Multiple universalities in order-disorder magnetic phase transitions

H. D. Scammell and O. P. Sushkov
School of Physics, The University of New South Wales, Sydney, NSW 2052, Australia
(Dated: November 15, 2018)

Phase transitions in isotropic quantum antiferromagnets are associated with the condensation of bosonic triplet excitations. In three dimensional quantum antiferromagnets, such as TiCuCl₃, condensation can be either pressure or magnetic field induced. The corresponding magnetic order obeys universal scaling with thermal critical exponent \( \phi \). Employing a relativistic quantum field theory, the present work predicts the emergence of multiple (three) universalities under combined pressure and field tuning. Changes of universality are signalled by changes of the critical exponent \( \phi \). Explicitly, we predict the existence of two new exponents \( \phi = 1 \) and \( \phi = 1/2 \) as well as recovering the known exponent \( \phi = 3/2 \). We also predict logarithmic corrections to the power law scaling.

PACS numbers: 64.70.Tg, 74.20.De

Pressure and magnetic field induced condensate phases in quantum magnetic systems have become instrumental to our understanding of universal, critical-phenomena. A great effort (experimental, numerical and theoretical) has been devoted to uncovering and categorising the universal features of critical magnetic condensate phases. The present work considers three dimensional (3D) quantum antiferromagnets (QAF), where the combined interplay between pressure, magnetic field and temperature \( (p,B,T) \) remains theoretically unexplored, yet offers an exiting arena for theorists and experimentalists alike to uncover new universal behaviour. In Figure 1 we present the generic phase diagrams of dimerised QAFs such as TiCuCl₃, KCuCl₃, and CsFeCl₃. Panel (a) shows the magnon Bose condensation (BEC) line in the field-pressure diagram, and panel (b) shows the antiferromagnetic (AFM) transition line in the temperature-pressure diagram. It is also instructive to look at Figure 2 which shows the 3D \( (p,B,T) \) phase diagram. The point of primary interest is the critical field-critical temperature power law,

\[
a : \delta B_{BEC} \sim T^{\phi}, \quad b : \delta T_N \sim B^{1/\phi},
\]

The shift of the BEC transition line at small temperature is shown schematically in Fig. 1a; while the shift of the AFM/Néel transition line at small field is in Fig. 1b.

It is widely believed that at \( p < p_c, \phi = 3/2 \) is the universal BEC exponent, which can be obtained from the scaling arguments on the dilute Bose gas [1,2] or explicitly for magnon BEC [3,4]. For a review see [5]. On the other hand, experiment (on TiCuCl₃ and KCuCl₃ [6,9]) and numerics [10] show \( 1.5 \leq \phi \lesssim 2.3 \), depending crucially on which temperature range is used for fitting [5,11]. We understand recent data on 3D QAF CsFeCl₃ [12], taken along the thick blue-red solid lines in Fig. 2 as a hint for a significant and unexpected evolution of the index \( \phi \) along the line.

The primary goal of the present work is to derive the evolution of the critical index \( \phi \) across the phase diagram. Another goal is to explain why the index depends on the fitting range; even if \textit{a priori} the range seems to be very narrow. We will show that answers to both questions are related to the quantum critical point \( (p,B,T) = (p_c,0,0) \). Ultimately, the quantum critical point (QCP) governs the evolution of the critical index
φ across the phase diagram. This is illustrated in Fig. 2.

Previous theoretical approaches were concentrated at the BEC transition, p < p_c. They employed a dilute Bose gas model \[4\] 5] and/or bond-operator technique \[13]. In the end, these techniques rely on the Hartree-Fock-Popov approximation, yet it is known that the Hartree-Fock-Popov approximation breaks down in the vicinity of a critical point \[14]. In the present work we employ a quantum field theory approach which naturally describes quantum critical points.

The quantum phase transition (QPT) between ordered and disordered phases is described by the effective field theory with the following Lagrangian \[15\] 16],

\[
\mathcal{L} = \frac{1}{2} (\partial_\mu \vec{\varphi} - \vec{\varphi} \times \vec{B})^2 - \frac{1}{2} (\nabla \cdot \vec{\varphi})^2 - \frac{1}{2} m_0^2 \varphi^2 - \frac{1}{4} \alpha_0 \varphi^4.
\]

(2)

The vector field \( \vec{\varphi} \) describes staggered magnetisation, \( B \) is an external applied field, and for now we set \( g J_B = 1. \)

We now briefly outline the mean-field phase transitions captured by this Lagrangian. Consider first \( B = 0 \), the pressure induced QPT results from tuning the mass term, \( m_0^2 \), for which we take the linear expansion \( m_0^2(p) = \gamma^2 (p_c - p) \), where \( \gamma^2 > 0 \) is a coefficient and \( p \) is the applied pressure. Varying the pressure leads to two distinct phases: (i) for \( p < p_c \), we have \( m_0^2 > 0 \), and the classical expectation value of the field is zero \( \varphi^2 = 0 \). This describes the magnetically ordered, antiferromagnetic phase. Varying \( m_0^2 \) from positive to negative spontaneously breaks the O(3) symmetry of the system.

