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Quantum Lifshitz Field Theory of a Frustrated Ferromagnet

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We propose a universal non-linear sigma model field theory for one dimensional frustrated ferromagnets, which applies in the vicinity of a "quantum Lifshitz point", at which the ferromagnetic state develops a spin wave instability. We investigate the phase diagram resulting from perturbations of the exchange and of magnetic field away from the Lifshitz point, and uncover a rich structure with two distinct regimes of different properties, depending upon the value of a marginal, dimensionless, parameter of the theory. In the regime relevant for one dimensional systems with low spin, we find a metamagnetic transition line to a vector chiral phase. This line terminates in a critical endpoint, beyond which there is at least one multipolar or "spin nematic" phase. We show that the field theory is asymptotically exactly soluble near the Lifshitz point.

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The study of order in all its variety anchors the field of condensed matter physics. Some current goals at the vanguard of this enterprise include characterizing "hidden" orders, determining the mechanism behind "competing" or "intertwined" orders, and understanding quantum phase transitions between different orders. These problems arise in diverse systems ranging from frustrated quantum magnets to correlated electron materials like the cuprates.

Here we describe a unification of the three above themes in a tangible context within quantum magnetism. Specifically, we study a *quantum Lifshitz* transition between a ferromagnet and a spiral magnet or quantum paramagnet, which is realized for example in the well-studied Frustrated Ferromagnetic Heisenberg Chain (FFHC):

$$H_{FFHC} = \sum_n \left[-\boldsymbol{S}_n \cdot \boldsymbol{S}_{n+1} + \beta \boldsymbol{S}_n \cdot \boldsymbol{S}_{n+2} - h S_n^z\right]. \quad (1)$$

With increasing frustration β, Eq. (1) has a Lifshitz point at $\beta = 1/4$, $h = 0$. Numerical studies of the FFHC have previously demonstrated that metamagnetism and a rich sequence of *multipolar* phases – a type of hidden order which does not appear in spin-spin correlation functions – appear in the vicinity of this point for non-zero applied magnetic field h. The simplest of these phases is the (spin) angular momentum $p = 2$ multipole, or quadrupolar state, also known as a spin nematic, which breaks spin rotational symmetry but preserves invariance with respect to time reversal [1]. As such, the spin nematic is characterized by an order parameter bilinear in the microscopic spins. It can be understood as a state of bound, condensed pairs of magnons[2–8]. The spin nematic has been sought experimentally in a number of quasi-one-dimensional materials which approximately realize the FFHC [9–16].

Theoretically, the proliferation of multipolar phases with $p \geq 2$ near the Lifshitz point in the FFHC is most extraordinary, and begs theoretical explanation. We provide a universal theory for the Lifshitz point, formulated as a non-relativistic Non-Linear Sigma Model (NLSM) with dynamic critical exponent $z = 4$. An asymptotically exact analytic solution of the Lifshitz NLSM produces the line of the first-order metamagnetic transitions which terminate at the metamagnetic endpoint, beyond which the transition from the saturated state turns continuous. We demonstrate that at least the $p = 2$ nematic phase is described by the NLSM, and speculate that higher multipoles may also be captured in the same framework.

Lifshitz non-linear sigma model: Instead of focusing on a specific microscopic model such as the FFHC in Eq. (1), we introduce a universal quantum field theory description which is based on translational symmetry and SU(2) spin-rotation invariance. Since we are interested in continuous transitions out of a ferromagnet, whose magnetization is O(1) and quantized given SU(2) symmetry, we expect that locally there is a (possibly fluctuating) magnetization, even close to and on both sides of the quantum critical point. Hence we propose that the low-energy properties of the system are described by a non-linear sigma model (NLsM) formulated in terms of unit vector $\hat{m} = (\hat{m}_1, \hat{m}_2, \hat{m}_3)$ which describes magnetization density. The action is

$$S = \int dx d\tau \big\{ is\mathcal{A}_B[\hat{m}] - \delta|\partial_x \hat{m}|^2 + \kappa|\partial_x^2 \hat{m}|^2 + \lambda|\partial_x \hat{m}|^4 - h\hat{m}_3 \big\}. \quad (2)$$

Here s is the spin and $\mathcal{A}_B$ is the Berry phase term describing those spins. It can be written in various ways, for example [17],

$$\mathcal{A}_B = \int_0^1 du\, \hat{m} \cdot \partial_\tau \hat{m} \times \partial_u \hat{m} = \frac{\hat{m}_1 \partial_\tau \hat{m}_2 - \hat{m}_2 \partial_\tau \hat{m}_1}{1 + \hat{m}_3}, \quad (3)$$

where we introduced a fictitious auxiliary coordinate u such that $\hat{m}(u = 0) = \hat{z}$ and $\hat{m}(u = 1) = \hat{m}$ is the physical value. The main important point is that $\mathcal{A}_B$ contains a single derivative with respect to imaginary time τ.

