Decoupled phase of frustrated spin-1/2 antiferromagnetic chains with and without long range order in the ground state

Manoranjan Kumar$^1$ and Z.G. Soos$^2$

$^1$S. N. Bose National Centre for Basic Sciences, Block-JD, Sector-III, Kolkata 700098, India.

$^2$Department of Chemistry, Princeton University, Princeton NJ 08544

(Dated: May 22, 2014)

The quantum phases of one-dimensional spin $s = 1/2$ chains are discussed for models with two parameters, frustrating exchange $g = J_2 > 0$ between second neighbors and nonfrustrating power-law exchange with exponent $\alpha$ and distance dependence $r^{-\alpha}$. The ground state (GS) at $g = 0$ has long-range order (LRO) for $\alpha < 2$, long-range spin fluctuations for $\alpha > 2$. The models conserve total spin $S = S_A + S_B$, have singlet GS for any $g$, $\alpha \geq 0$, and decouple at $1/g \to 0$ to linear Heisenberg antiferromagnets on sublattices A and B of odd and even-numbered sites. Exact diagonalization of finite chains gives the sublattice spin $\langle S^z_A \rangle$, the magnetic gap $E_m$ to the lowest triplet state and the excitation $E_2$ to the lowest singlet with opposite inversion symmetry to the GS. An analytical model that conserves sublattice spin has a first order quantum transition at $g_c = 1/4\ln 2$ from a GS with perfect LRO to a decoupled phase with $S_A = S_B = 0$ for $g \geq 4/\pi^2$ and no correlation between spins in different sublattices. The model with $\alpha = 1$ has a first order transition to a decoupled phase that closely resembles the analytical model. The bond order wave (BOW) phase and continuous quantum phase transitions of finite models with $\alpha \geq 2$ are discussed in terms of GS degeneracy where $E_0(g) = 0$, excited state degeneracy where $E_0(g) = E_m(g)$, and $\langle S^z_A \rangle$. The decoupled phase at large frustration has nondegenerate GS for any exponent $\alpha$ and excited states related to sublattice excitations.

PACS numbers: 75.10.Pq, 75.10.Jm, 64.70.Tg, 73.22.Gk

Email: soos@princeton.edu, manoranjan.kumar@bose.res.in

I. INTRODUCTION

One-dimensional (1D) spin chains have provided a wealth of quantum many-body problems over the years, starting with Bethe's treatment $^1$ of the linear Heisenberg antiferromagnet (HAF) with exchange $J_1 > 0$ between adjacent $s = 1/2$ sites. The linear HAF has been extensively studied and generalized $^2$.$^4$. Second-neighbor exchange $J_2 > 0$ is frustrating in chains with either sign of $J_1$. Magnetic frustration has recently been reported in copper oxides that contain $s = 1/2$ chains of Cu(II) ions with $J_1 > 0$ $^5$ or $< 0$ $^6$. Increasing $g = J_2/J_1$ in the $J_1 - J_2$ model generates a continuous quantum transition from the HAF ground state to a bond order wave (BOW) phase that has been established by multiple theoretical methods $^2$.$^9$ but to the best of our knowledge, the BOW phase of spin chains has not been realized experimentally. The characterization of the BOW phase is limited: The ground state is doubly degenerate, inversion symmetry is broken and there is a finite energy gap $E_m$ between the singlet ground state and lowest triplet state. We discuss in this paper spin chains with frustrating $J_2 > 0$ and variable-range nonfrustrating exchange that narrow and eventually suppress the BOW phase.

Laflencie, Affleck and Berciu $^{10}$ studied chains with nonfrustrating exchange $J_r(\alpha) \approx (-1)^{r-1}/r^\alpha$ between spins $p$ and $p + r$. Power laws $\alpha < \alpha_c \approx 2$ leads to 1D models whose ground state has long-range order (LRO) while $\alpha > \alpha_c$ leads to a spin liquid with long-range spin correlations. There are exact field theory results $^{11}$ at $\alpha = 2$. Sandvik $^{12}$ combined frustrating second-neighbor exchange $g = J_2 > 0$ with variable-range $J_r(\alpha)$ in spin chains that are characterized by two parameters, frustration $g$ and exponent $\alpha$

$$H(g, \alpha) = H_1(\alpha) + gH_2. \quad (1)$$

$H_2$ is always a linear HAF with unit exchange between neighbors in sublattices A and B of even and odd numbered sites,

$$H_2 = H_A + H_B = \sum_p \vec{s}_p \cdot \vec{s}_{p+2}. \quad (2)$$

$H_1(\alpha)$ has nonfrustrating exchanges $J_r(\alpha)$ with normalization $\sum_r |J_r(\alpha)| = 1$,

$$H_1(\alpha) = \sum_{r=1}^{2n-1} J_r(\alpha) \sum_{p=1}^{4n} \vec{s}_p \cdot \vec{s}_{p+r} + J_{2n}(\alpha) \sum_{p=1}^{2n} \vec{s}_p \cdot \vec{s}_{p+2n} \quad (3)$$

in a chain of $N = 4n$ spins with periodic boundary conditions (PBC).
The $J_1 - J_2$ model sketched in Fig. 1 is the short-range (1/$\alpha = 0$) limit of $H(g, \alpha)$ with $J_r = \delta_{1r}$. Using exact diagonalization (ED) of finite systems, Sandvik \cite{12} constructed an approximate quantum phase diagram of $H(g, \alpha)$ in the $(g, 1/\alpha)$ plane: increasing $g$ leads to a first order transition for $\alpha < \alpha_c \approx 1.8$, a continuous transition for $\alpha > \alpha_c$. We also use ED and focus on systems with large frustration $g$ where we identify and characterize a decoupled phase for any $\alpha$. We compare our phase diagram in the $(g, 1/\alpha)$ plane with Sandvik’s in Section III.

All models $H(g, \alpha)$ conserve total spin $S$ and have inversion symmetry $\sigma$ at sites. The ground state is always a singlet, $S = 0$. Two excitations have special roles in the following: the magnetic gap $E_m(g, \alpha)$ to the lowest triplet state, $S = 1$, and the gap $E_\sigma(g, \alpha)$ to the lowest singlet with opposite inversion symmetry to the GS. In finite systems with fixed $\alpha$, the relation $E_\sigma(g, \alpha) = 0$ defines points $g$ at which the GS is doubly degenerate and states with broken inversion symmetry can readily be constructed. The BOW phase of extended systems has $E_\sigma(g, \alpha) = 0$ over some interval $[g^*, g^{**}]$. Since $E_m(g, \alpha)$ is known to open very slowly on entering a BOW phase \cite{8,13}, phase boundaries $g^*$ in finite systems have been inferred from level crossing, the excited-state degeneracy $E_m(g^{**}, \alpha) = E_\sigma(g^{**}, \alpha)$. For the $J_1 - J_2$ model, Okamoto and Nomura \cite{8} obtained $g^{**} = 0.2411$ for the BOW phase, also called the dimer phase \cite{2} or a valence bond solid (VBS) \cite{12}. The excited-state degeneracy \cite{14} leads in the $J_1 - J_2$ model to $g^{**} = 2.02(3)$ for the boundary of the decoupled phase that is the focus of this paper. We find narrower BOW phases when $H_1(\alpha)$ has exchange beyond $J_1$ but no LRO. In Section II we solve exactly a model with uniform exchange that undergoes a first order quantum transition to a decoupled phase at $g_c = 1/4n2$. Models $H(g, \alpha)$ with variable $\alpha$ allow a more complete characterization of systems with strong frustration.

