Critical and tricritical behavior of the d=3 Blume-Capel model: Results from small-scale Monte Carlo simulations

CompPhys24

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Summary

1. Blume-Capel model
   - Second order line transition: Ising universality class
   - Tricritical point $d_u = 3$: Tricritical universality class + log corrections
2. Quantities and numerical simulations
   - Observables
   - Lee-Yang zeros
   - Cumulant method, density of zeros
   - Numerical details
3. Results
   - Critical Ising scaling behavior
   - Tricritical Ising scaling behavior
4. Conclusion

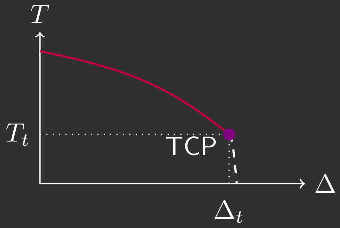
Blume-Capel model

The Blume-Capel model in $3D$

$$\mathcal{H} = -J \sum_{<i,j>} \sigma_i \sigma_j + \Delta \sum_i \sigma_i^2 - H \sum_i \sigma_i$$

Spin variables $\sigma_i = \{-1, 0, 1\}$, Δ is the crystal field coupling (controls the density of vacancies), H is the external magnetic field.

- Second order line: *Ising universality class.*
- Tricritical point at $\Delta_t = 2.84479(30)$, $T_t = 1.4182(55)$ †.
- First order line transition.



- Upper critical dimension $d_{uc} = 3$ at the tricritical point! MFT exponents are expected.

†M. Deserno. Phys. Rev. E, 56, 5204-5210 (1997)

Critical exponents along the second order line transition

Scaling hypothesis:

$$f^{\mathrm{sing}}(t,h) = L^{-d} f^{\mathrm{sing}}(L^{y_t} t, L^{y_h} h)$$

Ising universality class in 3D: Conformal bootstrap methods give[†]:

y_t	y_h
1.587374(4)	2.48180(14)

Table: 3D Ising universality class

Second order line of 3D Blume Capel model has been studied in several papers [‡].

†F. Kos, D. Poland, and D. Simmons-Duffin, Journal of High Energy Physics (2014)
‡N.G. Fytas and P.E. Theodorakis. The European Physical Journal B, vol. 86, no. 2 (2013). ; M. Hasenbusch. Physical Review B, vol. 82, no. 17 (2010). ; J. Zierenberg, N.G. Fytas and W. Janke. Physical review. E, Statistical, nonlinear, and soft matter physics. 91. (2015)

Critical exponents at the tricritical point

Tricritical Ising universality class → $d_u = 3$ is the upper critical dimension! The critical exponents take their tricritical mean-field values and multiplicative logarithmic corrections emerge.

Scaling hypothesis at the upper critical dimension:

$$f_{\text{tri}}^{\text{sing}}(t, g, h) = L^{-d}\mathcal{F}(L^{y_t}(\ln L)^{\hat{y}_t}t, L^{y_g}(\ln L)^{\hat{y}_g}g, L^{y_h}(\ln L)^{\hat{y}_h}h)$$

Tricritical point → ϕ^6 Landau expansion† :

$$y_g = 2 \;\; ; \quad y_h = \frac{5}{2} \;\; ; \quad y_t = 1,$$
$$\hat{y}_g = \frac{1}{3} \;\; ; \quad \hat{y}_h = \frac{1}{6} \;\; ; \quad \hat{y}_t = \frac{4}{15}$$

†I. D. Lawrie and S. Sarbach, Phase Transitions and Critical Phenomena, Vol. 9 (edited by C. Domb and J. L. Lebowitz, 1984

Quantities and numerical simulations

Observables

Magnetic susceptibility χ, magnetocaloric susceptibility coefficient χ_T, specific-heat-like quantity χ_2, magnetocaloric-like coefficient χ_{12}

$$\chi = \frac{\langle M^2\rangle - \langle |M|\rangle^2}{k_\mathrm{B}T}, \quad \chi_T = |\langle E|M|\rangle - \langle E\rangle\langle |M|\rangle|$$

$$\chi_2 = \frac{\langle E_\Delta^2\rangle - \langle E_\Delta\rangle^2}{k_\mathrm{B}T}, \quad \chi_{12} = |\langle E_\Delta|M|\rangle - \langle E_\Delta\rangle\langle |M|\rangle|$$

