Frustrated Spin-Peierls Chains

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Abstract

We study the phase diagram, ground state properties, and excitation gaps of a frustrated spin-Peierls chain, i.e. a spin-Peierls chain with both nearest neighbor exchange $J_1$ and next nearest neighbor exchange $J_2$. The phase diagram is calculated using a bosonization Renormalization-Group (RG) method. We propose a (bosonic) bond-operator mean field approximation to calculate the ground state properties and excitation gaps.

I. INTRODUCTION

A theoretical understanding of the frustrated spin-Peierls chains (i.e. frustrated $J_1 - J_2$ Heisenberg chains with spin-lattice interaction) is important for a number of reasons: First, there are a number of quasi-one-dimensional systems which can be described by a spin-Peierls model at low temperatures, and in some of these systems, such as $CuGeO_3$ materials and some MX materials, the competition between nearest neighbor $J_1$ and next nearest neighbor $J_2$ plays an important role. Second, the frustrated spin-Peierls model poses interesting theoretical problems. The frustrated $J_1 - J_2$ Heisenberg model has been studied in the literature. Majumdar showed that at $J_2/J_1 = 1/2$ the ground state is dimerized and the exact ground state wave function is

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\[\Psi_1 = [1, 2][3, 4] \cdots [2N - 1, 2N]\]
\[\Psi_2 = [2N, 1][2, 3] \cdots [2N - 2, 2N - 1],\]  

(1)

where \([i, j]\) denotes the normalized singlet combination of the spins on sites \(i\) and \(j\). Later it was shown by Haldane\(^5\) that dimerization exists at \(J_2/J_1 > J_c \approx 1/6\). For \(J_2/J_1 < J_c\), the system is in a gapless spin liquid phase. This result was confirmed by numerical studies on finite chains\(^6\). The critical value \(J_c\) found by numerical studies\(^7,8\) is \(J_c \approx 0.3\). With spin-lattice interaction, there is dimerization even without \(J_2\) frustration due to the Peierls instability. The interplay of \(J_2\) frustration and spin-Peierls mechanism is an interesting subject.

In this work, we consider the frustrated spin-Peierls system described by the Hamiltonian:

\[H = \sum (J_{1,i} \vec{\mathbf{S}}_i \cdot \vec{\mathbf{S}}_{i+1} + J_2 \vec{\mathbf{S}}_i \cdot \vec{\mathbf{S}}_{i+2}) + \frac{1}{2} \sum_i (M_i \dot{u}_i^2 + K u_i^2),\]  

(2)

where \(J_{1,i} = J_1 - \beta u_i\). In Sec. II, we recalculate the critical value \(J_c\) for the \(J_1 - J_2\) Heisenberg model using Haldane’s method and obtain \(J_c \approx 0.4\). We also study the RG equations for the spin-Peierls system in the adiabatic limit and find that the spin-lattice interaction is always relevant and opens a finite gap. In Sec. III, we use a bond-operator mean field approximation to calculate the dimerization magnitude, the ground state energy and the excitation gap. We find that this approximation can produce a very accurate ground state energy for the \(J_1 - J_2\) model for \(J_2/J_1 < 0.6\), and the ground state energy and gap calculated by this solution is exact at \(J_2/J_1 = 1/2\). Since our approximation is based on the dimerization of the system, we believe our mean-field approximation should be reliable for the spin-Peierls system. Our results are summarized in Sec. IV.

**II. SCALING THEORY**

**A. Frustrated \(J_1 - J_2\) Model**

Here we first discuss the frustrated \(J_1 - J_2\) model studied by Haldane\(^5\) for the \(S = \frac{1}{2}\) spin system

\[H_s = \sum J_1 (S_{i}^{x} S_{i+1}^{x} + S_{i}^{y} S_{i+1}^{y} + \gamma S_{i}^{z} S_{i+1}^{z}) + J_2 \vec{\mathbf{S}}_i \cdot \vec{\mathbf{S}}_{i+2},\]  

(3)

where the anisotropy parameter \(\gamma\) is introduced.

