Field-induced quantum disordered phases in $S = 1/2$ weakly-coupled dimer systems
with site dilution

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In the present paper we discuss the rich phase diagram of $S = 1/2$ weakly coupled dimer systems with site dilution as a function of an applied uniform magnetic field. Performing quantum Monte Carlo simulations on a site-diluted bilayer system, we find a sequence of three distinct quantum-disordered phases induced by the field. Such phases divide a doping-induced order-by-disorder phase at low fields from a field-induced ordered phase at intermediate fields. The three quantum disordered phases are: a gapless disordered-free-moment phase, a gapped plateau phase, and two gapless Bose-glass phases. Each of the quantum-disordered phases have distinct experimental signatures that make them observable through magnetometry and neutron scattering measurements. In particular the Bose-glass phase is characterized by an unconventional magnetization curve whose field-dependence is exponential. Making use of a local-gap model, we directly relate this behavior to the statistics of rare events in the system.

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The $T = 0$ field-induced ordering transition in spin-gap antiferromagnets is one of the most intensively studied quantum phase transitions in condensed matter systems, both theoretically and experimentally. Examples of field-induced ordering can be found in Haldane chains, and frustrated $S = 1/2$ weakly-coupled dimer systems arranged in spin ladder, coupled bilayers, and in more complex $3d$ geometries. The application of a uniform field overcomes the spin gap brings these systems from a gapped $S = 0$ state to a state with finite magnetization parallel to the field and (in $d > 1$) spontaneous finite staggered magnetization transverse to the field. From the theoretical point of view, such an ordered state is very well understood as the result of Bose-Einstein condensation for the $S = 1$ triplet quasiparticles created by the field, with the spontaneous antiferromagnetic ordering corresponding to long-range phase coherence of the condensate. An alternative way of driving quantum-disordered spin-gap systems into a spontaneously ordered state is by doping the magnetic lattice with non-magnetic impurities, as unambiguously observed in almost all of the above cited cases, namely in Haldane chains, coupled spin ladders, and $3d$ weakly coupled dimers. The effect of non-magnetic impurities is the formation of local free $S = 1/2$ moments exponentially localized around the impurities. In the weakly coupled dimer systems they roughly correspond to unpaired spins, while in doped Haldane chains they correspond to the edge spins of the chain fragments. The overlap between two exponentially localized moments produces an effective coupling between them which decays exponentially with the impurity-impurity distance. Despite the fact that the impurities are randomly located, such couplings are perfectly unfrustrated and have staggering signs so that they induce spontaneous long-range Néel order in the free moments, giving rise to a paradigmatic order-by-disorder phenomenon.

An intriguing question concerns the fate of the ground state of the system in presence of both site dilution and an applied magnetic field. This situation, which is obviously of direct experimental relevance for all the real systems cited before, offers in principle the possibility of investigating two well distinct physical phenomena. On the one side, it is interesting to study how the order-by-disorder phase of the site-diluted system is altered and eventually destroyed by the application of a field, which plays in this case a disordering role for the system. At the same time, the spin gap for the clean system can be orders of magnitude larger than the typical energy scale of the effective interactions between the $S = 1/2$ free moments. This means that, after destruction of the ordered state of the free moments, the system can still be driven by an increasing field through a further transition to an ordered state similar to the one of the clean case, involving this time the spins which are far from the impurities. This offers the invaluable perspective of investigating a phenomenon of Bose-Einstein condensation in presence of lattice disorder, for which the appearance of an intermediate novel disordered phase, the Bose-glass phase, has been predicted long ago, but it has so far eluded the experimental observation.

In this paper we investigate a specific example of site-diluted spin-gap antiferromagnets in a magnetic field, namely a bilayer system in the strong interlayer coupling regime. We choose this specific geometry for two main reasons. One is that a $2d$ arrangement of weakly coupled dimers is the lowest-dimensional structure displaying genuinely ordered phases at $T = 0$ and genuine order-disorder quantum phase transitions, and at the same time quantum effects remain significant due to the reduced dimensionality, in particular quantum localization effects which are at the core of the Bose glass phase. One the other hand, a system of weakly coupled Heisenberg bilayers is a faithful magnetic model for BaCuSi$_2$O$_6$, in which the $S = 1/2$ Cu$^{2+}$ ions can be in principle doped with...
$S = 0$ Mg$^{2+}$ or Zn$^{2+}$ ions, thus leading to site dilution of the magnetic lattice.

![Diagram showing the sequence of ground-state phases in the Heisenberg bilayer in zero field.](image)

**FIG. 1**: Sequence of ground-state phases in the Heisenberg bilayer in a uniform field $h$ (in dimensionless units, see text). Upper panel: clean case; lower panel: site-diluted case. The numerical values are referred to a bilayer with $J/J' = 8$, and, for the lower panel, with 20% of vacant sites. For the phases indicated with an acronym: OBD = order-by-disorder, BG = Bose glass. The light-shaded regions correspond to ordered (and gapless) phases, the medium-shaded regions to gapped disordered phases, and the dark-shaded regions to gapless disordered phases.

Making use of Stochastic Series Expansion (SSE) quantum Monte Carlo (QMC) techniques, we can investigate the detailed evolution of the ground state of the doped system upon growing the applied magnetic field. The main results of the paper are the following. At a field much smaller than the clean-system gap, the order-by-disorder phase is destroyed, but the subsequent field-induced disordered phase, despite having a finite correlation length, is gapless as the free moments induced by the impurities are still far from being saturated. We dub this novel quantum phase the disordered-free-moment phase. For still higher fields, the full polarization of the free moments leads to a plateau in the magnetization, and a gap proportional to the field opens in the spectrum of the system. By further increasing the field towards the lower critical value of the clean case, the gap closes again and the magnetization starts to rise exponentially slowly in the field as the system enters a second unconventional quantum phase, namely the aforementioned Bose-glass phase. The Bose-glass phase is then turned into a long-range ordered (superfluid) phase for the bosonic quasiparticles appearing on dimers far from non-magnetic impurities, namely triplet quasiparticles for lower field and a dilute gas of hardcore triplet bosonic quasiparticles, corresponding to the elementary excitations of the soft triplet mode, appears in the ground state of the system, and it naturally forms a Bose-Einstein condensate with finite superfluid density. The long-range phase coherence of the condensate is reflected in the appearance of a spontaneous staggered magnetization $m^x_S = (-1)^{x+i} \langle S_i^x \rangle$ transverse to the field, with the singular phenomenon of antiferromagnetic order induced by a uniform field.

