Letter

Quantum-critical scaling at the Bose-glass transition of the 3*d* diluted Heisenberg antiferromagnet in a field

Yuchen Fan [1,2] Rong Yu [1,3,*] and Tommaso Roscilde [4,†]

[1] *Department of Physics and Beijing Key Laboratory of Opto-electronic Functional Materials and Micro-nano Devices, Renmin University of China, Beijing 100872, China*

[2] *Beijing National Laboratory for Condensed Matter Physics and Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China*

[3] *Key Laboratory of Quantum State Construction and Manipulation (Ministry of Education), Renmin University of China, Beijing 100872, China*

[4] *Univ. Lyon, Ens de Lyon, CNRS, Laboratoire de Physique, F-69342 Lyon, France*

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The nature of the superfluid-to-Bose-glass (SF-BG) quantum phase transition, occurring in systems of interacting bosons immersed in a disordered environment, remains elusive. One fundamental open question is whether or not the transition obeys conventional scaling at quantum critical points (QCPs): this scaling would lock the value of the crossover exponent ϕ—dictating the vanishing of the superfluid critical temperature upon approaching the QCP—to the value of quantum critical exponents for the ground-state transition. Yet such a relation between exponents has been called into question by several numerical as well as experimental results on the SF-BG transition. Here we revisit this issue in the case of the $S = 1/2$ Heisenberg antiferromagnet on a site-diluted cubic lattice, which lends itself to efficient quantum Monte Carlo simulations. Our results show that the model exhibits a percolation transition in zero applied field, with the correlation length exponent $\nu = 0.87(8)$ and $\phi = 1.1(1)$ consistent with 3*d* percolation. When applying a sufficiently strong magnetic field, the dilution-induced transition decouples from geometric percolation, and it becomes a SF-BG transition; nonetheless, the ν and ϕ exponents maintain values consistent with those of the percolation transition. These results contradict the conventional scaling, which predicts $\phi \geqslant 2$; and they suggest a possible relationship between the SF-BG transition and percolation of phase coherence.

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Introduction. Quantum localization in strongly correlated systems is a central topic of current research in condensed matter and statistical physics [1–6] for its wide-ranging consequences on both the equilibrium physics of the system and nonequilibrium dynamics, with the possible breakdown of thermalization [7,8]. In this paper we shall specifically focus on the localization transition in bosonic systems, which is relevant to a wide variety of physical platforms, ranging from ^{4}He in porous media [9], to ultracold atoms in disordered optical potentials [10] to disordered superconductors [11]. The central question in this domain concerns the nature of the ground-state quantum phase transition (QPT) [1,2] from the long-range ordered, superfluid (SF) phase to the localized, Bose-glass (BG) phase. The nature of the QPT remains a subject of debate, as it appears to defy the conventional scenario for critical scaling. The seminal study of Ref. [2] postulated that the finite-temperature free energy in the vicinity of the QPT obeys a conventional scaling form, admitting the temperature and the control parameter of the QPT as the unique instability directions for the fixed point governing the quantum critical behavior. This has the result that, on the SF side of the transition, long-range order persists in 3*d* up to a critical temperature T_c, which vanishes upon approaching the quantum-critical point (QCP) as $T_c \sim |g - g_c|^\phi$ (with g the control parameter of the QPT), with a crossover exponent $\phi = \nu z$. Here ν is the correlation-length exponent at the QCP, and z the dynamical critical exponent. The finite compressibility of the BG phase leads to the prediction that $z = d$ [2] with d the number of dimensions. Combined with the Harris criterion for criticality in disordered systems [6], mandating that $\nu \geqslant 2/d$, this leads to the conclusion that $\phi \geqslant 2$.