Using the Jordan-Wigner transformation, Hamiltonian \(^3\) transforms into the spinless Fermion Hamiltonian
\[ H_s = -\frac{J_1}{2}(e_i^c c_{i+1} + H.C.) + J_1 \gamma (n_i - 1/2)(n_{i+1} - 1/2) + J_2 (n_i - 1/2)(n_{i+2} - 1/2) + [e_i^c (n_{i+1} - 1/2)c_{i+2} + H.C.] \] (4)

In the continuum limit, this Hamiltonian becomes

\[ \frac{H_s}{(J_1 a_0)} = \int dx (i\psi_+^\dagger \nabla \psi_+ - i\psi_-^\dagger \nabla \psi_-) + g_4 (\rho_+ \rho_+ + \rho_- \rho_-) + 2g_2 (\rho_+ \rho_-) - g_3 (\psi_+^\dagger (x) \psi_- (x + a_0) \psi_- (x + a_0) + H.C.), \] (5)

where \( g_4 = \gamma + 2J_2 / J_1 \), \( g_2 = 2\gamma + 2J_2 / J_1 \), and \( g_3 = \gamma - 3J_2 / J_1 \). Here our coefficients \( g_i \) are different from Haldane’s. The crucial difference is in the \( g_3 \) term. The difference comes from the term \( \psi_+^\dagger (x) \psi_- (x + 2a_0) \psi_+^\dagger (x + a_0) \psi_- (x + a_0) \). This term is written as \( (\psi_+^\dagger \nabla \psi_+^\dagger) \psi_- \nabla \psi_- \) in Ref. 3, which has opposite sign to the term from \( \psi_+^\dagger (x) \psi_- (x) \psi_+^\dagger (x + 2a_0) \psi_- (x + 2a_0) \). However, by direct bosonization\( ^{14,15} \), both expresses contribute negative Umklapp term: \( \cos (4\phi) \). Here \( \phi \) is the boson phase field:

\[ \phi (x) = -\frac{i\pi}{L} \sum_{p \neq 0} \frac{1}{p} e^{-\alpha|p|/2-ixp} [\rho_+ (p) + \rho_- (p)] - (N_+ + N_-) \frac{\pi x}{L}, \] (6)

where \( N_\pm \) are the number operators. Thus we have \( g_3 = \gamma - 3J_2 / J_1 \) instead of \( g_3 = \gamma - 6J_2 / J_1 \).

The scaling theory for model (3) is well known\( ^{17,18} \). The phases for the isotropic model \( \gamma \sim 1 \) are identified by Haldane\( ^{14,15} \) as Neel state, gapless spin liquid, and dimer state (with a finite gap). The scaling diagram shown in Fig. (4) is calculated numerically by integrating the scaling equations. The critical value of \( J_2 / J_1 \) is calculated numerically by locating the intersection of the phase boundary curve and curve 1/\( K_\rho = [(\pi + 13/3\gamma - 4/3g_3)/(\pi - \gamma)]^{1/2} \). The critical value we obtained is \( J_c \sim 0.447 \) instead of 0.16. The critical value calculated by Density-Matrix-Renormalization-Group method using 300 sites\( ^4 \) is \( J_c = 0.298 \). Since we only used the lowest order scaling equations and the critical point of \( J_2 / J_1 \) is not close to 1/\( K_\rho = 2.0 \), the value of \( J_c \) calculated here is not accurate. The true critical value of \( J_c \) should be close to the numerical value\( ^4 \) 0.3.
B. Frustrated Spin-Peierls Model

The lattice part of the Hamiltonian (2) can be written as follows (after rescaling $u$ and going to the continuum limit):

$$H_p = \int dx \left( \frac{1}{2\rho_I} \Pi_{2k_f}^2 + 1/2k u_{2k_f}^2 + \frac{\gamma_0 u_{2k_f}}{\pi \alpha} \cos(2\phi) \right),$$  \hspace{1cm} (7)

where $\alpha$ is the cutoff and $\phi$ is the boson field defined in Eq.(6). We have use the following equation to derive Eq.(7):

$$\psi_\pm(x) = \frac{1}{(2\pi \alpha)^{1/2}} \exp[\pm 2i\phi_\pm(x)]$$  \hspace{1cm} (8)

with the definition

$$\phi_\pm(x) = \frac{1}{2} \left( \phi(x) \mp \int_{-\infty}^x \partial_0 \phi(x') dx' \right).$$  \hspace{1cm} (9)