The action S contains all leading terms in gradients of $\hat{m}$. The parameter δ ($\propto \beta - 1/4$ in the FFHC) tunes the zero field criticality: a trivial fully ordered ferromagnetic (FM) state with constant $\hat{m}$ and no fluctuations obtains for $\delta < 0$, while the system is non-trivial for $\delta > 0$. The absence of fluctuations for $\delta < 0$ is due to the $\mathcal{A}_B$ term, which makes the dynamics completely different from the commonly studied relativistic NLsM's. Further, note that there are two terms, κ and λ, quartic in derivatives, which is crucial in the following. The λ term has been ignored in previous field theoretic approaches[18, 19].

The action (2) needs a condition for stability against large gradients of $\hat{m}$. Starting from constraint $\hat{m}\cdot\hat{m}=1$, it is easy to obtain $|\partial_x^2\hat{m}|^2 > |\partial_x\hat{m}|^4$, which is enough to show stability is present so long as $\lambda+\kappa>0$. This means *negative* λ in (2) is allowed so long as $\lambda > -\kappa$.

The action describes several distinct dynamical regimes. For $\delta<0$, the excitations above the ground states are quadratically dispersing spin waves, $\omega \sim k^z$, characterized by the dynamical critical exponent $z=2$, which is easily seen by equating the linear τ derivative in $\mathcal{A}_B$ with the second spatial derivative in the δ term. For $\delta=0$, the dynamics changes to $z=4$. For $\delta>0$, the theory is more non-trivial, and there is even a $z=1$ regime (see below).

Asymptotic solubility: Physically, the absence of fluctuations in the FM state suggests a saddle point approximation may apply near to it. Indeed, a simple rescaling $x\to\sqrt{\kappa/\delta}\,x'$ and $\tau\to\kappa\tau'/\delta^2$ transforms the action into suggestive form (we defined $v=-\lambda/\kappa$ and $h'=h\kappa/\delta^2$)

$$S=\sqrt{\frac{\kappa}{\delta}}\int dx'd\tau'\,\{is\mathcal{A}'_B[\hat{m}]-\mathrm{sign}(\delta)|\partial_{x'}\hat{m}|^2+|\partial_{x'}^2\hat{m}|^2 -v|\partial_{x'}\hat{m}|^4-h'\hat{m}_z\}, \quad (4)$$

which shows that near the critical point, when $\delta/\kappa \ll 1$, the action is large in dimensionless terms so that a saddle point analysis becomes asymptotically correct on approaching the Lifshitz point. Because $|\delta|$ appears only in the prefactor of the action in Eq. (4), the phase diagram at the saddle point level and only the dimensionless parameters v and h' control the saddle point. Note that $v<1$ defines the stability region of the theory.

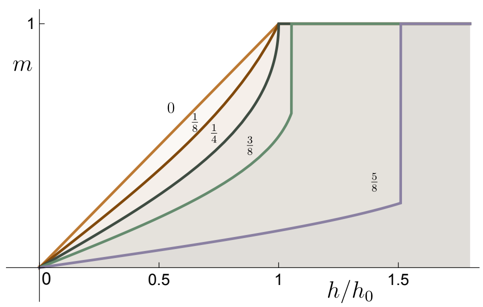

FIG. 1. Saddle point result for the magnetization $m(h)$ for different values of interaction parameter v, which is shown next to each curve.

