THE FRUSTRATED HEISENBERG ANTIFERROMAGNET ON THE CHECKERBOARD LATTICE: The spin-$\frac{1}{2}$ J_1–J_2 model

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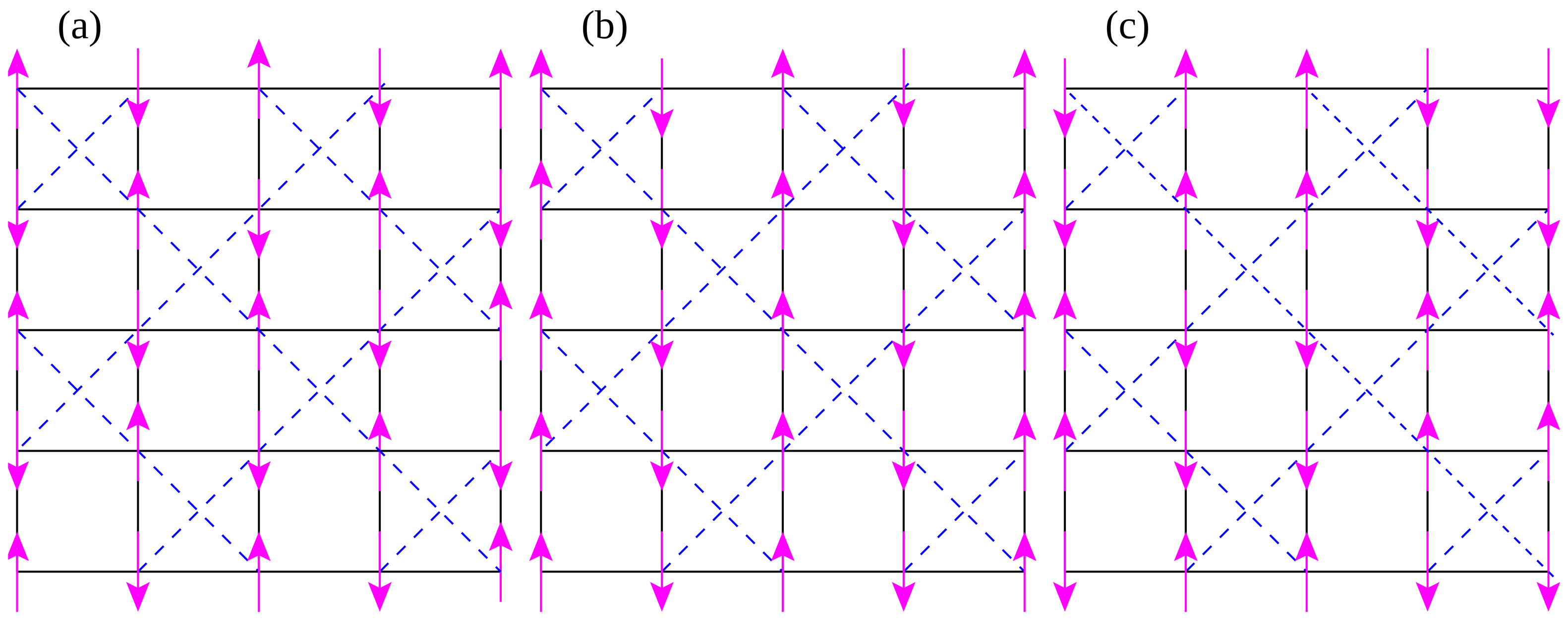
1. Introduction

- One of the prime theoretical interests in frustrated quantum magnets lies in the possibility that they might exhibit disordered quantum paramagnetic states and/or spin-liquid behaviour. Among the most highly frustrated systems are those composed of tetrahedra coupled into 2D or 3D lattice networks. Prominent among the latter are the pyrochlores, whose basic structure is one of vertex-sharing tetrahedra.
- Using the coupled cluster method (CCM) we study the zero-temperature ground-state phase diagram of the spin-$\frac{1}{2}$ anisotropic planar pyrochlore (or crossed chain) model [1].
- The CCM is one of the most powerful and most universally applicable techniques of quantum many-body theory. It has been applied successfully to many lattice quantum spin systems [2,3]. Two of the unique strengths of the CCM are:
  - its ability to deal with highly frustrated systems as easily as unfrustrated ones, and
  - its use from the outset of infinite lattices, which leads in turn to its ability to yield accurate phase boundaries even near quantum critical points.

