Geometric Frustration and Dimensional Reduction at a Quantum Critical Point

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We show that the spatial dimensionality of the quantum critical point associated with Bose-Einstein condensation at $T = 0$ is reduced when the underlying lattice comprises layers coupled by a frustrating interaction. Our theoretical predictions for the critical behavior correspond very well with recent measurements in $BaCuSi_2O_6$ [S. E. Sebastian *et al.*, Nature (London) **441**, 617 (2006)].

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The universality class of a critical point (CP) depends on a few properties such as the symmetry of the underlying model, range of the interactions, number of components of the order parameter (OP), and the space dimensionality d [1]. For highly anisotropic systems such as weakly coupled layers, the universality class changes when the system approaches the CP. A dimensional crossover takes place: the effective dimensionality is reduced *beyond* a certain distance from the CP, determined by the weak interlayer interaction. Sufficiently close to the CP the transition is, however, three dimensional. In contrast, the dimensional reduction (DR) discussed here occurs when the system *approaches* a Gaussian quantum critical point (QCP). This qualitative difference results from the nature of the interlayer coupling that vanishes right at the QCP for a chemical potential tuned Bose-Einstein condensation (BEC). We argue this effect is relevant for the field tuned QCP of a *geometrically frustrated* quantum magnet.

Although geometric frustration has previously been invoked [2] as a mechanism for DR, zero-point fluctuations are expected to restore the interlayer coupling [3], as shown by Maltseva and Coleman [4]. We show, however, that this coupling is suppressed near the BEC-QCP, relevant to spin dimer systems in a magnetic field. In this case, the spatial dimensionality of the Gaussian QCP is $d = 2$. Interactions between either thermally excited or quantum condensed bosons induce a crossover to $d = 3$ away from the QCP. Key to this result is the supression of zero-point phase fluctuations of the OP near a chemical potential tuned BEC. First experimental evidence of this phenomenon was found recently by critical exponents measurements of a field induced QCP in $BaCuSi_2O_6$ [5].

We first present rigorous results for a chemical potential tuned BEC of interacting bosons on a body-centered tetragonal (bct) lattice. Later we apply these results to $S = \frac{1}{2}$ spins forming dimers on a bct lattice, thereby offering a quantitative explanation for the observation of DR [5] in the similar $BaCuSi_2O_6$ system [6,7].

We start from the Hamiltonian of interacting bosons

$$H_B = \sum_{\mathbf{k}} (\varepsilon_{\mathbf{k}} - \mu) a^\dagger_{\mathbf{k}} a_{\mathbf{k}} + u \sum_i n_i n_i, \tag{1}$$

where $n_i = a^\dagger_i a_i$ is the local number operator of the bosons and $a^\dagger_{\mathbf{k}} = \sum_i a^\dagger_i e^{i\mathbf{k}\cdot\mathbf{R}_i}/\sqrt{N}$. The tight binding dispersion for nearest-neighbor boson hopping on the bcc lattice is

$$\varepsilon_{\mathbf{k}} = \varepsilon_{\parallel}(\mathbf{k}_{\parallel}) + 2t_{\perp}\gamma(\mathbf{k}_{\parallel})\cos k_z, \tag{2}$$

where $\mathbf{k}_{\parallel} = (k_x, k_y)$ refers to the in-plane momentum. $\varepsilon_{\parallel}(\mathbf{k}_{\parallel}) = t_{\parallel}(2 + \cos k_x + \cos k_y)$ is the in-plane dispersion, while $\gamma(\mathbf{k}_{\parallel}) = \cos\frac{k_x}{2}\cos\frac{k_y}{2}$. For $t_{\parallel}, t_{\perp} > 0$, and $t_{\parallel} > t_{\perp}/2$, a BEC takes place at $\mathbf{K}_{\parallel} = (\pi, \pi)$. Since $\gamma(\mathbf{K}_{\parallel}) = 0$, the dispersion $\varepsilon_{\mathbf{k}}$ at the condensation momentum is independent of k_z. For an ideal Bose gas ($u = 0$) this implies complete layer decoupling at $T = 0$. Only excitations at finite T with in-plane momentum away from the condensation point can propagate in the z direction. This behavior changes for finite interactions ($u > 0$). States in the Bose condensate scatter and create virtual excitations above the condensate that can propagate in the z direction and couple to condensate states in other layers [4]. The condensed state of interacting bosons is then truly 3D, even at $T = 0$.