The saddle point of Eq. (2) with minimum action describes a cone (umbrella) state:

$$\hat{m}_{\mathrm{sp}}=(\varphi\cos qx,\varphi\sin qx,\sqrt{1-\varphi^2}), \quad (5)$$

with $0\le\varphi\le 1$ and q functions of the parameters of the action. Solutions with both sign of q are degenerate, which reflects spontaneous breaking of reflection symmetry and chiral order: $\hat{z}\cdot\hat{m}_{\mathrm{sp}}\times\partial_x\hat{m}_{\mathrm{sp}}=\varphi^2 q\neq 0$. For sufficient large field, $h>h_c$, the solution is simply the ferromagnetic one, with $\varphi=0$. On reducing the field, there are two possible behaviors. For $\lambda>-\kappa/4$ ($v<1/4$), a continuous transition occurs at the critical field $h_c=h_0=\delta^2/(2\kappa)$. The "order parameter" φ, which represents the local moment transverse to the magnetic field, increases smoothly from zero below h_0. This corresponds to the point of local instability of the FM phase to single magnons, which Bose condense when their energy vanishes at h_0. For $\lambda<-\kappa/4$ ($v>1/4$), the transition occurs discontinuously at $h_c>h_0$, at which point the ferromagnetic state is still locally stable. The order parameter jumps to a non-zero value φ_c for $h=h_c-0^+$. This is a metamagnetic transition, described by

$$\varphi_c^2=\frac{2\sqrt{v}-1}{v}, h_c=\frac{\delta^2}{8\kappa\sqrt{v}(1-\sqrt{v})}, q_c^2=\frac{\delta}{4\kappa(1-\sqrt{v})}, \quad (6)$$

which hold for $1/4<v<1$. Due to the aforementioned scale invariance, the metamagnetic line extends for all δ at the saddle point level. The saddle point gives direct predictions for experiment such as the magnetization $m=\sqrt{1-\varphi^2}$ shown in Fig. 1.

Quantum corrections: Fluctuations beyond the saddle point have several types of effects. One innocuous effect is that of phase fluctuations within the "cone phase": configurations of form of Eq. (5) with $qx\to qx+\theta$ have small action when $\theta(x,\tau)$ has small space-time gradients. Fluctuations of θ are thereby described by a free $z=1$ boson theory with central charge $c=1$, which converts the long-range cone order into power-law spin correlations, but preserves the chiral order. These properties characterize a "vector chiral" phase (VC), identified previously in the FFHC.

A more drastic effect of fluctuations is to move the phase boundaries and even introduce new phases. We show below that quantum fluctuations lower the energy difference between the cone and FM states, eventually inducing a metamagnetic endpoint. To proceed, we write the magnetization $\hat{m}$ in the *co-moving* system of coordinates

$$\hat{m}=\sqrt{2-\frac{\bar{\eta}\eta}{s}}[\frac{\bar{\eta}+\eta}{2\sqrt{s}}\hat{e}_1+i\frac{\bar{\eta}-\eta}{2\sqrt{s}}\hat{e}_2]+(1-\frac{\bar{\eta}\eta}{s})\hat{e}_3, \quad (7)$$

where the rotating dreibein $\hat{e}_j(x)$ are chosen as follows: $\hat{e}_1\times\hat{e}_2=\hat{e}_3\equiv\hat{m}_{\mathrm{sp}}$. The fields $\bar{\eta},\eta$ describe magnons, transverse fluctuations of the magnetization. To quadratic order the action in Eq. (2) becomes $S=\int d\tau\left[\int dx\,\bar{\eta}\partial_\tau\eta+H_{\mathrm{fluct}}\right]$, which shows that $\bar{\eta},\eta$ are canonical Bose operators, and $H_{\mathrm{fluc}}(\bar{\eta},\eta)$ is a Hamiltonian. Fourier transforming it into momentum space shows that H_{fluc} contains both normal and anomalous terms:

$$H_{\mathrm{fluc}}=\sum_k 2A_k\bar{\eta}_k\eta_k+B_k(\eta_k\eta_{-k}+\bar{\eta}_k\bar{\eta}_{-k}). \quad (8)$$

Here coefficients A_k,B_k are functions of momentum k and depend on parameters δ,κ,v,h and φ of the saddle point action. Diagonalization of (8) with the help of a standard Bogoluiubov transformation gives us the desired correction: the zero-point energy $\delta\mathcal{E}_{\rm cone} = \frac{1}{N}\sum_k\{\sqrt{A_k^2 - B_k^2} - A_k\}$.

