Magnetic field-induced transition in a quantum magnet described by the Quantum Dimer Model

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The effect of a magnetic field on a gapped quantum magnet is described within the framework of the Quantum Dimer Model. A minimal model describing the proliferation of itinerant spinons above a critical field is proposed and investigated by Lanczos exact diagonalizations and quantum Monte Carlo simulations. For both square and triangular lattices, it is shown that spinons are fully polarized and Bose-condensed. This offers a novel scenario of a Quantum Critical Point in the dimer-liquid phase (triangular lattices) characterized by the continuous appearance of a spinon superfluid density, contrasting with the usual triplet condensation picture. The possible role of other spinon kinetic terms neglected in the model are discussed.

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Quantum (spin) disordered magnets are currently a very active field of research in Condensed Matter Physics. They are characterized by the absence of magnetic ordering down to very low temperatures and, for some of them of interest here, by a spin gap to triplet excitations. In this context, the magnetic field is a particularly relevant external parameter as it can drive the system to a Quantum Critical Point (QCP) at which the spin gap vanishes [1]. In the conventional picture, the QCP can be viewed as the Bose condensation of triplets. Numerous examples of such QCP can be found in quasi-one dimensional magnets like the CuHpCl spin ladder [2], in two dimensional layered frustrated magnets like e.g. the Copper-Borate system [3] or in the interesting three dimensional BaCuSiO dimer compound [4].

The resonating valence bond (RVB) liquid describes the paradigm for magnetically disordered systems. Indeed, RVB states describe pure quantum phases, which have no classical counterparts and, therefore, cannot be adiabatically connected to any band theory, based on Hartree-Fock or more sophisticated density functional approaches. Moreover, as suggested by Anderson in a cornerstone paper [5], an RVB insulator could be intimately connected to high-temperature superconductors. In this field, an important step forward was done by Rokhsar and Kivelson, who formulated the RVB concept by introducing a simple microscopic Hamiltonian, the so-called Quantum Dimer Model (QDM) [6]. Simplifying the original electronic problem, they proposed an effective theory describing the dynamics of short-range dimers, that become the fundamental entities of the problem. The QDM relies on two approximations which are believed not to alter significantly its physical relevance (and could be relieved at the price of bringing an enormous extra complexity): (i) only nearest-neighbor singlets are considered and (ii) different dimer configurations are taken to be orthogonal to each other, hence producing singlets to “classical” dimers. However, quantum mechanics still enters in an essential way in the possibility to flip plaquettes with parallel dimers. On the square lattice, the ground state of the QDM always shows lattice symmetry breaking. This fact has encouraged the (wrong) surmise that “fully” disordered ground state (in the sense of a state with neither SU(2) nor lattice symmetry breaking) cannot be stabilized in this framework. In this respect, the discovery that a gapped and disordered state can be obtained on the triangular lattice opened the way to an enormous number of investigations [7, 8]. Recently, the zero-temperature properties of the QDM on the triangular and square lattices have been considered in great detail by numerical calculations [11, 10].

In the QDM, both charge and spin excitations are frozen and the elementary excitations have topological character [11, 12, 13]. Some effort has been done in order to introduce charged spinless excitations in the doped QDM, the so-called holons. The exact nature of these objects has been widely debated [11, 14, 15]. Much more subtle is the problem of inserting spinons, namely chargeless spin-1/2 objects, since, in this case, one faces a serious problem of non-orthogonality [11]. In fact SU(2) valence-bond configurations with unpaired spins at different locations are not orthogonal to one another, in contrast to the holon case. The magnetic field offers a formidable tool to experimentally investigate such issues since it plays the role of a chemical potential w.r.t. the spinon density.

In this Letter, we address the issue of spinon doping in both (lattice) ordered and disordered dimer backgrounds. Physically, this is achieved by the action of a magnetic field. On a general basis, we first derive all types of terms that should govern the spinon dynamics. Then, we propose a simplified model where the (up or down) spinon can hop along plaquette diagonals (while its neighboring dimer rotates by 90 degrees) and where the dimer dynam-
ics is that of the standard QDM. By using Lanczos exact diagonalizations, we show that, within this model, for a finite magnetic field, all spinons are fully polarized, the energy gain being of kinetic origin as in the well known Nagaoka effect \[16\]. The magnetization profiles are then computed using Green’s function Monte Carlo. We find a new type of QCP characterized by Bose-Condensation of spinons in contrast to the usual scenario of triplet condensate. The behavior of the magnetization at the QCP depends on the nature of the (spin) disordered ground state at zero field.