### I. BILAYER HEISENBERG ANTFERRROMAGNET IN A FIELD: CLEAN CASE

The Hamiltonian of the $S = 1/2$ Heisenberg antiferromagnet on a bilayer reads

$$
\mathcal{H} = J' \sum_{\langle ij \rangle} \sum_{\alpha=1,2} S_{i,\alpha} \cdot S_{j,\alpha} \\
+ J \sum_i S_{i,1} \cdot S_{i,2} - g_\mu_B H \sum_{i,\alpha} \epsilon_{i,\alpha} S_{i,\alpha}^z .
$$

Here the index $i$ runs over the sites of a square lattice, $(ij)$ are pairs of nearest neighbors on the square lattice, and $\alpha$ is the layer index. $J$ is the interlayer coupling and $J'$ the intralayer one. Hereafter we will express the field in reduced units $h = g_\mu_B H / J$.

This model has been extensively studied in the past, both analytically and numerically. For $h = 0$ the system is in a Néel ordered ground state if $g = J/J' < g_c = 2.52$, while for $g > g_c$ the ground state is a total singlet with no long-range magnetic order and a finite gap to all triplet excitations. In the limit of $g \gg g_c$ the ground state can be approximately represented as a collection of singlets on the strong interlayer bonds (dimers), so that the quantum-disordered phase of the model is generally indicated as the dimer-singlet phase. In what follows we will focus on a bilayer system with $g = 8$, namely, in absence of disorder and magnetic field, the system is deep in the dimer-singlet regime.

Applying a uniform magnetic field (see Fig. 1) has the effect of lowering the energy of the $S > 0$ states aligned with the field, up to a critical value $h^{(0)}_{c1} \approx 1 - 2/g + O(g^{-2})$, corresponding to the singlet-triplet gap $\Delta$, where the lowest triplet becomes degenerate with the singlet state, and the system develops a finite uniform magnetization along the field. At this field value a dilute gas of hardcore triplet bosonic quasiparticles, corresponding to the elementary excitations of the soft triplet mode, appears in the ground state of the system, and it naturally forms a Bose-Einstein condensate with finite superfluid density. The long-range phase coherence of the condensate is reflected in the appearance of a spontaneous staggered magnetization $m^x_S = (-1)^{x+i} \langle S_i^x \rangle$ transverse to the field, with the singular phenomenon of antiferromagnetic order induced by a uniform field.
more bilayers are weakly coupled in a 3d structure, as in the case of BaCuSi2O6, the field-induced staggered magnetization persists up to a finite critical temperature $T_c$, whose scaling with the applied field is well described by the mean-field theory for a diluted repulsive Bose gas.

When increasing the field even further, the gas of hard-core quasiparticles approaches the maximum density of one particle per dimer, in which case the ordered ground state is better described by a Bose-Einstein condensate of singlet quasiholes in the ‘triplet sea’. Eventually the hole condensate is completely removed by increasing the field beyond an upper critical value $k_{\text{F}}(d) = 1 + 4/g$, at which the uniform magnetization reaches its saturation.

II. SITE-DILUTED HEISENBERG BILAYER: ORDER BY DISORDER

In this section we discuss how the dimer-singlet ground state of the Heisenberg bilayer is transformed under site dilution of the lattice with a concentration $p$ of vacancies well below the percolation threshold of the lattice $p^* = 0.5244(2)$\cite{22}. The Hamiltonian of the site-diluted Heisenberg bilayer reads

$$
\mathcal{H} = J' \sum_{i} \sum_{\alpha=1,2} \epsilon_{i,\alpha} S_{i,\alpha} \cdot S_{i,\alpha} + J \sum_{i} \epsilon_{i,1} S_{i,1} \cdot S_{i,2} - hJ \sum_{i,\alpha} \epsilon_{i,\alpha} S_{i,\alpha}^z \, .
$$

The variables $\epsilon_{i,\alpha}$ take the values 0 or 1 with probability $p$ and $1-p$ respectively. In this section we focus on the case $h = 0$. Starting from $N_{\text{tot}}$ spins the elimination of a fraction $p$ of them leaves $p(1-p)N_{\text{tot}}$ unpaired spins (namely spins that are missing their dimer partner) and $(1-p)^2N_{\text{tot}}$ spins involved in intact dimers. Normalizing to the number of surviving spins, $N = (1-p)N_{\text{tot}}$, we obtain a global fraction $p$ of unpaired spins.

The presence of an unpaired spin on a given site introduces a significant local perturbation of the dimer-singlet state of the system. In fact the coupling $J'$ of the unpaired spin to the neighboring intact dimers can cause spin flips of the unpaired spin and simultaneous creation of a triplet excitation in the intact dimers, which are then polarized in the original direction of the unpaired spin. This flip-flop process, albeit weak if the energy gap to triplet excitations is large, effectively spreads the overall $S = 1/2$ magnetic moment of the unpaired spin over the neighboring intact dimers, within a volume of the order of $\xi_0^{d}$ where $\xi_0$ is the correlation length in the clean limit. This can be easily seen in first order perturbation theory, as discussed in the Appendix A. The large-distance tail of the wavefunction of the spread $S = 1/2$ free moment in 2d, centered around the $r = 0$ site of the unpaired spin, reads

$$
\psi(r) \approx \frac{J'z}{\Delta} e^{-r/\xi_0} \frac{e^{-r/\xi_0}}{r} \, .
$$

where $\Delta$ is the triplet gap of the clean system.

Due to their spatial spread, the induced $S = 1/2$ magnetic moments can overlap and thus effectively interact across regions of intact dimers. Given that the wavefunction overlap is exponentially decaying with the inter-moment distance, we should expect the interaction strength $J_{\text{eff}}$ to decay the same way. The leading contribution to the effective interaction can be calculated within second order perturbation theory\cite{22,23} in a similar fashion to the RKKY interaction between magnetic impurities in a metal; the details of the calculation in the 2d case are given in Appendix A. The resulting effective interaction between two impurities located at sites $(i, \alpha)$ and $(j, \beta)$ at a distance $r = |r_i - r_j|$ is $H_{\text{eff}} = J_{\text{eff}} S_{i,\alpha} \cdot S_{j,\beta}$, where, in the large-$r$ limit

$$
J_{\text{eff}}(i, j; \alpha, \beta) \approx (-1)^{\sigma} \frac{J_1}{r} e^{-r/\xi_0} \, ,
$$

with

$$
J_1 = \frac{(zJ')^2}{4\pi\Delta} \, ,
$$

and $\sigma = x_i + y_i + x_j + y_j + \alpha + \beta$. Due to this staggering factor, such interactions form an unfrustrated network which induces long-range antiferromagnetic ordering of the free moments. The resulting ordered phase will be denoted in the following as the order-by-disorder phase.

