The introduction of randomness in strongly correlated fermionic and bosonic systems on a lattice offers a large showcase of novel quantum behavior \[1,2,3\]. In quantum spin systems with an ordered ground state, the generic effect of geometric disorder is an enhancement of local quantum fluctuations through the reduction of the connectivity of the lattice \[4\], which may lead to quantum disordered phases \[5\]. On the other hand, in spin systems with a gapped quantum-disordered ground state, geometric randomness can induce local magnetic moments giving rise to long-range order through an order-by-disorder mechanism \[6\]. In the case of superfluid interacting bosons, the presence of an increasing amount of disorder can destroy superfluidity through quantum localization, inducing a disordered, yet gapless Bose-glass phase with a finite compressibility \[2\].

Recently, the strong connection between lattice bosons and quantum spin models has been pointed out in the context of unfrustrated \( S = 1/2 \) weakly-coupled dimer systems. For sufficiently weak inter-dimer couplings, the spin system has a singlet ground state with a finite gap to triplet excitations. The application of a uniform magnetic field leads to the closing the triplet gap, accompanied by-disorder mechanism \[3\]. In the case of superfluidity, the clean system with large \( J/g \) ratio can be well described by an effective model of hardcore TQPs \[4\]. Off-diagonal long-range order corresponds to the appearance of a finite staggered magnetization in the plane perpendicular to the field. When the magnetization is half-saturated, the relevant degrees of freedom of the condensate become hardcore singlet quasi-holes (SQHs) in the triplet sea, which disappear completely at an upper critical field \( h_1^{(0)} \) fully polarizing the system. For \( h < h_1^{(0)} \) \( (h > h_2^{(0)} \) the system is therefore a band insulator, with an empty (full) band of TQPs. The validity of the description of the ordered phase as a Bose-Einstein condensate has been extensively investigated both theoretically and experimentally \[5,6,7,8\].

By virtue of the bosonic picture, it is intriguing to envision the possibility of a Bose-glass phase for weakly coupled dimer systems in a magnetic field upon introduction of lattice disorder \[10\]. This opens up the appealing perspective of unambiguously realizing such a phase in a quantum spin system, profiting of the high level of control with which disorder can be introduced in a magnetic lattice \[11\]. The focus of this Letter is the extent and the major signatures of such a phase in a realistic model.

In what follows we investigate the \( S = 1/2 \) Heisenberg antiferromagnet in a magnetic field and with site dilution, whose Hamiltonian reads:

\[
H = J' \sum_{\langle ij \rangle} \sum_{\alpha=1,2} \epsilon_{i,\alpha} \epsilon_{j,\alpha} S_{i,\alpha} \cdot S_{j,\alpha} \\
+ J \sum_i \epsilon_{i,1} \epsilon_{i,2} S_{i,1} \cdot S_{i,2} - g \mu_B H \sum_{i,\alpha} \epsilon_{i,\alpha} S_{i,\alpha}^z \quad (1)
\]

Here the index \( i \) runs over the sites of a square lattice, \( \langle ij \rangle \) 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. The variables \( \epsilon_{i,\alpha} \) take the values 0 or 1 with probability \( p \) and \( 1-p \) respectively, \( p \) being the concentration of non-magnetic sites. Hereafter we will express the field in reduced units \( h = g \mu_B H/J \). We have investigated the above Hamiltonian making use of Stochastic Series Expansion quantum Monte Carlo based on the directed-loop algorithm \[12\]. and considering \( L \times L \times 2 \) lattices with \( L \) up to 40. The \( T = 0 \) limit is reached through a \( \beta \)-doubling approach \[3\]. Disorder averaging is performed by using typically 200 different disorder realizations.

In the clean limit \( (p = 0) \) and at zero field, the Hamiltonian of Eq. \[14\] is in a gapped dimer-singlet phase for \( J/J' > 2.5 \) \[13\]. Hereafter we will specialize to the case of a bilayer with \( J/J' = 4 \), namely well inside the dimer-singlet phase. As discussed in the introduction, the clean system with large \( J/J' \) ratio can be well described by an effective model of hardcore TQPs which hop from dimer to dimer with amplitude \( J'/2 \), nearest-neighbor repulsion \( J'/2 \), and chemical potential \( J(h - 1) \) controlled by the field \[14\]. Increasing the field leads to the closing the triplet gap, accompanied
by the condensation of TQPs. We have investigated this
scenario numerically, by studying the field evolution of
the uniform magnetization \( m_u^x = \langle S^x \rangle \), the uniform sus-
ceptibility \( \chi_u = \frac{m_u^x}{h} \), the staggered magnetization
\( m_s^x = \frac{1}{4} \sum_{\alpha\beta} \sqrt{\langle -1 \rangle L^2} \langle S^x_{\alpha\beta} S^x_{\alpha+L/2,\beta} \rangle \), and the
superfluid density \( \Upsilon = T/2 \langle W^2 + W_2^2 \rangle \), where \( W_{x/y} \)
is the worldline winding number in the \( x/y \) direction.