In terms of the boson field $\phi(x)$ the total Hamiltonian is expressed by

$$H = H_0 + H_p + H_I,$$  \hspace{1cm} (10)

where
\[ H_0 = \frac{1}{2\pi} \int dx \left[ (\bar{v}K_\rho)(\partial_\tau \phi)^2 + (\frac{\bar{v}}{K_\rho})\partial_x \phi \right]^2, \]

\[ H_p = \frac{1}{2} \int dx \left[ \frac{1}{\rho I} \Pi_{2k_f}^2 + ku_{2k_f}^2 \right], \]

\[ H_I = \frac{2g_3}{(2\pi\alpha)^2} \int dx \cos(4\phi) + \frac{\gamma}{\pi\alpha} \int dx \cos(2\phi)u_{2k_f} \]

and

\[ \bar{v} = \left[ (1 + \frac{g_4}{\pi})^2 - \frac{(g_2)^2}{\pi} \right]^{1/2} \]

\[ K_\rho = \left[ \frac{\pi + g_4 - g_2}{\pi + g_4 + g_2} \right]^{1/2}. \]

With the Fermion-phonon interaction, the scaling theory is much more complicated. The analysis is only possible in high phonon frequency limit \( \Delta \ll \omega_{2k_f} \) or in the adiabatic limit \( \Delta \gg \omega_{2k_f} \), where \( \Delta \) is the gap in the spinless Fermion spectrum. In this paper, we will concentrate on the adiabatic limit, which is valid for many compounds. For completeness, we first discuss the high phonon frequency limit.

(a) \( \omega_{2k_f} \to \infty \)

In this limit, the phonon degrees of freedom can be integrated out completely and the result is to introduce an effective attractive electron-electron interaction: \(-\gamma^2/k/(2\pi\alpha)^2 \cos(2\phi)\). Then the phonon effect is to renormalize the Umklapp interaction:

\[ \tilde{g}_3 = g_3 - \frac{\gamma^2}{k}. \]

The phase boundary between the spin liquid and dimerized state is changed accordingly. For weak electron-phonon coupling \( \gamma^2/k \ll 1 \), the dimerization critical point changes from \( J_c \to J_c - \gamma^2/k/3 \). For strong electron-phonon coupling \( \gamma^2/k > 1 \), the system is always dimerized.

(b) **finite high phonon frequency limit** \( \omega_{2k_f} \gg \Delta \)

For high phonon frequency \( \omega_{2k_f} \gg \Delta \) and weak electron-phonon interactions, we can still integrate out the phonon degree of freedom and obtain a phonon-induced retarded attractive electron-electron interaction:

\[ \frac{\delta g_3}{(2\pi\alpha)^2} \cos(4\phi) = -\gamma^2/k \int dt \int dt' \tilde{\psi}(x,t)\psi(x,t)D_0(t - t')\tilde{\psi}(x,t')\psi(x,t') \]

\[ = -\frac{\gamma^2/k}{(2\pi\alpha)^2} \cos(4\phi) - \left( \frac{\gamma^2}{k} \right) \sum_{n=1}^{\infty} \left[ \frac{\partial^n}{\partial t^n} J(x,t) \right]^2 \frac{1}{\omega^{2n}}. \]

where
\[ J(x, t) = \bar{\psi}(x, t)\psi(x, t) \]
\[ = \psi_+(x, t)\psi_-(x, t) + \psi_+^\dagger(x, t)\psi_-(x, t) \]

and \( D_0(t) = \omega/2 \exp(-i|t|\omega) \) is the bare phonon Green’s function. All the terms containing explicit derivatives are superficially irrelevant operators. So for finite high frequency phonons and weak electron-phonon interaction, the retardation effects will be scaled out at \( l^* \sim v_f/\omega_{2k_f} \) or \( E_f(l^*) \sim \omega_{2k_f} \). The critical theory is governed by the limit \( \omega_{2k_f} \to \infty \).