Creating a pair of spinons in a gapped quantum magnet (described by a QDM) will cost a finite energy (called \(\Delta_B\) later on). However, a finite density \(x\) of (partially polarized) spinons could be stabilized by the Zeeman energy \(-g\mu_B H \sum_i S_i^z = -\frac{1}{2} N (n_\uparrow - n_\downarrow), n_\uparrow (n_\downarrow)\) being the densities of up (down) spinons in the system, \(x = n_\uparrow + n_\downarrow\) and \(N\) is the number of sites. Therefore, as a preliminary work, we need to establish the form of the kinetic processes for the spinons moving in the fluctuating dimer background. At the microscopic level, such terms will \(a\ priori\) arise from the non-orthogonality of the basis set. Since the derivation for a true frustrated microscopic model is beyond the scope of this work, we simply consider here the (non-frustrated) Heisenberg model on the square lattice to get insights on the generic form of these matrix elements \[17\]. Notice that a similar type of derivation has been carried out for a realistic but more complex model in a different context \[18\].

Following the same procedure as for the derivation of the QDM in the absence of spinons \[14\], we calculate the largest contributions of the matrix elements, \(H_{\text{e,c}'} = (c'|H_{\text{Heis}}|c)\), where \(|c\rangle\) and \(|c'\rangle\) are typical dimer configurations, including spinons. A careful analysis gives four elementary kinetic processes and their overlap weights, as displayed in Fig. 1. Interestingly, the processes involving a spin-flip of two spinons \(\text{term 3)}\) or two-spinon creation or annihilation \(\text{term 4)}\) have both positive and negative signs depending on the orientation of the spinons. This introduces a serious sign problem into the quantum Monte Carlo approach. In addition, the term 4), in contrast to the holon-doped case, does not conserve the number of “dopants”.

Hereafter, we consider a simplified version of the QDM-spinon model, by retaining only the dimer flips (as in the usual QDM) and the spinon hopping \(2\). This model has only negative off-diagonal matrix elements and should be tractable by appropriate quantum Monte Carlo. In a second step, we shall discuss the possible role of the terms we have left behind. Note that in the case of a frustrated magnet, we expect the same type of processes although their magnitudes should depend on the precise microscopic magnetic interactions. Therefore, the QDM Hamiltonian is defined here by

\[
H_0 = v \sum_c N_c |c\rangle\langle c| - J \sum_{\langle c,c'\rangle} |c\rangle\langle c'| + t \sum_{\langle c,c'\rangle} |c'\rangle\langle c|. \tag{1}
\]

The sum on \(\langle c\rangle\) runs over all configurations of the Hilbert space, \(N_c\) is the number of flippable plaquettes, the sum on \(\langle c', c\rangle\) runs over all configurations \(|c\rangle\) and \(|c'\rangle\) that differ by a single plaquette dimer flip, and the sum on \(\langle c'', c\rangle\) runs over all configurations \(|c\rangle\) and \(|c''\rangle\) that differ by a single spinon hopping between nearest neighbors (triangular lattice) or next-nearest neighbors (square lattice), see Fig. 1. The coupling to the external magnetic field is also added to the above Hamiltonian.

To get insights on the ground-state properties of this system, we first exactly diagonalized (by standard routines or a Lanczos algorithm) a \(4 \times 4\) square cluster with periodic boundary conditions and with 4 and 6 doped spinons. Eigen-energies are labeled according to the total spin \(S\). The lowest-energy levels for four and six spinons on a \(4 \times 4\) square lattice in the subspace of zero magnetic field. The couplings are \(t/J = 0.2\) and \(v/J = 0.5\) and states are classified according to the total spin \(S\).
energy gain w.r.t. the singlet subspace is of kinetic origin. Obviously, the fully polarized state is further stabilized by a finite magnetic field so that this property should be valid for all fields and dopant concentration making quantum Monte Carlo simulations available. Note however that the neglected processes 3) and 4) of Fig. 1 might change the relative stability of the fully polarized state w.r.t. some lower spin states and this will be discussed later on. In this way, technically, the spin variable does not play any role and, therefore, one can borrow here the results obtained in the context of the monomer-doped QDM [20, 21], but accounting for the extra term involving the magnetic field \(-h N x /2 (n_{1} = x)\). It is of interest to notice that, in contrast to the case of hole-doping where Fermi statistics plays a role [15], “spinon-doping” do not introduce any minus-sign problem (here \(J > 0\)). In other words, since an electron destruction operator can be written as \(c_{\sigma} = f_{\uparrow} b_{\sigma}\) in term of a fermionic holon-creation operator \(f_{\uparrow}\) and a bosonic spinon-destruction operator \(b_{\sigma}\), the physical holon-doped and “spinon-doped” QDM simply differ from the statistic of the bare doped monomers.