We note that finite $g^{**}$ for the $J_1 - J_2$ model disagrees with the field theory of White and Affleck \cite{9} or of Itoi and Qin \cite{13}. Both start with small $g$ and infer finite $E_m$ for arbitrarily large $g$, albeit $E_m$ is exponentially small and has different $g$ dependence in the two treatments. At large frustration, it is natural to consider $H(g, \alpha)/g$ in Eq. 1 as an HAF on each sublattice. The $J_1 - J_2$ model in Fig. 1 then has nearest-neighbor $J_1 = 1/g$. Each spin $s_{2p}$ in sublattice A is coupled to two spins, $s_{2p+1}$ and $s_{2p-1}$, in sublattice B, and vice-versa. In the two-leg spin ladder, each spin in one leg (sublattice) is coupled to one spin in the other leg. Barnes et al. \cite{10} conclude that arbitrarily small $J_2 = 2/g$ at rungs opens a finite gap in two-leg ladders, just as does any dimerization $J_1 = (1 \pm \delta)$ along the chain \cite{4,17}. Either $\delta$ or $J_2$ leads to two spins per unit cell and breaks inversion symmetry at sites. We contrast in Section III the magnetic gaps $E_m$ of the $J_1 - J_2$ model and two-leg ladders.

In addition to the excitations $E_m(g, \alpha)$ and $E_\sigma(g, \alpha)$, we will focus on the GS expectation value of sublattice spin,

$$\langle S_A^2 \rangle = \langle S_B^2 \rangle = -4n \sum_{p=1}^{n} \langle \vec{s}_1 \cdot \vec{s}_2 \rangle$$

where we have used $S = 0$ and PBC. Correlation functions between spins in different sublattices are governed by $H_1(\alpha)$ at $g = 0$ and become vanishingly small at large $g$. Sublattice spin is an approximate or hidden symmetry since states with different $S_A, S_B$ are orthogonal. The GS is a linear combination of states centered on $\langle S_A^2 \rangle^{1/2}$ that shift to smaller $S_A$ with increasing frustration.

The paper is organized as follows. The model solved in Section II has uniform exchanges in $H_1$ and conserved $S_A$ and $S_B$. The GS has perfect LRO for $g < g_c(4n)$ that depends weakly on size and goes to $g_c(1/4n2)$ in the infinite chain. Increasing $g$ induces a first order transition to the decoupled phase that corresponds to non-interacting HAFs on sublattices. Accordingly, $E_\sigma$ and $E_m$ are directly related to HAF excitations. In Section III we present ED results for models $H(g, \alpha)$ that do not conserve $S_A$ or $S_B$. A first order transition to the decoupled phase is inferred for models with LRO at small frustration based on almost identical $\langle S_A^2 \rangle$, $E_\sigma$ and $E_m$ as in the uniform-exchange model. The BOW and decoupled phases of the $J_1 - J_2$ model are related to degeneracies of ground states at $E_\sigma = 0$ and of excited states at $E_\sigma = E_m$. The BOW/decoupled boundary of $H(g, \alpha)$ is estimated in the $(g, 1/\alpha)$ plane. The magnetic gap $E_m$ in the decoupled phase is contrasted to $E_m$ of the two-leg ladder using the density matrix renormalization group (DMRG). In Section IV we briefly discuss the decoupled phase.

II. FRUSTRATED CHAIN WITH UNIFORM EXCHANGE

In this Section, we solve a 1D model with $4n$ spins that conserves sublattice spins $S_A$ and $S_B$. Extensive results for finite and infinite linear HAFs are directly
applicable in this case. The $H_1$ part, Eq. 3 is taken to have uniform AF exchange $J_z = 2/(4n - 1)$ between spins in opposite sublattices, as in the Lieb-Mattis model \cite{18}, and also uniform exchange $-J_z$ between all spins on the same sublattice. The $(4n - 1)/2$ exchanges $|J_z|$ per site are normalized to unity. Uniform exchange makes it straightforward to express $H_1$ for $4n$ spins as

$$H_1(4n) = \frac{S^2 - 2S^2_S - 2S^2_B + 3n}{(4n - 1)}$$  \hspace{1cm} (5)

The integer ranges are $0 \leq S \leq 2n$, $0 \leq S_A, S_B \leq n$, and the index $\alpha$ has been omitted. The GS is evidently always in the $S = 0$ sector. In the absence of frustration, the GS is a linear combination of $2n + 1$ sublattice states with $S_A = S_B = n$ and $z$ components $M_B = -M_A$. The degeneracy of states with fixed $S, S_A$ and $S_B$ is lifted by $gH_2$ with frustrating $J_2 = g$. There are two $J_2$ contributions in Eq. 11 $g$ from $H_2$ and $-2/(4n - 1)$ from $H_1$. All eigenstates of the model are products of HAF eigenstates on sublattices. Increasing frustration generates energy shifts and numerous level crossings that can be followed explicitly.

We classify the HAF eigenvalues in Eq. 2 as $E_i(S_A, 2n) + E_j(S_B, 2n)$ where $i, j = 0, 1, 2, \ldots$ are eigenvalues with sublattice spins $S_A$ and $S_B$. The lowest energy $E_0(S, 2n)$ in each sector is sufficient. The singlet GS for $4n$ spins in the singlet sector $S_A = S_B$ has energy

$$E(0, S_A, g) = -\frac{4S_A(S_A + 1) - 3n}{4n - 1} + 2gE_0(S_A, 2n).$$  \hspace{1cm} (6)

There is perfect ferromagnetic order with $S_A = n$ at small $g$, where $E_0(n, 2n) = n/2$, and the GS transforms as $\sigma = 1$. The GS is doubly degenerate at $E(0, n, g) = E(0, n - 1, g)$: the GS in the sector with $S_A = S_B < n$ is odd under inversion. Repeating the argument shows that the GS for $S_A = n - m$ is even, odd under inversion for even, odd $m$. Since inversion symmetry changes $n$ times between $S_A = n$ and $S_A = 0$, the GS for $S_A = 0$ transforms as $\sigma = (-1)^n$ and corresponds to the product $|G\rangle|G\rangle$, the singlet GS of each sublattice.