We use this corrected energy to identify a metamagnetic endpoint. A metamagnetic endpoint occurs at $\delta = \delta_c$ if, for $\delta > \delta_c$, the cone state remains higher in energy than the FM state for all $h \geq h_0$, while for $\delta < \delta_c$, the cone state has lower energy than the FM one for some range of fields $h_0 < h < h_c$. Hence the endpoint is determined by the condition that the energy of the cone state equals that of the FM state at $h = h_0$, i.e. $\Delta E = \Delta\mathcal{E} - \delta\mathcal{E}_{\rm cone} = 0$ at $h = h_0$ where the first term $\Delta\mathcal{E} = \mathcal{E}_{FM} - \mathcal{E}_{\rm cone}$ represents the saddle point energy difference, and the last is the Bogoliubov correction.

Before analyzing this in detail, we note that from Eq. (4), the fluctuation corrections to the energy are expected to be reduced from the saddle point value by a factor of $\sqrt{\delta/\kappa}$, which is assumed small for consistency of the approach. Hence they can affect the balance between cone and FM states only when the energy difference between the two is already small at the saddle point level. Therefore we now focus on the regime close to the onset of metamagnetism, and let $v = 1/4 + \epsilon$ in what follows, with $\epsilon \ll 1$. In this limit, $\Delta\mathcal{E}(h_0) = \frac{256}{27}\kappa\epsilon^3(\delta/\kappa)^2$.

The fluctuation correction $\delta\mathcal{E}_{\rm cone}$ contains a regular cutoff-dependent part and a singular universal term. The former may be absorbed into a renormalized coupling $v \to \tilde{v}$ and likewise ϵ. The latter represents a physically distinct contribution to the cone state energy. For the lattice FFHC it was obtained previously in [20]. We obtain $\delta\mathcal{E}^{\rm sing}_{\rm cone} = s^{-1}\int_{-\infty}^{\infty}\frac{dk}{2\pi}\frac{100\delta^3\epsilon^2}{\kappa^2k^2+2\kappa\delta} = (25\sqrt{2}/s)\kappa\epsilon^2(\delta/\kappa)^{5/2}$.

Now combining the saddle point and corrections, we find that the total energy $\Delta E = \Delta\mathcal{E}(h_0) - \delta\mathcal{E}^{\rm sing}_{\rm cone}$ is seen to change sign at $\delta_c \approx 0.07\kappa s^2\epsilon^2$, indeed indicating a metamagnetic endpoint. Since $\delta_c \ll 1$ with $\epsilon \ll 1$, this is within the regime of validity of the field theory.

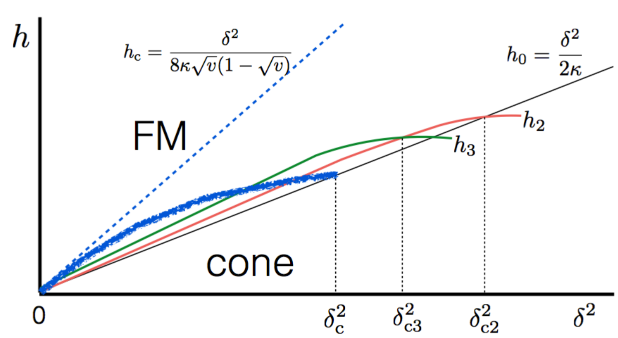

FIG. 2. Stability curves (schematic). The thin dashed (blue) line shows the critical h_c field of the first order transition within the classical saddle point approximation. The wide brushed (blue) line indicates h_c as modified by quantum fluctuations. It crosses the thin (black) single-magnon instability field h_0 at $\delta = \delta_c$. The red (green) solid lines denote the critical magnetic fields $h_2(h_3)$ describing two-(three-) magnon condensation instabilities. The $h_3(\delta)$ curve is a conjecture.

Quantum few-body physics: Considering the above result, we see that for $\delta > \delta_c$, the effective attraction between magnons is too weak to induce collapse. Nonetheless, here we argue that it still is strong enough to produce bound states of a finite number of magnons, which leads to distinct multipolar phases in a range $\delta_c < \delta < \delta_{c2}$, that set in at $h > h_0$.

