Quantum Phase Diagram for a Planar Pyrochlore Antiferromagnet

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We study a spin-half Heisenberg antiferromagnet on a checkerboard geometry, the two-dimensional version of the pyrochlore lattice. Ground-state properties and low-energy excitations for this highly frustrated model are investigated by means of perturbative expansions, spin-wave theory and by applying a contractor renormalisation analysis. We examine the validity of previously conjectured zero-temperature phase diagrams and the nature of quantum critical points separating valence bond crystalline and Néel-ordered phases.

1. Introduction

Classical spin systems often display a macroscopically degenerate ground-state in the presence of geometric frustration and one might therefore expect exotic phases to be stabilised, via an "order from disorder" mechanism, in the presence of quantum fluctuations, especially in the extreme quantum limit of $S = 1/2$. Interest in frustrated quantum magnets can be traced back to Anderson's conjecture [1] on the possibility of a spin-liquid ground-state for the spin-half antiferromagnet on the triangular lattice. Although the particular model considered by Anderson was later shown to display more conventional Néel order, many other frustrated magnets have been proposed as candidates for displaying exotic phases. In particular, the highly frustrated spin-half Heisenberg models defined on the pyrochlore lattice, comprised of corner-sharing tetrahedra, and on its planar projection known as the checkerboard lattice, shown in Fig. 1, have attracted considerable interest.

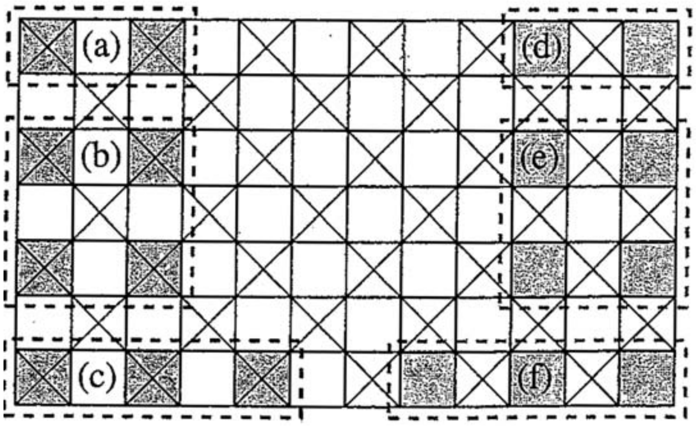

Fig. 1. The checkerboard lattice considered in the present work. Nearest-neighbour spins interact via coupling J (horizontal and vertical full lines) and the frustrating coupling $J_\times$ (diagonal dashed lines) connects spins joined in every other plaquette. Dashed lines indicate the clusters employed in performing the CORE expansion [(a)-(c) crossed expansion and (d)-(f) uncrossed expansion].

The Hamiltonian for the planar pyrochlore antiferromagnet reads

$$\mathcal{H} = J \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j + J_\times \sum_{[i,j]} \vec{S}_i \cdot \vec{S}_j \ . \qquad (1)$$

J is the nearest-neighbour coupling and $J_\times$ (diagonal lines in Fig. 1) connects spins along the diagonals of every other square plaquette in the lattice. Two limiting cases are well understood: for $J_\times = 0$ the model reduces to the Néel-ordered antiferromagnet on the square lattice and for $J = 0$ the system is comprised by decoupled chains, exactly solvable via the Bethe Ansatz. The point $J_\times = J$ has been investigated in a number of recent works [2-4] and there is strong evidence for a quadrumerised valence bond solid (VBS) ground-state (P-VBS in Fig. 2). Starykh *et al.* [5] have recently applied a strong coupling analysis in the limit $J_\times / J << 1$ and found evidence for a second VBS phase, termed *crossed-dimers VBS* phase (CD-VBS in Fig. 2), later supported by numerical results [6]. Furthermore, based on symmetry arguments, Starykh *et al.* [5] conjectured on the existence of a long-range ordered phase for intermediate couplings (D-Néel in Fig. 2) and proposed the phase diagram depicted in Fig. 2.