The above argument for "dimensional restoration" due to interactions does not apply in case of chemical potential tuned BEC. In this case, the number of bosons at $T = 0$ is zero before the BEC sets in ($\mu < 0$). The absence of particles makes their interaction mute and this situation persists arbitrarily close to the QCP. While the Bose condensed state for $\mu > 0$ and the entire regime for $T > 0$ is 3D, the decoupling for ($\mu < 0$, $T = 0$) has dramatic consequences. We show that the BEC-transition temperature varies as

$$T_c \propto \mu \ln\left(\frac{t_{\parallel}}{\mu}\right) \Big/ \ln\ln\frac{t_{\parallel}}{\mu}, \tag{3}$$

whereas $T_c \propto \mu^{2/d}$ holds instead for an isotropic Bose

system in $d > 2$. Despite the fact that different layers are coupled at finite T the BEC-transition temperature, Eq. (3), depends on μ just like the Berezinskii-Kosterlitz-Thouless (BKT) transition temperature of a 2D system [8].

The one-loop renormalization group (RG) calculation used to obtain this result (analogous to Ref. [8]) shows a classical thermodynamic 3D XY transition, instead of a BKT transition. We conclude, therefore, that the $T = 0$ QCP of chemical potential tuned BEC with 3D dispersion, Eq. (2), is strictly 2D. The system then crosses over to be 3D for $\mu > 0$ or $T > 0$, where the density of bosons becomes finite and boson-boson interactions drive the crossover to $d = 3$. The transition temperature of this 3D BEC is given by the 2D result, Eq. (3). It is important to stress that the vanishing density for ($\mu < 0$, $T = 0$) implies that these results are not limited to weakly interacting bosons [9].

The detailed derivation of Eq. (3) using the RG approach will be presented in [10]. Here we present a heuristic derivation of the same result based on an approach introduced by Popov [8,11]: infrared divergencies are cutoff for momenta $k < k_0 \simeq \sqrt{\mu/t_\parallel}$. We analyze the interacting Bose system in the disordered phase and perform an expansion in the interlayer hopping amplitude $t_\perp/t_\parallel$. Dominant interactions at low density are given by ladder diagrams [see Fig. 1(a)], yielding a renormalized boson interaction [12]:

$$v_0^{-1} = \frac{1}{4}\int_{k_0} \frac{d^2k_\parallel}{4\pi^2 \varepsilon_\parallel(\mathbf{k}_\parallel)} \propto \frac{\ln k_0^{-1}}{t_\parallel}, \tag{4}$$

for $u \to \infty$ (hard-core bosons). The bare interlayer coupling leads to scattering of bosons between different layers. The corresponding scattering matrices between neighboring layers, v_1 [see Fig. 1(b)], and second neighbor layers, v_2 [see Fig. 1(c)] are then given as ($l = 1, 2$)

$$v_l \simeq -\left(\frac{t_\perp}{t_\parallel}\right)^{2l} \frac{t_\parallel}{\ln k_0^{-1}}, \tag{5}$$

where the overall negative sign results from the fact that the lowest order contribution to $v_{1,2}$ are of order v_0^2.

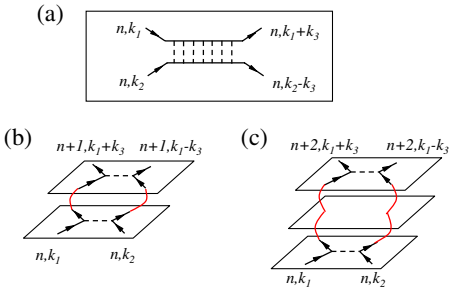

FIG. 1 (color online). (a) Ladder diagrams that provide the dominant contribution to the intralayer scattering in the low density regime [12]. (b) and (c) leading order diagrams that contribute to the coherent interlayer hoppings $t^*_{\perp,1}$ and $t^*_{\perp,2}$.

These interlayer coupling lead to new nonlocal interaction terms $v_l n_i n_{i+l\mathbf{e}_z}$ in the low energy theory, and result from $T = 0$ quantum fluctuations of the interacting Bose system. Pairs of boson propagate as virtual excitations between layers and mediate the nonlocal boson-boson coupling [4]. It is crucial to observe that no coherent boson hopping $t^*_{\perp,l} a^\dagger_{\mathbf{k}_\parallel,n} a_{\mathbf{k}_\parallel,n+l}$ between layers emerges for $T = 0$.