Next consider non-zero \( B \) at fixed \( p < p_c \): For \( B < B_c = m_0 \), the system has O(2) symmetry, and the degeneracy of the triplet modes is lifted by Zeeman splitting. The field induced QPT results from tuning \( B > m_0 \). The condensate field is \( \varphi^2 \) determined by the order-disorder (BEC or AFM) transition line one can approach the transition starting from either the ordered or disordered phase. In this work we start from the latter; all results are derived starting from disordered phase.

There are three magnetic excitations with ladder polarisation \( \sigma = -, 0, + \). The polariation is the projection of angular momentum on the direction of magnetic field. In Figure 3 we summarise the results for the evolution of the three mode gaps through the field and pressure quantum phase transitions, separately. Explicit parameters correspond to those found in Ref. \[19\] for TlCuCl\(_3\).

![Figure 3](image-url)

**FIG. 3:** Excitation gaps \( \Delta_\sigma \): (Left) pressure driven at fixed field \( B = 0.2 \) meV and \( T = 0 \). (Right) field driven at \( p = 0 \) kbar and \( T = 1.5 \) K. Solid lines are theoretical results derived in this paper. Markers indicate experimental data for TlCuCl\(_3\) \[17\] 18].

*Beyond mean-field:* Everywhere in the text \( m_0^2 = \gamma^2 (p_c - p) \) and \( \alpha_0 \) represent the zero temperature mass tuning parameter and coupling constant without quantum fluctuation corrections. Taking into account quantum and thermal fluctuation corrections due to interaction term \( \frac{1}{4} \alpha_0 \varphi^4 \), we will denote the renormalized parameters \( m_0^2 \to m_{\Lambda, \sigma}^2 \) and \( \alpha_0 \to \alpha_\Lambda \). The explicit form for \( m_{\Lambda, \sigma}^2 = m_{\Lambda, \sigma}^2(p,T,B) \) depends on the location within the phase diagram, and polarisation \( \sigma \). Full details are presented in Supplementary Material C and D, while expressions are presented below. The strength of the coupling \( \alpha_\Lambda \) determines the strength of all interactions in the theory, and is dependent on the energy scale \( \Lambda \). Generally, the one-loop renormalized coupling takes the form \[19\] 21]

\[
\alpha_\Lambda = \frac{\alpha_0}{1 + 11 \alpha_0/(8 \pi^2) \ln(\Lambda_0/\Lambda)}.
\]

(3)

Specifically for the problem at hand, the coupling runs with scale \( \Lambda = \max\{m_{\Lambda, \sigma}, B, T\} \). Accordingly, there is just a single point on the phase diagram at which all energy scales vanish \( \Lambda \to 0 \); the quantum critical point \((p_c, 0, 0)\), see Fig. 2. At this point the coupling runs to zero \( \alpha_\Lambda \to 0 \) (asymptotic freedom). The running of the coupling constant will play an essential role in resolving our main goals/questions: Why the index \( \phi \) depends on the location within the phase diagram, and: why the expected index \( \phi = 3/2 \) in the BEC regime depends on the fitting range.

In the disordered phase the Euler-Lagrange equation with \( t \) results in the following dispersion

\[
\omega_\sigma^2 = \sqrt{k^2 + m_{\Lambda, \sigma}^2} + \sigma B.
\]