The above picture has been severely cast into doubt by the first quantitative tests of the scaling theory for the SF-BG transition, which have been mostly performed on its magnetic incarnation [12]. A broad family of gapped magnetic systems exhibits a magnetic analog of the commensurate-incommensurate transition of strongly interacting bosons [13] when subject to a strong magnetic field [14,15]; and this transition takes the nature of a SF-BG transition when disorder is introduced in the system [12]. The magnetic SF-BG transition has been investigated in a variety of doped compounds [16–20] and theoretical models thereof [20,21], the most extensively studied case being the one of $NiCl_{2(1-x)}Br_{2x} \cdot 4SC(NH_2)_2$ (Br-DTN) [20–23]. All these studies have concluded that $\phi < 2$, with the most in-depth investigations giving $\phi \approx 1.1$, at least in the range of T_c that were accessible to both experiments and numerics [20]. This is in open contradiction with the $\phi \geqslant 2$ prediction, casting one or more

*rong.yu@ruc.edu.cn
†tommaso.roscilde@ens-lyon.fr

hypothesis behind it into doubt. The Harris criterion $\nu \geqslant 2/3$ [6] is confirmed by all the studies of the 3d SF-BG transition [21,23–25], giving $\nu \approx 0.7 - 0.9$. The prediction $z = d$, while called into question by several studies in $d = 2$ [26–28], appears to be confirmed by all the available studies of the 3d SF-BG transition [21,23–25]. Therefore a possible conclusion is that the SF-BG transition does not obey conventional scaling, and several generalized two-argument scaling Ansätze have been put forward [21].

Meanwhile, a large-scale numerical study [25] found that $\phi \approx 2.7$ for the disordered link-current model (a dual model to the disordered Bose-Hubbard model) and for disordered hardcore bosons at zero average chemical potential. In particular Ref. [25] puts forward a density criterion $|n(T)/n_c - 1| \ll 1$ identifying the putative temperature range to observe the correct ϕ exponent, where $n(T)$ is the finite-T boson density and n_c its value at the QCP; and arguing that the observation of $\phi \approx 1.1$ is the result of an analysis of T_c values in a temperature range not complying with this criterion. Nonetheless this argument is contradicted by the fact that existing data consistent with $\phi \approx 1.1$ [20] are also complying with the density criterion [29].

Here we revisit the ϕ exponent problem at the 3d SF-BG transition by looking at the $S = 1/2$ Heisenberg antiferromagnet on a site-diluted cubic lattice and in a uniform magnetic field, which lends itself to very efficient quantum Monte Carlo (QMC) simulations of the transition on very big lattices and at very low temperatures. Long-range magnetic order can be destroyed in the ground state by a sufficiently large dilution x (density of empty sites), and in zero applied field this transition is found to have a percolative nature, exhibiting a crossover exponent $\phi = 1.1(1)$ consistent with the one for 3d percolation, $\phi_p = 1.12(2)$ [30–32]. The transition becomes a SF-BG one in a finite field, but the crossover exponent is found to maintain a value consistent with the percolation one. Our data reverse the conclusions of Ref. [25], in that an exponent $\phi \gtrsim 2$ can only fit our T_c data in an intermediate temperature range, but it cannot account for the lowest-temperature regime we access. Moreover our results suggest the existence of a strong link between the Bose-glass transition and percolation at least for what concerns the finite-temperature behavior. Yet a simple geometrical percolation picture of the SF-BG transition is definitely not supported by our data, because the boson density is not percolating across the system in the vicinity of the transition, and ordering is fundamentally supported by weak links [22].

Model and ground-state phase diagram. We study the $S = 1/2$ Heisenberg antiferromagnet defined on a site-diluted cubic lattice, whose Hamiltonian reads

$$\mathcal{H} = J \sum_{\langle i,j \rangle} \epsilon_i \epsilon_j \boldsymbol{S}_i \cdot \boldsymbol{S}_j - H \sum_i \epsilon_i S_i^z; \quad (1)$$

here $\boldsymbol{S}_i$ is an $S = 1/2$ quantum spin operator on each site i; H is the applied magnetic field; and ϵ_i takes values 1 and 0 randomly, with probabilities $1 - x$ and x respectively—where x is the dilution concentration. This model is also equivalent to hardcore bosons with hopping $J/2$, nearest-neighbor repulsion J, and a uniform chemical potential H, defined on the same lattice [33]. In the following we take J as the energy unit