As we consider larger δ, the semiclassical analysis becomes inadequate, and a full quantum treatment of the action in Eq. (2) becomes necessary, which is daunting due to its non-polynomial nature (implicit in the NLsM constraint). In principle, by using Eq. (7) with $\hat{e}_\mu = \hat{x}_\mu$, one can expand and truncate the action to $\mathcal{O}(\eta^{2n})$ for an exact treatment of n-magnon states, since higher order terms, if properly normal-ordered, annihilate these states. This leads to a quantum Hamiltonian for bosonic fields $\overline{\eta}, \eta$ with an unconventional kinetic energy and up to n-body momentum dependent interactions. Due to the complexity of this problem, we have limited ourselves to the $n = 2$ case. This expansion yields

$$H = \sum_k \epsilon_k\overline{\eta}_k\eta_k + \frac{1}{2L}\sum_{kpp'} V(k,p,p')\overline{\eta}_{k/2+p}\overline{\eta}_{k/2-p}\eta_{k/2-p'}\eta_{k/2+p'}, \tag{9}$$

with $\epsilon_k = (h + 2\kappa k^4 - 2\delta k^2)/s$ and $V(k,p,p')$ in [21].

One can gain some insight by focusing on the minima of ϵ_k, which occur at $k = \pm q$, with $q = \sqrt{\delta/(2\kappa)}$. We therefore define new fields $\psi_{a,k} = \eta_{(2a-3)q+k}$ for $|k| \ll q$ and $a = 1, 2$. Then, Fourier transforming back to real space, one obtains, *assuming all the scattered magnons remain near the two minima*,

$$H = \int dx \left\{ \sum_{a=1}^{2}\overline{\psi}_a(\epsilon_0 - \frac{\partial_x^2}{2m})\psi_a + \frac{1}{2}\gamma_1\left[(\overline{\psi}_1\psi_1)^2 + (\overline{\psi}_2\psi_2)^2\right] + \gamma_2\overline{\psi}_1\psi_1\overline{\psi}_2\psi_2 \right\}, \tag{10}$$

where $\epsilon_0 = h/s - \delta^2/(2\kappa s)$, $m = s/8\delta$, $\gamma_2 = \delta^2(5 - 4v)/(\kappa s^2)$ and $\gamma_1 = \delta^2(1-4v)/(2\kappa s^2)$. Observe that for $v > 1/4$, when the saddle point analysis found metamagnetism, the *intra*-valley interaction γ_1 is negative, i.e. *attractive*. As is well known, bosons with attractive delta-function potential, such as described by the γ_1 term in (10), undergo collapse [20, 22, 23] – the ground state of the system is given by the N-body bound state in which all N bosons of the system participate. This collapse corresponds to the metamagnetic transition. In reality an infinite collapse is prevented by three-body interactions, and moreover the saddle point condition is renormalized with increasing δ as we found above, leading to the metamagnetic endpoint.

We can investigate renormalizations at the two-body level from Eq. (9). In particular, taking the *full* dispersion and momentum-dependent interactions, we solve the two-body Schrödinger equation for the minimum energy state. The general form for such a state is $|\psi, k\rangle = \int\frac{dq}{2\pi}\Psi(q;k)\overline{\eta}_{k/2+q}\overline{\eta}_{k/2-q}|0\rangle$, where $|0\rangle$ is the boson vacuum, i.e. the ferromagnetic state, k is the (conserved) center of mass momentum, and the two-magnon wavefunction obeys

$$(\epsilon_{k/2+p} + \epsilon_{k/2-p} - E)\Psi(p;k) + \int \frac{dp'}{2\pi} V(k,p,p')\Psi(p';k) = 0. \tag{11}$$

This equation can be solved exactly [21]. We obtain the minimum energy state for $k = \pm 2q$, which corresponds to a pair of magnons from the same minima, and find the binding energy $\epsilon_b = 2\epsilon_q - E$ given by the relation

$$\sqrt{\epsilon_b} \approx \sqrt{\epsilon_{b0}} \left[1 - \left(\frac{\delta}{\delta_{c2}} \right)^{1/2} \right] + \mathcal{O}(\delta^{5/2}), \tag{12}$$

where $\epsilon_{b0} = \epsilon^2\delta^3/(8\kappa^2 s^3)$ is just the naïve binding energy one would obtain from the delta-function interaction model, $\epsilon_{b0} = m\gamma_1^2/4$, and the term in the brackets represents the leading correction. This defines a critical value $\delta_{c2} = \frac{128}{625}\kappa s^2\epsilon^2 \approx 0.2\kappa s^2 \epsilon^2$, such that the two-magnon bound state disappears for $\delta > \delta_{c2}$.