(4)

where \( m_{\Lambda, \sigma} \) is the renormalised mass. Note that the \( \sigma B \) term is not renormalised. This is a consequence of a Ward identity (Larmor theorem). While the stationary states \( \{t\} \) have a fixed ladder polarisation, technically it is more convenient to calculate fluctuation corrections in the Cartesian basis \( \vec{\varphi} = (\varphi_x, \varphi_y, \varphi_z) \). Let us denote by \( \mathcal{V} \)
the part of the Lagrangian \( \Sigma \) independent of derivatives. Then, using a Wick decoupling of the interaction term \( \frac{1}{4} \alpha_0 \varphi^4 \), in the single loop approximation we find

\[
\frac{\partial^2 \mathcal{V}}{\partial \varphi^2} = m_0^2 - B^2 + 3\alpha_0 \langle \varphi_x^2 \rangle + \alpha_0 \langle \varphi_y^2 \rangle + \alpha_0 \langle \varphi^2 \rangle \quad \frac{\partial^2 \mathcal{V}}{\partial \varphi_x^2} = m_0^2 - B^2 + \alpha_0 \langle \varphi_x^2 \rangle + 3\alpha_0 \langle \varphi_y^2 \rangle + \alpha_0 \langle \varphi^2 \rangle \\
\frac{\partial^2 \mathcal{V}}{\partial \varphi_y^2} = m_0^2 + \alpha_0 \langle \varphi_x^2 \rangle + \alpha_0 \langle \varphi_y^2 \rangle + 3\alpha_0 \langle \varphi^2 \rangle
\]

where \( \langle \varphi_x^2 \rangle \) is the loop integral over the Green’s function of field \( \varphi_x \). An explicit calculation shows \( \langle \varphi_x^2 \rangle = \langle \varphi_y^2 \rangle \), hence from equations (5), we have rather trivially satisfied the O(2) Ward identity:

\[
\frac{\partial^2 \mathcal{V}}{\partial \varphi_x^2} - \frac{\partial^2 \mathcal{V}}{\partial \varphi_y^2} = 0.
\]

Further details are presented in Supplementary Material A and B.

Quantum corrections corresponding to (5) come from the scale \( \Lambda < q < \Lambda_0 \). Hence they must be accounted via single loop renormalization group (RG). The thermal part of (5) comes from \( q \sim T \), hence here the simple single loop approximation is sufficient. All in all, calculations presented in Supplementary Material D give

\[
\frac{\partial^2 \mathcal{V}}{\partial \varphi_i^2} = m_{\Lambda,\pm}(T) - B^2 \\
\frac{\partial^2 \mathcal{V}}{\partial \varphi_x^2} = m_{\Lambda,0}(T)
\]

where \( \varphi_i = \{ \varphi_x, \varphi_y \} \), and the renormalised masses are

\[
m_{\Lambda,\pm}^2 = m_0^2 \left[ \frac{\alpha_\Lambda}{\alpha_0} \right]^{\frac{1}{2}} + \Sigma_T \\
m_{\Lambda,0}^2 = m_0^2 \left[ \frac{\alpha_\Lambda}{\alpha_0} \right]^{\frac{1}{2}} + \alpha_\Lambda \sum_k \frac{1}{\omega_k^0} \left( n(\omega^+_k) + n(\omega^-_k) + 3n(0) \right)
\]

\[
\Sigma_T = \alpha_\Lambda \sum_k 1/\omega_k^0 \left( 2n(\omega^+_k) + 2n(\omega^-_k) + n(0) \right).
\]

Here \( n(\omega_k) = 1/(\sqrt{\omega_k^2 - T^2}) - 1 \), and we introduce the function \( \Sigma_T \) for brevity. Obviously, expansions of Eq.’s (7) in powers of \( \Lambda \) contain only even powers. Interestingly these expansions are different for \( m_{\Lambda,\pm} \) and \( m_{\Lambda,0} \). Therefore the relation \( \omega^+_k - \omega^-_k = \omega^0_k - \omega_k^0 \), which is exact at \( T = 0 \), does not hold at non-zero \( T \). At non-zero \( T \) the relation is valid only up to the linear in \( B \) approximation.

In a magnetic field, the condition of condensation follows from Eq. (4), \( m_{\Lambda,\pm} - B = 0 \). Using (7) this equation can be rewritten as

\[
\Sigma_T = B^2 - m_0^2 \left[ \frac{\alpha_\Lambda}{\alpha_0} \right]^{\frac{1}{2}} + \omega_0^2
\]

There are three distinct cases: (I) Above the critical pressure, \( p = p_c \); (II) below the critical pressure, when \( T_c = T_{N-critical} \). At zero magnetic field, the critical temperature in case (I), Eq. (8), is identical to the equation for the Néel temperature derived in Ref. [19].

