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Exotic phenomena in doped quantum magnets

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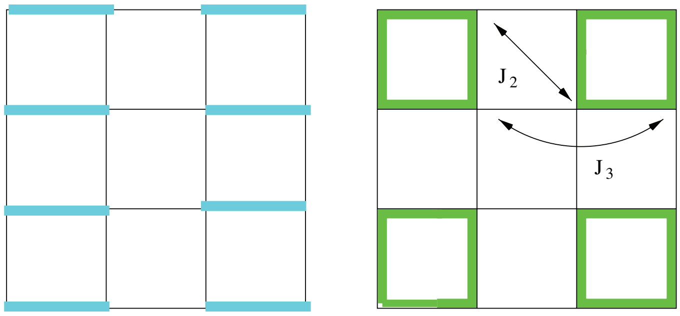
Abstract
We investigate the properties of a two-dimensional frustrated quantum antiferromagnet on a square lattice, especially at infinitesimal doping. We find that next nearest neighbour (NN) J_2 and next–next NN J_3 interactions together destroy the antiferromagnetic long-range order and stabilize a quantum disordered valence bond crystalline *plaquette* phase. A static vacancy or a dynamic hole doped into this phase liberates a spinon. From the profile of the spinon wavefunction around the (static) vacancy we identify an intermediate behaviour between complete deconfinement (behaviour seen in the kagome lattice) and strong confinement (behaviour seen in the checkerboard lattice) with the emergence of two length scales, a spinon confinement length *larger* than the magnetic correlation length. When finite hole hopping is introduced, this behaviour translates into an extended (mobile) spinon–holon bound state with a very small quasiparticle weight. These features provide clear evidence for a nearby 'deconfined critical point' in a doped microscopic model. Finally, we give arguments to support the idea that the doped plaquette phase has superconducting properties.

(Some figures in this article are in colour only in the electronic version)

1. Introduction: the plaquette valence bond crystal

Magnetic frustration is believed to be the major tool to drive a two-dimensional (2D) quantum antiferromagnet (AF) into exotic quantum disordered $SU(2)$-symmetric phases such as the spin liquid (SL) state characterized by the absence of ordering of any kind, and possibly observed in the 2D kagome lattice [1]. The valence bond crystal (VBC) which, in contrast, breaks lattice symmetry (see figure 1 for pictures of such states), seems to be a serious alternative in some other frustrated quantum magnets as suggested by robust field theoretical arguments [2],



(a) (b)

Figure 1. Examples of simple VBC states, (a) columnar phase and (b) plaquette phase, where 2(4) spins are paired up in dimer- (plaquette-) singlets. In both cases the ground state is 4-fold degenerate. The J_2 and J_3 couplings (depicted on (b)) are shown to stabilize the plaquette phase.

early numerical computations of frustrated quantum AFs on the square lattice with diagonal J_2 bonds [3] and in the 2D checkerboard lattice [4] (with diagonal bonds only on half of the plaquettes).

The 'deconfined critical point' (DCP) was recently proposed to describe a new class of quantum criticality characterizing the AF to VBC transition [5]. Here we argue that the two-dimensional (2D) spin-1/2 AF J_1–J_2–J_3 Heisenberg model [6] on the square lattice 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) NN AF couplings is a strong candidate for exhibiting such a transition. Recent investigations of this model along the pure J_3 axis [7, 8] or for both J_2 and J_3 finite [9] provide an accumulation of evidence in favour of the existence of a VBC phase with strong plaquette correlations similar to the diagram in figure 1(b).

Extensive exact diagonalizations of the model within its full Hilbert space and within a restricted Hilbert space of NN ($SU(2)$) dimer configurations reported in [9] strongly support the existence of a plaquette VBC phase along the $J_2 + J_3 = 1/2$ line of parameter space (see figure 2). We shall provide here a selection of these data to illustrate this point. Dimer–dimer correlations (not shown) reveal a strong signal of VBC order of some kind. Summing up these spatial correlations with appropriate phase factors provides quantitative estimates of both the 'generic' VBC and the 'specific' columnar VBC structure factors (normalized to give the squares of the corresponding order parameters). Such estimates are displayed in figure 3; the upper line is obtained by an extrapolation to infinite size of the dimer structure factor constructed by summing up the correlations of the horizontal dimers (only) with an alternating sign along columns (in order to provide a signal for all types of VBC phases). Clearly, a large VBC order parameter is seen with a value close to the one of a pure plaquette phase (dotted line), at least close to the pure J_3 axis. The data sets at the bottom are obtained by summing up the dimer correlations with opposite sign for vertical and horizontal dimers (also omitting the short-distance contributions) to filter the signal of columnar order only. The small values of the latter data strongly suggest that the VBC order is a plaquette order rather than a columnar order. Note, however, that the VBC signal weakens significantly when approaching the pure J_2 axis.