We find $g_0(4n)$ at which the ordered state is degenerate with the GS in the sector $S = S_A < n$. The points are defined by $E(0, n, g) = E(0, S_A, g)$

$$g_0(4n) = \frac{1}{4n - 1} \left( 1 - \frac{S_A(S_A + 1)/(n(n + 1))}{\epsilon(S, 2n)/1} \right)$$  \hspace{1cm} (7)

where $\epsilon(S, 2n) = E_0(S, 2n)/2n$ is an energy per site and $S = 0, 1, 2, \ldots, n - 1$. ED for $2n$-spin HAFs yields exact $g_0(4n)$ in Table 1 up to $4n \approx 60$. Increasing $g$ leads directly from $S_A = n$ to $S_A = 1$ at $g_1(4n)$ and then to $S_A = 0$ at $g_0(4n)$. Exact results in Eq. 8 for the infinite chain place the first-order transition at

$$g_c = \frac{1}{4n^2}.$$  \hspace{1cm} (8)

TABLE I: Ground state degeneracies of the frustrated chain with $N = 4n$ spins and uniform exchange. The GS with $S_A = n$ and $S_A = 0$ or 1 are degenerate at $g_0(4n)$ or $g_1(4n)$, respectively; the GS at $S_A = 0$ and 1 are degenerate at $g_0(4n)$.

| $N = 4n$ | $g_0$ | $g_1$ | $g_{10}$ |
|----------|-------|-------|---------|
| 16       | 0.47189 | 0.46789 | 0.51020 |
| 20       | 0.45013 | 0.44710 | 0.49735 |
| 24       | 0.43544 | 0.43308 | 0.48873 |
| 28       | 0.42486 | 0.42299 | 0.48341 |
| 32       | 0.41689 | 0.41539 | 0.47756 |
| 36       | 0.41063 | 0.40944 | 0.47382 |
| 40       | 0.40570 | 0.40467 | 0.47058 |
| 400      | 0.36518 | 0.36510 | 0.44864 |
| $\infty$| 0.36067 | 0.36067 | 0.40528 |

The Bethe ansatz was used by Hulthen \cite{11} to find the GS energy per site of the extended HAF; it has more recently been applied to finite systems of $N = 4n$ spins. Woynarovich and Eckle\cite{12} found logarithmic corrections to the lowest energy per site in sector $S$. To leading order in $1/n$,

$$\epsilon(S, 2n) - \epsilon(0, 2n) = \frac{\pi^2 S^2}{8n^2} \left( 1 - \frac{1}{2n2n} \right).$$  \hspace{1cm} (9)

The $n = 100$ entries in Table I illustrate the convergence of $g_1(4n)$ and $g_0(4n)$. It follows from substituting Eq. 9 into Eq. 7 that the infinite chain also has $g_1 < g_0 < g_s$, $S \geq 2$.

The degeneracy $E(0, 1, g) = E(0, 0, g)$ between the GS in the singlet sector with $S_A = S_B = 1$ and 0 occurs at

$$g_{10}(4n) = \frac{4}{(4n - 1)\epsilon_{ST}(2n)}.$$  \hspace{1cm} (10)

The singlet-triplet gap, $\epsilon_{ST}(2n) = E_0(1, 2n) - E_0(0, 2n)$, appears frequently in the following. ED returns the $g_{10}$ entries in Table I to leading order for large systems, $\epsilon_{ST}$ is given by setting $S = 1$ and multiplying Eq. 9 by $2n$, and then substituting in Eq. 10

$$g_{10}(4n >> 1) = \frac{4}{\pi^2} \left( \frac{4n}{4n - 1} \right) \frac{1}{(1 - 1/2n2n)}.$$  \hspace{1cm} (11)

The absolute GS for $g > g_{10}(4n)$ is $E(0, 0, g)$ for chains of any length. The eigenstate $|G\rangle|G\rangle$ has $S_A = S_B = 0$, vanishing spin correlations between sublattices in Eq. 4 and hence no possibility of a BOW phase. The system of 400 spins in Table I shows slow convergence to $g_{10} = 4/\pi^2$.

The interval between $g_1(4n)$ and $g_{10}(4n)$ is not relevant in the context of the infinite chain, in which $|S_A^2| = n(n + 1)$ for arbitrarily large $n$ drops to $S_A^2 = 2$ at $g_c = 1/4n2n$ and vanishes for $g \geq g_{10} = 4/\pi^2$. The discontinuity at $g_c$ marks a first order transition to the
decoupled phase. Spin correlations between the sublattices vanish rigorously for \( g \geq 4/\pi^2 \). The degeneracy at \( g_{10}(4n) \) involves states of opposite inversion symmetry, as does degeneracy at \( g_1(4n) \) for even \( n \). For odd \( n \), however, the GS in the sectors \( S_A = n \) and \( 1 \) are both even under inversion. They are mixed and lead to an avoided crossing in finite models that do not conserve \( S_A \).

Next we find \( E_m(g) \) and \( E_\sigma(g) \), the excitation energy to the lowest triplet and the lowest singlet with reversed inversion symmetry. It follows from Eq. \( [5] \) that the lowest triplet for \( g < g_{10}(4n) \) is obtained by changing \( S \) from 0 to 1 without changing \( S_A \) or \( S_B \); hence \( E_m(g, 4n) = 2/(4n - 1) \) is constant, independent of \( g \) up to \( g_{10}(4n) \). When the GS energy is \( E(0, 0, g) \), the lowest triplet has \( S = 1, S_A + S_B = 1 \). It is doubly degenerate, \( |G\rangle|T\rangle \) or \(|T\rangle|G\rangle \) in obvious notation, with a triplet on either sublattice. The magnetic gap is \( E_m(g, 4n) = g\epsilon_{ST}(2n) - 2/(4n - 1) \quad g \geq g_{10}(4n) \).

The second term is the contribution from Eq. \( [5] \)

The lowest singlet excitation for \( g > g_1(4n) \) is
\[
E_\sigma(g, 4n) = \left| E_0(0, 1, g) - E_0(0, 0, g) \right| = \left| 2g\epsilon_{ST}(2n) - \frac{8}{(4n-1)} \right|. \tag{13}
\]
The excitations \( E_m(g) \) in Eq. \( [12] \) and \( E_\sigma(g) \) in Eq. \( [13] \) are equal at \( g = 3g_{10}(4n)/2 \). It is instructive to rewrite the excitations using Eq. \( [10] \)

\[
E_m(g, 4n) = \frac{4}{4n-1} \left( g - \frac{1}{g_{10}(4n)} \right) \quad g \geq g_{10}(4n)
\]

\[
E_\sigma(g, 4n) = \frac{8}{4n-1} \left| \frac{g}{g_{10}(4n)} - 1 \right| \quad g \geq g_1(4n). \tag{14}
\]
The V-shaped dependence of \( E_\sigma(g, 4n) \) on either side of \( g_{10} \) is evident, as are the related slopes with increasing \( g \). These features are used in Section III to interpret \( E_m \) and \( E_\sigma \) in models that do not conserve \( S_A \). It is still convenient to refer to products of \( |G\rangle \) or \(|T\rangle \). Although no longer exact \( 1/g = 0 \) eigenstates, the actual eigenstates can be expanded in terms of sublattice eigenstates.