Consider case (I): \( p > p_c \). In this case according to Eq. (11) the Néel temperature varies in a weak magnetic field. To calculate \( \Sigma_T \) at \( B \to 0 \) we take the critical line dispersions \( \omega^+_k = \omega^-_k = \omega_k^0 = k \). Hence \( \Sigma_T = \frac{2\pi k^2}{\alpha_\Lambda} T^2 \), where \( T = T_{NO} + \delta T_N \). \( T_{NO} \) is the Néel temperature in zero magnetic field. Hence using Eq. (8) we find

\[
(I) : \quad \delta T_N = \frac{6}{5\alpha_\Lambda} \frac{B^2}{T_{NO}} \quad \text{at} \ B \ll T_{NO}.
\]

So the critical index in Eq. (11) is \( \phi = 1/2 \).

In Ref. [19] the set of parameters describing \( TiCuCl_3 \) was determined

\[
p_c = 1.01 \text{ kbar}, \quad \gamma = 0.68 \text{ meV/kbar}^{1/2}, \quad \frac{\alpha_0}{8\pi} = 0.23, \quad \Lambda_0 = 1 \text{ meV}.
\]

When fitting experimental data in Ref. [19] the thermal line-broadening had been accounted via \( \omega = k \to \omega = \sqrt{k^2 + \xi^2 T^2} \), \( \xi = 0.15 \). Therefore, if we use the set of parameters (10) to determine the value of the running coupling constant \( \alpha_\Lambda \), Eq. (10), the coefficient in (9) has to be corrected accordingly: \( \frac{\alpha_\Lambda}{8\pi} \to 1.14 \frac{\alpha_\Lambda}{8\pi} \). In Fig. 4 we illustrate Eq.(9) by dashed yellow line originating from \( T_{NO} = 2.8 \text{K} \). The coupling constant is \( \alpha_\Lambda/8\pi = \alpha_{T_{NO}}/8\pi = 0.107 \). For comparison, the solid blue line originating from 2.8K represents exact solution of Eq.(8) with coupling constant running along the line.

Consider case (II); tuning exactly to the quantum critical point, \( p = p_c \), \( T_{NO} = 0 \). Again, to calculate \( \Sigma_T \) at \( B \to 0 \) we have to take the critical line dispersions \( \omega^+_k = \omega^-_k = \omega_k^0 = k \) and hence again \( \Sigma_T = \frac{2\pi^2 k^2}{\alpha_\Lambda} T^2 \). Substitution into (8) gives

\[
(II) : \quad B_c = \sqrt{\frac{4\alpha_\Lambda}{\pi^2}} \frac{T}{12} \quad \text{at} \ B_c \ll T.
\]

The condition \( B_c \ll T \) is satisfied at sufficiently low temperatures since the coupling constants decays logarithmically, \( \alpha_\Lambda \propto 1/\ln \left( \frac{2\pi k}{\Delta} \right) \). Hence in this case (II), the critical index of Eq. (11) is \( \phi = 1 \), and we find that, in addition to the exponent, there is nontrivial logarithmic scaling. In Fig. 4 we illustrate the asymptotic (11) by dashed yellow line originating from \( B = T = 0 \). The solid blue line originating from the same point represents exact solution of Eq.(8).

Finally we consider the BEC case (III), \( p < p_c \). In this case only the \( \omega^-_k \) dispersion branch is critical, \( \omega^-_k \approx \frac{k^2}{2\Delta} \), where \( \Delta = 0 \) is the gap at \( B = 0 \). The other two branches are gapped. Calculation of \( \Sigma_T \) gives \( \Sigma_T = \alpha_{\Lambda,\pm} \frac{c(3/2)}{\pi \sqrt{2\pi}} \sqrt{\Delta} T^{3/2} \), where \( \zeta \) is Riemann’s \( \zeta \)-
The set of parameters (10) was determined in Ref. [19]. In Fig. 4 we plot the predicted critical field in TlCuCl₃ vs temperature at various pressures. For comparison in Fig. 5 we present a similar experimental plot for quantum antiferromagnet CsFeCl₃ published very recently [12]. Unfortunately we cannot perform exact quantitative calculations (including all pre-factors) for CsFeCl₃. Existing data for this compound are not sufficient to perform analysis similar to [19] for TlCuCl₃. However, the data [12] supports the proposed multiple critical exponent theory.

In summary, employing a quantum field theoretic approach, our work predicts multiple critical exponents, and their corresponding logarithmic corrections, on the pressure, magnetic field and temperature - phase diagram for 3D quantum antiferromagnets in vicinity of the quantum critical point. For TlCuCl₃ we demonstrate remark-
able agreement with existing data, and provide quantitative predictions for future experiments. We also resolve the long standing problem relating to the observed critical exponent in Bose-Einstein condensation of magnons.