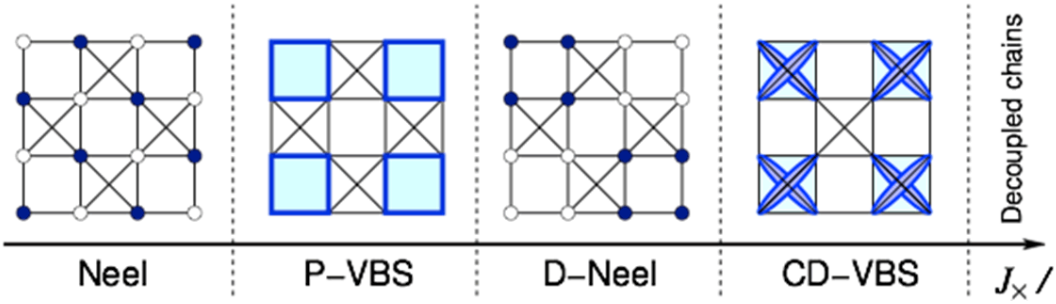

Fig. 2. Quantum phase diagram for the checkerboard antiferromagnet proposed by Starykh *et al.* [5], based on a strong coupling analysis, previously obtained numerical results at $J_\times / J = 1$, and symmetry considerations. Up (down) spins are represented by open (filled) circles and singlets are depicted as filled squares (P-VBS) or ellipsis (CD-VBS).

In the present work, we investigate the quantum phase diagram for the checkerboard antiferromagnet by combining linked-cluster expansions [7] and the Contractor Renormalisation (CORE) algorithm [8]. The so obtained results for ground-state properties and low-lying excited states are compared with spin wave calculations and previous findings.

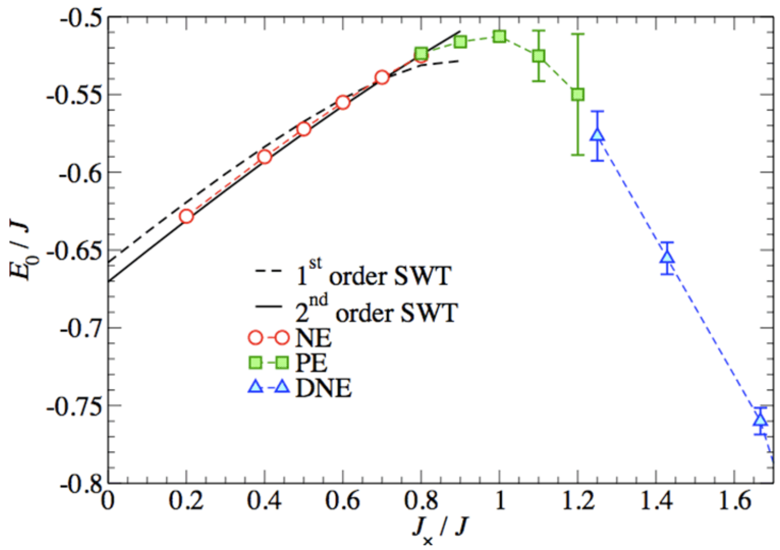

Fig. 3. Ground-state energy as a function of $J_\times / J$ around the isotropic limit ($J_\times / J = 1$). Results have been obtained from linear (first order) SWT, second-order modified SWT and four different linked cluster expansion: Néel (NE), plaquette (PE) and *diagonal* Néel (DNE).

2. Perturbative Expansions

We have derived three different linked-cluster expansions [7] for the ground-state properties of the model Eq. (1). A *Néel expansion* (NE) is valid for small values of $J_\times$ / J and assumes a perfectly ordered Néel unperturbed state. A *plaquette expansion* (PE), starting from the plaquette VBS state depicted in Fig. 2 (P-VBS), is adequate for couplings around $J_\times / J = 1$ [2-4]. Finally, an expansion for higher values of $J_\times$ / J, termed *diagonal-Néel expansion* (DNE), assumes the ordered state depicted as "D-Néel" in Fig. 2 as the unperturbed state.

Data for the ground-state energy obtained by extrapolating the series from the various expansions are shown in Fig. 3. Also shown are the results obtained from linear and modified second-order spin-wave theory (SWT). The plot suggests that the quantum phase transition between Néel and plaquette VBS phases takes place around $J_\times / J \sim 0.8$, consistently with our results for the staggered magnetisation shown in Fig. 4 (a smaller estimate for this critical point, $J_\times / J \sim 0.6$, was obtained in Ref. [6]). Additionally, our results shown in Fig. 3 also suggest that the transition between the "plaquette VBS" and diagonal "Néel phases" takes place around $J_\times / J \sim 1.2$, a value consistent with the one obtained in Ref. [6], $J_\times / J \sim 1.1$.

