Spinon deconfinement in doped frustrated quantum antiferromagnets

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Spinon confinement around a vacancy in frustrated quantum antiferromagnets

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(Dated: June 30, 2005)

The confinement of a spinon liberated by doping frustrated quantum two-dimensional Heisenberg antiferromagnets with a non-magnetic impurity is investigated. For a static impurity, an intermediate behaviour between complete deconfinement (kagome) and strong confinement (checkerboard) is identified, with a spinon confinement length significantly *larger* than the short magnetic correlation length of the host and a reduced Z factor ($J_1-J_2-J_3$ model on the square lattice). This translates into an extended spinon-holon boundstate for mobile vacancies, allowing one to relate features of the hole spectral function measured by ARPES to features accessible in real space by NMR experiments on impurity-doped systems.

PACS numbers: 75.10.-b, 75.10.Jm, 75.40.Mg

The search for exotic spin liquids (SL) has been enormously amplified after the discovery of the high critical temperature (high-T_C) cuprate superconductors. Indeed, Anderson suggested that the Resonating Valence Bond (RVB) state is the relevant insulating parent state that would become immediately superconducting under hole doping [1]. Such a RVB state is characterized by short range magnetic correlations and no continuous (spin) or discrete (lattice) broken symmetry. Another major characteristic of this SL phase is the deconfinement [2] of the S=1/2 excitations (spinons) in contrast to ordered magnets which have $S = 1$ spin waves. Upon doping, some scenarii predict a 2D Luttinger liquid [3], i.e. a state which exhibits spin-charge separation, a feature generic of one-dimensional correlated conductors.

Magnetic frustration is believed to be one of the major ingredient that could drive a two-dimensional (2D) quantum antiferromagnet (AF) into exotic non-magnetic phases. The Valence Bond Solid (VBS), an alternative class of magnetically disordered phases which break lattice symmetry, seems to be a strong candidate in frustrated quantum magnets as suggested by robust field theoretical arguments [4]. Indeed, early numerical computations of the frustrated quantum AF on the square lattice with diagonal bonds have revealed increased dimer correlations, possibly long-range, for large frustration [5, 6, 7]. Moreover, strong evidence for a VBS (plaquette rather than columnar) exists also in the 2D checkerboard lattice [8] (with diagonal bonds only on half of the plaquettes). On the contrary, the 2D Kagomé lattice [9] shows no sign of ordering and no gap in the singlet spectrum, the signature of a form of SL phase [10, 11].

Investigation of hole doping in frustrated magnets [12] has revealed stricking differences between VBS and SL phases. Viewing these phases as (liquid or solid) fluctuating singlet backgrounds, removing an electron at a given site or, as in Angular Resolved Photoemission Spectroscopy (ARPES) experiments, in a Bloch state of given momentum naturally breaks a spin dimer and liberates a spinon, i.e. a S=1/2 polarisation in the vicinity of the empty site (holon). The single hole spectral function shows a sharp peak (resp. a broad feature) characteristic of a holon-spinon boundstate (resp. holon-spinon scattering states) in the checkerboard VBS phase (resp. Kagomé SL phase). Interestingly enough, such a property does not depend crucially on whether the holon mass is finite (e.g. ARPES injected hole) or "infinite" (e.g. static impurity introduced by chemistry). The simple physical pictures behind these two typical behaviors are depicted in Fig. 1(a) and (b) for a confining columnar dimer phase and a SL phase respectively.

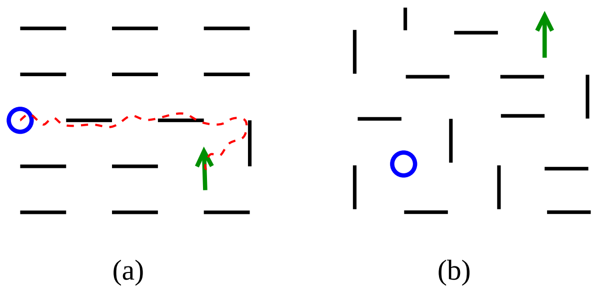

FIG. 1: (Color on-line) Schematic picture of a vacancy (or doped hole) in a frustrated magnet. The segments stand for singlet bonds and the arrow represents the spinon liberated in the process. (a) Holon-spinon BS in a columnar VBS bound by a "string" potential (dotted line). (b) Deconfined holon and spinon in an (hypothetical) SL host.