As shown in Fig. 1, a field-induced ordered phase with
\( m_s^x, \Upsilon \neq 0 \) is clearly observed between \( h_{c1}^{(0)} = 0.47(1) \) and
\( h_{c2}^{(0)} = 2 \), in between a dimer-singlet phase \((h < h_{c2}^{(0)})\) and a
fully polarized phase \((h < h_{c1}^{(0)})\).

We now turn to the case of the doped system, \( p \neq 0 \).
From the purely geometric point of view, the lattice un-
dergoes a percolation transition at \( p^* = 0.5244(2) \) which
we estimated through classical Monte Carlo calculations
based on a recently proposed algorithm [15].

The magnetic behavior in turn displays a rich se-
quence of phases well below the percolation transition.
Fig. 2 shows the zero-temperature phase diagram, where
boundary lines between ordered and disordered phases
have been estimated through the linear scaling of the
disorder-averaged correlation length, \( \xi_{xx(yy)} \sim L \).

In what follows, we will discuss the phase diagram
making use of both the bosonic and the magnetic
language. Strictly speaking, the conventional bosonic map-
ning onto hardcore TQPs breaks down in presence of im-
purities, since some of the spins become unpaired, as they
miss their partner on the neighboring layer. A bosonic
mapping is however still possible in which bosons corre-
spond to \( | \uparrow \uparrow \rangle \) states on intact dimers and to \( | \uparrow \rangle \) states
on unpaired spins. Site dilution of the spin model re-
fects in correlated diagonal and off-diagonal disorder of
the bosonic model [10].

In the dimer-singlet phase the introduction of vacan-
cies in the magnetic lattice leads to the appearence of
local \( S = 1/2 \) moments. It is straightforward to iden-
tify these moments with unpaired spins, but in fact they
occupy a larger volume \( \sim \xi_0^2 \) where \( \xi_0 \) is the correla-
tion length in the clean limit \( p = 0 \) [17], thus spreading
also over intact dimers. Those moments are coupled
through an effective unfrustrated antiferromagnetic net-
work, which can sustain long-range order at \( T = 0 \). This
gives rise to an order-by-disorder phenomenon, which
is expected to persist for any doping concentration up
to percolation \( p^* \). The network of local moments has
a broad distribution of effective couplings, which scale
exponentially with the inter-moment distance \( r \) [18],
\( J_{\text{eff}} \sim \exp[-r/\xi_0] \). The application of a moderate field
\((h < h_{c1}^{(0)})\) can easily destroy the antiferromagnetic order

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{fig1}
\caption{Field dependence of the uniform magnetization \( m_u^x \),
transverse staggered magnetization \( m_s^x \), and superfluid den-
sity \( \Upsilon \) at \( T = 0 \) for the bilayer antiferromagnet with \( J/J' = 4 \)
in the clean limit \( (p = 0) \).}
\end{figure}

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{fig2}
\caption{Ground-state phase diagram of the site-diluted bi-
layer Heisenberg antiferromagnet with \( J/J' = 4 \).
(a) \( m = 0.05 \) \quad (b) \( m = 0.05 \)
\end{figure}

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{fig3}
\caption{(a)-(b): Real-space images of the dimer magnetiza-
tion \( m_i = \langle S^x_i + S^z_i \rangle \) on intact dimers in a 40x40x2 bilayer
with \( J/J' = 4 \), dilution \( p = 0.1 \) and at inverse temperature
\( \beta J = 256 \), for \( h = 0.56 \) (a) and \( h = 0.6 \) (b). The radius of
the dots is proportional to the dimer magnetization. The mag-
netization of unpaired spins is omitted for clarity. The most
visible localized states are highlighted in (a), while the back-
bone of the percolating magnetized network is highlighted in
(b). (c): Superfluid density as a function of the field for the
specific sample considered.}
\end{figure}
by polarizing a majority of the effective magnetic moments \( \mathbf{19} \), bringing the system into a partially polarized quantum-disordered phase. In particular, those dimers which are immediately close to an unpaired spin (roughly within a distance of \( \xi_0 \)) are also partially polarized, even if the field is lower than the dimer gap and the bilayer gap. In the bosonic picture, this means that TQPs are present in the ground state, localized around unpaired spins and only weakly penetrating clean regions of intact dimers, which mostly remain unmagnetized. They form a “gossamer” superfluid network with exponentially suppressed links for small fields, but for larger particle numbers this network turns into an insulating one due to the complete filling of some of its islands.