Here, we aim to assess the number of spinons that are present in the ground state, once an external magnetic field \(h\) is applied and competes with the dimer binding energy \(\Delta_{B}\). Indeed, \(-h\) plays the role of a chemical potential and controls the spinon density which gives the reduced magnetization. It is natural to introduce the effective energy cost \(\Delta_{B}^{\text{eff}} = \Delta_{B} - h\) of breaking a dimer into two unbound static spinons under a finite magnetic field. Note that the spontaneous appearance of spinons in the ground-state (which defines the QCP) should appear for fields lower than the characteristic field \(h = \Delta_{B}\) since spinons acquire extra kinetic energy compared to dimers (in other words, the actual critical value of \(\Delta_{B}^{\text{eff}}\) is positive). This study can be done by considering the energy per site \(\epsilon(x)\) of the holon-doped model [21], from which the Legendre transform \(F(x) = \epsilon(x) + \frac{1}{2} \Delta_{B}^{\text{eff}} x\) can be constructed. The actual \(\epsilon(x)\) has been obtained by using the Green’s function Monte Carlo method [22], for both the square and the triangular lattices [21]. The actual spinon concentration \(x_{0}\) for a given value of \(\Delta_{B}^{\text{eff}}\) is obtained by minimizing \(F(x)\) with respect to \(x\). Notice that \(x_{0}\) is nothing else but the ratio of the magnetizations \(M/M_{\text{sat}}\), with \(M_{\text{sat}}\) the value at saturation, i.e., when the whole system is filled by spinons.

The fact that the monomer-doped model may or may not show phase separation (PS), opens the way to two different scenarios for the behavior of the system as a function of the magnetic field. Let us first recall that, on the square lattice, as soon as \(v/J < 1\), the ground state is unstable in the presence of an infinitesimal monomer concentration and phase-separates between undoped (macroscopic) domains and regions with a concentration \(x_{c}\) of monomers. Instead, in the triangular lattice, the infinitesimally doped system is stable for \(v/J \gtrsim 0.9\), whereas it phase-separates for smaller values of the dimer-dimer repulsion [21]. Such different behaviors are reflected in the phase diagram of Fig. 3 in the \((h - \Delta_{B}, t)\) plane by continuous or first-order transitions between the regions with and without magnetization. Remarkably, the transition curves \(t = t^{\text{cr}}(h)\) have linear behaviors and, for a given lattice structure, the slope does not depend upon the ratio \(v/J\). Three different values of the dimer-dimer repulsion \(v/J\) have been chosen for the triangular lattice, two of them inside the stability region of the RVB liquid of the undoped system \((v/J = 1\) and \(0.95\)), whereas the latter one \((v/J = 0.85\) corresponds to a region where the doped ground state phase separates, due to local dimer ordering.

The behavior of the magnetization vs magnetic field can be understood on simple grounds. In a stable system, the compressibility is finite, implying that the second derivative of \(\epsilon(x)\) is positive (i.e., \(\epsilon(x)\) is a concave up function of \(x\)). In this case, \(\epsilon(x) \simeq \epsilon(0) + a x + b x^{2}/2\), where \(b > 0\) from the stability criterion. Moreover, the linear coefficient is generally negative, i.e., \(a = -|a|\). On the other hand, PS is signaled by an infinite compressibility and a vanishing second derivative of \(\epsilon(x)\). This leads to a precise form of the energy in the thermodynamic limit, namely \(\epsilon(x) = \epsilon(0) + a x + b x^{2}/2\) for \(x \leq x_{c}\) and \(\epsilon(x) \simeq \epsilon(x_{c}) + a(x - x_{c}) + b(x - x_{c})^{2}/2\) for \(x \geq x_{c}\). Notice that the correct behavior of the stable case may be found from the previous one by imposing \(x_{c} = 0\). By minimizing \(F(x)\) we then find a general expression for the reduced magnetization,

\[
\frac{M}{M_{\text{sat}}} = x_{c} + \frac{|a|}{b} + \frac{1}{2b} (h - \Delta_{B}),
\]

for \(h > 2|a| - \Delta_{B}\) and \(M = 0\) otherwise. Therefore, in a stable system (i.e., \(x_{c} = 0\), by increasing the magnetic field, there is a continuous transition between the
Fig. 4, we show the behavior of gapped phase to a phase with a finite spinon density. In panel Fig. 4a, we consider the case of the triangular lattice at \( v = 0.95 \). The same as in a), but for the square lattice and at \( v = 0.80 \). Dashed lines show the region where a first order transition occurs. Error-bars are of the size of the symbols.

In panel Fig. 4b, we consider the case of the square lattice and at \( v/J = 0 \), namely starting from a \( h \rightarrow 0 \) RVB liquid phase. A Bose-condensation of spinons is found, characterized by a second-order phase transition for all the values of \( t/J \) considered, hence confirming the analytical arguments.

In summary, a simple extension of the QDM including spinon doping is introduced to account for the Zeeman effect of an applied magnetic field. This model involves two semi-phenomenological parameters, the hopping amplitude \( t \) for a spinon to hop (and exchange with a dimer) and the bare energy cost \( \Delta_B \) to break up a dimer into two spinons. Interestingly, the phase diagram of this model can be obtained from large-scale Green’s function Monte Carlo methods \([21]\) showing, as a function of the field, either a first order transition (square lattice) or a new type of Quantum Critical Point (triangular lattice) characterized by Bose-Condensation of spinons.

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