In this Letter we study the problem of a single vacancy (named "impurity" or "hole") introduced in the 2D spin-1/2 AF J_1-J_2-J_3 Heisenberg model on the square lattice at zero temperature defined by

$$H = \sum_{\langle ij \rangle} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j \tag{1}$$

where the J_{ij} exchange parameters are limited to first

(J_1), second (J_2) and third (J_3) N.N. AF couplings. The classical phase diagram of this model [13, 14, 15] is very rich (see Fig. 2) showing four ordered states – Néel, collinear ($\mathbf{q} = (\pi, 0)$) and two helicoidal – separated by continuous or discontinuous boundaries.

The effects of quantum fluctuations on this classical phase diagram is still an open question. For the pure $J_1 - J_2$ model and $J_2/J_1 \lesssim 0.4$, the classical (π, π) Néel behavior is essentially conserved [5, 16]. On the other hand, for $J_2/J_1 \gtrsim 0.6$ an *order by disorder* mechanism [17] selects two collinear states at $\mathbf{q} = (\pi, 0)$ and $(0, \pi)$. In the parameter range where frustration is largest, $0.4 \lesssim J_2/J_1 \lesssim 0.6$, many approaches (including spin-wave theory [16], exact diagonalizations [5], series-expansion [18] and large-N expansions [2]) have now firmly established that quantum fluctuations destabilize the classical ordered ground state and lead to a magnetically disordered singlet ground state. However, its precise nature is still controversial : a columnar valence bond solid with both translational and rotational broken symmetries [4], a plaquette state with no broken rotational symmetry [6] or even a spin-liquid with no broken symmetry [19] have been proposed.

Similar questions apply to the $J_3 \neq 0$ case. First of all, as remarked by Ferrer [15], the end point of the classical critical line $(J_2+2J_3)/J_1 = 1/2$ on the J_3 axis is substantially shifted to larger values of J_3 when quantum fluctuations are switched on. But even for the pure $J_1 - J_3$ model, in the region of large frustration $J_3/J_2 \sim 0.5$, a non-classical and still controversial phase appears between the Néel (π, π) and the spiral (q, q) phases : VBS columnar state [20], spin-liquid [21] or a succession of a VBS and Z_2 spin-liquid phases [22].

In the large frustration regime $(J_3 + J_2)/J_1 \sim 0.4 - 0.6$ of the phase diagram further insights on the nature of the singlet ground state can be obtained using a truncated (non-orthogonal) short range resonating valence bond set of states as a basis for diagonalization of the hamiltonian. Both the ground state energy and wave function provided by this method [23, 24] can be directly compared with exact diagonalizations for small clusters. Moreover, it gives access to substantially larger bidimensionnal clusters and is able to describe both VBS and spin-liquid states. It appears [25] that in the vicinity of $(J_3 + J_2)/J_1 \sim 0.5$, (i) a very good description of the ground state can be obtained in terms of nearest neighbor dimer coverings of the square lattice, (ii) the scaling analysis of the dimer susceptibility computed up to 50 sites shows a non-vanishing signal at the thermodynamic limit, increasing as J_3/J_2 increases, strongly suggesting a VBS order [7]. Therefore, a confinement of a spinon near a vacancy is also expected in this model.

In the following, a static vacancy introduced at a given site O of the lattice is simply modelled by setting to zero all the couplings J_{ij} involving site O and the computations are performed by Lanczos ED of a cluster of 32 sites