2. The J_1–J_2 checkerboard model

$$H = J_1 \sum_{\langle i,j\rangle} \mathbf{s}_i \cdot \mathbf{s}_j + J_2 \sum_{\langle\langle i,k\rangle\rangle} \mathbf{s}_i \cdot \mathbf{s}_k \,.$$

- The model is equvalently described as a frustrated J_1–J_2 Heisenberg antiferromagnet (HAFM) on the 2D checkerboard lattice, with nearest-neighbour exchange bonds of strength $J_1 > 0$ and next-nearest-neighbour bonds of strength $J_2 \equiv \kappa J_1 > 0$.
- **Special cases:**
  - $\kappa = 0$ $\leftrightarrow$ square-lattice HAFM
  - $\kappa = 1$ $\leftrightarrow$ isotropic checkerboard lattice HAFM
  - $\kappa \to \infty$ $\leftrightarrow$ decoupled 1D HAFM chains



(a) Néel state, (b) striped state - columnar and (c) Néel* state. The NN J_1 bonds are shown as solid (black) lines and the NNN J_2 bonds are shown as dashed (blue lines).

- **Energy scale:** Henceforth we set $J_1 \equiv 1$.
- **Classical ground states:**
  - $\kappa < 1$ $\leftrightarrow$ Néel state
  - $\kappa > 1$ $\leftrightarrow$ infinitely degenerate family of AFM (crossed) diagonals, from which the fourfold set of (row and columnar) striped states and (doubly degenerate) Néel* states are selected by quantum fluctuations to $O(1/s)$
- Using the above 3 antiferromagnetic (AFM) classical ground states as CCM model or reference states we present results for the gs energy, average on-site magnetization, susceptibilities to plaquette valence-bond crystal (PVBC) and crossed-dimer valence-bond crystal (CDVBC) ordering.

3. CCM Formalism

- **General formalism**

$$He^S|\Phi\rangle = Ee^S|\Phi\rangle\,; \quad \langle\Phi|\tilde{S}e^{-S}H = E\langle\Phi|\tilde{S}e^{-S}\,,$$

$$S = \textstyle\sum_{I\neq 0} \mathcal{S}_I C_I^+\,; \quad \tilde{S} = 1 + \sum_{I\neq 0} \tilde{\mathcal{S}}_I C_I^-\,.$$

- $|\Phi\rangle \leftrightarrow$ model state. C_I^+ and $C_I^- \equiv (C_I^+)^\dagger \leftrightarrow$ complete set of multiparticle creation and destruction operators, where $C_0^+ \equiv 1 \equiv C_0^-$ and $C_I^-|\Phi\rangle = 0 = \langle\Phi|C_I^+\,; \quad \forall I \neq 0$.
- $I \leftrightarrow$ multi-configurational set-index.
- The ket- and bra-state correlation coefficients $(\mathcal{S}_I, \tilde{\mathcal{S}}_I)$ are calculated by requiring the energy expectation value $\bar{H} \equiv \langle\tilde{\Psi}|H|\Psi\rangle$ to be minimized with respect to each of them $\Rightarrow$

$$\langle\Phi|C_I^- e^{-S}He^S|\Phi\rangle = 0\,; \quad \langle\Phi|\tilde{S}e^{-S}[H, C_I^+]e^S C_I^+|\Phi\rangle = 0\,;\ \forall I \neq 0\,,$$

and the ground-state (gs) energy is given by

$$E = \langle\Phi|e^{-S}He^S|\Phi\rangle\,.$$

- **Specific formalism for quantum spin-lattice systems**
  - In order to treat each site identically, we perform a mathematical rotation of the local axes of each spin so that all spins on each model state align along the negative z axis. In the rotated frames, we have $|\Phi\rangle = |\downarrow\downarrow\downarrow\cdots\rangle$, and $C_I^+ \to s_{i_1}^+ \cdots s_{i_k}^+$ (where on each lattice site i_n we have at most one spin-raising operator for $s = 1/2$).
  - The order parameter is the average local on-site magnetization,

$$M \equiv -\frac{1}{N}\langle\tilde{\Psi}|\textstyle\sum_{i=1}^{N} s_i^z|\Psi\rangle\,; \quad \text{where } s_i^z \text{ is expressed in the local rotated spin coordinates.}$$