(c) adiabatic limit \( \omega_{2k_f} \to 0 \)

In the adiabatic limit, we should “integrate” out the electronic degree of freedom first and then study the effective phonon system. To this end, we can use the following strategy to study the spin-Peierls system in the mean-field approximation for the phonon effect: we can first study the electronic Hamiltonian by assuming a mean lattice dimerization \( u_2 \), then we can calculate \( u_0 \) by minimizing the electron-lattice total energy. In this adiabatic limit, the electronic Hamiltonian we want to study is:

\[
H = \frac{1}{2\pi} \int dx \left[ (\bar{v}K_\rho)(\partial_\tau \phi)^2 + \left( \frac{\bar{v}}{K_\rho} \right) \partial_x \phi \right]^2 + \frac{2g_3}{(2\pi\alpha)^2} \int dx \cos(4\phi) + \frac{\gamma u u_0}{\pi\alpha} \int dx \cos(2\phi). \tag{15}
\]

In lowest order, the scaling equation can be derived using the Coulomb gas analogy \[ \text{[4,8]} \]. The resulting equations are:

\[
\frac{dY_g}{d\ln \alpha} = 2Y_g(1 - 2K_\rho) + \frac{1}{2}Y_{ph}^2 \tag{16}
\]
\[
\frac{dY_{ph}}{d\ln \alpha} = Y_{ph}(2 - K_\rho + Y_g) \tag{17}
\]
\[
\frac{dK_\rho}{d\ln \alpha} = -\frac{K_\rho^2}{2}(Y_{ph}^2 + Y_g^2), \tag{18}
\]

where \( Y_g = g_3/\pi \) and \( Y_{ph} = \gamma u u_0 \alpha \). The scaling diagram Fig.(2) following from Eq.(16)-(18) is calculated numerically by standard ordinary differential equations integration.
In the Coulomb gas analogy, the system is equivalent to a Coulomb gas of four kinds of particles (i.e., two fugacities \( Y_g \) and \( Y_{ph} \)) with charges \((\pm e_0, \pm 2e_0)\). Here \( \beta e_0 = (2\theta)^{-1} \). The activities \( \lambda_i \) of these particles are \( \exp(-\beta \lambda_1) = Y_g / (2\alpha)^2 \) for \((\pm 2e_0)\) particles and \( \exp(-\beta \lambda_2) = Y_{ph} / (2\alpha) \) for \((\pm e_0)\) particles. The transition from the gapless phase to the gapped phase is of Kosterlitz-Thouless type. If there is no coupling between these two fugacities, the two coupling constants \( Y_{ph} \) and \( Y_g \) define two separate transition “temperatures” approximately at \( |Y_g| = |1 - 1/\theta| \) and \( |Y_{ph}| = |1 - 1/(4\theta)| \), corresponding to the breaking of pairs \((-2e_0, 2e_0)\) and \((-e_0, e_0)\), respectively. For each of the fugacities, the scaling trajectories are well known, see Fig. 1 for the scaling diagram of \( 1/K_{\rho} - Y_g \), the scaling diagram of \( 1/K_{\rho} - Y_{ph} \) can be obtained by rescaling 1/4 of \( 1/K_{\rho} \) axis in Fig. 1.

The coupling between the fugacities contributes to the scaling equations in two respects: (1) \( K_{\rho} \) is renormalized by \( Y_{ph} \) and \( Y_g \) simultaneously; see Eq.\( (18) \); (2) the close “pairs” with nonzero net charge will contribute to the renormalization of \( Y_{ph} \) and \( Y_g \). Physically, it is easy to see that the transition from gapless to gapped phases is controlled by the unbinding of \((e_0, -e_0)\) pairs, since the unbinding of \((e_0, -e_0)\) pairs has a lower transition temperature. So the scaling process is dominated by the \( Y_{ph} \) scaling (for initial \( Y_{ph} \neq 0 \)) (see Fig. 2): the separatrix line is through the point \((Y_{ph} = 0, Y_g = 0, 1/K_{\rho} = 1/2)\). The gapless spin liquid phase exists only at \( 1/K_{\rho} < 1/2 \). Since for general value of \( J_1 \) and \( J_2 \), \( 1/K_{\rho} > 1 \), the system is always in the gapped phase.