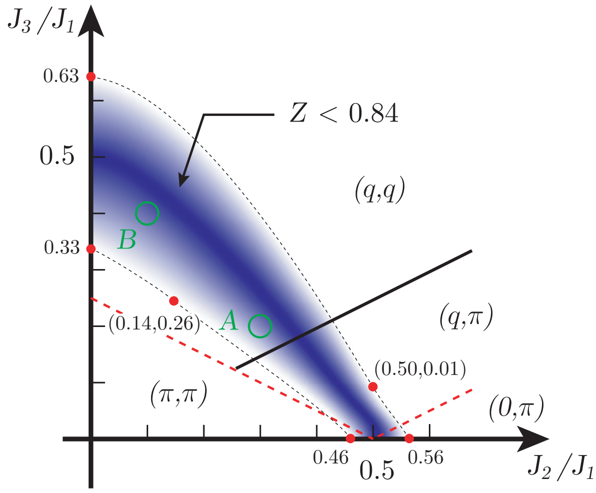

FIG. 2: (Color on-line) Classical phase diagram for the J_1-J_2-J_3 model. Second order (discontinuous) transitions are indicated by dashed (solid) lines. The shaded (blue online) region shows the approximate location of the minimum of the spectral weight Z in the quantum version. The area where $Z < 0.84$ on a 32-site cluster is delimited by dashed lines and red dots.

(i.e. $\sqrt{32} \times \sqrt{32}$) which respects all point group symmetries of the infinite lattice. Such an impurity acts, theoretically, as a local probe of the host. It can be viewed alternatively as a localized holon ($S = 0$ and charge $Q = e$) so that the form of the surrounding spin density is expected to provide valuable insights on spin-charge confinement or deconfinement.

The single impurity Green function $G(\omega) = \langle \Psi_{\rm bare}|(\omega - H)^{-1}|\Psi_{\rm bare}\rangle$ is computed by (i) constructing the (normalized) "bare" initial state $|\Psi_{\rm bare}\rangle = 2c_{O,\sigma}|\Psi_0\rangle$ from the host GS $|\Psi_0\rangle$ by removing an electron of spin σ and (ii) using a standard Lanczos continued-fraction technique. Most of the ω-integrated spectral weight (normalized to 1) of Im$G(\omega)$ is in fact contained in the lowest energy pole of weight $Z = |\langle \Psi_{\rm gs}|\Psi_{\rm bare}\rangle|^2$ where $|\Psi_{\rm gs}\rangle$ is the (normalized) GS of the system with one vacancy at site O. Results shown in Fig. 3(a,b) show however that Z is significantly suppressed in the region where a magnetically disordered state is expected. We show in Fig. 2 the region corresponding to a weight between 0.79 and 0.84 on the 32-site cluster.

We believe that the reduction of Z signals a tendancy of the spinon to *move away* from the original site next to the vacancy to an average distance $\xi_{\rm conf} > 1$. Additional evidences in favor of this scenario are obtained from a careful inspection of the average local spin density $\langle S_i^z \rangle$ around the vacancy in both the "bare" wavefunction and the true GS. Results are provided in Fig. 4(a,b) for parameters corresponding to the two typical A and B points of the phase diagram of Fig. 2. Note that, in fact, $\langle S_i^z \rangle$ in $|\Psi_{\rm bare}\rangle$ gives the initial spin-spin correlation $\langle S_O^z S_i^z \rangle_0$

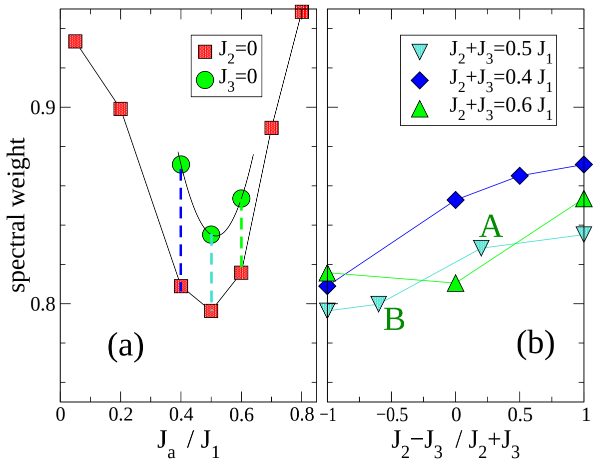

FIG. 3: (Color on-line) Static hole (vacancy) spectral weight vs AF exchange parameters. (a) vs J_2/J_1 for $J_3 = 0$ and vs J_3/J_1 (for $J_2 = 0$) as indicated on plot. (b) Along three different lines $(J_2 + J_3)/J_1$ = cst in the 2D (J_2/J_1,J_3/J_1) parameter space. A and B refer to the points in the phase diagram of Fig. 2.