- **Approximation schemes to truncate the expansions of S and $\tilde{S}$**
  - **LSUB**m: includes all multi-spin-flip configurations defined over all lattice animals of size $\leq m$.
  - Number of **LSUB**m fundamental configurations, N_f:

Method	N_f		
	Néel	striped	Néel*
LSUB4	27	54	79
LSUB6	632	1225	2441
LSUB8	21317	41324	86590
LSUB10	825851	1598675	3373495

  - **Extrapolations:** The results are extrapolated heuristically to the $m \to \infty$ limit as,

$$E(m)/N = a_0 + a_1 m^{-2} + a_2 m^{-4}$$

$$M(m) = b_0 + b_1 m^{-1} + b_2 m^{-2}\,; \quad \text{LSUB}\infty(1) \leftrightarrow \text{for non-frustrated spin systems, and}$$

$$M(m) = c_0 + b_1 m^{-1/2} + a_2 m^{-3/2}\,; \quad \text{LSUB}\infty(2) \leftrightarrow \text{for highly fustrated spin systems.}$$

References

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[2] R. F. Bishop, Theor. Chim. Acta 80, 95 (1991).
[3] D. J. J. Farnell and R. F. Bishop, in *Quantum Magnetism*, U. Schollwöck, J. Richter, D.J.J. Farnell and R.F. Bishop (Eds.), *Lecture Notes in Physics* **645** (Springer, Berlin, 2004).

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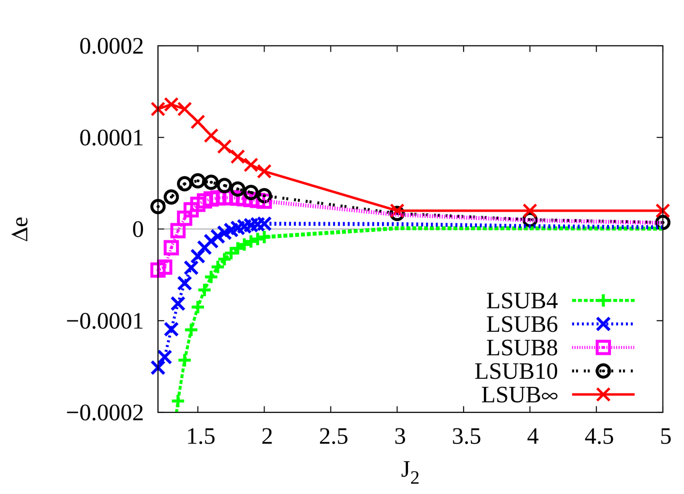
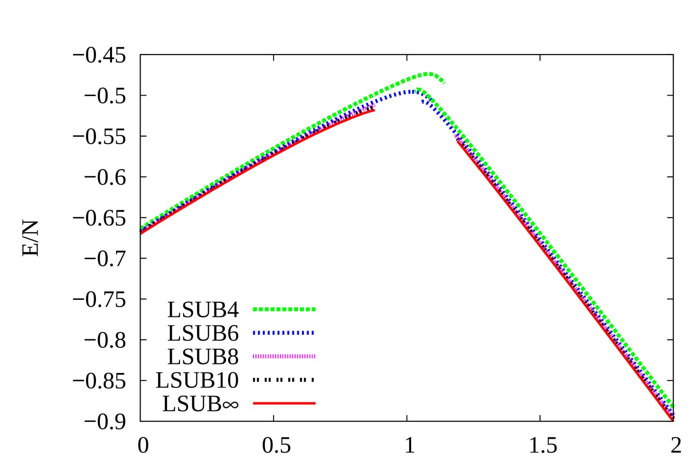
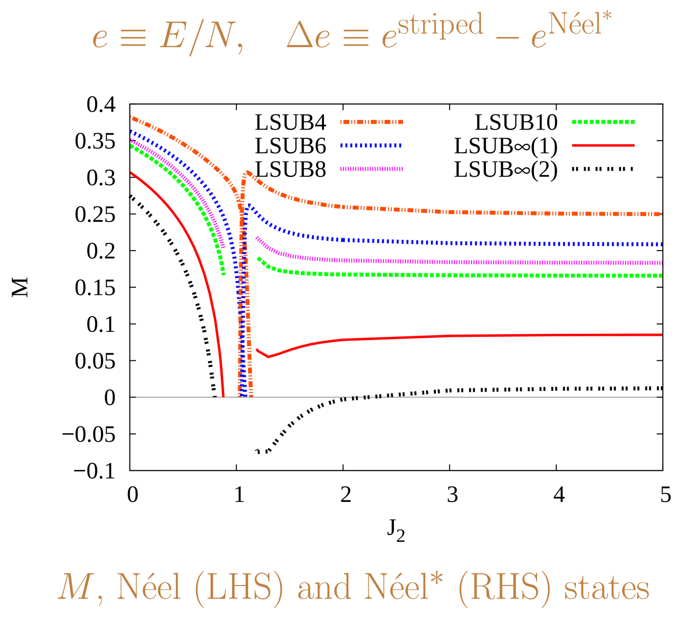
4. GROUND-STATE ENERGY AND MAGNETIZATION ($J_1 = 1$)