The order of magnitude of the interaction is mainly set by the ratio $(J')^2/\Delta$. Given that $\Delta \sim J$, this means that in the strong interlayer coupling regime $g \gg 1$ the order-by-disorder phenomenon has a characteristic energy scale for excitations which can be orders of magnitude smaller than the energy $(\sim J)$ for the excitations living far away from the impurities, namely in locally clean regions of the system. A more precise estimate of the typical energy scale for the effective interactions between the free moments is obtained by averaging Eq. 4 over its probability distribution. Here we simply consider pairs of closest-neighboring spins, discarding longer-range pairs due to the exponential decay of their mutual coupling. In the continuum limit, the probability for an unpaired spin to have its closest neighbor within a disk of radius $R$ is given by

$$
P(R) = 2p \, e^{-2p\pi R^2} \, .
$$

This probability distribution is normalized on the infinite disk. The corresponding probability distribution for the $J_{\text{eff}}$ couplings (here taken without the staggering sign) is then

$$
\tilde{P}(J_{\text{eff}}) = \frac{P(R(J_{\text{eff}}))}{|J_{\text{eff}}(R(J_{\text{eff}}))|} = \frac{4\pi p R \xi_0}{J_{\text{eff}}(1 + \xi_0/R)} e^{-2p\pi R^2} \Theta(J_1 e^{-1/\xi_0} - J_{\text{eff}}) \, .
$$
where the upper cutoff on $J_{\text{eff}}$ descends from the lower cutoff on the inter-moment distance $R = 1$ (corresponding to one lattice spacing), and it is necessary to regularize the distribution. The strength $J'$ of the inter-moment coupling for $R = 1$ is actually underestimated by the asymptotic formula Eq. (4). To take this into account one can in principle introduce the corrected distribution\footnote{\textcopyright 2022 American Physical Society.}} \(\tilde{P}(J_{\text{eff}}):\)
\[
\tilde{P}(J_{\text{eff}}) = \hat{P}(J_{\text{eff}}) + 4p \delta(J_{\text{eff}} - J').
\] (8)

We notice however that unpaired spins lying at the distance of a single lattice spacing will have a strong tendency to form a singlet state and therefore not to participate to the long-range Néel ordered state of the system (see also the discussion in Sec. IV). Therefore, when estimating the characteristic energy scale associated with the Néel ordered state of the free moments, we can discard the singular part of the distribution, obtaining therefore the following average effective coupling \(\langle J_{\text{eff}} \rangle:\)
\[
\langle J_{\text{eff}} \rangle = \int dJ_{\text{eff}} \hat{P}(J_{\text{eff}}) \approx 2\sqrt{2}\pi p J_1 e^{-1/\xi_0}. \tag{9}
\]

### III. QMC Method and Results

![FIG. 2: Zero-temperature field scan for the site-diluted Heisenberg bilayer with $g = 8$ and $p = 0.2$.](image)

In this section we present our numerical results for the Hamiltonian Eq. (2) in a finite field $h$. The method we use is the Stochastic Series Expansion (SSE) QMC based on the directed-loop algorithm\footnote{\textcopyright 2022 American Physical Society.}. Despite using a finite-temperature QMC approach, we can systematically study the ground-state physics of the model by efficiently cooling the system to its physical $T = 0$ limit via a successive doubling of the inverse temperature\footnote{\textcopyright 2022 American Physical Society.}. $L \times L \times 2$ lattices up to $L = 40$ have been considered. Here the size refers to the lattice before depletion. All the results for $p > 0$ have been averaged over at least 200 disorder realizations.

Fig. 2 shows the $T = 0$ field dependence of the most relevant observables for a site-diluted Heisenberg bilayer in the strong interlayer coupling regime $g = 8$, and with depletion $p = 0.2$. Plotted are the uniform magnetization along the field $m_u = \langle S^z_i \rangle$, the uniform susceptibility $\chi_u = dm_u/dh$, the staggered magnetization transverse to the field $m_s = 1/4 \sum_{\alpha\beta} (-1)^{L/2+\alpha+\beta} \langle S^x_{i+L/2,\alpha} S^x_{i+L/2,\beta} \rangle$ and the spin stiffness (superfluid density) $\Upsilon = k_B T/(2J) \langle W_1^2 + W_2^2 \rangle$, where $W_{1,2}$ are the winding numbers in the two lattice directions of the worldlines appearing in the SSE representation of the quantum partition function\footnote{\textcopyright 2022 American Physical Society.}.\footnote{\textcopyright 2022 American Physical Society.}

It is straightforward to observe that non-magnetic impurities introduce an extremely rich field dependence of the magnetic observables, which differs substantially from the one observed in the clean case\footnote{\textcopyright 2022 American Physical Society.}.\footnote{\textcopyright 2022 American Physical Society.}. Here we describe the alternation of phases induced by the field, postponing the details of the two novel quantum-disordered phases (disordered-free-moments and Bose-glass phase) to the following sections.

In zero field, long-range order is expected due to an order-by-disorder mechanism, as discussed in Sec. III. To estimate the average energy scale associated with the ordered phases through Eq. (9) we need the information the correlation length $\xi_0$ and the gap $\Delta$ in the clean case $p = 0$. From QMC simulations for the $p = 0$ case we obtain $\xi_0 \approx 0.5$, through second moment estimation\footnote{\textcopyright 2022 American Physical Society.}. Moreover we can estimate the gap through the critical field $h_{c1}^{(0)}$ that induces long-range antiferromagnetic order in the clean system. We obtain $h_{c1}^{(0)} = 0.745(2)$ the scaling of the uniform magnetization $m_u$, which becomes finite at the critical point. The resulting estimate for $\langle J_{\text{eff}} \rangle$ is then: $\langle J_{\text{eff}} \rangle \approx 6 \times 10^{-3}J$. In presence of a field, the zero-field Néel-ordered state of the free moments will turn into a canted XY-ordered state, and eventually the field will destroy the antiferromagnetic order of the free moments leading to their full polarization. Nonetheless, due to the peculiar features of the long-range interactions between the free moments, the canted XY-ordered phase and the fully polarized phase are not contiguous, but they are separated by an intermediate, novel phase.

