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Interaction between static holes in a quantum dimer model on the kagome lattice

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Abstract

A quantum dimer model (QDM) on the kagome lattice with an extensive ground-state entropy was recently introduced (Misguich *et al* 2003 *Phys. Rev.* B **67** 214413). The ground-state energy of this QDM in the presence of one and two static holes is investigated by means of exact diagonalizations on lattices containing up to 144 kagome sites. The interaction energy between the holes (at distances up to seven lattice spacings) is evaluated and the results show no indication of confinement at large hole separations.

1. Introduction

Quantum dimer models (QDM) can provide some effective descriptions of the low-energy singlet dynamics of frustrated quantum antiferromagnets [1]. A basis of the Hilbert space of these models is made up by all (nearest-neighbour) dimer coverings of the lattice and the Hamiltonian allows these dimers to move along local resonance loops. Two kinds of phase are well understood for these models in two dimensions: dimer crystals [1] and resonating-valence-bond (RVB) dimer liquids [2, 3]. Crystals are characterized by long-ranged dimer–dimer correlations and spontaneous lattice symmetry breaking and RVB liquids show no broken symmetry but topological order and $\mathbb{Z}_2$-vortex excitations [4]. Importantly also, these two phases can be distinguished by the behaviour of holes (or spinons) when the system is 'doped'; that is, we allow sites which are not occupied by any dimer. Holes experience a mutual interaction which grows linearly with their separation in a dimer crystal and this interaction confines them in pairs. On the other hand, they propagate independently in a RVB liquid background. A first and simple step is to consider QDM with *static* holes (non-magnetic impurities or spinons). In that case a relevant quantity is the ground-state energy as a function of the hole positions. This energy goes to a constant when two holes are far apart in a deconfined system whereas it grows linearly in a confined system[1].

[1] QDM at Rokhsar–Kivelson points [1] are an exception: the ground-state energy remains exactly zero whatever the positions of the holes.

We recently proposed a QDM on the kagome lattice which does not simply fall into either of these two categories [5]. This model, hereafter called the μ model, was introduced from the observation that the dimer kinetic energy terms arising from an overlap expansion of the spin-$\frac{1}{2}$ Heisenberg model [1] generally have non-trivial *signs* as soon as the competition of resonance loops with *different lengths* is considered [6]. The Hamiltonian is

$$\mathcal{H} = -\sum_h \mu_h \tag{1}$$

where

$$\mu_h = \sum_{\alpha=1}^{32} (-1)^{n_\alpha} |d_\alpha(h)\rangle\langle\bar{d}_\alpha(h)| + \text{H.c.} \tag{2}$$

and h runs over the hexagons of the lattice and $|d_\alpha(h)\rangle$ is one of the 32 possible dimerizations of h (table 1). The sign n_α counts the parity of the number of dimers involved[2]. It was realized that such signs can lead to a new state, different from dimer crystals or RVB liquids. In our previous study [5] the following results were obtained:

(i) The μ model has an extensive ground-state entropy $\frac{1}{6}\log(2)$ per kagome site, that is 50% of the classical dimer entropy. This exponentially large degeneracy comes from a hidden, local, but non-Abelian symmetry of the model.
(ii) It is possible to choose a basis of the ground-state manifold such that dimer–dimer correlations are short ranged in each state. These ground states are thus dimer liquids.
(iii) On the basis of exact diagonalizations we argued that, in addition to the ground state having degeneracy, the spectrum is likely to be gapless and energy–energy correlations (as well as susceptibilities) are likely to be critical.

In the present work we investigate numerically the effect of static holes in the μ model. This issue is of particular importance, as Dommange *et al* [8] pointed out in a recent work that static holes in the spin-$\frac{1}{2}$ kagome antiferromagnet experience a short-distance repulsion and are probably deconfined at larger distances. Sindzingre *et al* [7] previously reached a similar conclusion about *spinon deconfinement* from an analysis of the value of the spin gap in a 24-site sample with two holes. We show in this paper that a somewhat similar behaviour is observed in the μ QDM.