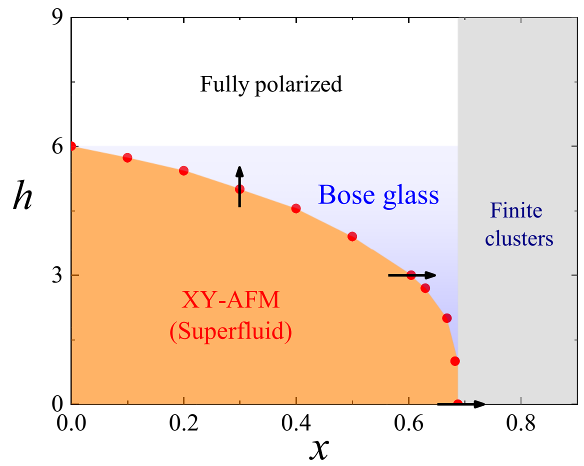

FIG. 1. Ground-state phase diagram of the $S = 1/2$ 3D site-diluted AFM Heisenberg model in the x-h plane. The dots give the QMC estimates of the order-disorder transition at $t = 10^{-3}$. Arrows illustrate the three different transitions analyzed in details in this paper.

and define a reduced temperature $t = T/J$ and a reduced field $h = H/J$ for convenience. We investigate this model using numerically exact QMC simulations, based on the stochastic series expansion (SSE) algorithm [34]. By using a β-doubling procedure [35], we simulate system sizes up to $L^3 = 26^3$ and with temperatures down to $t = 10^{-3}$. Our results are averaged over 2400–5300 disorder realizations (depending on the size). Compared to previous studies on $S = 1$ disordered spin models by some of us [20,21], the system sizes and disorder realization numbers studied here are at least twice as large, and the temperatures (in units of the interaction) are lower than all previous studies to our knowledge.

We characterize the equilibrium behavior of the system via the transverse static structure factor at wavevector $\boldsymbol{q}$, $\mathcal{S}^{xy}(\boldsymbol{q}) = L^{-3} \sum_{i,j} e^{i\boldsymbol{q}\cdot(\boldsymbol{r}_i - \boldsymbol{r}_j)} \langle S_i^x S_j^x + S_i^y S_j^y \rangle$, which is proportional to the momentum distribution of the hardcore bosons. Such a quantity allows us to define the squared order parameter characterizing the long-range antiferromagnetic phase in the XY plane as $m_s^2 = \mathcal{S}^{xy}(\boldsymbol{Q})/L^3$, where $\boldsymbol{Q} = (\pi, \pi, \pi)$ is the ordering wavevector; this quantity is proportional to the condensate density for bosons. A finite value of m_s^2 in the thermodynamic limit marks the phase with long-range antiferromagnetic order in the XY plane (AF-XY), which maps onto the SF phase for bosons. The correlation length can be determined by using the second-moment estimator $\xi = \frac{L}{2\pi} \sqrt{\frac{\mathcal{S}^{xy}(\boldsymbol{Q})}{\mathcal{S}^{xy}(\boldsymbol{Q}+(2\pi/L,0,0))} - 1}$. Throughout our paper, the critical temperatures $t_c(x, h)$ have been determined via the crossing points of ξ/L curves for different values of L, typically at fixed t and variable x or h.

The ground-state phase diagram, obtained via the ξ/L scaling at the lowest temperature $t = 10^{-3}$, is shown in Fig. 1 in the dilution-vs-field plane. Two fundamental features can be easily established: (1) at the percolation threshold $x_p = 0.6883923(2)$ [36], the site-diluted cubic lattice breaks up into finite clusters, so that long-range magnetic order is no longer sustainable for $x > x_p$; and (2) the clean system ($x = 0$) undergoes a polarization transition at the saturation