The extremely small value for $\langle J_{\text{eff}} \rangle$ compared with the gap in the clean case immediately suggests that an equally small field can suppress long-range antiferromagnetism. Estimating this field numerically is a formidable task, given that, to observe the $T = 0$ physics on reasonably large sizes, we need to be at $k_BT \ll \langle J_{\text{eff}} \rangle$. Our QMC simulations show unambiguously that no long-range order survives the extrapolation to the thermodynamic limit down to a field $h = 0.005$, as shown in Fig. 3. Therefore we set the value $h = 0.005$ as an upper bound for the destruction of the order-by-disorder phase.
corresponding to well below the saturation value for the free moments, and it is evident that it scales towards smaller values for increasing $L$, so that in the thermodynamic limit it will converge to a value well below the plateau one $m_u < pS = 0.1$.

Remarkably, the small field that destroys the order-by-disorder phase is able to only partially polarize the free moments localized around the unpaired spins, as shown in the inset of Fig. 3. In fact, immediately after the destruction of long-range order, the magnetization remains well below the saturation value for the free moments, corresponding to $m_u^* = pS = 0.1$. The state of partial polarization of the free moments persists up to a field $h = h_{\text{plateau}} \approx 0.36$ at which the magnetization reaches a plateau corresponding exactly to the value $m_u^*$. This means that, for $0.005 < h < h_{\text{plateau}}$, the free moments still preserve a finite projection on the $xy$ plane transverse to the field, and that the transverse spin components are quantum disordered. This quantum disordered state is gapless, given that the magnetization continues to grow with the field. To our knowledge this phase has no analog in what has been observed so far in clean systems, and we therefore dub it as disordered-free-moment phase. A possible scenario for the mechanism leading to quantum disorder in this phase is provided in Sec. IV.

For $h > h_{\text{plateau}}$ the system has fully polarized free moments, and it acquires a gap to all triplet excitations, corresponding to a vanishing of the uniform susceptibility. This state persists over a quite sizable field range: in this field interval the dynamics of the free moments is completely quenched by the fields, but intact dimers lying away from unpaired spins have a local gap which is still larger than the field. Therefore, by dynamically eliminating the extra degrees of freedom introduced by the unpaired spins, the field essentially restores a gapped disordered state which is the “dirty” counterpart to the dimer-singlet state in the clean limit. Interestingly, while the gap for the excitations of the free moments increases linearly with the field, the one for the excitation of the intact dimers in clean regions decreases, and eventually closes in a fashion similar to that of the clean limit, with the appearance of a dilute gas of triplet quasiparticles. The field value at which the gap to clean-region excitations closes is necessarily the same as the lower-critical field in the clean limit $h_{c1}^{(0)}$. In fact, in the thermodynamic limit there exists always an arbitrarily big clean region with probability

$$P(l) \sim \exp(-2|\ln(1-p)|l^2)$$

where $l$ is its characteristic linear size. This region, having an arbitrarily big size albeit with infinitesimal probability, is arbitrarily close to a clean system, and for $h > h_{c1}^{(0)}$ its local gap must close, thus accepting the appearance of the first triplet quasiparticles. This is fully consistent with our QMC results, where we observe a revival of the magnetization process after the plateau phase at $h \approx 0.76$ for lattice sizes up to $L = 32$, which is already in good agreement with $h_{c1}^{(0)} \approx 0.745$. It is important to point out that any finite-size estimate of the closure of the gap in a disordered system is an upper bound to the actual value, due to the fact that a rare clean region can be at most as big as the size of the entire finite-size system.

A fundamental difference with the closure of the gap in the clean case is provided by the fact that the first triplet quasiparticles appearing in the largest clean regions of the system are localized in such regions, and are not able to coherently propagate throughout the system. In fact, fully polarized free moments with a finite gap to spin-flips act as almost impenetrable scatterers for the triplet quasiparticles. On the other hand, intact dimers close to impurities have a lower coordination to the rest of the system and therefore they feature a local gap which is bigger than the one of the clean two-dimensional system, $h_{c1}^{(0)} J$, and closer to that of a single dimer, $J > h_{c1}^{(0)} J$. This means that they also act as energy barriers for triplet quasiparticles created in the clean regions. If $h > h_{c1}^{(0)} J$, the gas of triplet quasiparticles is extremely dilute, and we can neglect interactions among them. The state of the triplet quasiparticles at low filling in the site-diluted weakly coupled dimer system is therefore analogous to the ground state of an Anderson problem in two dimensions, which is always quantum localized regardless of the strength of disorder and of the dimensionality. Therefore, after the closure of the gap in the clean regions, the system of triplet quasi-particles form an Anderson-insulating state, which is usually denoted as Bose glass for interacting bosons\(^{22}\). Such state has no condensate and no superfluid fraction, corresponding to a vanishing transverse magnetization $m_s$ and to a vanishing spin stiffness $\gamma$, as clearly shown by our QMC results. Yet, it is a compressible state, namely it has a vanishing particle gap, corresponding to a finite susceptibility $\chi_u$.
in the magnetic language.

As the field is increased above \( h_{c1}^{(0)} \), the density of bosons increases, and the extent of locally gapless regions increases as well. The hard-core repulsion between the quasiparticles and their increased chemical potential eventually leads to a localization-delocalization transition, corresponding to the onset of superfluidity (\( \Upsilon > 0 \)) and to the appearance of long-range phase order (\( m_s > 0 \)). The Bose-glass-to-superfluid quantum phase transition happens at the critical field \( h_{c1} = 0.87(2) \), which we estimate through the study of the scaling of the correlation length, superfluid density and staggered magnetization.

The result for the dynamical critical exponent remarkably shows that the site-diluted Heisenberg bilayer fully realizes the theoretical picture of the transition from a Bose-glass state to a superfluid. In \( d = 2 \) the dynamical critical exponent is accidentally unchanged with respect to its clean value \( z = 2 \), but the other estimated exponents strongly differ from their mean-field values \( \beta = 1/2 \) and \( \nu = 1/2 \) which should hold in the clean limit, given that \( d+z = 4 \) is the upper critical dimension.