The logarithmic derivatives of the nth-order of the magnetization are studied $(K = 1/T)$

$$\left.\frac{\partial \ln\langle M^n\rangle}{\partial K} = \frac{\langle M^n \mathcal{H}\rangle}{\langle M^n\rangle} - \langle \mathcal{H}\rangle, \quad \frac{\partial \ln\langle M^n\rangle}{\partial \Delta} = K\left(\langle E_\Delta\rangle - \frac{\langle M^n E_\Delta\rangle}{\langle M^n\rangle}\right)\right\} \to L^{1/\nu}$$

FSS - Shift behavior (T-plane)

$$T_L \sim T_\mathrm{c} + aL^{-y_t}(1 + bL^{-\omega})$$

FSS - Shift behavior (Δ-plane)

$$\Delta_L \sim \Delta_\mathrm{t} + aL^{-y_g}(\ln L)^{\hat{y}_g}$$

Cumulant method for the Lee-Yang zeros

Cumulant method: A way to extract the Fisher zeros or Lee-Yang zeros from the energy/magnetization cumulants.
The magnetization cumulants are defined by the derivatives of the free energy with respect to the external field h

$$\langle\langle M^n(H)\rangle\rangle = (-1)^n N^{-1} \partial_H^n \ln \mathcal{Z} = \langle (M - \langle M\rangle)^n\rangle / N,$$

Different studies[‡] show that one can extract the first zero h_0 by studying

$$\mathrm{Im}[h_0] \approx \pm \frac{1}{K}\sqrt{2n(2n+1)\left|\frac{\langle\langle M^{2n}(0)\rangle\rangle}{\langle\langle M^{2(n+1)}(0)\rangle\rangle}\right|}, \quad \text{for } n >> 1$$

Finite-size Scaling

$$\langle\langle M^n(0)\rangle\rangle \sim L^{-d+ny_h}, \quad h_0 \sim L^{-y_h}$$

Density of zeros: an efficient approach to determine the order of the transition

The cumulative distribution function of the zeros is given by

$$G_L(r_j) = (2(j+1)-1)/2L^d,$$

where r_j is the $(j+1)^{\text{th}}$-zero of the partition function, j labels the zeros.
Lee-Yang zeros case: The cumulative density for finite systems behaves as†

$$G_L(h_j) \sim a_1 h_j (L)^{a_2} + a_3.$$

The value of a_2 determines whether the transition is of first or second order:
→ In the case of a first-order transition, $a_2 \sim 1$, and $a_1 \propto \Delta e$ for the Fisher zeros (or magnetization for the Lee-Yang zeros).
→ In the case of a second-order transition, $a_2 = d/y_h$ for the Lee-Yang zeros.
→ The term a_3 indicates a phase transition when it is very close to zero.

†W. Janke and R. Kenna, Journal of Statistical Physics 102, 1211 (2001)

Numerical details

Monte-Carlo simulations: Hybrid Wolff single-cluster update for the ± 1 spins and a single-spin-flip Metropolis update to account for the vacancies.
→ MC simulations at

$$(\Delta_{\rm c}, T_{\rm c}) = (0, 3.1952) \qquad (\Delta_{\rm t}, T_{\rm t}) = (2.8450, 1.4182)$$

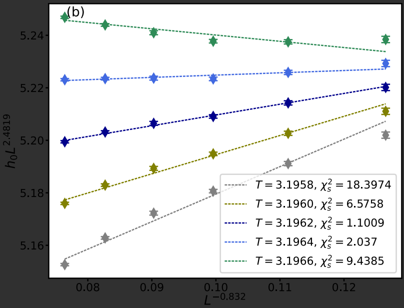
→ Histogram reweighting method, which allows us to extrapolate data obtained from simulations at fixed values of the crystal field (temperature) to nearby temperature (crystal-field) ranges
→ Periodic boundary conditions
→ System sizes: $L = 12 - 22$
→ We perform $900 \times N$ Monte Carlo steps per spin to ensure equilibration, followed by $900 \times 5 \times N$ Monte Carlo steps per spin for the collection of numerical data

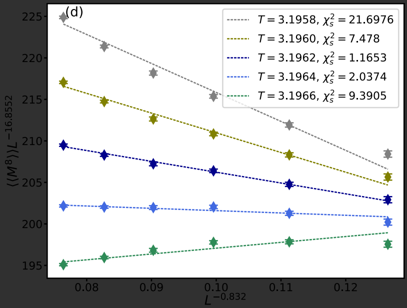
Results
Critical Ising scaling behavior

The Blume-Capel model in $3D$: critical point

Goal: At the critical point $\Delta_c = 0$, the goal is to locate accurately the location of the transition.