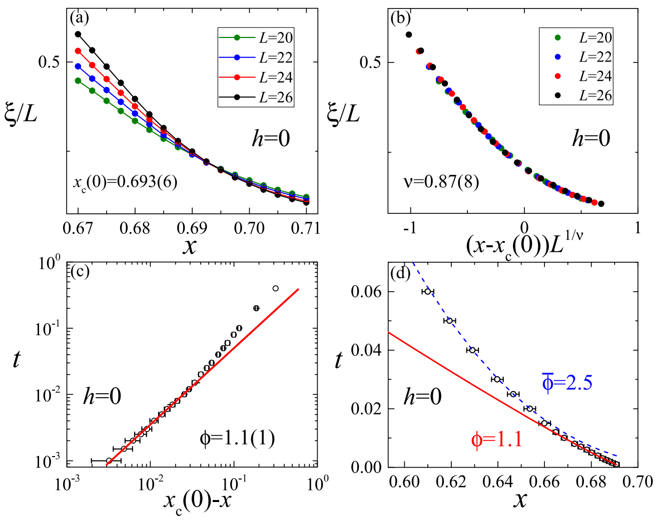

FIG. 2. Scaling at the zero-field magnetic transition. [(a),(b)] Finite-size scaling of the correlation length ξ at $t = 0.001$, leading to the estimates $x_c = 0.693(6)$ and $\nu = 0.87(8)$. [(c),(d)] Scaling of the finite-temperature transition line in the log-log (c) and normal (d) scales, respectively. Solid red lines are power-law fit $x_c = x_c(0) - At^{1/\phi}$ with $x_c(0) = 0.694(6)$ and $\phi = 1.1(1)$. The dashed blue line in panel (d) is a power-law fit with $\bar{\phi} = 2.5$ to the intermediate temperature data, giving $\bar{x}_c(0) \approx 0.732$.

field $h_c(x = 0) = 6$. Adding any finite amount of disorder to the system in the form of dilution alters the latter transition, introducing an intermediate BG phase [37], which necessarily erodes the SF phase, as the polarizing field is independent of the dilution. On the other hand, in zero field a magnetic percolation transition can occur, which is purely driven by the geometry of the underlying lattice. Such a transition persists up to a multicritical field $h^* \approx 1$, at which the SF-BG transition line and the magnetic percolation line meet.

Zero-field magnetic transition and percolation. We first focus on the zero-field transition induced by dilution x. Upon diluting the cubic lattice one may wonder whether quantum fluctuations are able to destroy long-range order for $x < x_p$, but this turns out not to be the case—as clearly shown in Fig. 2(a). There the scaling analysis of the correlation length at the lowest temperature ($t = 10^{-3}$) indicates a critical point of 0.693(6), consistent with x_p (see below for the $t = 0$ extrapolation). Moreover the estimated correlation length exponent $\nu = 0.87(8)$—obtained from the collapse of different data sets according to the scaling Ansatz $\xi/L = F(|x - x_c|L^{1/\nu})$ [Fig. 2(b)]—is also found to be consistent with the percolation value $\nu_p = 0.876(1)$. As shown in the Supplemental Material (SM) [38], adding corrections to scaling allows us to collapse the ξ/L curves by using $x_c = x_p$, as well as to collapse curves for m_s^2 with the 3d percolation exponent $\beta_p = 0.418(1)$ [36]. We conclude that corrections to scaling, while necessary for the correct estimate of quantum critical exponents, only lead to a small ($\lesssim 1\%$) shift in the estimate of the critical point. Therefore, in order to minimize the number of fitting factors, we shall not apply them in the rest of the work. Our data are therefore fully consistent with a magnetic percolation transition occurring at $x_c = x_p$. These results generalize to three dimensions the ones (both theoretical [35] as well as experimental [39]) already obtained for the magnetic percolation transition of the 2d version of this model.

