a stable approach to the analysis of phase transition order and strength. A complementary analysis of Lee-Yang zeros leads to scaling relations between even and odd critical exponents at higher-order transitions of a general type. Finally, a finite-size scaling analysis shows that the conventional formal identification of $\nu$ with $1/d$ that holds at first-order transitions extends to $\nu = m/d$ for discontinuous transitions of $m^{\rm th}$ order.



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