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The spin-Peierls instability in a spin-$\frac{1}{2}$ XY chain in the non-adiabatic limit

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Abstract. The spin-Peierls instability in a spin-$\frac{1}{2}$ XY chain coupled to dispersionless phonons of frequency ω has been studied in the non-adiabatic limit. We have chosen the Lang–Firsov variational wavefunction for the phonon subsystem to obtain an effective spin Hamiltonian. The effective spin Hamiltonian is then solved in the framework of the mean-field approximation and bond operator technique. We observed two types of phase transitions, one is from the spin liquid phase to the dimerized phase and the other is from the dimerized phase to the antiferromagnetic phase as we vary the spin–phonon coupling from a very low value. The variation of lattice distortion, dimerized order parameter and energy gap with spin–phonon coupling parameter have also been investigated here.

1. Introduction

The discovery of the spin-Peierls transition in $CuGeO_3$ [1] has sparked an intense effort to study the properties of this quasi-one-dimensional magneto-elastic system where the coupling of the magnetic to the lattice degrees of freedom leads to a phase transition into a dimerized phase. This magneto-elastic transition is due to the competition between the gain in magnetic energy due to dimerization and the loss in the elastic energy of the lattice distortion. Recently quite a large number of experimental [2–5] and theoretical [6–13] works have been performed to investigate the various aspects of the spin-Peierls systems. Except for a few [14–16], most of the theoretical investigations rely on the adiabatic treatment of the phonons. In adiabatic approaches one assumes that the phonons responsible for the distortion have low energy with respect to the characteristic energies for the spin systems (e.g. the gap $= \Delta$). The experimental evidence for $CuGeO_3$ indicates that the application of the adiabatic approximation to these systems is not sufficient. Regnault *et al* [17] investigated the spin dynamics of the spin-Peierls system $CuGeO_3$ by inelastic neutron scattering. Their result confirmed the existence of a gap (Δ) in the magnetic excitations at $\Delta = 2$ meV $= 23$ K and the Heisenberg exchange parameter was estimated to be $J_1 = 10.6$ meV $= 115$ K. Braden *et al* [18] found by symmetry that four optical phonons are possible candidates for the spin-Peierls distortion in $CuGeO_3$. Among these four modes two, one of energy 330 K and the other of energy 150 K are experimentally found to be suitable candidates for the spin-Peierls distortion. In both cases we find that the phonon frequency is larger than J as well as Δ. When $\omega > \Delta$ the spin–phonon interaction is unretarded and non-adiabatic effects or quantum lattice fluctuations become important. Fradkin and Hirsch [19] considered the Su–Schrieffer–Heeger model [20] of electron–phonon interaction for spinless fermions and spin-$\frac{1}{2}$ electrons in one dimension to investigate the stability of the Peierls-dimerized ground

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state against quantum fluctuations. In that work they showed by renormalization group arguments and by quantum Monte Carlo simulation that for spinless fermions quantum lattice fluctuations destroy the long-range dimerization order when the fermion–phonon coupling constant is small and predicted a transition from an undimerized ground state to a dimerized phase when the fermion–phonon interaction is larger than a critical value. Campbell and Bishop [21] independently confirmed the findings of Fradkin and Hirsch. Recently Caron and Moukouri [14] using the density matrix renormalization group (DMRG) method studied the XY spin chain coupled to dispersionless phonons and showed that quantum fluctuations reduce the spin-Peierls gap and even destroy the dimerization when the phonon frequency becomes appreciably larger than the gap.

The coupled spin–phonon system for all values of the coupling parameter is a very difficult problem. However, one may gain considerable insight into the stability problem by simply considering limiting situations. By analysing the stability of these limits a qualitative picture of possible phases (or the ground state) will emerge. In the present work we will investigate the effect of spin–phonon interaction in the non-adiabatic limit, i.e. when phonons are certainly fast. In this case we will treat the phonons as fast variables and derive an effective interacting fermion model.

We propose to study an XY spin chain whose magnetic interaction depends on the bond length. The reason for this study is twofold: (i) the undeformed spin chain Hamiltonian can be solved exactly, (ii) the model contains the essential elements for the spin-Peierls transition, that is coupling to intermolecular motion. In the future it will be of interest to study the Heisenberg chain with a next-nearest-neighbour frustration term to make the model a more realistic match to the inorganic spin-Peierls systems.