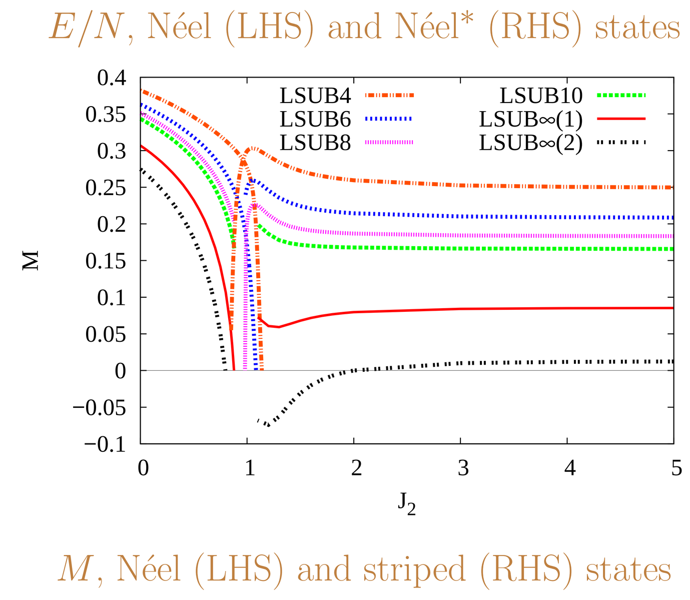
$e \equiv E/N$, $\quad \Delta e \equiv e^{\text{striped}} - e^{\text{Néel*}}$