We conclude the discussion of the uniform exchange model by noting that the infinite chain has a first order quantum transition at modest frustration \( g_c = 1/4n2 \). The GS has perfect LRO up to \( g_c \). The decoupled phase has \( S_A = S_B = 1 \) in the interval \( g_c < g < g_{10} = 4/\pi^2 \) and \( S_A = S_B = 0 \) for \( g > g_{10} \) when all spin correlation functions in Eq. \( [4] \) are zero. The infinite chain has \( E_m(g) = 0 \) for all \( g \geq 0 \).

### III. FRUSTRATED CHAINS WITH VARIABLE RANGE EXCHANGE

We present ED results for models \( H(g, \alpha) \) that do not conserve sublattice spin. The GS is degenerate under inversion at frustration \( g_j \) where \( E_\sigma(g_j, 4n) = 0 \). It is convenient to retain the labeling \( g_{s}(4n) \) and \( g_{10}(4n) \) in Eqs. \( [7] \) and \( [11] \) used for the model with uniform exchange.

We start with a model with LRO at \( g = 0 \) and a first order transition to the decoupled phase that closely resembles the uniform model. Next we consider the \( J_1 - J_2 \) model without LRO at \( g = 0 \) and continuous transitions with increasing \( g \) from spin liquid to BOW to decoupled phase. We then consider intermediate \( \alpha \) to construct an approximate the GS phase diagram in the \( (g, 1/\alpha) \) plane.

#### A. Model with LRO

The Hamiltonian \( H(g, \alpha) \) in Eq. \( [11] \) has nonfrustrating exchanges in Eq. \( [5] \). It differs from the model studied by Sandvik only in the \( J_{2n} \) terms, which are double counted in Eq. \( [1] \) of ref. \( [12] \). Since \( J_{2n} \) contributions decrease with size \( n \) or increasing exponent \( \alpha \), numerical difference due to double counting are limited to small \( n \) and \( \alpha \). The normalization condition \( \sum_r |J_r| = 1 \) leads to

\[
J_{r \neq 2}(\alpha) = \left( \frac{-1}{\alpha} \right) \left( 1 + \frac{1}{2} \frac{1}{2n} \right)^{\alpha} + \sum_{s=3}^{2n-1} \frac{1}{s!} \right)^{-1}. \tag{15}
\]

Since frustrating \( J_2 = g \) is entirely in \( gH_2 \), the model with \( \alpha = 0 \) and finite \( n \) in Eq. \( [15] \) is slightly different from the model with uniform exchange.

The following results are for \( \alpha = 1 \), a model with \( [10] \) LRO at \( g = 0 \). Excitation energies \( E_m(g) \) and \( E_\sigma(g) \) are shown in Fig. \( [2] \) as a function of \( g \) for \( 4n = 24 \) sites (top panel) and 20 sites (bottom panel). As anticipated for LRO systems with a first order transition, we have \( E_\sigma(g) = 0 \) at two points \( g_1 \) and \( g_0 \) when \( n \) is even and one point \( g_{10} \) when \( n \) is odd. Inversion symmetry at sites reverses twice for 24 sites, once for 20 sites. The first order transition is at \( g_1 = 0.404 \) for 24 spins and the avoided crossing is at \( g = 0.411 \) for 20 spins. The degeneracy at \( g_{10} \) corresponds to changing from \( S_A = 1 \) to 0 in the model with uniform exchange. The GS in the \( \sigma = 1 \) and \( -1 \) sectors cross at \( g_{10} \) for \( 4n = 20 \), in contrast to the avoided crossing in Fig. \( [2] \) of ref. \( [12] \) for the \( \alpha = 1 \) model with \( [20] 4n = 28 \).

The separation \( g_{10} - g_1 = 0.065 \) for the \( \alpha = 1 \) model is comparable to \( g_{10}(24) - g_1(24) = 0.056 \) in Table\( \[1 \] \) for uniform exchange. In accord with Eq. \( [12] \) for uniform exchange, \( E_m(g) \) is almost constant up to \( g_1 \); it is doubly degenerate for \( g \geq g_{10} \) and linear with increasing \( g \). The slopes \( dE_m/dg \) are within 1\% of \( \epsilon_{ST}(12) = 0.356 \) for 24 sites and \( \epsilon_{ST}(10) = 0.423 \) for 20 sites. Likewise for the lowest singlet excitation, \( |T\rangle\langle T| \), the slope of \( E_\sigma(g) \) between \( g_{10}(4n) \) and \( 2g_{10}(4n) \) is slightly larger than
sublattice. The ground state is doubly degenerate at \( g_{10} \) where \( E_\sigma(g_{10}) = 0 \) and at \( E_\sigma(g) \) for 24 spins. As expected, \( \rho_p \) is constant on each sublattice, slightly less than \( 1/2n \) on one and slightly positive on the other. The deviations from Eq. (17) are less 0.1% at \( g = 1 \), less than 0.01% at \( g = 2 \). The

\[ J_1 - J_2 \] model. Somewhat larger systems are accessible in principle with current computational resources.

The \( \alpha = 1 \) model has almost perfect LRO at \( g = 0 \), \( s_A(0, 4n) = 0.486 \), in agreement with larger systems studied in ref. [10] using multiple methods. As anticipated in Section II, \( s_A(g, 4n) \) is discontinuous when \( E_\sigma(g) = 0 \) and changes rapidly but continuously for 20 spins at the avoided crossing. The size dependence of \( s_A(g_{10}, 4n) \) shown in Fig. 3 is consistent with a discontinuity at \( g_1 \) in the infinite system and \( s_A(g_{10}) \approx 0 \) for \( g > g_{10} \). Both results can be understood in terms of a GS with LRO at small \( g \) and a first order transition to the decoupled phase.

All properties of frustrated spin chains of \( 4n \) spins are given at \( 1/g = 0 \) by exact HAF eigenstates for \( 2n \) spins. The triplet \( |T\rangle \) with \( S^2 = 1 \) and energy \( E_0(1, 2n) \) has equal spin density \( \rho_p = s_z = 1/2n \) at all sites. The spin density at site \( p \) of the degenerate triplets \( |G\rangle|T\rangle \) and \( |T\rangle|G\rangle \) at \( 1/g = 0 \) is

\[ \rho_p(4n) = \frac{1}{4n}(1 \pm (-1)^p). \]  

The plus sign corresponds to a triplet on the sublattice of even-numbered sites and \( \rho_p = 0 \) for odd \( p \); the minus sign has the triplet on the odd-numbered sublattice. The \( \alpha = 1 \) spin densities at \( g_{10} \) are shown in the top panel of Fig. 3 for 24 spins. As expected, \( \rho_p \) is constant on each sublattice, slightly less than \( 1/2n \) on one and slightly positive on the other. The deviations from Eq. (17) are less 0.1% at \( g = 1 \), less than 0.01% at \( g = 2 \). The

\[ 2\epsilon_{ST}(2n) \] in either case, \( dE_\sigma/dg = 0.741 \) for 24 sites and 0.884 for 20 sites.