In the superfluid phase we notice that all the quantities shown in Fig. 2 display a feature at a field \( h \) corresponding approximately to half filling of the intact dimers with triplet quasiparticles, namely to a magnetization \( m_s = S(1+p)/2 = 0.3 \). The uniform magnetization shows a kink, which reflects in a peak of the uniform susceptibility; the staggered magnetization \( m_s \) and the superfluid density \( \Upsilon \) also show a kink. This singular behavior is not observed at all in the clean system\(^\text{22} \) at half filling. Such a feature is probably to be attributed to weakly coordinated dimers or small clusters of dimers present in the system, whose response to a field is step-like when the field exceeds their local gap. See also Sec. \( \text{I} \) for further discussion.

Given the hardcore nature of the triplet quasiparticles, a filling of at most a triplet quasiparticle per intact dimer can be reached by the system. When the density of quasiparticles gets close to its maximum value, the system can be more conveniently regarded as a dilute gas of singlet quasiholes in the triplet sea, living on intact dimers which are not fully polarized. Interestingly, the intact dimers belonging to clean regions can be fully polarized only by a field close to the saturation field of the clean limit \( h \lesssim h_{c2}^{(0)} = 1+4/g \). On the contrary, intact dimers which are in regions of lower local coordination are more easily polarized, because their local saturation field is closer to that of an isolated dimer, \( h = 1 \). This means that singlet quasiholes get gradually expelled from regions close to the impurities and get localized in the clean regions, analogously to what had happened to the triplet quasiparticles for \( h \gtrsim h_{c1}^{(0)} \). The superfluid state of the singlet quasiholes gets therefore destroyed by the field, and the system undergoes a second superfluid-to-Bose-glass transition at a critical field \( h_{c2} = 1.36(2) < h_{c2}^{(0)} = 1.5 \). After

\[
m_s = L^{-\beta/\nu} F_{m_s}[L^{1/\nu}(h - h_{c1})].
\]
a second extended Bose-glass phase for $h_{c2} < h < h_{c2}^{(0)}$, the system of triplet quasiparticles reaches unitary filling, and at this point the system becomes a band insulator (or, alternatively, a Mott insulator with infinite on-site repulsion). Such state corresponds to the saturation of the magnetization, $m_u = S = 1/2$. It is important to point out that, in the thermodynamic limit, full saturation is only attained at the clean critical field $h_{c2}^{(0)}$ and not before: in fact, in an infinite system there exists always an arbitrarily big clean region whose local saturation field is arbitrarily close to that of the perfectly clean system.

**IV. FIELD DESTRUCTION OF ORDER BY DISORDER: THE DISORDERED-FREE-MOMENT PHASE**

As pointed out in the previous section, the resulting disordered-free-moment phase has the markedly unconventional feature of displaying a gapless spectrum and absence of spontaneous long-range order. Here we propose a physical scenario for the explanation of such phase.

To simplify the picture of the free moments, we imagine them to be fully equivalent to a system of randomly located spins on a square lattice and interacting with exponentially decaying Heisenberg couplings. Fig. 5 sketches such system in the simpler case of a single layer - the case of a bilayer is anyway completely analogous. In the classical limit $S \to \infty$, the system of randomly located spins in a weak enough magnetic field has a canted antiferromagnetic ground state (Fig. 5 upper panel), in which the spin components transverse to the field are staggered according to a 2-sublattice structure. Locally it might happen that isolated spins minimize their energy by fully aligning with the field and losing therefore their transverse components. Nonetheless, the remaining clusters of partially polarized spins, even if separated by fully polarized ones, will preserve the long-range antiferromagnetic order of their transverse components because they are directly coupled through long-range interactions that go across the polarized regions. This means that, in the classical limit, the system has long-range order up to the field that roughly equals the strongest coupling $(J_{eff})_{max}$ and thus polarizes all the spins.

Quantum mechanically it is easy to imagine a substantially different ground state. A fundamental phenomenon introduced by quantum fluctuations is the formation of local singlets between spins that lie close to each other on different sublattices and are therefore strongly coupled through $J_{eff} \sim J'$. If all the other spins are sufficiently far apart, it is evident that the close-lying spins will have a strong tendency to form a singlet as long as their singlet-to-triplet gap is much larger than the sum of the interactions with all the other spins, $J_{eff} \gg \sum' J_{eff}$ where $\sum'$ runs over all spins but the one lying close. The formation of a local singlet decouples the spins involved in it from the rest of the system. If two other spins exist nearby which are lying on different sublattices, are close enough to each other (but not as close as the previous two ones) and far from the others, they will also have a tendency to form a singlet with a smaller gap, etc. In one-dimensional bond disordered antiferromagnets this argument leads to the prediction of a gapless random-singlet phase without long-range order, where singlets exist to all energy scale. Interestingly, in two dimensions the above reasoning is only valid for close-lying spin pairs, namely only over a short length scale. Due to the higher coordination in a two-dimensional lattice, when two spins are sufficiently far from each other the long-range singlet formation becomes unfavourable with respect to the appearance of long-range Néel order. Indeed, in Ref. 38 it has been shown that, in zero-field, a model of randomly located spins with exponentially decaying couplings always displays long-range order regardless of the concentration of the spins. The ground state of

In this section we focus on the field destruction of the long-range ordered phase of the free moments.
the system is evidently very inhomogeneous, with closely-lying spins forming approximately singlets and partially isolated spins being instead involved in a long-range ordered Néel state. A notable feature of this ground state is that short-range singlets have a triplet gap which can be substantially larger than the typical energy associated with the Néel state formed by the other spins. Therefore not only the state is highly inhomogeneous, but it also displays a broad range of energy scales.

Accepting this sketchy view of the ordered state of randomly located spins in zero field, it is trivial to argue what happens in presence of a field. Due to the large spread in energy scales, the response to an applied field will be very inhomogeneous. As in the classical case, the partially isolated spins will be the first to be polarized by the field, thus minimizing their Zeeman energy. But, according to what noticed before, these spins are also the ones that are involved in the long-range ordered state. If there is a net energy separation between the characteristic energy of the Néel state \( J_{\text{Néel}} \) for these spins and the characteristic energy of the singlet states of the close-lying spins \( J_{\text{eff}} \), there exists also a field value \( J_{\text{Néel}}/J < h < J_{\text{eff}}/J \) which destroys the Néel state of the isolated spins by polarizing them, but does not polarize the close-lying spins. This field would then correspond to the one which drives the order-by-disorder phase into the disordered-free-moment phase. The surviving unpolarized singlets are responsible for the magnetization not being fully saturated. Their maximum spatial range is fixed by the field value, since singlets cannot survive when the coupling energy \( J_{\text{eff}} \) is overcome by the Zeeman energy \( hJ \). Therefore we expect the antiferromagnetic correlations in this phase to be short-ranged, as our QMC data seem to suggest, although a direct analysis of this point is deferred to future work\(^{27}\). Such a quantum-disordered state is clearly gapless, given that the surviving singlets have in-field gaps that roughly span the continuous interval \([0, J'(1 - h)]\).