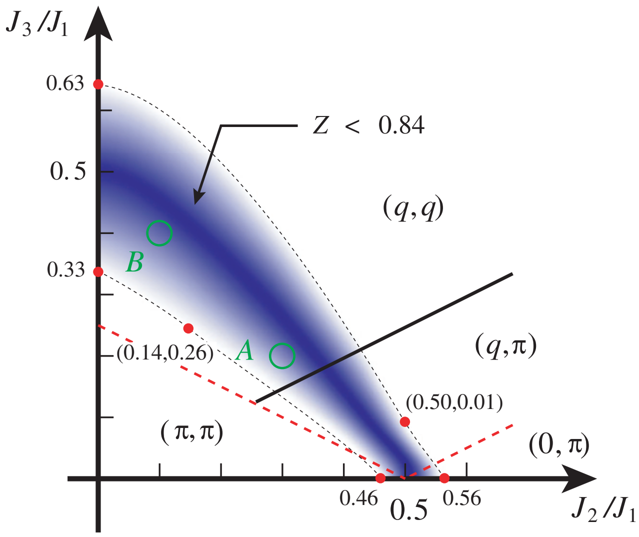


Figure 2. Classical phase diagram for the J_1–J_2–J_3 model. Second-order (discontinuous) transitions are indicated by dashed (solid) lines (see [6] for more details). The shaded (blue online) region shows the approximate location of the minimum of the impurity spectral weight Z ($0.79 < Z < 0.84$) in the quantum version. From [10].

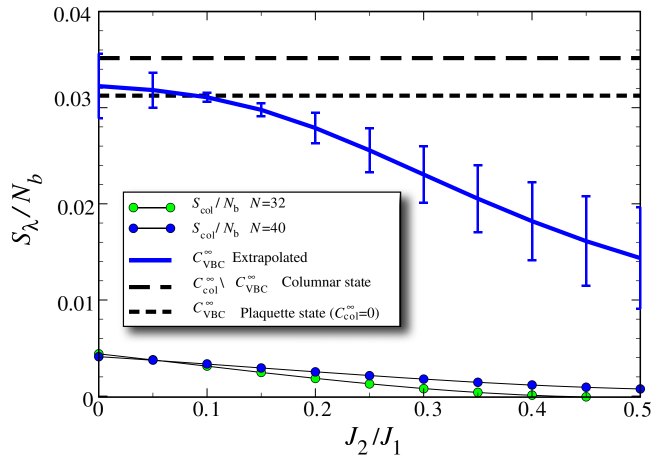


Figure 3. VBC (extrapolation) and columnar (for 32 and 40 site clusters) structure factors along a simple cut $J_2 + J_3 = 1/2$ in parameter space (see text). The dashed lines correspond to the value of both structure factors expected in pure columnar dimer and plaquette states. From [9].

2. Doping the plaquette VBC

We shall now test the properties of the plaquette VBC by removing an electron at a given site (e.g. by chemical substitution with an inert atom) or, as in ARPES experiments, in a Bloch state of given momentum. This process naturally liberates a spinon, i.e. a $S = 1/2$ polarization in the vicinity of the empty site (holon). A new length scale ξ_{conf} corresponding to the average distance between vacancy and spinon emerges naturally in a VBC phase and is to be identified with the correlation length over which VBC order sets in. Interestingly, it has been predicted

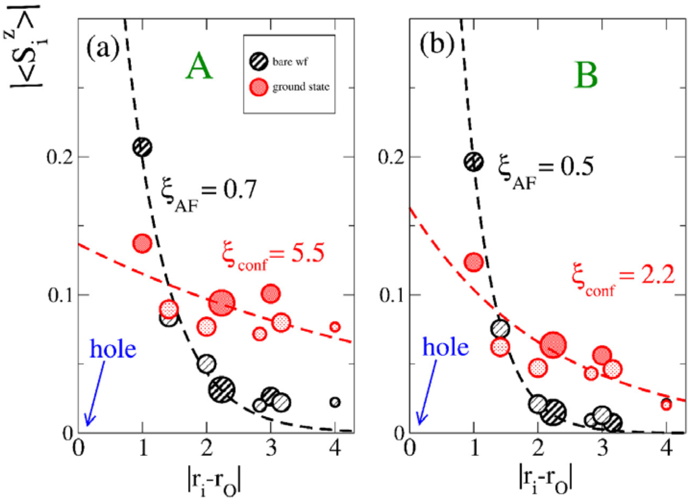


Figure 4. Modulus of the spin–spin correlation (black) and of the spin polarization in the vicinity of the vacancy (red) (summed up on equivalent sites) versus distance for both $J_2/J_1 = 0.3$ and $J_3/J_1 = 0.2$ (a) and $J_2/J_1 = 0.1$ and $J_3/J_1 = 0.4$ (b) corresponding to points A and B in the phase diagram of figure 2. Fits using exponential forms are shown by dashed lines. The areas of the dots are proportional to the number of equivalent sites (entering in the fits). Dark and light symbols correspond to positive and negative values respectively. From [10].