Since we have used the bosonization procedure, \( g_i \) and \( \gamma u_0 \) are treated as small parameters. Consequently, we can not expect that the above scaling theory is correct for large \( g_3 \).
or large $J_2/J_1$. Most importantly, since we used a continuum model, “lattice-effects” can not be recovered. From analytical results\textsuperscript{4} we know that in the special limit $J_2/J_1 = 1/2$, the ground state is a perfect dimer configuration which should be true only for a discrete model. Intuitively, we may expect that if we keep $J_2$ finite and $J_1 \to 0$, the system behaves as two decoupled gapless spin liquids. This phase does not occur in the above scaling phase diagram. Nevertheless, from the scaling theory, we can know that for the $J_1 - J_2$ Heisenberg model, there is a gapped phase at $J_2/J_1 > J_c$ (but not $J_2/J_1 \to \infty$), and from the exact results at $J_2/J_1 = 1/2$, the ground state in this gapped phase is dimerized. For the frustrated spin-Peierls model (in the adiabatic limit), from the scaling theory, there is always a gap due to spin lattice coupling.

III. BOND-OPERATOR MEAN FIELD SOLUTION

From Ref.\textsuperscript{4}, we know the ground states of the $J_1 - J_2$ model at $J_2/J_1 = 1/2$ are degenerate dimer states with wave functions

$$
\Psi_1 = [1, 2][3, 4] \cdots [2N - 1, 2N] \\
\Psi_2 = [2N, 1][2, 3] \cdots [2N - 2, 2N - 1].
$$

12342i-12i2N-12N

\textbf{FIG. 3.} Dimerization of the Chain

The bond-operator representation depends on the dimerization of the valence bond. Let us choose a dimer pattern as in Fig 3. For each pair of spins connected in the dimer pattern, we can use four bond spin operators which are defined by the singlet $|s\rangle$ and triplet $|t_{i \in \{1,2,3\}}\rangle$ states:

$$
|s\rangle = \hat{s}^\dagger |0\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle) \\
|t_1\rangle = \hat{t}_1^\dagger |0\rangle = \frac{-1}{\sqrt{2}}(|\uparrow\uparrow\rangle - |\downarrow\downarrow\rangle)
$$

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\[ |t_2\rangle = \frac{i}{\sqrt{2}}(|\uparrow\uparrow\rangle + |\downarrow\downarrow\rangle) \]
\[ |t_3\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle) \]  

(20)

The representations of the four bond operators \( \hat{s}_n \) and \( \hat{t}_{n,i} \in \{1,2,3\} \) is a faithful representation of the original spin operators and these bond operators can be treated as boson operators. Their relation to the spin operators \( \tilde{S}_n \) is as follows:

\[
\tilde{S}^\alpha_{2n} = \frac{1}{2}(-\hat{s}^\dagger_n \hat{t}_{n,\alpha} - \hat{t}^\dagger_n \hat{t}_{n,\alpha} + i\epsilon_{\alpha\beta\gamma} \hat{t}^\dagger_n \hat{t}_{n,\alpha} - i\epsilon_{\alpha\beta\gamma} \hat{t}^\dagger_n \hat{t}_{n,\alpha}) \\
\tilde{S}^\alpha_{2n-1} = \frac{1}{2}(-\hat{s}^\dagger_n \hat{t}_{n,\alpha} + \hat{t}^\dagger_n \hat{t}_{n,\alpha} - i\epsilon_{\alpha\beta\gamma} \hat{t}^\dagger_n \hat{t}_{n,\alpha} - i\epsilon_{\alpha\beta\gamma} \hat{t}^\dagger_n \hat{t}_{n,\alpha}).
\]  

(21)

Using the bond operators, the Hamiltonian becomes:

\[ H = H_0 + H_1 + H_2 + H_3, \]  