H_B is invariant with respect to the discrete Z_2 symmetry: $k_x \to -k_x + 2\pi$ and $k_z \to k_z + \pi$. As long as this symmetry is intact, no term $t^*_{\perp,1}\cos(k_z)$ in the dispersion is allowed, while coherent hopping between second neighbor layers with $t^*_{\perp,2}\cos(2k_z)$ does not break the Z_2 symmetry. To determine these coherent interlayer hoppings $t^*_{\perp,l}$ we perform a mean field (MF) theory of the low energy problem with interlayer interactions v_l. We approximate $v_l n_i n_{i+l\mathbf{e}_z} \to v_l \langle a_i^\dagger a_{i+l\mathbf{e}_z}\rangle a_i^\dagger a_{i+l\mathbf{e}_z}$ and obtain

$$t^*_{\perp,l} = v_l \int \frac{d^2k_\parallel}{4\pi^2} \langle a^\dagger_{\mathbf{k}_\parallel,n} a_{\mathbf{k}_\parallel,n+l}\rangle. \tag{6}$$

The expectation values of $\langle a^\dagger_{\mathbf{k}_\parallel,n} a_{\mathbf{k}_\parallel,n+l}\rangle$ are determined self-consistently. As expected, we find $t^*_{\perp,2}(T = 0) = 0$ and $t^*_{\perp,1}(T) = 0$. The former result reflects that coherent motion is forbidden at $T = 0$, while the latter is caused by the Z_2 symmetry, forcing the hopping between nearest neighbor layers to vanish at all T. The solution of Eq. (6) for the coherent second neighbor hopping is

$$t^*_{\perp,2} \simeq v_2 \left(\frac{t_\perp}{t_\parallel}\right)^2 \frac{T}{t_\parallel} \ln \frac{T}{t_\parallel k_0^2}. \tag{7}$$

Using the above result for v_2 it then follows $t^*_{\perp,2} \simeq (\frac{t_\perp}{t_\parallel})^6 \times \frac{T \ln T/\mu}{\ln t_\parallel/\mu}$. Since the density of bosons is $\rho \simeq T \ln(T/\mu)/t_\parallel$, thermally excited bosons induce a coherent hopping between second neighbor layers $t^*_{\perp,2} \propto \rho/\ln(t_\parallel/\mu)$. While this hopping is small, the finite T transition will be 3D XY with T_c given by the MF condition:

$$\mu_c = v_0 \rho, \tag{8}$$

and as usual for strongly anisotropic systems, its value is given by the characteristic temperature scale of the in-plane ordering. Since $t^*_{\perp,2} \ll \epsilon_\parallel(k_0)$, the $d = 2$ fluctuations dominate the value of T_c at very low densities resulting in Eq. (3). Similarly, we obtain $d = 2$ expressions for

$$\rho(T = 0, \mu) \propto \mu \ln \frac{\mu}{t_\parallel}, \qquad \rho(T, \mu = 0) \propto \frac{T}{t_\parallel} \ln\left(\ln \frac{t_\parallel}{T}\right). \tag{9}$$

Based on these results we next address the origin of DR in the frustrated magnet $BaCuSi_2O_6$ [5]. We start from a Heisenberg Hamiltonian of $S = \frac{1}{2}$ spin dimers on a bct lattice, closely approximating $BaCuSi_2O_6$ [6,7]. The dominant Heisenberg interaction, $J\sum_{\mathbf{i}} \mathbf{S}_{i1} \cdot \mathbf{S}_{i2}$, is between spins on the same dimer i. Since there are two low energy states in an applied magnetic field, the singlet and the $S^z_{i1} + S^z_{i2} = 1$ triplet, we can describe the low energy sector