Upon increasing the field beyond \( h_{c1}(0) \), the picture of TQPs exponentially localized around vacancies start to change substantially. Continuous regions of intact dimers, which occur with probability exponentially small in the size of the region, begin to respond to a field similarly to what would happen in the clean case. Some of the intact dimers with a lower local coordination, nonetheless, have a higher local gap which a field \( h \approx h_{c1}(0) \) is not able to close, so that they remain non-magnetized up to higher fields. In the bosonic picture, this means that TQPs begin to appear in the bulk of the clean regions, but they are exponentially localized due to disorder. This picture clearly corresponds to that of a Bose-glass phase \( \mathbf{2} \). Such a phase extends up to a critical field \( h_{c1} \) at which the increased population of bosons, together with the hardcore repulsive interaction, leads to a localization-delocalization transition and to superfluidity, as shown in Fig. 3. There the density distribution of the TQPs is imaged by the dimer magnetization \( m_i = \langle S^z_{i,1} + S^z_{i,2} \rangle \). As the figure shows, superfluidity occurs via quantum percolation of the collective bosonic state throughout the lattice, while single particle states would all be exponentially localized in 2D.

From the numerical data, we observe that the Bose-glass phase extends over a field region that increases with the dilution \( p \). In particular, beyond an upper critical dilution, \( p_c \approx 0.36 \), no field-induced order survives. This happens well below the lattice percolation threshold \( p^* \). Therefore there is quite a large region of doping completely dominated by quantum disorder.

As the field is increased even further for \( p < p_c \), singlet quasi-holes (SQHs) become the relevant degrees of freedom. They undergo a similar superfluid-to-Bose-glass transition at a field \( h_{c2} \) without major alterations with respect to the TQP case. In particular the magnetization does not reach full saturation until the clean upper critical field \( h_{c1}(0) \), given that (exponentially rare) large clean areas cannot be fully polarized before \( h_{c1}(0) \) is reached.

A typical field scan through the phase diagram is shown in Fig. 4 for a dilution \( p = 0.2 \). The field is seen to quench the order-by-disorder spontaneous transverse magnetization and to drive the system towards a partially polarized state without fully polarizing the local free moments, whose magnetization continues to grow even beyond the transition. Eventually for large enough fields all the local moments get fully polarized by the field, leading to a magnetization plateau at \( m = ps = p/2 \) \( \mathbf{20} \). In the Bose-glass phase the uniform magnetization is seen to change concavity and to start to grow slowly, as the clean regions are gradually magnetized. A simple analysis can be made based on a “local-gap” model, for which the overall magnetization is the sum of the magnetizations of uncorrelated clusters of intact dimers with different local gaps \( \mathbf{10} \). The result is that the growth over the plateau value is exponentially activated, \( m^z_u - ps \sim \exp \left[ -c \left( h - h_{c1}(0) \right)^{-1} \right] \), where the exponential behavior comes from the exponential tail of the size distribution of clean regions, and it is a direct evidence of the dominant behavior of rare events in the Bose-glass phase. Similarly, an exponential saturation is observed for \( h \rightarrow h_{c2} \) in the upper Bose-glass region.

Let us now turn to the finite-temperature signatures of each phase. The zero-temperature XY ordered phase turns into a quasi-long-range ordered phase at finite \( T \) up to a Berezinskii-Kosterlitz-Thouless (BKT) transition temperature \( T_{\text{BKT}} \), at which the superfluid density vanishes and the transverse structure factor \( S(x, x') = \langle 1/N \rangle \sum_{i,\alpha,\beta} (-1)^{i+j+n+i+j} \langle \delta z_i(x) \delta z_j(x') \rangle \) becomes finite. We estimate the transition temperature \( T_{\text{BKT}} \) through BKT scaling of the superfluid density and of the transverse structure factor \( \mathbf{21} \). The transition temperature as a function of the field is shown in Fig. 5. Due to disorder and quantum fluctuations, \( T_{\text{BKT}} \) is almost two order of magnitudes lower than the interlayer exchange coupling \( J \), and its slightly asymmetric field dependence mimics that of the \( T = 0 \) order parameter.
Turning on the temperature from a $T = 0$ disordered phase, on the other hand, we observe interesting differences between the quantum disordered phase for $h < h_{c1}^0$ and the Bose-glass phase for $h_{c1}^0 < h < h_{c1}$ and $h_{c2} < h < h_{c2}^0$. In the clean limit $p = 0$, the gapped disordered phases for $h < h_{c1}^0$ and $h > h_{c2}^0$ show the common feature of thermal activation, with transverse structure factor $S(\pi, \pi)$, transverse correlation length $\xi_{xx(\pi)}$, and uniform magnetization $m_\pi^z$ increasing as $T$ grows above 0. Such a behavior is easily understood: upon increasing the temperature, the system is able to explore more correlated states with finite magnetization sitting beyond the energy gap. In the presence of site dilution, the temperature activation of correlations turns into a slow decrease as $T$ increases in the low-field regime dominated by the unpaired spins (see inset of Fig. 5). For high enough fields, and in particular in the Bose-glass phase, the temperature activation of correlations is restored up to a temperature $T^*_2$ for $S(\pi, \pi)$ and $T^*_\xi$ for $\xi$ at which both quantities hit a maximum, showing then a crossover to a decreasing dependence typical of a conventional paramagnetic phase. In contrast to the clean disordered phases, the Bose-glass phase is gapless. Nonetheless some clusters of intact dimers resist being magnetized for $h_{c1}^{(0)} < h < h_{c1}$ or they are fully polarized already for $h_{c2} < h < h_{c2}^{(0)}$. This means that the observed temperature activation in that field range can be associated with those portions of the system visiting states with higher transverse correlations, linked to the presence of bosonic TQPs/SQHs. In the bosonic language, this can be suggestively pictured as a partial delocalization of the trapped quasiparticles into those regions, assisted by thermal fluctuations.