The paper is organized as follows. In section 2 we obtained an effective fermionic Hamiltonian for the XY model in the presence of the spin–phonon interaction. The effective Hamiltonian is then solved within the mean-field approximation taking into account the dimerization as well as antiferromagnetic ordering. The results of the numerical solution and its implications are discussed in section 3. In section 4 we solved this effective Hamiltonian with the help of the bond operator technique. Finally we present our conclusion in section 5.

2. Formulation

We start with the XY model in the presence of the spin–phonon interaction on a linear chain

$$H = \sum_l [(J + g(b_l^\dagger + b_l - b_{l+1}^\dagger - b_{l+1})](S_l^X S_{l+1}^X + S_l^Y S_{l+1}^Y) + \omega \sum_l b_l^\dagger b_l \quad (1)$$

where l denotes the site index of the N site linear chain, S_l^X and S_l^Y are components of the local XY spin of value $\frac{1}{2}$, $b_l(b_l^\dagger)$ is the annihilation (creation) operator for the vibration of a molecule at site l and J is the magnetic exchange interaction between the nearest-neighbour spins. Here ω accounts for the dispersionless vibrational spectra for molecular motion along the chain direction and g is the spin–phonon interaction [22].

We transform the spin operator to a spinless fermion representation using the Jordan–Wigner transformation [23]

$$S_l^X + \mathrm{i}S_l^Y = S_l^+ = \exp\left(-\mathrm{i}\pi \sum_j^{l-1} d_j^\dagger d_j\right) d_l^\dagger \quad (2)$$

$$S_l^X - \mathrm{i}S_l^Y = S_l^- = \exp\left(\mathrm{i}\pi \sum_j^{l-1} d_j^\dagger d_j\right) d_l \quad (3)$$

$$S_l^z = \tfrac{1}{2} + d_l^\dagger d_l \tag{4}$$

to make use of the growing understanding of a one-dimensional Fermi system.

After the Jordan–Wigner transformation, the Hamiltonian (1) can be written in terms of fermion operators $d_l^\dagger$ and d_l as

$$H = \frac{1}{2}J\sum_l P_l + \frac{1}{2}g\sum_l (b_l^\dagger + b_l)(P_l - P_{l-1}) + \omega\sum_l b_l^\dagger b_l \tag{5}$$

where

$$P_l = d_l^\dagger d_{l+1} + d_{l+1}^\dagger d_l. \tag{6}$$

In the adiabatic approximation the spin–phonon interaction deforms the lattice to undergo the Peierls instability. To take into account the lattice distortion due to spin–phonon coupling, in our case we choose a variational wavefunction $|\psi\rangle_{ph} = U|0\rangle$ with

$$U = \exp\left(\frac{\lambda}{2\omega}\sum_l (b_l^\dagger - b_l)(P_l - P_{l-1})\right) \tag{7}$$

for the phonon subsystem, where $|0\rangle$ is the zero-phonon state and U describes a modified Lang–Firsov transformation [24, 25]. In this formalism the effective fermion Hamiltonian is written as

$$H_{eff} = \langle 0|H_T|0\rangle \tag{8}$$

with

$$\begin{aligned} H_T = U^{-1}HU = {} & \frac{J}{2}\sum_l U^{-1}P_l U + \frac{g-\lambda}{2}\sum_l (b_l^\dagger + b_l)(P_l - P_{l-1}) \\ & -4g'^2\sum_l n_l + 4g'^2\sum_l n_l n_{l+1} + g'^2\sum (1-2n_l)(d_{l-1}^\dagger d_{l+1} + d_{l+1}^\dagger d_{l-1}) \\ & +\omega\sum_l b_l^\dagger b_l \end{aligned} \tag{9}$$

where

$$n_l = d_l^\dagger d_l \tag{10}$$

$$g'^2 = \left(\frac{g\lambda}{2\omega} - \frac{\lambda^2}{4\omega}\right). \tag{11}$$