We define \( s_A(g, 4n) \leq 1/2 \) to quantify sublattice spin as the GS expectation value

\[ s_A(g, 4n) = \langle S_A^2 \rangle^{1/2} / (4n(n + 1))^{1/2}. \]  

\( s_A(g, 4n) \) decreases with frustration and is double-valued at \( E_\sigma(g_j) = 0 \). Figure 3 shows \( s_A(g, 4n) \) with increasing \( g \) for 20 and 24 sites. Dotted lines for \( g > g_{10}(4n) \) refer to the excited state \( |T\rangle|T\rangle \). The \( s_A(g_{10}, 4n) \) values in Table I at modest frustration \( g \approx 0.5 \) are already close to \( 1/[2n(n + 1)]^{1/2} \), the exact result at \( 1/g = 0 \). The \( \sigma = 1 \) eigenstates near the transition contain small admixtures of sublattice spin. The \( \alpha = 1 \) model requires matrix elements for all \( J_r \) in Eq. (3) \( r = 1, 2, \ldots, 2n \) that make it tedious to evaluate \( \langle S_A^2 \rangle \). The results in Table I go to 24 spins for the \( \alpha = 1 \) model and to 28 spins for the

![FIG. 2: Excitation energies \( E_m \) and \( E_\sigma \) as functions of frustration \( g \) in models with exchanges with \( \alpha = 1 \) in Eq. (13) and 4n = 24 or 20 spins; \( E_m \) is to the lowest triplet, \( E_\sigma \) to the lowest singlet with reversed inversion symmetry. The ground state is doubly degenerate at \( g_{10} \) where \( E_\sigma(g_{10}) = 0 \) and at \( E_\sigma(g) \) for 24 spins. For \( g > g_{10} \), the triplet is doubly degenerate and the excited singlet is \( ^1T\rangle|T\rangle \), a triplet on each sublattice.

![FIG. 3: Solid lines: Ground state expectation value \( s_A(g, 4n) \) in Eq. (13) with increasing frustration \( g \) in models with 20 and 24 spins and exchanges \( \alpha = 1 \) in Eq. (13) Dotted lines for \( g \geq g_{10} \) are \( s_A(g, 4n) \) for the excited singlet \( ^1T\rangle|T\rangle \).]
neighbors, and the infinite chain has

Spin correlation functions are now limited to nearest

the exact GS is known for any even number of spins.

is of order 4

FIG. 4: Spin density $\rho_p$ at site $p$ in the lowest triplet of 24 spin
chains at frustration $g_{10}$, the largest $g$ at which the ground
state is degenerate. The upper panel has exchanges $\alpha = 1$ in
Eq. 15 (top); the lower panel is the $J_1 - J_2$ model.

decoupled phase found rigorously for uniform exchange
readily accounts for the $\alpha = 1$ model.

B. $J_1 - J_2$ model

The linear HAF with $J_1$ between nearest neighbors
and frustration $g = J_2/J_1$ is a prototypical model with
a BOW phase \footnote{\bibitem{Okamoto} Okamoto and Nomura
placed the continuous transition to the BOW phase at
g* = 0.2411 by extrapolation of the excited state degeneracy $E_\sigma(g, 4n) = E_m(g, 4n)$ up to $4n = 24$ spins. The GS
is nondegenerate for $g < g^*$. There is no LRO at $g = 0$ but
there are long-range spin correlation functions that
go as $10$.

$$\langle \hat{s}_0, \hat{s}_p \rangle = \frac{(-1)^p \sqrt{\ln p}}{p}.$$  \hspace{1cm} (18)

The exact values \footnote{\bibitem{Dagotto} Dagotto et al.,
Phys. Rev. Lett. 57, 2510 (1986).} of $\langle \hat{s}_0, \hat{s}_1 \rangle$ and $\langle \hat{s}_0, \hat{s}_3 \rangle$ are
$1/4 - \ln 2 = -0.443147...$ and $-0.15074...$, respectively,
and all correlations between spins in opposite sublattices
are negative. It follows that $\langle S^z_A \rangle$ for $4n$ spins in Eq. 11
is of order $4nhn4n$ at $g = 0$.

The $J_1 - J_2$ model has multiple GS degeneracies
\footnote{\bibitem{SSH} Su, Schrieffer, and Heeger, Phys. Rev. B
20, 3361 (1979).} $E_\sigma(g, 4n) = 0$ with increasing $g$. The first one at
$g_{MG} = 1/2$ is the Majumdar-Ghosh point \footnote{\bibitem{Okamoto} Okamoto and Nomura,
Phys. Rev. B 24, 4038 (1981).} where the exact GS is known for any even number of spins.
Spin correlation functions are now limited to nearest
neighbors, and the infinite chain has $\langle S^z_A \rangle = 3n/2$, or
$3/8$ per site. In contrast to the transition from $S_A = n$
to $S_A = 1$ in models with LRO at $g = 0$, the symmetry
changes at $g_j(4n), j = n, n-1, ...$, occur sequentially
with increasing $g$ up to $28$ spins, the largest $4n$ system we
solved. The upper panel of Fig. 3 shows $E_\sigma(g, 24)$ and
$E_m(g, 24)$ as a function of frustration, with six arrows
at $g_j(24)$. The magnitude of $E_\sigma(g, 4n)$ is remarkably
small between $g \approx 0.45$ and $\approx 1.2$. A finer energy scale
is needed to see $E_\sigma$ in the BOW phase. The lower panel
shows $E_\sigma$ and $E_m$ for $4n = 20$ spins, with five arrows at
$g_j(20)$. The behavior at large frustration is qualitatively
similar to the $\alpha = 1$ model in Fig. 2. The triplet is
doubly degenerate for $g > g_{10}$. The slopes $dE_m/dg$ and
$dE_\sigma/dg$ are within 5% and 8% of $\epsilon_{ST}(2n) and 2\epsilon_{ST}(2n)$, respectively, between $g_{10}(4n)$ and $g = 2$.