2. μ model with holes

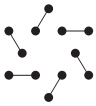
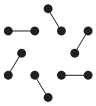
Like any QDM, the μ model can be extended to include static holes. These holes can equally represent charge degrees of freedom or neutral spinons (unpaired spin in a dimer background). The new Hamiltonian $\mathcal{H}'$ contains all the kinetic terms of $\mathcal{H}$ except those where the resonance loop passes through a missing site. Consider a hole which belongs to two hexagons 1 and 2 (figure 1). No loop of μ_1 or μ_2 survives in $\mathcal{H}'$ because they would all pass through the missing site. As for hexagons 3 and 4, one half of their resonance loops pass through the hole and must be removed. In the presence of a hole the operators μ_3 and μ_4 thus only contain 16 resonance loops (instead of 32). However, these two modified operators satisfy the *same algebraic relations* [5] *as the hole-free* μ. For any hexagon $h \neq 1, 2$ and for $i = 3$ or 4 we have $\mu_i^2 = 1$ and

$$\mu_i\mu_h = \mu_h\mu_i \qquad h \text{ not a neighbour of } i \tag{3}$$

$$\mu_i\mu_h = -\mu_h\mu_i \qquad h \text{ neighbour of } i. \tag{4}$$

[2] In the absence of that sign the model reduces to that of [3] and can be solved exactly; it has a RVB liquid ground state with topological order and gapped $\mathbb{Z}_2$-vortex excitations.

Table 1. The eight different classes (up to rotations) of dimerizations of a hexagon of the kagome lattice.

α	n_α	$\lvert d_\alpha\rangle$	$\lvert \bar{d}_\alpha\rangle$	$(-1)^{n_\alpha}$
1	3			-1
$2,\cdots,4$	4			$+1$
$5,\cdots,10$	4			$+1$
$11,\cdots,16$	4			$+1$
$17,\cdots,19$	5			-1
$20,\cdots,25$	5			-1
$26,\cdots,31$	5			-1
32	6			$+1$

These relations are easy to check with the help of the arrow representation of dimer coverings of the kagome lattice [3, 5, 9]. It is also easy to check that the argument leading to an exponential degeneracy $\sim 2^{N/6}$ of the energy levels [5] holds even in the presence of these static holes. As a first result we thus find that the extensive ground-state entropy of the μ model survives in the presence of holes. This also allows one to use the reduced representation of the Hilbert space which was used in [5] to compute the spectrum in the absence of holes. The spectrum is non-degenerate in this representation, which has a dimension $\sim 2^{N/6}$ (instead of $2^{N/3+1}$ as for the dimer Hilbert space). The ground state of systems up to 48 hexagons (144 kagome sites) can be obtained with a standard Lanczos algorithm. The result was checked (with and without holes) against direct calculations in the dimer Hilbert space for small systems ($N \leqslant 48$). We investigated samples with $N = 36$, 48, 60, 72, 84, 108 and 144 kagome sites ($N_h = 12$, 16, 20, 24, 28, 36 and 48 hexagons). Periodic boundary conditions are used and the shapes of these clusters are the same as those of [5].

Interestingly this representation allows one to compute the spectra of even a system pierced by a *single* hole. Strictly speaking the QDM is not defined on such an *odd* sample, but the non-degenerate representation of the μ algebra mentioned above can still be constructed. This trick is useful for estimating the energy cost Δ of a *single hole* in a given sample.

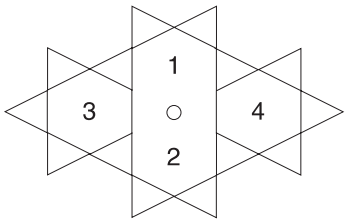


Figure 1. The hole forbids all resonance loops on hexagons 1 and 2 and suppresses some of the loops around 3 and 4.

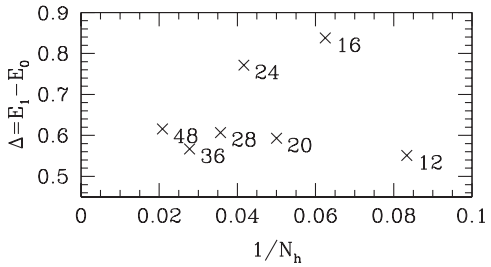


Figure 2. The energy cost Δ of a single hole in the μ QDM as a function of the number of hexagons N_h.

3. Single-hole ground-state energy

The ground-state energy in the absence of holes is denoted as E_0; E_1 is the energy with a single hole (two neighbouring μ removed). If $\langle \mu_i \mu_j \rangle$ correlations are neglected, the ground-state energy would increase by $2\langle \mu \rangle \simeq 0.88$ around each hole (the ground-state energy is estimated to be $\simeq -0.44$ per hexagon in the thermodynamic limit [5]). In fact, removing two neighbouring μ operators increases the ground-state energy by $\Delta = E_1 - E_0 \sim 0.6$ (figure 2). It is easy to understand why the actual hole gap Δ is smaller than the naive estimate above. Because of the anti-commutation relations between nearby μ operators (equation (4)), the system cannot simultaneously achieve a minimal energy (i.e. $\mu = 1$) on two neighbouring hexagons. Removing some μ operators therefore decreases the frustration on their neighbours, which can acquire in turn a larger expectation value (lower energy). This larger 'polarization' of the hexagons around the hole will enhance the frustration on their neighbours, and the corresponding μ will have to reduce (slightly) their expectation value compared with the bulk value. This mechanism produces spatial oscillations in $\langle \mu \rangle$ (data not shown), oscillations which have the same wavevector as the correlations which dominate in the bulk [5].