Our findings are directly relevant to experimental investigations of site-diluted weakly coupled dimer systems in a magnetic field. The particular case of an Heisenberg antiferromagnet on coupled bilayers is realized by BaCuSi$_2$O$_6$ [8], in which doping of the magnetic Cu$^{2+}$ ions with non magnetic Zn$^{2+}$ and Mg$^{2+}$ can lead to site dilution of the magnetic lattice. The picture of quantum localization of bosonic quasiparticles applies nonetheless to other spin gap systems with different geometries, such as Sr$_2$Cu(BO$_3$)$_2$ [22] or Ti(K)CuCl$_3$ [7]. The quantities we have investigated clearly show a characteristic sequence of phases, with disorder suppression of magnetism and onset of a novel Bose-glass phase, and they are directly accessible to magnetometry and neutron scattering experiments.

We acknowledge fruitful discussions with C. Batista, M. Jaime, N. Laflorencie, B. Normand, N. Prokof’ev, H. Saleur, and T. Vojta, and we particularly thank O. Nohadani and S. Wessel for carefully reading our manuscript. This work is supported by DOE. Computational facilities have been generously provided by the HPC Center at USC.

[1] D.S. Fisher Phys. Rev. B 50, 3799 (1994).
[2] M.P.A. Fisher et al., Phys. Rev. B 40, 546 (1989).
[3] E.F. Shender and S.A. Kivelson, Phys. Rev. Lett. 66, 2384 (1991).
[4] A.W. Sandvik, Phys. Rev. B 66, 024418 (2002).
[5] R. Yu et al., Phys. Rev. Lett. 94, 197204 (2005).
[6] T.M. Rice, Science 298, 760 (2002).
[7] Ch. Rüegg et al., Nature (London) 423, 62 (2003).
[8] M. Jaime et al., Phys. Rev. Lett. 93, 087203 (2004); S.E. Sebastian et al., cond-mat/0502374.
[9] T. Nikuni et al., Phys. Rev. Lett. 84, 5868 (2000).
[10] O. Nohadani et al., cond-mat/0506033.
[11] O.P. Vajk et al., Science 295, 1691 (2002).
[12] O.F. Syljuåsen and A.W. Sandvik, Phys. Rev. E 66, 046701 (2002).
[13] A.W. Sandvik and D.J. Scalapino Phys. Rev. Lett. 72, 2777 (1994).
[14] T. Giamarchi and A.M. Tsvelik, Phys. Rev. B 59, 11398 (1999).
[15] M.E.J. Newman and R.M. Ziff, Phys. Rev. Lett. 85, 4104 (2000).
[16] T. Roscilde and S. Haas, in preparation.
[17] A.W. Sandvik et al., Phys. Rev. B 56, 11701 (1997).
[18] M. Sigrist and A. Furusaki, J. Phys. Soc. Jpn. 65, 2385 (1996).
[19] H.-J. Mikeska et al., Phys. Rev. Lett. 93, 217204 (2004).
[20] For the specific model considered the magnetization reaches the value $p/2$ only beyond $h_{c1}^{(0)}$, which means that the plateau shrinks an horizontal inflection point and the overall quantum disordered phase for $h < h_{c1}^{(0)}$ is gapless. For a larger $J/J'$ an extended magnetization plateau appears below $h_{c1}^{(0)}$, so that the disordered phase for $h < h_{c1}^{(0)}$ becomes gapped [13].
[21] A. Cuccoli et al., Phys. Rev. B 67, 104414 (2003).
[22] S.E. Sebastian et al., Phys. Rev. B 71, 212405 (2005).