with hard-core bosons. The triplet state corresponds to an effective site i occupied by a boson while the singlet state is mapped into the empty site [13,14]. The resulting low energy effective Hamiltonian corresponds to a gas of interacting (infinite u) canonical bosons, as in Eq. (1). The number of bosons (triplets) equals the magnetization along the z axis. The chemical potential $\mu = g\mu_B(H - H_c)$ is determined by the applied magnetic field H and the critical field $g\mu_B H_c = J - 2J'$. The hoppings $t_\parallel = J'$ and $t_\perp = J^\perp$ are determined by the interdimer exchange interactions between spins on the same bilayer, $J' \simeq 6$ K [14–16] and on adjacent bilayers, $J^\perp < J'$. The modulation of the $BaCuSi_2O_6$ lattice structure along the c axis leads to an alternation of two nonequivalent bilayers A and B, with intradimer interactions $J_A = 49.5(1)$ K and $J_B = 54.8(1)$ K [7,16]. This alternation reduces the magnitude of the residual nonfrustrating interlayer couplings characteristic to all real systems [17], while the principal treatment of $BaCuSi_2O_6$ presented here remains unaffected.

The correspondence between the quantum spin model for $BaCuSi_2O_6$ with the boson model of Eq. (1) allows us to interpret T_c of Eq. (3) as the phase boundary as a function of $\mu = g\mu_B(H - H_c)$. At this phase transition, we also expect that the Z_2 symmetry will be broken as well. It is interesting to analyze the dimensional crossover and the coupling between second neighbor layers directly in the spin language. For classical spins $\mathbf{S_i}$ at $T = 0$, the frustrated nature of $J^\perp$ produces a perfect decoupling of the OP's (XY staggered magnetization) on different layers. However, this decoupling is unstable to quantum or thermal fluctuations [4]. Either of these fluctuations induces an effective interlayer coupling via an order from disorder mechanism as illustrated in Fig. 2. When the sum of the four spins on a given plaquette, $\mathbf{S}_P$, is exactly equal to zero, the coupling between that plaquette and the spins which are above ($\mathbf{S}_T$) and below ($\mathbf{S}_B$) cancels out. However, phase fluctuations can produce a net total spin on the plaquette, $\mathbf{S}_P \neq 0$. Since $\mathbf{S}_P$ is antiferromagnetically coupled with $\mathbf{S}_T$ and $\mathbf{S}_B$ [see Fig. 2(b)], an effective ferromagnetic (FM) interaction results between $\mathbf{S}_T$ and $\mathbf{S}_B$, i.e., between second neighbor layers.

The defining characteristic of the BEC quantum phase transition is that amplitude fluctuations of the OP drive it, in contrast to the XY transition driven by phase fluctuations. This difference is vital to the effective coupling at the QCP: it vanishes due to its quadratic dependence on the amplitude of the OP. The remarkable consequence is a DR of the Gaussian QCP from $d = 3$ to $d = 2$.

Our previous analysis shows that the nonuniversal prefactors of Eqs. (3) and (10) can be accurately determined using a strictly $d = 2$ theory. The RG and MF approaches used to describe the quasicondensate phase of a weakly interacting 2D Bose gas [11] give the right universality class and generic T vs μ dependence, yet are quantitatively inadequate for realistic densities. The limitation of these treatments arises from the insensitivity of the size of the critical region ΔT (where fluctuation corrections of the BKT transition are important) to the smallness of the interaction: $\Delta T/T_c \sim 1/\ln t_\parallel/v_0$. This limitation is, however, overcome by our use of Monte Carlo (MC) simulations to obtain the nonuniversal constants in Eq. (3), and the results of Prokof'ev and Svistunov [18] who computed these constants for realistic low densities and weak interactions, obtaining the following expression for the phase boundary of the quasicondensate [18]:

$$\mu_c = \frac{v_0 T}{\pi J'} \ln \frac{J' \xi_\mu}{v_0}, \tag{10}$$

where $\xi_\mu = 13.2 \pm 0.4$. In Fig. 3(a), we compare the experimental data for $BaCuSi_2O_6$ [5] with the result of Eq. (10) and Monte Carlo (MC) simulations of hard-core bosons on a square lattice ($L \times L$ with $L = 32$) with hopping $t_\parallel = J' = 6$ K [15,16]. Similar MC results were reported previously in Ref. [19]. The agreement is good for $T \lesssim 200$ mK ($\rho \lesssim 0.02$) but, as expected, there is a significant deviation at higher temperatures (densities). The significant underestimation of T_c by the MC result at higher temperatures indicates that neglecting the effective interlayer tunneling is no longer valid in $BaCuSi_2O_6$ for $\rho \gtrsim 0.02$. Figure 3(b) shows a similar comparison for $\rho(\mu, T \simeq 0)$ and $\rho(\mu = 0, T)$ [see Eqs. (10)]. Again, we compare the experimental data against the MC simulation because the MF approximation that leads to Eqs. (10) is adequate to determine the generic μ and T dependence, but cannot reproduce the nonuniversal constants. Our theory also predicts a linear dependence of the specific heat $C(T, H_c)$ and the nuclear relaxation time $1/T_1(T, H_c)$ as a function of T at the QCP of $BaCuSi_2O_6$.