We find that the relation $E_\sigma(g, \alpha) = 0$ is not limited to
finite $J_1 - J_2$ models. On the contrary, Sandvik \footnote{\bibitem{Sandvik} Sandvik,
Phys. Rev. B 39, 12 630 (1989).} states that the degeneracy is not exact except in the $J_1 - J_2$
model at the special point $g_{MG} = 1/2$. The discrepancy
is not due to ED but to motivation. ED is necessarily
performed at fixed values of $g$ that are typically on a grid.
The GS symmetry changes in calculations that keep track
of inversion at sites. It is then natural to search for the
exact $(g, \alpha)$ at which the GS is degenerate by choosing
$g$ more precisely. The lowest two singlets are both even
under inversion at the center of bonds, which suggests an
avoided crossing and less reason for refining $g$ in search
of exact degeneracy. The symmetry operators of course commute with $H(g, \alpha)$ but not with each other. Hence
inversion symmetry at sites or at bonds leads to different
linear combinations of degenerate eigenstates.

Degenerate GS at $g_{MG}$ are products of singlet-paired
spins on successive sites, either $\ket{K_1} = \ket{1, 2}(3, 4)\cdots(2n - 1, 2n)$ or $\ket{K2} = \ket{2, 3}(4, 5)\cdots(2n, 1)$. Such states are
the familiar Kekulé diagrams of organic chemistry or the de-
egenerate GS of polyacetylene in the Su-Schrieffer-Heeger
(SSH) model \footnote{\bibitem{Su} Su, Schrieffer, and Heeger, Phys. Rev. B
20, 3361 (1979).} (SSH) model \footnote{\bibitem{Okamoto} Okamoto and Nomura,
Phys. Rev. B 24, 4038 (1981).}. The gap $\epsilon_{ST}$ that opens at $g^*$ is rigor-
ously known \footnote{\bibitem{Okamoto} Okamoto and Nomura,
Phys. Rev. B 24, 4038 (1981).} to be finite in the infinite chain at $g_{MG}$.
It is already large \footnote{\bibitem{Okamoto} Okamoto and Nomura,
Phys. Rev. B 24, 4038 (1981).} at $g_{10}(4n) = g_{MG}$ and remains large
up to $g_{10}(4n)$, clearly exceeding finite-size effects in Fig. 5.
The elementary excitations of the BOW phase are
topological spin solitons \footnote{\bibitem{Okamoto} Okamoto and Nomura,
Phys. Rev. B 24, 4038 (1981).} or domain walls generated by
spin correlations that closely resemble \footnote{\bibitem{Okamoto} Okamoto and Nomura,
Phys. Rev. B 24, 4038 (1981).} SSH soli-
tons generated by electron-phonon coupling. The BOW
phase extends beyond $g_{10}(4n)$ in Fig. 5 by the GS
degeneracy at the largest frustration. We suppose that the BOW
phase terminates at $g^{**} \approx 2.02(3)$ at the excited-state
degeneracy \footnote{\bibitem{Okamoto} Okamoto and Nomura,
Phys. Rev. B 24, 4038 (1981).} $E_\sigma = E_m$. As discussed below, finite-size
effects are larger at $g^{**}$ than at $g^*$.

The evolution of $s_A(g, 4n)$ with increasing frustration
is shown in Fig. 6 for 20 and 24 spins; $s_A(g, 4n)$ for the
excited state $\ket{T}^\dagger \ket{T}$ is the dotted line for $g > g_{10}(4n)$.
As expected, $s_A(g, 4n)$ decreases with increasing $g$ and is
discontinuous when the GS is degenerate. Table \footnote{\bibitem{Okamoto} Okamoto and Nomura,
Phys. Rev. B 24, 4038 (1981).} lists both values of $s_A(g_{10}, 4n)$. The excited state at $g_{10}$ is
already within 5% of the $1/g = 0$ limit. The $J_1 - J_2$ model has stronger but still modest mixing of $1/g = 0$ states at $g_{10}$ than the $\alpha = 1$ model. The $J_1 - J_2$ spin densities of the degenerate triplets at $g_{10}$ in Fig. 3 again follow Eq. (17) with $\rho_p$ slightly less than $1/2n$ on one sublattice and slightly positive on the other. The spin densities at $g = 2$ are $\rho_p = 0.082$ and 0.002. At $g_{MG} = 1/2$, the overlap of the VB diagrams for $4n$ spins is $\langle K1|K2 \rangle = 2^{-(2n-1)}$. Aside from finite-size effects that are already less than 1% at $4n = 20$, we obtain

$$s_A(1/2, 4n) = \left( \frac{3}{8n+1} \right)^{1/2}.$$  \hspace{1cm} (19)

The infinite chain has continuous $s_A(g)$ over the entire range $g \geq 0$.

C. Quantum phase diagram

Models with $\alpha = 2$, 3 and 4 have nonfrustrating exchange intermediate between $\alpha = 1$ and $1/\alpha = 0$. We find the GS degeneracies $g_m(4n)$ where $E_m = 0$ and the excited state degeneracies $g^*$ and $g^{**}$ where $E_\sigma = E_m$ that delimit the BOW phase. These points are used to construct an approximate quantum phase diagram in the $(g, 1/\alpha)$ plane.

Fig. 7 shows the phase diagram of $H(g, \alpha)$ for $\alpha = 0$ to 4 and the $J_1 - J_2$ model $(1/\alpha = 0)$ over the entire range of frustration $g \geq 0$. The diagrams for 24 and 20 spins illustrate the modest size dependence and differences between $4n$ with even and odd $n$. Open points indicate GS degeneracy $g_m$; closed points are $g^*$ and $g^{**}$; solid lines mark first order transitions at $g_1$ for 24 spins and the avoided crossing for 20 spins; dashed lines are the boundary between the BOW and decoupled phases at large $g$ and between the spin liquid and BOW phase at small $g$. The BOW phase terminates at a multicritical point, and the dotted line separates spin liquids from models with LRO. The BOW phase for $\alpha = 4$ closely resembles the $J_1 - J_2$ model, as might be expected since largest change is small, $J_3/J_1 = 1/16$. The width of the BOW phase, $g^{**} - g^*$, narrows for $\alpha = 3$ or 2 and $E_\sigma = 0$ is satisfied at fewer than $n$ points. The $\alpha = 1$ model has a first order transition and no BOW phase.

Sandvik [12] used additional values of $\alpha$ to estimate the multicritical point as $\alpha_c \approx 1.8$, $g_c \approx 0.41$. We have not varied $\alpha$ and took $\alpha_c = 1.8$ in Fig. 7, it will be challenging to be more accurate as long as ED is limited to about 30 spins. Our phase diagram in Fig. 7 is quite similar at small frustration to Fig. 4 of ref. [12] with VBS instead of BOW, AFM instead of LRO and QLRD($\pi$) instead of spin liquid. So far there is no consensus for naming phases. There are clear differences at large $g$, however. The VBS or BOW phase in Fig. 1 of ref. [12] does not terminate at either large $g$ or at small $\alpha$ and the line at large $g$ between VBS and VBS+QLRD($\pi/2$) separates phases with different $\alpha$. A BOW phase is rigorously excluded at $\alpha = 0$, the analytical model with a first order transition to the
decoupled phase.