that, in the vicinity of the DCP, confinement occurs on a much larger length scale $\xi_{\rm conf}$ than the spin–spin correlation length $\xi_{\rm AF}$ [5].

In figure 4 we compare the decay of the spin–spin correlation with distance to one of the spinon 'clouds' away from the vacancy, which can be fitted using exponential forms, hence enabling us to extract the corresponding length scales. The obtained very short magnetic correlation length $\xi_{\rm AF}$, below one lattice spacing, is to be contrasted with the strikingly large *confinement* length $\xi_{\rm conf}$ typically ranging from 2 to 6 lattice spacings. This is to be compared with two other behaviours observed in the kagome and in the checkerboard lattices [10] respectively: in the checkerboard lattice (which also exhibits a plaquette phase but a larger spin gap [4]) very short-ranged spin–spin correlations are seen while the spinon remains almost entirely confined on the NN sites of the vacancy. In contrast, on the kagome lattice, the spin-$1/2$ delocalizes on the whole lattice, a clear signature of deconfinement which is consistent with an SL ground state.

The quasiparticle weight Z can be deduced from the computation of the single hole Green function. Figure 2 shows that it is clearly reduced in the vicinity of the $J_2 + J_3 = J_{1/2}$ line where evidence for a plaquette VBC phase was found. This behaviour is in agreement with the above real-space picture which naturally implies that the extended spinon wavefunction of size $\xi_{\rm conf}$ has a reduced overlap Z with the bare wavefunction (of extension $\xi_{\rm AF}$). When the vacancy is given some kinetic energy (through an NN hopping as in the well-known t–J model), the Z factor of the hole drops further to very small values [10] showing that the hole motion strongly suppresses the effect of the remaining spinon–holon VBC string potential [11]. Typical spectral functions along the pure J_3 line are shown in figure 5. Note that a *complete* deconfinement was shown for a mobile hole on the kagome lattice [12] as evidenced by a fully incoherent spectral weight at low energies.

Lastly, we would like to comment on the possibility of superconducting pairing upon doping VBCs. In fact, pairing driven by a kinetic energy gain of the Cooper pair was discovered

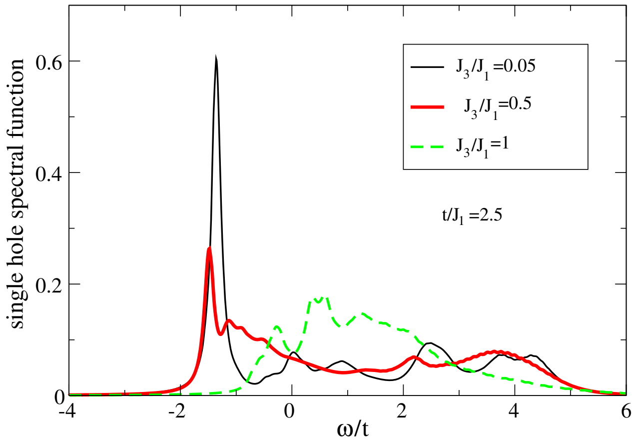


Figure 5. Single-hole spectral function (at momentum $(\pi, 0)$) for various values of the magnetic frustration and a realistic hole hopping of $t/J_1 = 2.5$ (on a 32-site cluster). Note that for $J_3/J_1 = 0.5$ the main low energy peak contains several poles in contrast to the $J_3 = 0.05$ case where a single pole is present.

in the robust plaquette phase of the checkerboard lattice [13]. On general grounds, one would also expect hole pairing in the doped J_1–J_2–J_3 quantum AF due to the long distance confining string of the VBC. However, short-range effects (as in the checkerboard lattice) could boost the weak pairing interaction.

3. Conclusions

To conclude, the confinement of a spinon liberated by introducing a vacant site or a mobile hole has been studied in the J_1–J_2–J_3 model where a plaquette VBC phase has been identified in some extended region of the phase diagram. In this region of large frustration, we have identified a new length scale related to the confinement of the spinon. Its large value compared to the spin–spin correlation length supports the field-theoretic 'deconfined critical point scenario' [5] for the Néel–VBC transition.

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