(22)

where

\[
H_0 = \sum_n (J_1 + u)(-\frac{3}{4}\hat{s}^\dagger_n \hat{s}_n + \frac{1}{4}\hat{t}^\dagger_n \hat{t}_{n,\alpha} + \frac{1}{2}NKu^2 - \sum_n \mu(\hat{s}^\dagger_n \hat{s}_n + \hat{t}^\dagger_n \hat{t}_{n,\alpha} - 1) \\
H_1 = \sum_n \frac{1}{4}(-J_1 + u + 2J_2)(\hat{t}^\dagger_{n,\alpha} \hat{t}^\dagger_{n+1,\alpha} \hat{s}_n \hat{s}_{n+1} + \hat{t}^\dagger_{n,\alpha} \hat{t}^\dagger_{n+1,\alpha} \hat{s}_n \hat{s}_{n+1} + H.C.) \\
H_2 = \sum_n \frac{1}{4}(J_1 - u + 2J_2)(-\hat{t}^\dagger_{n,\alpha} \hat{t}^\dagger_{n+1,\alpha} \hat{t}_{n,\beta} \hat{t}_{n+1,\beta} + \hat{t}^\dagger_{n,\alpha} \hat{t}^\dagger_{n+1,\alpha} \hat{t}_{n,\beta} \hat{t}_{n+1,\beta} + H.C.) \\
H_3 = \frac{1}{4}(J_1 - u)\epsilon_{\alpha\beta\gamma}(\hat{t}^\dagger_{n,\alpha} \hat{t}^\dagger_{n+1,\alpha} \hat{t}_{n+1,\gamma} \hat{s}_n + \hat{t}^\dagger_{n+1,\alpha} \hat{t}^\dagger_{n,\alpha} \hat{t}_{n,\gamma} \hat{s}_{n+1} + H.C.).
\]  

(23)

Here we have used a mean field approximation for the phonon part. Because of the \(-\frac{3}{4}\hat{s}^\dagger_n \hat{s}_n\) term in \(H_0\), it is clear that the \(s\) bosons will condense: \(\langle \hat{s}_n \rangle = s_0\). The terms in \(H_1\) and \(H_2\) suggest a nonzero value of \(\langle \hat{t}_\alpha \hat{t}_\alpha \rangle\). As \(J_2\) increases, the \(t_i\) bosons will also condense. Whether \(t_i\) condense or not, we can omit \(H_3\) in the mean field approximation.

Using this procedure, the Hamiltonian becomes:

\[
H = N[-\frac{3}{4}(J_1 + u)s_0^2 - \mu s_0^2 + \mu + Ku^2] + \frac{1}{4}(2J_2 + J_1 - u)B^2 - \frac{1}{4}(2J_2 + J_1 - u)A^2 + (J_2 + J_1/2 - u/2)A \cos k|\hat{t}^\dagger_{k,\alpha} \hat{t}_{k,\alpha} + \sum_k \frac{1}{4}(2J_2 + u - J_1)B \cos k|\hat{t}^\dagger_{k,\alpha} \hat{t}_{k,\alpha} + H.C. \\
+ \sum_k \frac{1}{4}(J_1 + u) - \mu + (J_2 + u/2 - J_1/2)s_0^2 \cos k.
\]  

(24)

The self-consistent equations (at zero temperature) are:

\[
A = s_0 + \frac{3}{N} \sum_k \frac{\epsilon_k}{2E_k} \cos k
\]
\[ B = s_0 + \frac{3}{N} \sum_k \frac{\Delta_k}{2E_k} \cos k \]

\[ s_0^2 + s_0 + \frac{3}{N} \sum_k \frac{\epsilon_k}{2E_k} = \frac{5}{2} \] (25)

and

\[ \epsilon_k = (J_1 + u)/2 + \frac{1}{4}(2J_2 + u - J_1)s_0^2 \cos k - \frac{1}{4}(2J_2 + u - J_1)(A + B) + \]

\[ \frac{1}{4}(2J_2 - u + J_1)A \cos k \]

\[ \Delta_k = \frac{1}{4}[(2J_2 + J_1 - u)B - (J_2 + u - J_1)s_0^2] \cos k \]

\[ 2Ku = s_0^2(1 - \frac{A + B}{2}) + \frac{A^2 - B^2}{4} - \frac{1}{4} \]

\[ E_k = \sqrt{\epsilon_k^2 - \Delta_k^2}. \] (26)

The self-consistent equations (25) and (26) can be solved iteratively. The numerical results are summarized in Fig. 4.