4. Two-hole ground-state energy

The difference between the energy $E_2(d)$ with two holes at distance d and the energy E_0 without holes is shown in figure 3. In the analysis of [5] it appeared that the μ model has significant local $\langle \mu_i \mu_j \rangle$ correlations with a period of three hexagons. It is therefore convenient to plot separately the data for N_h not a multiple of three and the others ($N_h = 12$, 24, 36 and 48), which do not frustrate the local order. At short distance, when the two holes belong to a common hexagon, only three μ operators are removed from $\mathcal{H}$ and the energy cost is roughly $E_2 - E_0 \sim \frac{3}{2}\Delta$. This happens for $d = 1, \sqrt{3}$ as well as for $d = 2$ when the two holes are on opposite sites of a hexagon. This is a short-distance effect because for $d > 2$ the number of μ suppressed is always four. In other words, when two holes sit on the same

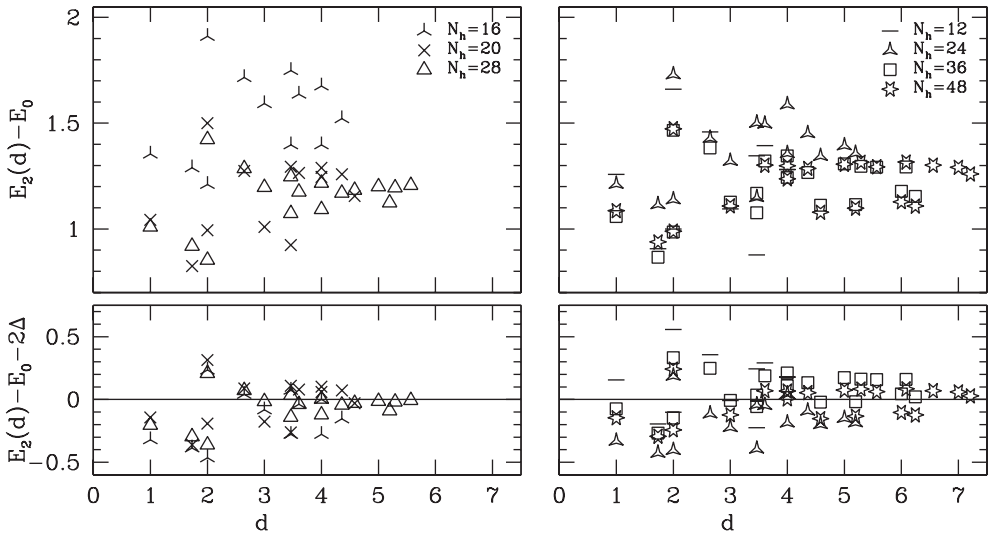


Figure 3. The energy $E_2(d)$ of the ground state of the μ QDM in the presence of two holes at distance d. In the top panels this energy is compared to the energy E_0 of the system without holes and in the lower panels $E_2(d)$ is compared to the hole-free energy E_0 corrected by twice the energy cost $\Delta = E_1 - E_0$ of a single hole.

hexagon they minimize the number of loops which are 'lost' for resonances[3]. At intermediate distances ($2 \leqslant d \leqslant \sqrt{12}$) the energy decreases with distance in a regular way for all samples. In this range of d the behaviour is thus reminiscent of the strong hole repulsion observed in the kagome Heisenberg model by Dommange *et al* [8].

For $d \geqslant 4$ the data suggest that the energy $E_2(d)$ goes to a constant. The values are indeed close to the energy $E_0 + 2\Delta$ (see the lower panels of figure 3) which is expected if the dimer background is not mediating any interaction between the holes. We therefore argue that the μ model is not confining static holes. It is interesting to note that in the samples which do not frustrate the local order (right-hand panels of figure 3) the hole–hole interaction seems to decay more slowly with distance than in the other samples. This rather slow decay is not incompatible with the interesting suggestion [8] of a $1/d$ behaviour. In addition, weak oscillations can be observed. They may be related to the oscillations of $\langle\mu\rangle$ mentioned in the previous section and to the (presumably) quasi-long-ranged correlations in $\langle\mu_i\mu_j\rangle^c$ discussed in [5].

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[3] This effect can also be found, to a smaller extent, in the two-hole energies of the spin-1/2 model [8]: comparing the two ways in which two holes can be at distance $d = 2$, the energy is always lower when they belong to the same hexagon. There is, however, no strong reduction of E_2 for $d = 1$ and $\sqrt{3}$ in the spin model as we have in the μ QDM.