We thank Christian Rüegg for a very important, stimulating discussion and Yaroslav Kharkov for drawing our attention to Ref. [12]. The work has been supported by the Australian Research Council grant DP160103630.

[1] M. P. A. Fisher, P. B. Weighman, G. Grinstein and D. S. Fisher, Phys. Rev. B 40 546 (1988).
[2] D. I. Uzunov: Physics Letters 87A (1981) 11.
[3] T. Giamarchi and A. M. Tsvelik, Phys. Rev. B 59, 11398 (1999).
[4] T. Nikuni, M. Oshikawa, A. Oosawa, and H. Tanaka Phys. Rev. Lett. 84, 5868 (2000).
[5] N. Kawashima, J. Phys. Soc. Jpn. 74, pp. 145-150 (2005)
[6] W. Shiramura, K. Takatsu, H. Tanaka, K. Kamishima, M. Takahashi, H. Mitamura, and T. Goto, J. Phys. Soc. Jpn. 66, 1900 (1997).
[7] T. Kato, K. Takatsu, H. Tanaka, W. Shiramura, M. Mori, K. Nakajima, and K. Kakurai, J. Phys. Soc. Jpn. 67, 752 (1998); A. Oosawa, T. Takamatsu, K. Tatani, H. Abe, N. Tsujii, O. Suzuki, H. Tanaka, G. Kido, and K. Kindo, Phys. Rev. B 66, 104405 (2002).
[8] A. Oosawa, M. Ishii, and H. Tanaka, J. Phys. Condens. Matter 11, 265 (1999); N. Cavadini, G. Heigold, W. Henggeler, A. Furrer, H.-U. Güdel, K. Krämer, and H. Mutka, Phys. Rev. B 63, 172414 (2001); Ch. Rüegg, N. Cavadini, A. Furrer, H.-U. Güdel, K. Krämer, H. Mutka, A. Wildes, K. Habicht, and P. Vorderwisch, Nature (London) 423, 62 (2003).
[9] H. Tanaka, A. Oosawa, T. Kato, H. Uekusa, Y. Ohashi, K. Kakurai and A. Hoser, J. Phys. Soc. Jpn. 70, 939 (2001).
[10] S. Wessel, M. Olshanii, and S. Haas, Phys. Rev. Lett. 87, 206407 (2001).
[11] O. Nohadani, S. Wessel, B. Normand, and S. Haas, Phys. Rev. B 69, 220402(R) (2004)
[12] N. Kurita and H. Tanaka Phys. Rev. B 94, 104409 (2016).
[13] Jesko Sirker, Alexander Weiße and Oleg P. Sushkov, J. Phys. Soc. Jpn. Vol. 74 (2005) Suppl. pp. 129?134
[14] For a review see H. Shi and A. Griffin: Phys. Reports 304 (1998) 1.
[15] S. Sachdev, Quantum Phase Transitions (Cambridge Univ. Press, 2011).
[16] Y. Kulik and O. P. Sushkov, Phys. Rev. B 84, 134418 (2011).
[17] Ch. Rüegg, N. Cavadini, A. Furrer, K. Krämer, H.-U. Güdel, P. Vorderwisch, and H. Mutka, Appl. Phys. A 74, S840 (2002).
[18] Ch. Rüegg, N. Cavadini, A. Furrer, H.-U. Güdel, K. Krämer, H. Mutka, A. Wildes, K. Habicht, and P. Vorderwisch, Nature 423, 62 (2003).
[19] H. D. Scannell and O. P. Sushkov, Phys. Rev. B 92, 220401(R) (2015).
[20] Due to a small anisotropy, the g-factor slightly depends on the direction of magnetic field with respect to the crystal axes. We use BEC data with magnetic field directed as per experiment.
[21] J. Zinn-Justin. Quantum Field Theory and Critical Phenomena (Oxford University Press, Oxford, 2002).
[22] A. Oosawa, H. Aruga Katori, and H. Tanaka, Phys. Rev. B 63, 134416 (2001).
[23] Y. Shindo and H. Tanaka: J. Phys. Soc. Jpn. 73 (2004) 2642.
[24] Ch. Rüegg, B. Normand, M. Matsumoto, A. Furrer, D. F. McMorrow, K. W. Krämer, H. U. Güdel, S. N. Gvasaliya, H. Mutka, and M. Boehm, Phys. Rev. Lett. 100, 205701 (2008).
[25] F. Yamada, T. Ono, H. Tanaka, G. Misguich, M. Oshikawa, and T. Sakakibara, J. Phys. Soc. Jpn. 77, 013701 (2008).