$$h_0 \sim aL^{-2.4819}(1 + bL^{-0.832}), \quad \langle\langle M^8 \rangle\rangle \sim aL^{16.8552}(1 + bL^{-0.832})$$



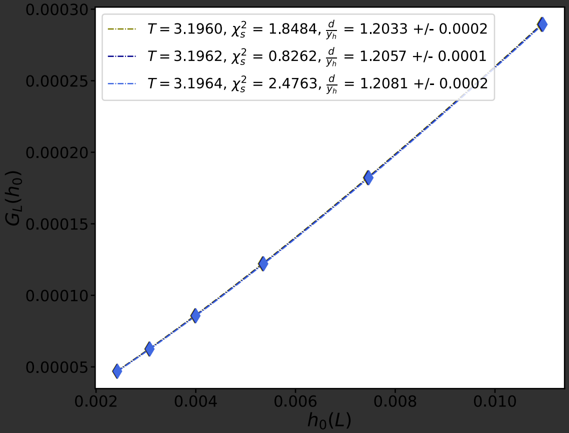


At $T = 3.1962$, the quality of the fit is good.

The Blume-Capel model in $3D$: critical point

FSS - Density of the LY zeros

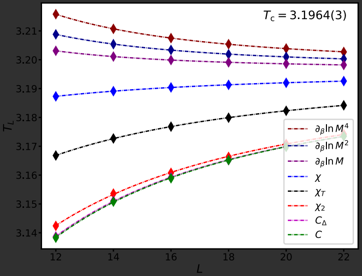
$$G_L(h_0) \sim a_1 h_0^{d/y_h} + a_3, \quad a_3 = 0 \textit{ in the vicinity of } T_c$$

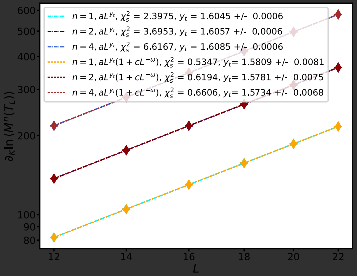


The Blume-Capel model in $3D$: critical point

FSS

$$T_L \sim T_c + aL^{-y_t}(1 + bL^{-\omega}), \qquad \partial_K \ln\langle M^n(T_L)\rangle \sim aL^{-y_t}(1 + bL^{-\omega})$$





→ Determination of T_c: The joint fit on all quantities in the left figure gives $T_c = 3.1964(3)$. $T_c = 3.1952(8)^\dagger$ obtained from the shift behavior of T_L of the C and χ peaks $(L = 8 - 24)$

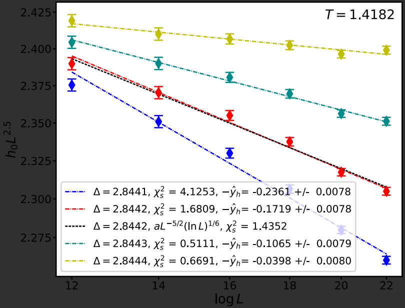
→ Determination of y_t: The best fit is for $= 1$ with corrections where $y_t = 1.5809(81)$, close to the expected value $y_t^{\text{ref}} = 1.587374(4)$

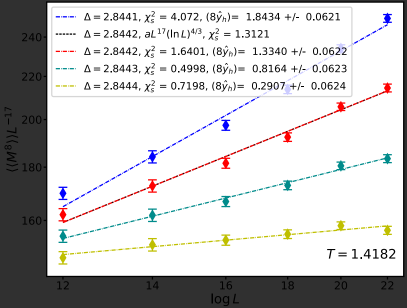
†N.G. Fytas and P.E. Theodorakis. The European Physical Journal B, vol. 86, no. 2 (2013).

The Blume-Capel model in $3D$: tricritical point

Goal: Extract the hatted exponent $\hat{y}_h$ from the LY zeros and the 8th cumulant at the estimated tricritcal temperature $T_t = 1.4182$

$$h_0 \sim L^{-5/2}(\ln L)^{-\hat{y}_h}, \quad \langle\langle M^8 \rangle\rangle \sim L^{17}(\ln L)^{8\hat{y}_h}$$





→ At $\Delta = 2.8442$, the estimated exponent $\hat{y}_h$ is really close to the expected value.