A recent mean-field study of the field destruction in site-diluted weakly-coupled dimer systems is presented in Ref. \(^{21}\). This study does not report any disordered-free-moment phase between the order-by-disorder phase and the plateau one, although the mechanism of local singlet formation is clearly mentioned, and the spins involved in local singlets are explicitly excluded from the mean-field treatment and from the disorder average (compare the discussion in Sec. \(^{11}\)). Therefore the conclusions of Ref. \(^{21}\) only apply to the free moments participating in the Néel state in zero field and do not exclude the existence of a disordered-free-moment phase as the one we have described.

V. BOSE GLASS PHASE AND RARE-EVENT STATISTICS

In this section we discuss in details the nature of the Bose-glass phase and of its unconventional magnetization behavior. As already pointed out in Sec. \(^{11}\) the characteristic feature of this phase is the appearance of quantum-localized triplet quasiparticles (singlet quasiholes) in rare clean regions, corresponding to locally magnetized (not fully polarized) intact dimers. Here we assume that clean regions hosting quantum-localized quasiparticles are completely uncorrelated from each other, which is consistent with the picture that the quasiparticles are unable to propagate coherently throughout the system. From the point of view of the response to a magnetic field, this means that each clean region behaves independently from the others, and it essentially behaves as a finite-size cluster with characteristic linear size \( l \) following the exponentially decaying distribution Eq. \(^{10}\) characteristic of the geometrical statistics of rare regions. In particular, the response to a magnetic field is dictated by the spectral properties of the cluster, namely by the value of the local gap \( \Delta(l) \). Treating the response of the system as the sum of independent responses of different finite-size clusters, governed by their local gap, represents the core assumption of a local-gap model for the Bose-glass phase (see Fig. \( \text{B} \)).

First we consider the low-field Bose-glass phase,
namely the one occurring for \( h \gtrsim h_{c1}^{(0)} \). In this field regime, a cluster with a gap \( \Delta(l) \) will only respond to a field larger or equal to the gap, namely it develops a total uniform magnetization of the type

\[
M_l(h) = [h - \Delta(l)]^\gamma \Theta[h - \Delta(l)].
\] (13)

where we approximate the stepwise magnetization curve of a finite cluster through a power law with an exponent \( \gamma \) whose knowledge is not essential for our conclusions, although we expect \( \gamma = 1 \) for clusters with a layer structure. For \( h_{c1}^{(0)} < h < h_{c2}^{(0)} \) the infinite clean system is gapless, so in this field range the gap on finite clusters is purely a finite-size one. We can assume that the finite-size correction to the zero-field gap of the infinite system, \( \Delta(\infty) = h_{c1}^{(0)} \), scales with inverse of the cluster volume, as expected in Heisenberg antiferromagnets undergoing spontaneous symmetry breaking.

\[
\Delta(l) \approx h_{c1}^{(0)} + \frac{c}{l^2}.
\] (14)

The above relation allows us to relate the probability distribution of local gaps to that of the cluster sizes, Eq. (10):

\[
\tilde{P}(\Delta) = \frac{P[l(\Delta)]}{|\Delta'[l(\Delta)]|} \sim (\Delta - h_{c1}^{(0)})^{3/2} \exp \left[ -\frac{2|\ln(1-p)|}{c(\Delta - h_{c1}^{(0)})} \right].
\] (15)

As expected, this distribution attributes an exponentially vanishing probability to nearly gapless clusters, reflecting the exponentially rare occurrence of large clean regions.

This local-gap model allows us then to extract the total magnetization of the clean clusters as the sum of the magnetizations of the individual clusters:

\[
m_u(h) - ps = \frac{1}{N(1-p)} \sum \text{clusters} M_{\text{cluster}}(h)
= \int d\Delta (\Delta - \Delta)^\gamma \Theta(\Delta - \Delta) \tilde{P}(\Delta).
\] (16)

Here the magnetization of the clean clusters is expressed as the global magnetization \( m_u(h) \) minus the saturated magnetization of the free moments, \( ps \), corresponding to the magnetization plateau.

The field dependence of the magnetization can be determined to leading order through a saddle-point approximation of the above integral over the probability distribution \( \tilde{P}(\Delta) \), which, for \( 0 < h - h_{c1}^{(0)} \ll 1 \), yields the following prediction:

\[
m_u(h) - ps \sim \exp \left[ -\frac{2|\ln(1-p)|}{c(h - h_{c1}^{(0)})} \right],
\] (17)

namely an exponentially slow magnetization, which reflects directly the statistics of the rare clean regions.

A completely analogous treatment of the field-dependence of the magnetization can be used for the high-field Bose-glass phase, \( h \lesssim h_{c2}^{(0)} \). In this case we introduce the conjugate magnetization \( \tilde{m}_u = S - m_u \) and the conjugate field \( \tilde{h} = h_{c2}^{(0)} - h \), such that \( \tilde{m}_u \) grows monotonically with \( \tilde{h} \). The in-field finite-size gap of the clusters for \( h \lesssim h_{c2}^{(0)} \) is taken as \( \Delta(l) = c'/l^2 \), and it derives from the fact that a finite-size cluster is fully polarized by a lower field than the one of the infinite system.

\[
S - m_u(h) \sim \exp \left[ -\frac{2|\ln(1-p)|}{c'(h_{c2}^{(0)} - h)} \right].
\] (18)

Fig. 7 shows the magnetization behavior in the two Bose-glass phases of the system. Remarkably the magnetization curve has a marked exponential dependence on the inverse of the distance of the field from the clean critical fields \( h_{c1}^{(0)} \) and \( h_{c2}^{(0)} \), reflecting directly the rare-event statistics. Also, such exponential dependence clearly appears to spread well beyond the Bose glass phase and to hold also in part of the superfluid phase. In particular we can relate the kink in the magnetization, leading to a blip in \( n_4 \) as seen in Fig. 2, to the point where the two exponential behaviors of the magnetization coming from \( h_{c1}^{(0)} \) and \( h_{c2}^{(0)} \) [Eq. (17) and Eq. (18)] meet each other roughly halfway at \( h \approx (h_{c1}^{(0)} + h_{c2}^{(0)})/2 \approx 1.12 \) in a discontinuous manner.