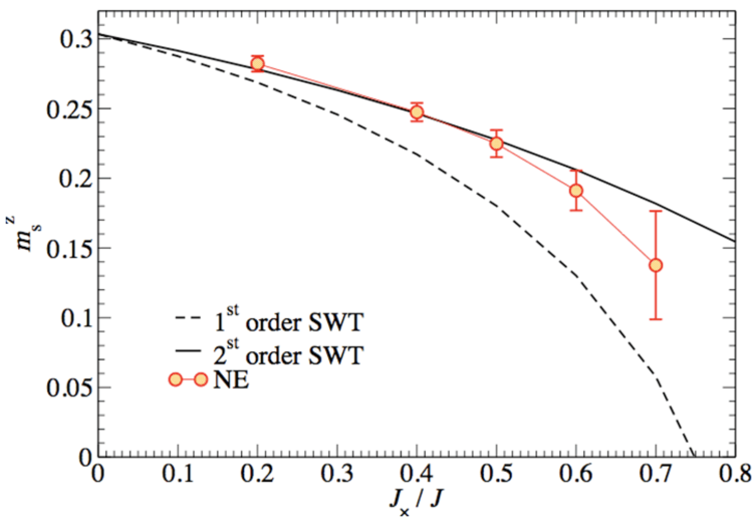

Fig. 4. Staggered magnetisation as a function of $J_\times$ / J in the Néel phase. Results have been obtained from first and second order SWT, and from a Néel expansion (NE).

3. Contractor Renormalisation: Preliminary Results

We also present preliminary results obtained from a CORE expansion. CORE was previously applied to the study of the checkerboard antiferromagnet by Berg *et al.* [4], but their analysis was restricted to $J_\times / J = 1$.

In Fig. 5 we plot an estimate for the gap for triplet excitations above the plaquette VBS ground-state as a function of $J_\times$ / J, as obtained from a low-order CORE calculation assuming the "uncrossed plaquettes" [4] as the elementary blocks [results are obtained from the cluster depicted in Fig. 1(d)]. The triplet gap is simply estimated as $\Delta_t / J = \mu_t - 4t_t$, where μ_t is the chemical potential and t_t is the nearest-neighbour hopping amplitude for triplets, both directly obtained from the effective CORE Hamiltonian. Δ_t / J vanishes for $J_\times / J \sim 0.55$, a value substantially smaller than the aforementioned estimate for the critical point separating Néel and plaquette VBS phases obtained from series expansions. However, we expect sizeable corrections from extended CORE calculations, considering the larger clusters shown in Fig. 1, and work along this direction is in progress.

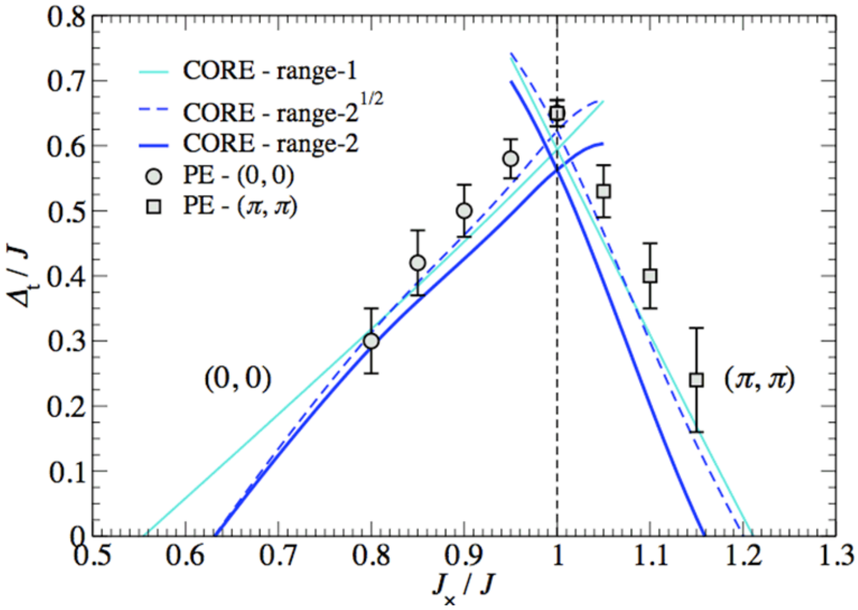

Fig. 5. Gap for triplet excitations above the plaquette VBS ground-state as a function of $J_\times / J$, obtained from a CORE expansion (lines) and from plaquette expansion (symbols).

4. Conclusions and Future Work

Summarising, we have investigated zero-temperature properties of the $S = 1/2$ antiferromgnetic Heisenberg model on the highly frustrated checkerboard lattice. By combining spin-wave theory, high-order perturbative expansions and the CORE technique, we find evidence for a rich quantum phase diagram, comprising both magnetically ordered and less conventional valence bond crystal phases.

Results presented here have been obtained as part of an ongoing research project that will be complemented by further analysis. We are currently devising a fourth series expansion, adequate to the study of the crossed-dimers VBS phase (CD-VBS in Fig. 2), and are extending the CORE expansion by considering longer ranged contributions and by applying a more sophisticated analysis to the effective Hamiltonians.

Acknowledgments

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