The critical dilution $x_c(t)$ for the 3d Heisenberg model at various finite temperatures can be systematically determined via the ξ/L scaling, and it is shown in Figs. 2(c) and 2(d). It clearly exhibits a power-law behavior $x_c(t) = x_c(0) - At^{1/\phi}$, stabilizing only in the lowest-temperature range we explored ($t \sim 10^{-3} \div 10^{-2}$). Fitting the data in this range delivers $x_c(0) = 0.694(6)$, deviating by $<1\%$ from x_p; and $\phi = 1.1(1)$. Most interestingly, a similar value for ϕ has been recently obtained in an extensive numerical study on the classical ($S = \infty$) Heisenberg model on the same diluted lattice [32]; and it has been shown to be consistent with the crossover exponent for percolation, $\phi = \nu_p \tilde{\zeta}_R = 1.12(2)$, where $\tilde{\zeta}_R = 1.28(2)$ dictates the scaling of the resistance of a resistor network defined on the critical percolating cluster [31]. The coincidence of the behavior of the quantum system and that of the classical system is not at all surprising, given that quantum effects are found not to change the percolative nature of the magnetic transition at zero temperature; and they are even less expected to affect the finite-temperature behavior. On the other hand we remark that an exponent $\phi \geqslant 2$ could be easily fitted to our results when discarding the lowest temperature results; but this approach would lead to an unphysical estimate of the zero-temperature transition at $x_c(0) > x_p$.

SF-BG transition and ϕ exponent. We now move to the central part of the work, namely the study of the crossover exponent ϕ at the SF-BG transition. To demonstrate the universality, we study the transition along two cuts of the SF-BG transition line: (i) varying h at $x = 0.3$, and (ii) varying x at $h = 3$. The critical field and dilution concentration for the lowest accessible temperature $t = 10^{-3}$ are determined from the scaling analysis of ξ/L to be $h_c(t = 10^{-3}, x = 0.3) = 4.998(3)$ and $x_c(t = 10^{-3}, h = 3) = 0.604(3)$, respectively, with an estimated $\nu = 0.9(1)$—see Figs. 3(a) and 3(c). The critical fields [$h_c(t)$] and concentrations [$x_c(t)$] at finite temperature, obtained with a similar scaling analysis, are shown in Figs. 3(b) and 3(d), and fitted to the power-law dependence $g_c(t) = g_c(0) - At^{1/\phi}$ $(g = h, x)$. Our data clearly indicate that $\phi = 1.1(1)$ in both cases—a detailed fitting analysis on variable temperature windows is presented in the SM [38]. The curve best fitting the points at the lowest temperatures $t = 10^{-3} \div 10^{-2}$ has nearly zero curvature (since ϕ is very close to unity). Yet the prediction of conventional scaling theory ($\phi \geqslant 2$) would instead require a finite curvature, which can be easily found by looking at higher temperatures. A $\phi = 2$ exponent can fit our data only if we *exclude* the points in the above-cited low-t range, leading to extrapolated $t = 0$ critical points, which are inconsistent with those [$h_c(t = 0, x = 0.3) = 5.007(3)$ and $x_c(t = 0, h = 3) = 0.606(5)$] obtained by using ϕ as a fitting parameter.

In addition to the analysis of the finite-temperature transition lines in the vicinity of the QCP, a completely alternative approach can be used to extract the ϕ exponent, based on the thermodynamic behavior along the so-called quantum critical (QC) trajectory, namely varying t at fixed $g = g_c(0)$. Along this trajectory the specific heat scales as $C(t) \sim t^{x_C}$, and the uniform magnetization behaves as $m(t) - m(0) \sim t^{x_m}$, where x_C and x_m are the associated scaling exponents. It has been shown that the relation $\phi^{-1} = x_C - x_m + 1$ holds for all