We have given reasons for extending the decoupled phase in Fig. 7 to first order LRO/decoupled transitions and to continuous BOW/decoupled transitions without any distinction for different $\alpha$. The sublattices of $H(g, \alpha)$ have weak interactions at large $g$. The coupling is weak even in the $J_1 - J_2$ model and $s_\perp(g, 4n)$ becomes arbitrarily small at large $g$. By continuity, we expect the same phase to be reached at $1/g << 1$ for any choice of $H(g, \alpha)$. The decoupled phase starts at the first order transition in systems with LRO at $g = 0$ and at $g^{**}$ in systems with a BOW phase and continuous transitions.

D. Magnetic gap

Density matrix renormalization group (DMRG) has been extensively applied to 1D spin systems $[9, 25–28]$. DMRG with open boundary conditions (OBC) breaks inversion symmetry at sites at the outset: an even number of spins is required for a singlet GS and even chains have inversion symmetry at the center of the central bond. As shown explicitly for a half-filled band of free electrons $[27]$, OBC generates $1/N$ corrections to the bond order of the central bond. OBC strongly breaks the GS degeneracies of the $J_1 - J_2$ model at $g_{J_1 - J_2}$.

At these points, the lowest singlet excitation for 16, 20 or 24 spins is slightly higher than $E_m$, thus reversing the order of excitations in addition to lifting the degeneracy.

It is convenient to study $H(g, \alpha)/g$ in Eq. 4 for $1/g \ll 1$. Then $H_2$ has decoupled HAFs on the sublattices for models with any exponent $\alpha$. In particular, the frustrated $J_1 - J_2$ model has $N$ exchanges $J_1 = 1/g$ between spins at adjacent sites $p, p + 1$ in Fig. 1 while the non-frustrated two-leg ladder has $N/2$ exchanges $J_\perp = 2/g$ between sites $2p - 1, 2p$. The $J_1 - J_2$ model has one spin per unit cell and inversion symmetry at both sites and centers of bonds. The two-leg ladder with $J_\perp > 0$ has two spins per unit cell and inversion only at bond centers.

DMRG results for $E_m$ are compared in Fig. 8 for $J_1 - J_2$ models and two-leg ladders, and are seen to be qualitatively different. The ladder has large $E_m = 0.49$ at $g = 2$ that decreases to $E_m = 0.20$ at $g = 4$. Finite $E_m$ is expected $[10]$ for finite $J_\perp$, nearly linear in small $J_\perp$, just as for finite dimerization $[4, 17]$ in chains with alternating $J_1 = (1 + \delta)$ and $J_2 = 0$. The $J_1 - J_2$ model returns $E_m \approx 0.03$ at $g = 2$, close to the BOW/decoupled boundary $g^{**}$, and $E_m < 0.01$ at $g = 3$ or 4, the limit $[27]$ of accuracy for DMRG with four spins added per step. Large $g$ in Fig. 8 brings out the contrasting behavior of $E_m$. While an exponentially small $E_m$ cannot be ruled out in the $J_1 - J_2$ model, DMRG is consistent with $E_m \approx 0$ in the decoupled phase and suggests that $g^{**}$ is slightly larger than 2.0, the value estimated from extrapolation of $E_m = E_\sigma$.

FIG. 7: Quantum phase diagram of $H(g, \alpha)$ in Eq. 1 in the $1/\alpha, g$ plane for chains of 20 and 24 spins; $g > 0$ is frustration and $\alpha$ in Eq. 13 specifies the nonfrustrating exchanges. Open points and solid points indicate ground-state degeneracy $E_\sigma = 0$ and excited state degeneracy, $E_m = E_\sigma$, respectively. Dashed lines are approximate boundaries of the BOW phase. Solid lines are approximate boundaries of the decoupled phase in models with LRO at $g = 0$; the dotted line separates models with long-range fluctuations and order at small frustration $[12]$.

FIG. 8: DMRG results the magnetic gap $E_m$ of $N = 4n$ spins for $J_1 - J_2$ models with $J_1 = 1/g, J_\perp = 1$ in Eq. 4 and for two-leg ladders with $J_\perp = 2/g$ at every rung.
The relation $E_\alpha = E_m$ for the BOW/decoupled boundary $g^{**}$ is less accurate due to finite size effects. Models with $2n$ spins are used to obtain $g^*(2n)$, which is then extrapolated; models of $4n$ spins are needed for $g^{**}(4n)$ in order to decouple to HAFs with an even number of spins rather than two radicals with $S = 1/2$ ground states. Even for large $N$, weak coupling between open shell radicals with degenerate GS is quite different from weak coupling of closed shell systems with nondegenerate GS. Indeed, Fadeev and Takhtajan [29] have pointed out that the HAF with odd $N$ and states with half-integer $S$ has unexpected and unexplored features. Different approaches are required for $1/g \ll 1$, including field theories designed for weakly coupled HAFs.

**IV. DISCUSSION**

The defining features of BOW phases are a doubly degenerate GS, broken inversion symmetry at sites and finite magnetic gap $E_m$ that opens slowly at a Kosterlitz-Thouless transition. The elementary excitations in spin chains are $s = 1/2$ solitons centered on sites in opposite sublattices. The frustrated spin chains $H(g, \alpha)$ in Eq. [I] do not meet these signatures at large $g$. To be sure, we cannot discriminate between exponentially small and zero $E_m$. But the energy spectrum at $1/g = 0$ is just the HAF spectrum. The GS is not degenerate at $1/g = 0$ and it is unlikely that arbitrarily small $1/g$ will place $1/|T|/|T|$ below $E_m$. Yet that is minimally required for GS degeneracy at any $1/g > 0$. Conversely, the lowest triplet state at small $g$ is not degenerate while the lowest triplet at large $g$ is doubly degenerate, $|T\rangle|G\rangle$ or $|G\rangle|T\rangle$ with both unpaired spins largely confined to one sublattice.

The principal goal of the present study is the identification of a decoupled phase at large frustration $g$ that is distinct from the BOW phase of the $J_1 - J_2$ model at intermediate $g$. GS is not degenerate in the decoupled phase; inversion symmetry is not broken; the lowest triplet is doubly degenerate. The magnetic gap $E_m$ is zero within numerical accuracy for $g > g^{**}$ and strictly so in the model with uniform exchange. The properties of the decoupled phase at $g > g_0$ in Table II or in Figs. [2-6] are already close to the $1/g = 0$ limit of decoupled HAFs on sublattices.

BOW phases occur in spin chains [7, 8, 14] with frustrated exchange or in half-filled 1D Hubbard models nearest-neighbor [13] or long-range [30] Coulomb interactions. Moderate interactions are required to avoid a first order transition that for $H(g, \alpha)$ is related to LRO at $g = 0$. Models without LRO have continuous transitions from spin liquid to BOW to decoupled at $g^{**}(\alpha)$ and $g^{**}(\alpha)$, respectively. As shown in Fig. [7] all spin chains have a decoupled phase at large $g$. By contrast, Sandvik’s phase diagram [12] at large $g$ distinguishes between models with and without LRO and does not terminate the BOW phase.