To compute the exponent of the next-order correction to Eq. (3) we note that the effective boson-boson interaction $v_0(\rho)$ is obtained as an expansion in the small parameter $\rho^{1/2}$ [12]: $\tilde{v}_0(\rho) = v_0(1 + \alpha\rho^{1/2} + \ldots)$. While the first term in this expansion is determined by the ladder diagrams of Fig. 1(a), higher-order diagrams contribute to the second term. The MF relation (8) implies that the next order correction to Eq. (10) is proportional to $T^{3/2}$. The value of u_1 determines the crossover between the linear

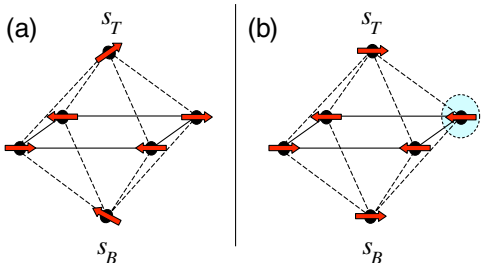

FIG. 2 (color online). (a) The perfect antiferromagnetic (AF) order of the four spins in the square plaquette precludes an effective coupling between S_B and S_T. (b) A phase fluctuation of the AF OP induces an effective ferromagnetic coupling between S_B and S_T. For $BaCuSi_2O_6$, each site represents a dimer.

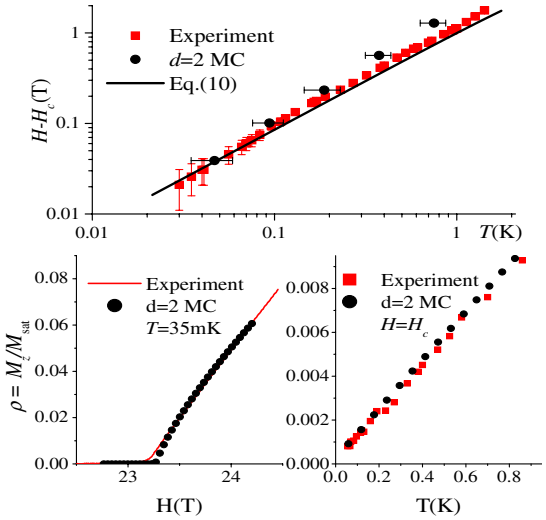

FIG. 3 (color online). (a) Phase boundary near the QCP measured in $BaCuSi_2O_6$ [5] compared to the curves obtained from a MC simulation and Eq. (10) for a $d = 2$ gas of hard-core bosons on a square lattice with $t_{\|} = J' = 6$ K. (b) Similar comparison for $\rho(T = 30\ \text{mK}, \mu = H - H_c)$ and $\rho(T = 30\ \text{mK}, H = H_c)$. We have neglected the density of bosons on the B bilayers because $J_2 - g\mu_B H \gg |t^*_{\perp,l}|$ as long as H is not close to $J_2/g\mu_B \simeq H_c + 3.4$ T.

regime consistent with a $d = 2$-QCP and the $T^{3/2}$ regime characteristic of a $d = 3$ BEC. Such a crossover was reported in $BaCuSi_2O_6$ [5]. We can demonstrate in general that the phase boundary equation of a d-dimensional bosonic system comprising $d - 1$-dimensional regions coupled via a frustrated interaction is $\mu_c \simeq AT^{(d-1)/2} + BT^{d/2}$ for low enough ρ.