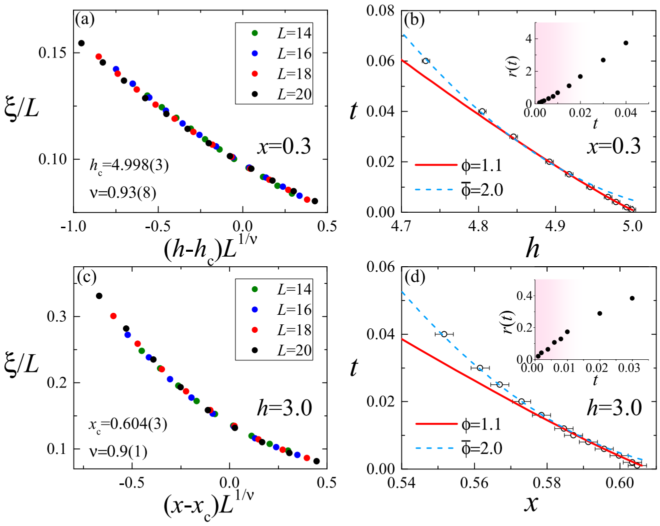

FIG. 3. Scaling at the SF-BG transition. [(a),(c)] Scaling plots of the correlation length ξ/L at $t = 0.001$ and the finite-temperature transition line by varying h at $x = 0.3$ (a) and by varying x at $h = 3$ (c). [(b),(d)] Temperature-dependent critical points $h_c(t)$ at $x = 0.3$ (b) and $x_c(t)$ data at $h = 3$ (d). The red lines show fits to the power-law behavior $g_c(t) = g_c(0) - At^{1/\phi}$ $(g = h, x)$. The blue lines are fits of the intermediate temperature data with fixed $\bar{\phi} = 2$. Insets of (b) and (d) are parameter $r(t)$ (see text) along the critical line; the pink-shaded region shows the temperature regime in which we observe $\phi \approx 1.1$.

scaling Ansätze proposed so far for the transition [21], including that of Ref. [2]. The x_C exponent can be most conveniently obtained via QMC from that governing the scaling of the thermal energy, $E(t) - E(0) \sim t^{x_E}$ with $x_E = x_C + 1$. Data of $E(t)$ and $m(t)$ at $x = 0.3$ and $h_c(0) = 5.007$ are shown in Figs. 4(a) and 4(b), respectively. From the power-law fit, we obtain $x_E \approx 2.58(4)$ and $x_m = 1.71(1)$, which leads to $\phi = 1.20(7)$, fully consistent with the analysis based on the transition lines.

We notice that the density factor $r(t) = |n(t)/n_c - 1|$ [40] can take widely different values over the temperature ranges that consistently lead us to the estimate $\phi \approx 1.1$ – $r \lesssim 1$ in Fig. 3(b), $r \lesssim 0.2$ Fig. 3(d), and $r \lesssim 4$ in the temperature range $t \leqslant 0.25$ exhibiting the QC trajectory behavior in Figs. 4(a) and 4(b). These results question the relevance of the density criterion $r \ll 1$ put forward by Ref. [25].

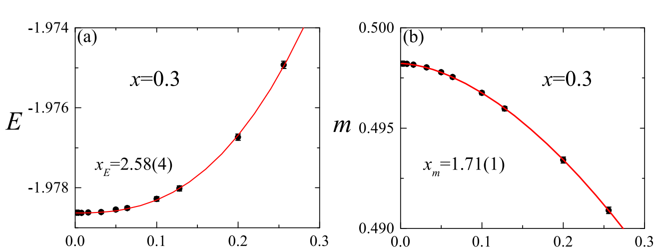

FIG. 4. Temperature evolution of the thermal energy per spin $E(t)$ (a) and the uniform magnetization $m(t)$ (b) along the QC trajectory at $x = 0.3$, $h_c(0) = 5.007$. The solid lines are power-law fits giving $x_E = 2.58(4)$ and $x_m = 1.71(1)$, respectively.

Discussion and conclusions. Using two independent approaches for the extraction of the crossover exponent at the SF-BG transition (via the vanishing of T_c; and via the thermodynamics along the QC trajectory) we unambiguously find a value of ϕ, which violates the prediction from conventional scaling theory, $\phi \geqslant 2$. On the other hand, our findings are consistent with experimental results on Br-DTN, as well as with extensive numerical studies of its model Hamiltonian [20,29]. Note that clear signs of saturation of the thermodynamic quantities to their $t = 0$ value (see data within the SM [38]) are observed at the lowest temperature ($t = 10^{-3}$) in our calculations, and correspondingly the critical values $x_c(t = 10^{-3})$ and $h_c(t = 10^{-3})$ for dilution and field are typically compatible with their extrapolated $t = 0$ value within the error bar. Therefore our results reach a rather satisfactory level of control on thermal effects, at least up to the system sizes we could access. The results of Ref. [25], concluding that $\phi \approx 2.7$, have full control on the position of the $t = 0$ QCP only for the disordered link-current model: remarkably this model has an additional (particle-hole) symmetry with respect to generic bosonic models with disorder. In the disordered hardcore-boson models studied by Ref. [25] (not possessing this symmetry) the position of the QCP is not evaluated directly, and one cannot conclude whether or not the asymptotic scaling regime was reached. As we have shown above, curves with $\phi \geqslant 2$ can be fitted to our data as well in an intermediate temperature range ($t \gtrsim 10^{-2}$), which is the one reached by Ref. [25] for hardcore bosons; but they are no longer working when going to even lower temperatures.