Frustration ensures the existence of the correlated phases with variable sublattice spin $(S^2_A)$. The model with uniform exchange has a first order transition at $g_c = 1/4n^2$ from $S^2_A = n(n+1)$ to $S^2_A = 2$. The divergence of $(S^2_A)/4n$ is linear or logarithmic, respectively, at $g = 0$ in spin chains with and without LRO. The $\alpha = 1$ model has a first order transition from a GS with LRO to the decoupled phase. The $J_1 - J_2$ model has $(S^2_A)/3n/2$ at $g_{MC} = 1/2$ in the BOW phase and continuous transitions to a spin liquid phase $g < g^*$ and the decoupled phase at $g > g^{**}$. The BOW phase narrows in models with intermediate $\alpha$ and terminates for $\alpha < \alpha_c \approx 1.8$. Accurate phase boundaries pose major challenges for all models and especially for systems with continuous transitions and a BOW phase.

**Acknowledgments:** ZGS thanks A.W. Sandvik for a stimulating discussion of spin chains. We thank the National Science Foundation for partial support of this work through the Princeton MRSEC (DMR-0819860). MK thanks DST India for partial financial support of this work.

[1] H. Bethe, Z. Phys. 71, 205 (1931); L. Hulthen, Ark. Mat., Astron. Fys. 26A, 11 (1938).
[2] M. Takahashi, Thermodynamics of One-Dimensional Solvable Models, (Cambridge University Press, Cambridge, 1999).
[3] I. Affleck, T. Kennedy, E.H. Lieb and H. Tasaki, Commun. Math. Phys. 115, 477 (1988).
[4] D. C. Johnston, R. K. Kremer, M. Troyer, X. Wang, A. Klumper, S. L. Budko, A. F. Panchula, and P. C. Canfield, Phys. Rev. B 61, 9558 (2000).
[5] M. Hase, H. Kuroe, K. Ozawa, O. Suzuki, H. Kitazawa, G. Kido, and T. Sekine, Phys. Rev. B 70, 104426 (2004); H. Kikuchi, H. Nagasawa, Y. Ajiro, T. Asano, and T. Goto, Physica B 284, 1631 (2000); N. Maeshima, M. Hagiwara, Y. Narumi, K. Kindo, T. C. Kobayashi, and K. Okunishi, J. Phys.: Condens. Matter 15, 3607 (2003).
[6] S.-L. Drechsler et al., Phys. Rev. Lett. 98, 077202 (2007); S. Park, Y.J. Choi, C.L. Zhang, and S-W. Cheong, Phys. Rev. Lett. 98, 057601 (2007); S. E. Dutton, M. Kumar, M. Mourigal, Z. G. Soos, J.J. Wen, C. L. Broholm, N. H. Andersen, Q. Huang, M. Zbir, R. Toft-Petersen, and R. J. Cava, Phys. Rev. Lett. 108, 187206 (2012).
[7] K. Okamoto and K. Nomura, Phys. Lett. A 169, 433 (1992).
[8] I. Affleck, D. Gepner, H. J. Schultz, and T. Ziman, J. Phys. A 22, 511 (1989); F. D. M. Haldane, Phys. Rev. B
[9] S. R. White and I. Affleck, Phys. Rev. B 54, 9862 (1996).
[10] N. Laflorencie, I. Affleck, and M. Berciu, J. Stat. Mech. P12001 (2005).
[11] F. D. M. Haldane, Phys. Rev. Lett. 60, 635 (1988); B.S. Shastry, Phys. Rev. Lett. 60, 639 (1988).
[12] A. W. Sandvik, Phys. Rev. Lett. 104, 137204 (2010).
[13] M. Nakamura, Phys. Rev. B 61, 16377 (2000); J. Phys. Soc. Jpn. 68, 3123 (1999).
[14] M. Kumar, S. Ramasesha, and Z. G. Soos, Phys. Rev. B 81, 054413 (2010).
[15] C. Itoi and S. Qin, Phys. Rev. B 63, 224423 (2001).
[16] T. Barnes, E. Dagotto, J. Riera, and E. S. Swanson, Phys. Rev. B 47, 3196 (1993).
[17] Z. G. Soos, S. Kuwajima, and J. E. Mihalick, Phys. Rev. B 32, 3124 (1985); M. Kumar, S. Ramasesha, D. Sen and Z.G. Soos, Phys. Rev. B 75, 052404 (2007).
[18] E. Lieb and D. Mattis, J. Math. Phys. 3, 749 (1962).
[19] F. Woynarovich and H-P. Eckle, J. Phys A: Math. Gen. 20, L97 (1987).
[20] A. W. Sandvik, private communication; Fig. 2 is for $N = 28$ rather than $N = 16$ in the caption; inversion $\sigma$ at the center of bonds was used and since the lowest two singlets transform at $\sigma = 1$, the GS touch but do not cross.
[21] M. Shiroishi and M. Takahashi, J. Phys. Soc. Jpn. 74, Suppl. p. 47, (2005).
[22] C. K. Majumdar and D. K. Ghosh, J. Math. Phys. 10, 1399 (1969).
[23] W. P. Su, J. R. Schrieffer, and A. J. Heeger, Phys. Rev. Lett. 42, 1698 (1979); Phys. Rev. B 22, 2099 (1980).
[24] B. S. Shastry and B. Sutherland, Phys. Rev. Lett 47, 964 (1981).
[25] S. R. White, Phys. Rev. Lett. 69, 2863 (1992); S.R. White, Phys. Rev. B 48, 10345 (1993).
[26] R. Chitra, S. Pati, H. R. Krishnamurthy, D. Sen, and S. Ramasesha, Phys. Rev. B 52, 6581 (1995).
[27] M. Kumar, Z. G. Soos, D. Sen and S. Ramasesha, Phys. Rev. B 81, 104406 (2010).
[28] U. Schollwöck Rev. Mod. Phys. 77, 259 (2005); J. Ren and J. Sirker Phys. Rev. B 85, 140410(R); R. Bursill, G. A. Gehring, D. J. J. Farnell, J. B. Parkinson, T. Xiang and C. Zeng, J. Phys. Condens. Matter 7, 8605 (1995); T. Hikihara, L. Kecke, T. Momoi, and A. Furusaki Phys. Rev. B 78, 144404 (2008); K. A. Hallberg, Advances in Physics, 55, 477, (2006).
[29] L. D. Faddeev and L. A. Takhtajan, Phys. Lett. 85A, 375 (1981).
[30] M. Kumar, S. Ramasesha, and Z. G. Soos Phys. Rev. B 79, 035102 (2009).