The local-gap model predictions of Eq. (17)-(18) is strikingly verified in both Bose-glass phases, as shown in Fig. 4(a): the exponential dependence of on \( \left( h - h_{c1}^{(0)} \right)^{-1} \), \( \left( h_{c2}^{(0)} - h \right)^{-1} \) is verified over about three orders of magnitude. In the low-field phase we still observe slight deviations from the perfectly exponential behavior close to \( h_{c1}^{(0)} \), most likely due to the presence of the free moments. The free moments are indeed fully polarized in this phase, with a gap to all excitations which grows linearly with the field distance from the onset of the plateau phase, \( \Delta_{\text{free-moments}} \sim h - h_{\text{plateau}} \). Yet, for \( h \gtrsim h_{c1}^{(0)} \), this gap might still not be big enough to completely rule out off-resonant exchanges of a triplet excitation between the clean regions and the free moments, mediated by the \( J' \) couplings between unpaired spins and intact dimers. When the density of triplets in the clean regions is very low, namely for \( m(h) - m_{\text{plateau}} \ll 1 \), this small effect might lead to visible deviations with respect to the predictions of the simple local-gap model. At high fields, on the other hand, the gap to excitations of the free moments is larger, and the above effect is expected to be suppressed, which is consistent with the excellent agreement we find between the numerical data and the magnetization of the local-gap model.
in very good agreement with the above prediction. This further demonstrates that the details of the exponential magnetization curve are very sensitive to the geometric features of the system. This result could in principle be used experimentally, e.g., to determine the doping concentration in a system, when its magnetization curve is compared with a reference system with known doping.

VI. EXPERIMENTAL IMPLICATIONS AND CONCLUSIONS

In this paper we have presented a complete picture of the extremely rich phase diagram displayed by site-diluted weakly-coupled dimer systems as a function of the applied field. We have shown that the field-induced Bose-Einstein condensation of triplet quasiparticles/singlet quasiholes appearing in the clean limit is strongly affected by disorder, which introduces a novel Bose-glass phase of quantum localized quasiparticles/quasiholes between the insulating (empty) phase and the condensate phase. The quantum phase transition to the ordered phase takes the nature of a localization-delocalization transition, and it numerically verifies the prediction for the dynamical critical exponent of the Bose-glass to superfluid transition. In the Bose glass phase, we show that rare event statistics dominates the response to the applied magnetic field, and the magnetization curve acquires an unconventional exponential dependence on the field reflecting the probability distribution of rare clean regions in the sample, as accurately predicted by a local-gap model. Finally, in zero field, disorder introduces free moments in the dimer-singlet state which show long-range antiferromagnetic ordering. We find that this antiferromagnetic state is destroyed by the field in an unconventional way, namely without full polarization of the free moments. A possible scenario for this mechanism involves the formation of finite-range singlets, reminiscent of the random-singlet phase in bond-disordered $S = 1/2$ Heisenberg spin chains. Such singlets survive the application of a small enough field which is on the contrary able to fully polarize the spins involved in the Néel ordered state. Further studies are being currently pursued to verify this scenario quantitatively.

We believe that our results have immediate experimental relevance for all unfrustrated spin gap systems in dimensions $d = 2$ and higher, and with a gap of the order of the strongest magnetic coupling in the system. As already mentioned in the introduction, it is generally accepted that the field-induced ordering in unfrustrated and magnetically isotropic spin gap systems has the common nature of a Bose-Einstein condensation of quasiparticle excitations. The disorder effects on such transition, here discussed in the specific example of the bilayer Heisenberg antiferromagnet, can be fully rephrased in the context of coupled Haldane chains, coupled spin ladders, and other two- and three-dimensional arrangements of weakly coupled $S = 1/2$.
dimers. The localization effects leading to the appearance of a Bose-glass phase are possibly more dramatic in quasi one-dimensional systems, leading to a larger extent in field values for the Bose-glass phase.

Candidate coupled-dimer compounds for the observation of the phase succession of Fig. 1 should display a significant difference between the intradimer coupling $J$ and the overall energy of the interdimer ones, $\sim zJ'/2$. Here $J'$ is the average energy of the interdimer couplings and $z$ is the dimer-lattice coordination number. This requirement leads to a zero field gap $\Delta \approx J - zJ'/2 \sim J$, which in turn results into a zero field correlation length $\xi_0 \lesssim 1$. If this condition is satisfied in the clean limit, as observed in the bilayer with $g = 8$, in the doped case the free moments induced in the system are very weakly interacting on average, $\langle J_{\text{eff}} \rangle/J \sim p(zJ'/J)^2 \exp(-1/\xi_0) \ll 1$, and their zero-field ordered state is destroyed by an applied field much smaller than the clean-limit gap $\Delta$. This guarantees a large separation of energy scales between the order-by-disorder phenomenon and the field-induced condensation of triplet quasi-particles, hence offering the possibility of clearly observing the intermediate phases (disordered-free-moment, plateau phase and Bose-glass). If the above requirement is not satisfied by the intrinsic parameters $J$, $J'$ and $z$ of the system, there is still the possibility of working at very low doping $p \ll 1$. Fortunately, the requirement $J \ll zJ'/2$ appears to be met by a variety of compounds. Among others: BaCuSi$_2$O$_6$, which has $zJ'/2J \approx 0.3$, Sr$_2$Cu(BO$_3$)$_2$ which has $zJ'/2J \approx 0.2 - 0.3$, Cu$_{12}$[(C$_5$H$_{12}$N$_2$)$_2$]Cl$_4$ with $zJ'/2J \approx 0.2$, (C$_5$H$_{12}$N$_2$)$_2$CuBr$_4$ with $zJ'/2J \approx 0.3$, etc. On the other hand, if the inter-moment coupling is too large, short-range antiferromagnetic correlations between the free moments might survive up to a field of the order of the gap, thus eliminating the plateau phase, as theoretically observed in the bilayer system with $g = 4$. If long-range antiferromagnetic order of the free moments persists up to fields of the order of the gap, the order-by-disorder phase might even merge with the ordered phase of the intact dimers, so that all disordered phases in between are washed out. This is the conclusion of a recent study on the Mg-doped TICuCl$_3$, which has indeed $zJ'/2J \sim 0.9$.