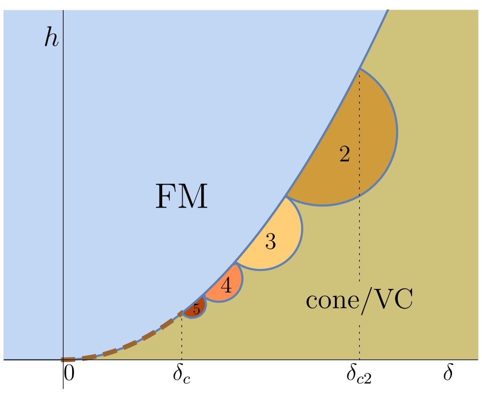

FIG. 3. Schematic phase diagram in $\delta - h$ plane. The dashed line is the metamagnetic transition emerging from the Lifshitz point at the origin. “FM” and “cone/VC” denote the fully polarized ferromagnetic and cone/vector chiral phases, respectively. Integers $n = 2, 3, 4, 5$ label multipolar phases comprised of the corresponding number of bound magnons. Phases with $n > 2$ are conjectural, and their appearance and number in the *universal* regime is an open question.

Importantly, we note that $\delta_{c2} > \delta_c$, which implies that in this interval the ferromagnetic state is unstable to two-magnon condensation for a non-zero range of fields $h > h_0$. In principle, we should now check for bound states of more than two magnons. Unfortunately, we have not been technically able to accomplish this. We speculate that in the range $\delta_c < \delta < \delta_{c2}$, bound states of increasing numbers of magnons appear with decreasing δ, at thresholds $\delta_{c,n}$, with $\delta_c < \delta_{c,n} < \delta_{c,n'}$ for $n > n'$ [24]. This would imply a sequence of distinct multipolar phases just below saturation in this intermediate range of δ, as shown schematically in Fig. 3. Note that the defining feature of the n^{th} multipolar phase is the presence of a gap for excitations with spin $S^z < n$. In one dimension, due to fluctuations, there is no true multipolar condensate, and each phase evolves smoothly from more condensate-like to spin-density-wave-like on reducing field [6, 25]. The presence of states with $n > 2$ is, as we indicated, speculative, and the physics governing the maximum n is an interesting open problem.

Microscopic calculation of v: The crucial dimensionless parameter v of the theory cannot be determined within our field theory approach. We found two ways to fix its value by comparing field theory predictions with those of complimentary microscopic calculations [21]. In the first, large spin $s \gg 1$ calculation, we use the standard spin-wave technique to calculate the leading spin-wave corrections to the ground state energy and the optimal spiral wave vector of the spin-s $J_1 - J_2$ chain. Comparing these results with the saddle point analysis, we find $v = 3/(2s)$. Hence $v < 1/4$ for large s, and thus metamagnetism occurs only for spin chains with $s < s_c = 6$, in agreement with earlier Bethe-Salpeter calculations [26, 27].

For the $s = 1/2$ chain, we match the value of the order parameter jump φ_c, (6), at the metamagnetic transition to the corresponding value of the magnetization $m_c = (\sqrt{7} - 1)/3$ reported in Ref. 20. This gives, via $m_c^2 = 1 - \varphi_c^2$, that $v_{s=1/2} = 1/(1+m_c)^2 \approx 0.42$. Given that $1/4 < v_{s=1/2} < 1$, our theory indeed predicts metamagnetism and multipolar phases for the FFHC, in agreement with numerical observations [7].

Generalizations and Outlook: The non-linear sigma model formulation can be easily extended to higher-dimensional Lifshitz points. This may provide a means to understand other frustrated ferromagnets and ferrimagnets, including possibly the kagomé lattice material volborthite [28, 29], which shows signs of nematic-like behavior below an unusually-wide $1/3$ magnetization plateau.

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[24] Note that strictly speaking the actual metamagnetic endpoint $\delta_{\rm c}^*$ is determined by the crossing of the renormalized first-order transition field $h_{\rm c}$ with $h_{\rm n_{max}}$, the field of the maximum-possible $n_{\rm max}$-complex condensation. Fig. 2 shows that $\delta_{\rm c}$ provides an upper bound on $\delta_{\rm c}^*$.

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