E/N, Néel (LHS) and Néel* (RHS) states



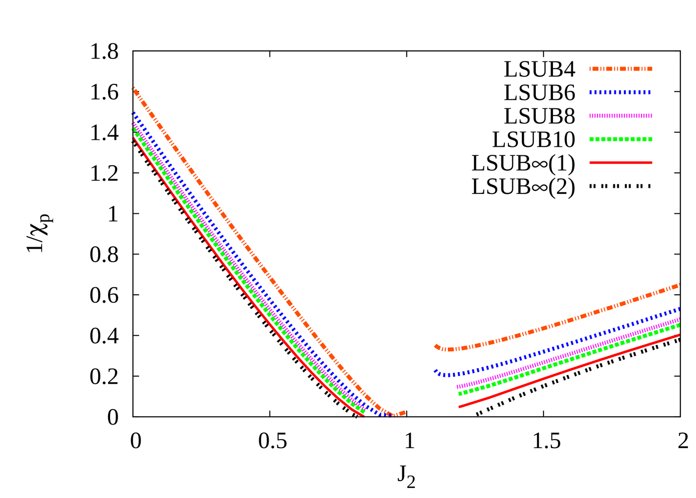
M, Néel (LHS) and Néel* (RHS) states

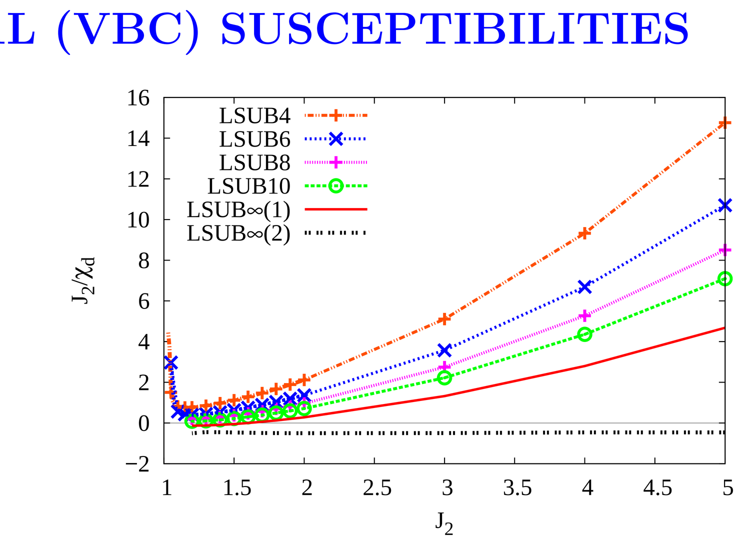


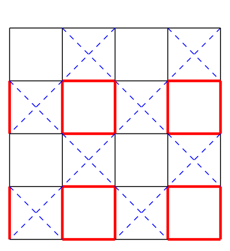
M, Néel (LHS) and striped (RHS) states

- Our calculations show that the AFM quasiclassical state with Néel ordering is the gs phase for $\kappa < \kappa_{c_1} \approx 0.80 \pm 0.01$, but that neither the striped nor Néel* states that form the gs phase for the classical version ($s \to \infty$) of the model (for $\kappa > 1$) survive the quantum fluctuations to form a stable magnetically-ordered gs phase for the $s = \frac{1}{2}$ case.

5. VALENCE-BOND CRYSTAL (VBC) SUSCEPTIBILITIES

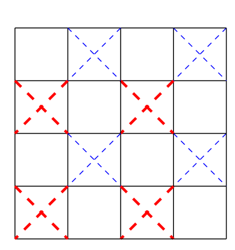






PVBC susceptibility

$$H \to H + F\,; \quad F \equiv \delta\,\hat{O}$$
$\hat{O} \leftrightarrow$ red bonds $(+)$, blue bonds $(-)$
$$E \to E(\delta)\,; \quad e(\delta) \equiv E(\delta)/N$$
$$\chi_F \equiv -\left(\partial^2 e(\delta)\right)/\left(\partial\delta^2\right)\big|_{\delta=0}$$



CDVBC susceptibility

$$\text{LSUB}\infty(1) \leftrightarrow \chi_F^{-1}(m) = x_0 + x_1 m^{-2} + x_2 m^{-4}\,; \qquad \text{LSUB}\infty(2) \leftrightarrow \chi_F^{-1}(m) = y_0 + y_1 m^{-y_2}$$

- We show that the quasiclassical Néel state becomes infinitely susceptible to PVBC ordering at or very near to $\kappa = \kappa_{c_1}$, and that the quasiclassical fourfold AFM states become infinitely susceptible to PVBC ordering at $\kappa = \kappa_{c_2} \approx 1.22 \pm 0.02$.
- In turn, we find that these states become infinitely susceptible to CDVBC ordering for *all* values of κ above a certain critical value at or very near to $\kappa = \kappa_{c_2}$. Our calculations thus indicate a Néel-ordered gs phase for $\kappa < \kappa_{c_1}$, a PVBC-ordered phase for $\kappa_{c_1} < \kappa < \kappa_{c_2}$, and a CDVBC-ordered phase for $\kappa > \kappa_{c_2}$. Both transitions are likely to be direct ones, although we cannot exclude very narrow coexistence regions confined to $0.79 \lesssim \kappa \lesssim 0.81$ and $1.20 \lesssim \kappa \lesssim 1.22$ respectively.