Our data show that the crossover ϕ exponent at the SF-BG transition is compatible with the one of $3d$ percolation, suggesting a link between the two phenomena. Nonetheless, the link, if existent, is rather complex, as the SF-BG quantum critical exponents are markedly different from the ones of percolation. As shown within the SM [38], a scaling analysis of $m_s^2 L^{2\beta/\nu}$ at the SF-BG transition for $x = 0.3$ leads to estimating the two critical exponents as $\nu = 0.9(1)$ and $\beta = 1.2(1)$: while the first exponent is compatible with ν_p of $3d$ percolation, the second one is definitely not compatible with β_p, even after taking into account corrections to scaling. Hence a more complex scenario of *quantum percolation* [22] is in order. Such a scenario is supported by a study of the magnetic participation ratio [22] (see the SM [38]), expressing the fraction of the diluted system effectively populated by hardcore bosons with density $n_i = 1/2 - S_i^z$; our numerical results show that this fraction is below the value associated with density percolation in the entire region surrounding the SF-BG transition. Hence percolation at the SF-BG transition can only be understood in the sense of phase correlations, spreading across weak links (akin to tunnel junctions), which are nearly devoid of bosons.

Reference [41] has proposed that criticality compatible with percolation might be seen as a transient crossover behavior upon approaching the SF-BG transition. Our results seem to exclude such a crossover. Indeed, as shown in the SM [38], we can extract a z exponent from the scaling of the spin stiffness, which appears to be compatible with $z = d = 3$ at $T = 0$ as expected for the true SF-BG QCP, but are instead incompatible with percolation [41]. These same data are in the temperature range in which we observe $\phi \approx 1.1$; hence we do not see much room for a further crossover to $\phi \geqslant 2$. Our results are instead compatible with two-argument scaling Ansätze [21], implying the existence of a dangerously irrelevant perturbation at the SF-BG fixed point, similarly to the one observed at the incommensurate SF-insulator transition in clean systems [13]. The physical origin of such a perturbation remains nonetheless to be identified.

Finally, the SF-BG transition we investigated can be potentially realized in any magnetic insulator realizing 3d Heisenberg antiferromagnetism (for $S = 1/2$ as well as higher spins), and subject to chemical doping of its magnetic ions—several examples of such systems (especially layered antiferromagnets exhibiting a 3d Néel transition) exist in the literature, e.g., $La_2Cu_{1-x}(Zn,Mg)_xO_4$ [39], $Rb_2Mn_{1-x}Mg_xF_4$ [42], $Mn_{1-x}Zn_xPS_3$ [43]. Our predictions are therefore testable via the high-field and low-temperature properties of such materials, as well as similar ones.

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[38] See Supplemental Material at http://link.aps.org/supplemental/10.1103/PhysRevB.109.L020405 for details about (1) the convergence of our results to their zero-temperature limit; (2) the scaling analysis of the correlation length and magnetization in zero field, showing that a consistent scaling collapse (including corrections to scaling) can be obtained using critical exponents and critical point from 3d percolation; (3) a windowing analysis of the extracted ϕ exponent from fits of the $t_c(h)$ and $t_c(x)$ data at the SF-BG transition; (4) a scaling analysis of m_s^2 at the SF-BG transition, showing that it is incompatible with percolation exponents; (5) the extraction of the z exponent from the scaling of the spin stiffness; and (6) the study of the magnetic participation ratio at finite temperature; which includes Refs. [44–47].

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