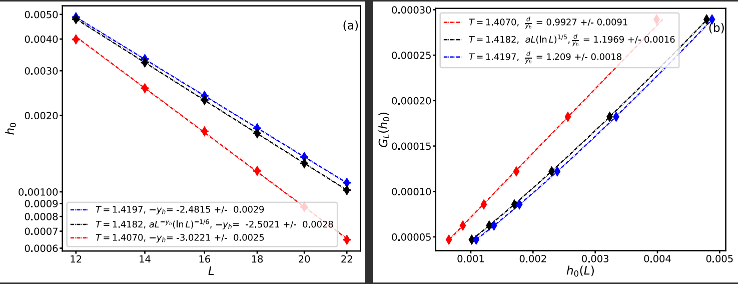
The Blume-Capel model in $3D$: Tricritical point

Observables	Reference exponent	Measured exponent	χ_s^2
h_0	$-1/6$	$-0.17(1)$	1.68
$\langle\langle M^4\rangle\rangle$	$2/3$	$0.62(3)$	1.52
$\langle\langle M^6\rangle\rangle$	1	$0.99(5)$	1.62
$\langle\langle M^8\rangle\rangle$	$4/3$	$1.33(6)$	1.64
$m(\Delta_L, T_{\rm t})$	$1/6$	$0.16(1)$	1.49

Table: A summary of the measured hatted exponents in this work at $\Delta_t = 2.8442, T_t = 1.4182$

The Blume-Capel model in $3D$: tricritical point

Goal: Let's study the crossover phenomena by studying the LY zeros near the TCP...

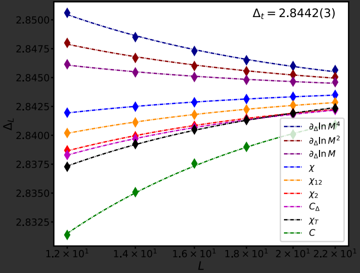


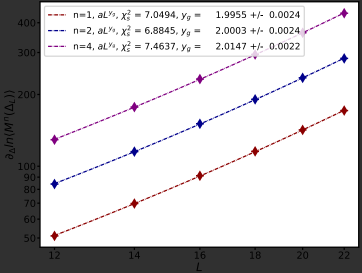
We expect

- $y_h = 2.48180(14)$ and $d/y_h = 1.2088(5)$ along the second order line.
- $y_h = 2.50$ and $d/y_h = 1.20$ at the tricritical point.
- $y_h = d = 3$ and $d/y_h = 1$ along the first order line.

The Blume-Capel model in $3D$: tricritical point

$$\Delta_L \sim \Delta_t + aL^{-y_g}(\ln L)^{\hat{y}_g}, \qquad \partial_\Delta \ln\langle M^n(\Delta_L)\rangle \sim aL^{-y_g}$$





→ Determination of Δ_t: the joint fit on all quantities in the left figure gives $\Delta_t = 2.8442(3)$. $\Delta_t = 2.8446(3)$ † obtained from the shift behavior of Δ_L of the specific-heat peaks ($L = 20 - 28$).

→ Determination of y_g: the extracted exponents are close to the expected but χ^2 is poor: fitting $\partial_\Delta \ln\langle M^n(\Delta_L)\rangle \sim aL^{-y_g}(\ln L)^{-1/3}$ improve the quality but the exponent deviates.

†J. Zierenberg, N. G. Fytas, and W. Janke, Physical Review E 91, 032126 (2015).

Conclusion

- It is possible to accurately determine the characteristics of a phase transition through small-scale numerical simulations for the 3d BC model.
- The study of the density of zeros can determine the tricritical point with precision, and the order of the transition.
- It is possible to determine the value of $\hat{y}_h$ thanks to the sensitivity of the zeros, even for small sizes.

$\rightarrow$ Next: study of the phase diagram of the 4D Blume-Capel model!