Our mapping of the spin problem to the boson model H_B is based on the assumption that only the lowest triplet and the singlet modes are important at low energies. The low density expansion for the boson problem is then well justified, as the XY symmetry of the original spins $\mathbf{S}_i$ is directly responsible for the charge conservation of H_B. Recently, it was shown by Rösch and Vojta [20] that the inclusion of the two higher triplet modes generates a small coherent second-neighbor hopping of low energy triplets between layers $t^*_{\perp,2} \simeq J^6_{\perp}/J^5$. This interesting effect restores the $d = 3$ character of the spin problem. For realistic values of $J = 49.5(1)$ K and $J_{\perp} < J'$, $J^6_{\perp}/J^5 < 0.1$ mK in $BaCuSi_2O_6$. This implies that the mechanism discussed in our Letter is still dominant for all experimentally accessible temperatures $T \gtrsim 30$ mK. Moreover, the U(1)-symmetry breaking terms induced by dipolar interactions will produce a crossover to a QCP with discrete symmetry at $T \sim 10$ mK [21], i.e., before the mechanism of Ref. [20] sets in. Finally, the inevitable presence of finite nonfrustrated couplings in real systems will eventually restore the 3D behavior below some characteristic temperature T_0 (for $BaCuSi_2O_6$ we estimate $T_0 < 30$ mK [17]). We stress that these considerations do not effect our theoretical results for H_B [Eq. (1)], which establish the existence of a nontrivial 3D interacting many body system with a strictly $d = 2$ QCP.

In summary, we demonstrate that the dimensionality of the BEC-QCP is $d = 2$ when the interlayer coupling is frustrated. However, this coupling is relevant for changing the thermodynamic phase transition from BKT to the 3D-XY universality class. These results explain quantitatively, and without free parameters, the DR manifested in the measured quantum critical exponents of $BaCuSi_2O_6$ [5].

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[1] H. E. Stanley, *Introduction to Phase Transitions and Critical Phenomena* (Oxford University, Oxford, 1987).
[2] O. Stockert *et al.*, Phys. Rev. Lett. **80**, 5627 (1998); N. D. Mathur *et al.*, Nature (London) **394**, 39 (1998).
[3] E. Shender, Sov. Phys. JETP **56**, 178 (1982); C. L. Henley, Phys. Rev. Lett. **62**, 2056 (1989).
[4] M. Maltseva and P. Coleman, Phys. Rev. B **72**, 174415 (2005).
[5] S. E. Sebastian *et al.*, Nature (London) **441**, 617 (2006).
[6] K. M. Sparta and G. Roth, Acta Crystallogr. Sect. B **60**, 491 (2004).
[7] E. Samulon *et al.*, Phys. Rev. B **73**, 100407(R) (2006).
[8] D. S. Fisher and P. C. Hohenberg, Phys. Rev. B **37**, 4936 (1988).
[9] S. Sachdev, *Quantum Phase Transitions* (Cambridge University Press, Cambridge, England, 1999).
[10] J. Schmalian and C. D. Batista (unpublished).
[11] V. N. Popov, Theor. Math. Phys. (Engl. Transl.) **11**, 565 (1972).
[12] S. T. Beliaev, Sov. Phys. JETP **34**, 299 (1958).
[13] T. Giamarchi and A. M. Tsvelik, Phys. Rev. B **59**, 11 398 (1999).
[14] M. Jaime *et al.*, Phys. Rev. Lett. **93**, 087203 (2004).
[15] S. E. Sebastian *et al.*, Phys. Rev. B **72**, 100404(R) (2005).
[16] Ch. Rüegg *et al.*, Phys. Rev. Lett. **98**, 017202 (2007).
[17] A weak structural distortion observed at ~100 K [7] provides such a mechanism. Inelastic neutron scattering (INS) indicates that the dimer axes is tilted, leading to a 10% change of the intradimer exchange coupling J (linear in the distortion) [16]. The resulting nonfrustrating interaction $\sim 0.01 J^{\perp} \simeq 10$ mK is quadratic in this distortion. We used preliminary INS measurements that indicate $J^{\perp} \sim 1$ K [Ch. Ruegg (private communication)].
[18] N. Prokof'ev and B. Svistunov, Phys. Rev. A **66**, 043608 (2002).
[19] K. Bernardet *et al.*, Phys. Rev. B **65**, 104519 (2002).
[20] O. Rösch and M. Vojta, arXiv:cond-mat/0702157.
[21] S. E. Sebastian *et al.*, Phys. Rev. B **74**, 180401(R) (2006).