**FIG. 4.** Ground state energy for $J_1 - J_2$ Heisenberg model (solid line) and frustrated spin-Peierls model (dashed line) at $K = 100$. 

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FIG. 5. Comparison of ground state energy from our mean-field approximation (solid line) and that from DMRG calculation (diamond) for $J_1 - J_2$ Heisenberg model.

In the limit $u_0 = 0$, the above Hamiltonian describes the $J_1 - J_2$ model studied earlier. We consider this case first. From equations (24)-(26), it is easy to show that at $J_2/J_1 = 1/2$ the ground is at $s_0 = 1$ and $A = B = 0$, i.e. the ground state is perfectly dimerized. The ground state energy is $-0.375J_1$ and the gap value is $0.25J_1$, which are exact. The ground state energy we calculated (Fig. 4) agrees with exact numerical results for $J_2/J_1 \sim 0 - 0.59J_1$ (see Fig. 5 for comparison to the calculation in Ref. 8). This is surprising since we do not expect dimerization for small $J_2$ without the spin-lattice interaction. Our interpretation is that at small $J_2$, although there is no dimerization, the ground state is still well described by fluctuating singlet valence bonds, so our mean-field bond operator approximation can give a rather accurate ground state energy. Since the spin-lattice coupling will enhance the dimerization, we can expect that the mean field ground state energy for the frustrated spin-Peierls model will also be accurate.

The lattice dimerization magnitude $u_0$ for the frustrated spin-Peierls model is shown in Fig. 6. Since the lattice dimerization magnitude $u_0$ only depends on the ground state of the system, we believe that this mean field result should be accurate. From Figs. 4 & 6 we can see that the dimerization of the lattice is enhanced by next nearest neighbor antiferromagnetic coupling $J_2$. 

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FIG. 6. Lattice dimerization magnitude $u$ for the frustrated spin-Peierls model at $K = 100$.

The gap calculated here (Fig. 7) is also reasonable comparing to the previous results for the $J_1 - J_2$ Heisenberg model\cite{7,8}. However there are two features of the mean-field gap for the $J_1 - J_2$ Heisenberg model which are incorrect: (i) We obtained a finite gap even for small $J_2/J_1$ values; and (2) The gap value starts to decrease immediately after $J_2/J_1 = 1/2$ in contrast to the DMRG results\cite{7} that the gap starts to decrease around $J_2/J_1 \sim 0.7$. The first incorrect feature is because we artificially assumed dimerization in the bond-operator representation even for small $J_2/J_1$. For $J_2/J_1 > 1/2$, bonding between next nearest neighbors becomes important and the description of this kind of bonding via nearest neighbor bonding will not be sufficient at the mean-field level. For $J_2/J_1 > 0.59$, the $t_i$ bosons start to condense, and the gap decreases to zero. Although the ground state energy and dimerization due to spin-lattice interaction can be calculated after the $t$ boson condensation, since we can not expect dimerization at large $J_2/J_1$ when next nearest neighbor valence bond becomes strong, the bond-operator representation is questionable in this $J_2/J_1$ region. The bond-operator mean-field approximation should work better for the frustrated spin-Peierls model, since even for $J_2/J_1 = 0$ there is then dimerization due to Peierls instability. Our bond-operator approximation calculation of the gap should be reliable for $J_2/J_1 \in [0, 0.59]$. 
FIG. 7. Energy gap for the for $J_1 - J_2$ Heisenberg model (solid line) and frustrated spin-Peierls model (dashed line) at $K = 100$.

IV. SUMMARY AND ACKNOWLEDGEMENT

In this work we have discussed the scaling behavior of a frustrated spin-Peierls system. The ground state energy, the excitation gap, and lattice dimerization magnitude have been calculated using a bond-operator mean-field approximation. We found that the dimerization of the spin-Peierls chain is substantially enhanced by the next nearest neighbor antiferromagnetic coupling $J_2$. In the most interesting region, $J_2/J_1 < 0.59$, our bond-operator mean field solution can describe the model rather accurately.

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