In the case of coupled Haldane chains with nonmagnetic doping, $S = 1/2$ moments are induced by the impurities at the edges of finite chain segments. To have a large energy separation between the inter-moment interaction and the Haldane gap, it is certainly necessary that the gap $\Delta \approx 0.4J$ be much larger than the characteristic energy of the interchain couplings, $zJ'\xi_0$, where $J'$ is the average interchain coupling, $z$ is the coordination number of the coupled chains, and $\xi_0 \sim 6$ is the correlation length of the isolated chain. Nonetheless, for weakly coupled chains the dominant coupling channel between the free moments is along the chain direction, namely it depends crucially on the average spacing between impurities along each chain $\sim 1/p$ compared with the characteristic decay length of the effective interactions, which is given by $\xi_0$ for small impurity concentrations. Therefore it is necessary that $1/p \gg \xi_0$, which roughly means $p \ll 0.1$. All these requirements have evidently been met by recent experiments on Pb(Ni$_{1-\delta}$Mg$_\delta$)$_2$V$_2$O$_8$ with $p \leq 0.02$. To our knowledge, this system stands as the only experimental example in which first the impurity-induced ordered phase is destroyed by the field through polarization of the free moments, and then order is induced again by the field through partial polarization of the clean chain segments. The temperature at which the experiments have been performed so far appears to be too high to resolve the predicted succession of disordered phases in between the two ordered ones, but further experiments at lower temperatures are a very promising test of the scenario presented in this paper.

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APPENDIX A: WAVEFUNCTION AND EFFECTIVE INTERACTION OF THE FREE MOMENTS IN 2$d$

In this appendix we perturbatively derive the wavefunction of the free moments, Eq. (B3), and their effective interaction in two dimensions, Eq. (B3). We first consider a single unpaired spin at site $i$ surrounded by intact dimers, and calculate the first-order perturbative correction to the ground state due to the coupling between the unpaired spin and the host matrix, $V_i = J' \sum_q S_i \cdot S_{i+\delta}$, where $\delta$ connects the site $i$ to its nearest neighbors. The unperturbed state of the system for $J' = 0$ is assumed as $|\Psi^{(0)}\rangle = |\uparrow_i\rangle |0\rangle$, where $|\uparrow_i\rangle$ is an arbitrary state of the unpaired spin and $|0\rangle$ is the unperturbed dimer-singlet state of the surrounding intact dimers. The perturbation term

$$V_i^{-+} = \frac{J'}{\sqrt{N}} \sum_q z\gamma_q S^{-}_i S^{+}_q e^{iq\cdot \mathbf{r}_i}$$

(A1)

flips the unpaired spin and transfers its magnetic moment to a triplet excitation of the intact dimers, namely it mixes up the unperturbed ground state $|\Psi^{(0)}\rangle$ with excited states of the form

$$|\Psi(k)\rangle = |\downarrow_i\rangle |k\rangle.$$  

(A2)

where $|k\rangle$ is the state of the intact dimers with one elementary triplet excitation at momentum $k$. Assuming
the following dispersion relation for the long-wavelength gapped modes of the unperturbed coupled dimer system

$$\epsilon(k) = \sqrt{\Delta^2 + v^2k^2}$$

(A3)

we obtain the first-order perturbed state

$$|\Psi^{(1)}\rangle = |\Psi^{(0)}\rangle + \frac{J'z}{\sqrt{N}} \sum_k \frac{M_k e^{i k \cdot r_i}}{\epsilon(k)} |\downarrow_i\rangle$$

$$= |\Psi^{(0)}\rangle + |\downarrow_i\rangle \sum_r \psi(r)|r\rangle$$

(A4)

with \(M_k \approx \gamma_k \langle k | S_k^+ | 0 \rangle\). In the last step we have introduced the localized triplet states \(|r\rangle = 1/\sqrt{N} \sum_q \exp(-i q \cdot r) |q\rangle\). In this form the amplitude \(\psi(r)\) takes the meaning of wavefunction of the free moment which is transferred by the perturbation from the unpaired spin to the host dimer system. Passing to the continuum limit, and neglecting the \(k\)-dependence of the matrix elements \(M_k \approx 1\), we obtain

$$\psi(r) = J'z \int d^2k \frac{e^{i k \cdot r}}{\epsilon(k)} = \frac{J'z}{\Delta \xi_0} \int_0^\infty \frac{k J_0(kr)}{\sqrt{r^2 + \frac{k^2}{\xi_0^2}}} \quad \text{(A5)}$$

where \(\xi_0 = v/\Delta\) is the correlation length of the unperturbed host dimers and \(J_0(x)\) is an ordinary Bessel function. The last expression contains an Hankel-Nicholson-type integral\(^{A3}\) whose solution is expressed through the modified Bessel function \(K_{1/2}\) in the form

$$\psi(r) = \frac{J'z}{\Delta \xi_0} \frac{\sqrt{2}}{\pi} \frac{K_{1/2}(r/\xi_0)}{\sqrt{r/\xi_0}} \quad \text{(A6)}$$

The asymptotic expression\(^{A6}\) of Eq. (A6) for large \(r\) gives Eq. (4).

The effective interaction between the free moments arises instead from second order perturbation corrections in the ground-state energy of the system\(^{19,21}\). Taking two unpaired spins at sites \(i\) and \(j\), they exchange a triplet excitation through second-order perturbations \(V_{i, r_i} V_{j, r_j}^\dagger\) and \(V_{j, r_j} V_{i, r_i}^\dagger\). These terms introduce a singlet-triplet splitting for the joint state of the unpaired spins which immediately gives the effective interaction strength \(J_{\text{eff}}(i, j; \alpha, \beta)\) in the form

$$J_{\text{eff}}(i, j; \alpha, \beta) = (-1)^\sigma \frac{(J'z)^2}{N} \sum_k \frac{|M_k|^2 \epsilon_k(r_i, -r_j)}{8 \epsilon(k)}$$

(A7)

where \(\sigma = x_i + y_i x_j + y_j + \alpha + \beta\). We then recover a similar expression to that encountered in Eq. (A6), which, in the continuum limit, can be evaluated through ordinary and modified Bessel functions as in Eq. (A5)-(A6). The final expression is

$$J_{\text{eff}}(i, j; \alpha, \beta) = (-1)^\sigma \frac{(J'z)^2}{4 \pi \Delta \xi_0} \frac{\sqrt{2}}{\Gamma(1/2)} \frac{K_{1/2}(r/\xi_0)}{\sqrt{r/\xi_0}} \quad \text{(A8)}$$

where \(r = |r_i - r_j|\). In the large-\(r\) limit we then recover Eq. (4).

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