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 [Phys. Rev. B 67, 214413 (2003)]. The ground-state energy of this QDM in 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 7 lattice spacings) is evaluated and the results show no indication of confinement at large hole separations.

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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 by all (nearest-neighbor) dimer coverings of the lattice and the Hamiltonian allows these dimer to move along local resonance loops. Two kinds of phases 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 $Z_2$-vortex excitations [4]. Importantly also, these two phases can be distinguished by the behavior 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 confine 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.
**Interaction between static holes in a quantum dimer model on the kagome lattice**

This energy goes to a constant when two holes are separated far apart in a deconfined system whereas it grows linearly in a confined system.‡

We recently proposed a QDM on the kagome lattice which does not simply fall in any of these two categories [5]. This model, hereafter called the $\mu$–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:

$$\mathcal{H} = - \sum_{h} \mu_h$$  \hspace{1cm} (1)

where

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

‡ QDMs at Rokhsar-Kivelson points [11] are an exception: the ground-state energy remains exactly zero whatever the positions of the holes.

**Table 1.** The 8 different classes (up to rotations) of dimerizations of an hexagon of the kagome lattice.

| $\alpha$ | $n_{\alpha}$ | $\langle d_{\alpha}\rangle$ | $\langle \bar{d}_{\alpha}\rangle$ | $(-1)^{n_{\alpha}}$ |
|----------|--------------|----------------|----------------|--------------|
| 1        | 3            | ![Diagram1](#) | ![Diagram2](#) | -1           |
| 2, ..., 4| 4            | ![Diagram3](#) | ![Diagram4](#) | +1           |
| 5, ..., 10| 4          | ![Diagram5](#) | ![Diagram6](#) | +1           |
| 11, ..., 16| 4        | ![Diagram7](#) | ![Diagram8](#) | +1           |
| 17, ..., 19| 5        | ![Diagram9](#) | ![Diagram10](#) | -1           |
| 20, ..., 25| 5        | ![Diagram11](#) | ![Diagram12](#) | -1           |
| 26, ..., 31| 5        | ![Diagram13](#) | ![Diagram14](#) | -1           |
| 32       | 6            | ![Diagram15](#) | ![Diagram16](#) | +1           |
Figure 1. The hole forbids all resonance loops on hexagons 1 and 2 and suppresses some of the loops around 3 and 4.

and \( h \) runs over the hexagons of the lattice and \( |d_\alpha(h)\rangle \) is one of the 32 possible dimerizations of \( h \) (table I). The sign \( n_\alpha \) counts the parity of the number of dimer involved\(^\S\). 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 \( \mu \)–model has an extensive ground-state entropy \( 1/6 \log(2) \) 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 so 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 degeneracy, the spectrum is likely to be gapless and that 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 \( \mu \)–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 behavior is observed in the \( \mu \)–QDM.

2. \( \mu \)–model with holes

As any QDM, the \( \mu \)–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 I). No loop of \( \mu_1 \) or \( \mu_2 \) survive 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 presence of a hole the operators \( \mu_3 \) and \( \mu_4 \) thus only contain 16 resonance loops (instead of 32). However these two

\(^\S\) In the absence of that sign the model reduces to that of reference \(^9\) and can be solved exactly, it has a RVB liquid ground-state with topological order and gapped \( Z_2 \)-vortex excitations.
modified operators satisfy the same algebraic relations as the hole-free \( \mu \)'s. For any hexagon \( h \neq 1, 2 \) and for \( i = 3 \) or \( 4 \) we have \( \mu_i^2 = 1 \) and:

\[
\begin{align*}
\mu_i \mu_h &= \mu_h \mu_i \quad \text{h not neighbor of } i \\
\mu_i \mu_h &= -\mu_h \mu_i \quad \text{h neighbor of } i
\end{align*}
\]  

These relations are easy to check with the help of the arrow representation of dimer coverings of the kagome lattice. It is also easy to check that the argument leading to an exponential degeneracy \( \sim 2^{N/6} \) of the energy levels holds even in the presence of these static holes. As a first result we thus find that the extensive ground-state entropy of the \( \mu \)-model survives in the presence of holes. This also allows to use the reduced representation of the Hilbert space which was used in reference 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 \( 2^{N/3+1} \) 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 (\( N \leq 48 \)). 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 reference.

Interestingly this representation allows to compute the spectra of a even 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 \( \mu \) algebra mentioned above can still be constructed. This trick is useful to estimate the energy cost \( \Delta \) of a single hole in a given sample.

### 3. Single hole ground-state energy

The ground-state energy in the absence of holes is noted \( E_0 \), \( E_1 \) is the energy with a single hole (two neighboring \( \mu \)'s removed). If \( \langle \mu_i \mu_j \rangle \) correlations are neglected, the ground-state energy would increase by \( 2 \langle \mu \rangle \approx 0.88 \) around each hole (the ground-state energy is estimated to be \( \approx -0.44 \) per hexagon in the thermodynamic limit). In fact removing
two neighboring $\mu$ 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 $\Delta$ is smaller than the naive estimate above. Because of the anti-commutation relations between nearby $\mu$ operators (equation 4) the system cannot simultaneously achieve a minimal energy (i.e. $\mu = 1$) on two neighboring hexagons. Removing some $\mu$ operators therefore decreases the frustration on their neighbors, 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 neighbors, and the corresponding $\mu$ 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 wave-vector as the correlations which dominate in the bulk [5].

4. Two-holes 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 Ref. [5] it appeared that the $\mu$-model has significant local $\langle s_i s_j \rangle$ correlations with a period of three hexagons. It is therefore convenient to plot separately the data for $N_h$ not multiple of three and the others ($N_p = 12, 24, 36$ and $48$), which do not frustrate the local order. At short distance, when the two holes belong to a common hexagon, only 3 $\mu$ operators are removed from $H$ 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 an hexagon. This is a short-distance effect because for $d > 2$ the number $\mu$ suppressed is always four.
In other words, when two holes sit on the same hexagon they minimize the number of loops which are “lost” for resonances \[\parallel\]. At intermediate distances \(2 \leq d \leq \sqrt{12}\) the energy decreases with distance in a regular way for all samples. In this range of \(d\) the behavior is thus reminiscent of the strong hole repulsion observed in the kagome Heisenberg model by Dommange et al. [8].

For \(d \geq 4\) 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 lower panels of figure[3] which is expected if the dimer background was not mediating any interaction between the holes. We therefore argue that the \(\mu\) model is not confining static holes. It is interesting to note that in the samples which do not frustrate the local order (right 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 \(1/d\) behavior. In addition, weak oscillations that 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 Ref. [5]

References

[1] Rokhsar D S and Kivelson S A 1988 Phys. Rev. Lett. 61, 2376
[2] Moessner R and Sondhi S L 2001 Phys. Rev. Lett. 86 1881
[3] Misguich G, Serban D and Pasquier V 2002 Phys. Rev. Lett. 89 137202
[4] Read and Chakraborty 1989 Phys. Rev. B 40 7133
[5] Misguich G, Serban D and Pasquier V 2003 Phys. Rev. B 67 214413
[6] Elser V and Zeng C 1995 Phys. Rev. B 51 8318
[7] Sindzingre P, Lhuillier C and Fouet J.-B. 2002, Advances in Quantum Many-Body Theory 6 90, cond-mat/0110283
[8] Dommange S, Mambrini M, Normand B and Mila F Preprint cond-mat/0306299
[9] Elser V and Zeng C 1993 Phys. Rev. B 48 13647

\[\parallel\] 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 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 \(\mu\)-QDM.