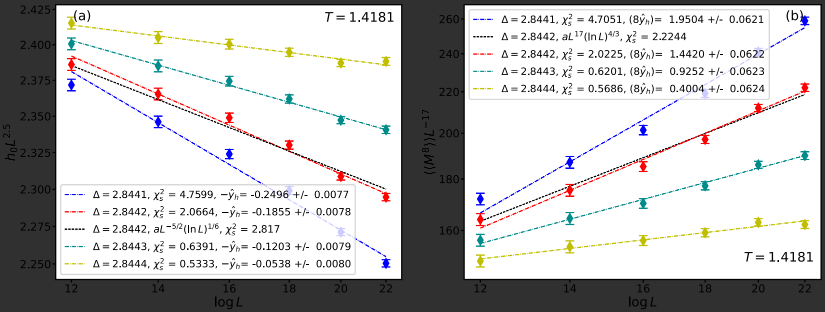
Acknowledgments

The End

The Blume-Capel model in $3D$: tricritical point

Goal: Extract the hatted exponent $\hat{y}_h$ from the LY zeros and the 8th cumulant at $T_t = 1.4181$

$$h_0 \sim L^{-5/2}(\ln L)^{-\hat{y}_h}, \quad \langle\langle M^8 \rangle\rangle \sim L^{17}(\ln L)^{8\hat{y}_h}$$



At $\Delta = 2.8442$, the estimated exponent $\hat{y}_h$ is really close to the expected value.

The Blume-Capel model in $3D$: tricritical point

Goal: Extract the hatted exponent $\hat{y}_h$ from the LY zeros and the 8th cumulant at $T_t = 1.4182$

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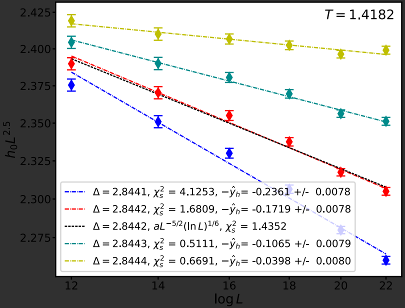

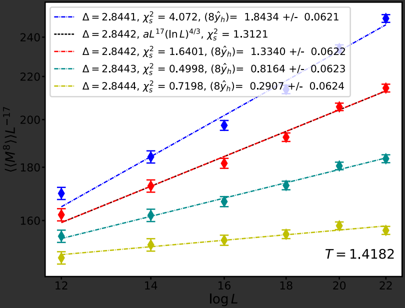

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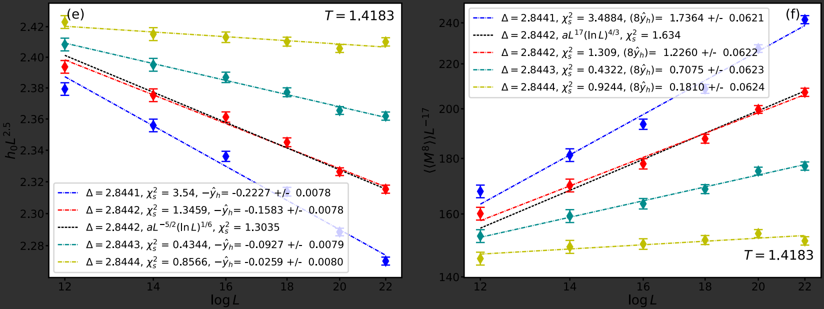
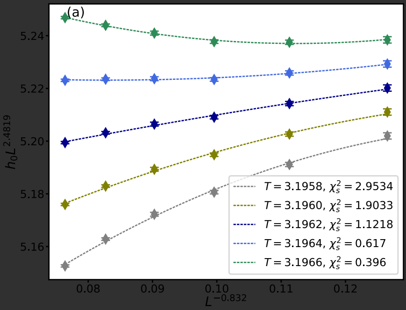


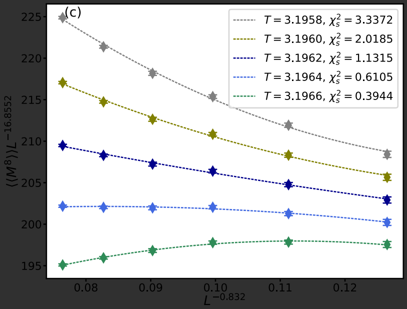
At $\Delta = 2.8442$, the estimated exponent $\hat{y}_h$ is really close to the expected value.

The Blume-Capel model in $3D$: critical point

Goal: At the critical point, the goal is to locate accurately the location of the transition.

$$h_0 \sim L^{-2.4819} a(1+bL^{-0.832}+cL^{-2(0.832)}), \;\; \langle\langle M^8 \rangle\rangle \sim L^{16.8552} a(1+bL^{-0.832}+cL^{-2(0.832)})$$





At $T = 3.1962$, the quality of the fit is really good.