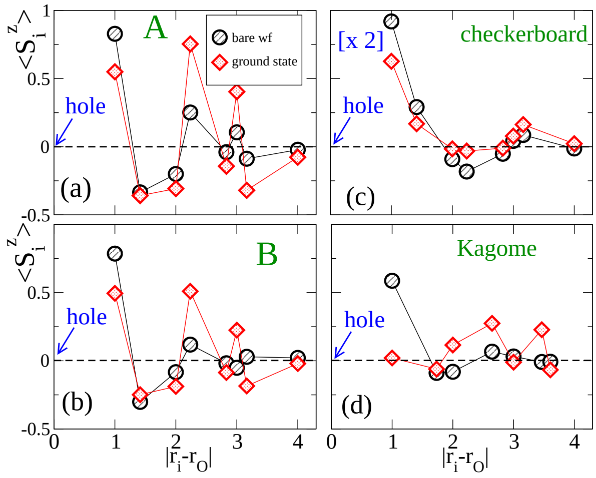

FIG. 4: (Color on-line) Spin polarization in the vicinity of the vacancy (summed up on equivalent sites and normalized to 1/2) for both the "bare" vacancy state $c_{O,\downarrow}|\Psi_0\rangle$ and the single vacancy GS as indicated on plots. J_1-J_2-J_3 model with $J_2/J_1 = 0.3$ and $J_3/J_1 = 0.2$ (a) and $J_2/J_1 = 0.1$ and $J_3/J_1 = 0.4$ (b) corresponding to points A ($Z \simeq 0.8283$) and B ($Z \simeq 0.7998$) in the phase diagram of Fig. 2. (c) same for the checkerboard lattice (32 site cluster) apart from a multiplicative factor of 2. (d) same for the Kagomé lattice (30 site cluster).

(apart from a $2 \times (-1)^\sigma$ trivial multiplicative factor) in the host GS. It is instructive to see that points A and B are characterized by very short magnetic correlation lengths, typically $\xi_{\rm AF} \simeq 2$ and 1 for A and B, respectively. It is important to notice that a large staggered component, i.e. of wavevector (π,π), is always accompanying the uniform polarization. Moreover, no sign of incommensurability is seen in the oscillations of Fig. 4 although a spiral phase of incommensurate wavevector is expected at the classical level. Interestingly, $\langle S_i^z\rangle$ in the "relaxed" state, i.e. $|\Psi_{\rm gs}\rangle$ state, shows important changes: (i) In contrast to the case of the unfrustrated Heisenberg antiferromagnet ($J_3 = J_2 = 0$) [26], the spin density *decreases* on the four nearest neighbor sites of the vacancy and (ii) a clear maximum, both in the uniform and staggered components, appears at a typical distance $\xi_{\rm conf}$ significantly larger than $\xi_{\rm AF}$, typically $\xi_{\rm conf} \sim 3$ lattice spacing from the vacancy. Unfortunately, larger systems would be needed to estimate more quantitatively the confinement length. However, our computation giving a lower bound of $\xi_{\rm conf}$ clearly proves that the long-range VBS order leads to a moderate confinement of the spinon so that a non-trivial spin structure can be seen in the vicinity of a vacancy. Similar data are shown in Fig. 4(c) and (d) for the Heisenberg model on the checkerboard and the Kagomé lattices respectively. Clearly, the results for the checkerboard lattice show some qualitative similarities with the J_1–J_2–J_3 model on the square lattice although with pronounced quantitative differences: (i) the spin-spin correlations on the checkerboard lattice is incommensurate and very short-ranged and (ii) the spinon is almost entierely confined on the N.N. site of the vacancy. In contrast, on the Kagome lattice, the spin-1/2 delocalizes on the whole lattice, a clear signature of deconfinement.

The previous findings could have important implications on the interpretation of the Nuclear Magnetic Resonance (NMR) experiments on doped 2D quantum anfiferromagnets. Indeed, the substitution of a S=1/2 atom by a non-magnetic one (e.g. Zn^{2+} for Cu^{2+}) which acts as a vacant site can be exactly described by our previous model. Moreover, the local spin densities $\langle S_i^z\rangle$ on the magnetic sites around a vacancy (spinless atom) can be directly accessed by NMR. It is important to notice that these densities correspond to those of the "relaxed" state i.e. $|\Psi_{\rm gs}\rangle$. It should be stressed then that, if the spin-spin correlations are short range, NMR probes the spinon "wavefunction" and not the host spin correlations. The later could be quite different, in particular when a clear separation of length scales occurs, i.e. $\xi_{\rm conf} > \xi_{\rm AF}$. Note that newly developped spin-polarized Scaning Tunneling Microscopy (SP-STM) techniques might allow to probe such atomic-scale spin structure [27] around a vacancy on a surface.

Lastly, we briefly examine the case of a mobile hole. This typically mimics the case of an ARPES experiment in a Mott insulator where a single photo-induced hole is created or the case of a small chemical doping by non-magnetic atoms. The hole motion described as in a t–J model is characterized by a hole hopping amplitude t. For the unfrustrated t–J model, the hole dynamics has been successfully analysed in term of holon-spinon bound-

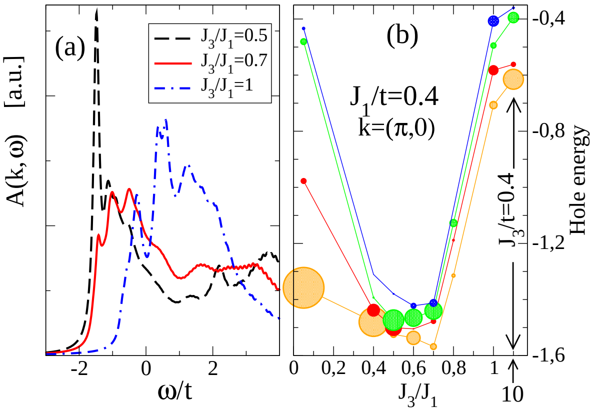

FIG. 5: (Color on-line) (a) Mobile hole spectral spectral function vs ω for $J_1/t = 0.4$ and hole momentum $\mathbf{k} = (\pi, 0)$. Data for several values of J_3/J_1 are shown. (b) Four lowest energy poles of $A(\mathbf{k}, \omega)$ vs the ratio J_3/J_1. The GS energy of the undoped AF sets the energy reference. $J_1/t = 0.4$ ($J_3/t = 0.4$) for $J_3 \leq J_1$ ($J_3 > J_1$). Areas of dots are proportionnal to spectral weights.

state [28] with a reduced quasiparticle weight. Typical spectral functions are shown in Fig. 5(a,b) for increasing frustration (we assume here $J_2 = 0$ and vary J_3) and a fixed ratio of J_1/t. For maximum frustration $0.5 \leq J_3/J_1 \leq 0.8$, the weight of the quasiparticle peak (at the bottom of the spectrum) is redistributed on several poles. Such a striking feature is consistent with a weakening of the binding between the two constituents of the hole or, somewhat equivalently, with a spatially extended holon-spinon boundstate. This scenario agrees with the previous real space picture discussed above for the case of a vacant site. Such a behavior bears also some similarity with the case of the t-J model on the checkerboard lattice showing a strongly reduced (but finite) single hole QP weight [12]. In contrast, on the Kagomé lattice the hole spectral function was found to be completely incoherent, the evidence for spin-charge separation [12].

To conclude, the confinement of a spinon liberated by introducing a vacant site (or a mobile hole) has been studied in various frustrated Heisenberg AF. In the non-magnetic phase of the $J_1-J_2-J_3$ model, an intermediate behavior between a strong confinement (as in the checkerboard Heisenberg model) and a complete deconfinement (as in the Heisenberg model on the Kagomé lattice) is observed, suggesting the existence of a new length scale related to the confinement of the $S = 1/2$ object . An interesting connection between this real-space picture and features in the hole spectral function is established. Similarly, observations in ARPES experiments on frustrated Mott insulators and in NMR or SP-STM on lightly substituted systems could be correlated.

We thank IDRIS (Orsay, France) for allocation of CPU-time on the NEC-SX5 supercomputer. D.P. acknowledges the Institute for Theoretical Physics (EPFL, Switzerland) for partial support. This work was supported by the Swiss National Fund and by MaNEP.

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