In the above equation b_l and $b_l^\dagger$ are the creation and annihilation operators for the phonon system vibrating about the displaced equilibrium position $(\lambda/\omega)(P_l - P_{l-1})$ of the lattice. Clearly, λ is proportional to a lattice displacement created by the spin–phonon interaction which has to be determined variationally. When $\lambda = g$ the transformation is exactly the Lang–Firsov [24] transformation where the fermion–phonon term is diagonalized exactly and the fermion hopping term is renormalized by dressed phonons. To obtain an effective fermionic Hamiltonian we take the average over the zero-phonon state of the transformed phonon subsystem and neglect terms of the order of λ^4/ω^4 and higher. In this approximation the effective Hamiltonian is

$$\begin{aligned} H_{eff}(\lambda) = {} & \frac{J}{2}\left(1 - \frac{3\lambda^2}{4\omega^2}\right)\sum_l (d_l^\dagger d_{l+1} + d_{l+1}^\dagger d_l) + \frac{J\lambda^2}{8\omega^2}\sum_l (d_l^\dagger d_{l+3} + d_{l+3}^\dagger d_l) \\ & -4g'^2\sum_l n_l + 4g'^2\sum_l n_l n_{l+1} + g'^2\sum (1-2n_l)(d_{l-1}^\dagger d_{l+1} + d_{l+1}^\dagger d_{l-1}) \\ & +\mathrm{O}(\lambda^4). \end{aligned} \tag{12}$$

Now, the above effective Hamiltonian (12) is too complicated to solve exactly. Therefore one has to look for approximate methods. We calculate the ground-state energy $E_{eff}(\lambda)$ of the effective Hamiltonian (13) in the framework of mean-field theory. We assume solutions which break the symmetry between even and odd sites with respect to the number of fermions on the site and to the corresponding hopping probability. Both of these kinds of order open a gap at the Fermi momentum at half-filling (i.e. when the total spin S_z is zero) and lower the ground-state energy. We will consider four variational parameters such as n_e, n_o, h_e and h_o (where e denotes even sites and o implies odd sites). All these variables are not independent because they are subject to the fermion number conservation constraint

$$n = \frac{\langle d_{2l}^{\dagger} d_{2l} + d_{2l+1}^{\dagger} d_{2l+1}\rangle}{2} = \frac{(n_e + n_o)}{2}. \tag{13}$$

For half-filling ($S_z = 0$) $n = \frac{1}{2}$. The three remaining variational parameters are then the antiferromagnetic order parameter

$$m = \frac{\langle d_{2l}^{\dagger} d_{2l} - d_{2l+1}^{\dagger} d_{2l+1}\rangle}{2} = \frac{(n_e - n_o)}{2} \tag{14}$$

the dimerized order parameter

$$\gamma = \frac{\langle d_{2l}^{\dagger} d_{2l+1} - d_{2l+1}^{\dagger} d_{2l+2}\rangle}{2} = \frac{(h_e - h_o)}{2} \tag{15}$$

and the average hopping probability

$$h = \frac{\langle d_{2l}^{\dagger} d_{2l+1} + d_{2l+1}^{\dagger} d_{2l+2}\rangle}{2} = \frac{(h_e + h_o)}{2}. \tag{16}$$

Here $\langle\ \rangle$ implies the expectation value over the ground state. Within the limitation of the Hartree–Fock approximation our effective Hamiltonian can be written as

$$\begin{aligned} H_{eff} = {} & \frac{J}{2}\left(1 - \frac{3\lambda^2}{4\omega^2}\right)\sum_l (d_l^{\dagger} d_{l+1} + d_{l+1}^{\dagger} d_l) + \frac{J\lambda^2}{8\omega^2}\sum_l (d_l^{\dagger} d_{l+3} + d_{l+3}^{\dagger} d_l) \\ & + 8g'^2\gamma \sum_l (-1)^l (d_l^{\dagger} d_{l+1} + d_{l+1}^{\dagger} d_l) + 8g'^2 \sum (\frac{1}{2} - (-1)^l m) n_l) \\ & - 4g'^2(\frac{1}{4} - m^2 - 2\gamma^2)N - 2g'^2 N + \mathrm{O}\left(\frac{\lambda^4}{\omega^4}\right). \end{aligned} \tag{17}$$

To diagonalize the Hamiltonian (18) we transform the operators from coordinate space to momentum space

$$c_j^{\dagger} = \frac{1}{\sqrt{N}} \sum_k c_k^{\dagger} \mathrm{e}^{\mathrm{i}kj} \tag{18}$$

$$c_j = \frac{1}{\sqrt{N}} \sum_k c_k \mathrm{e}^{-\mathrm{i}kj}. \tag{19}$$

Due to the reduced symmetry, each k state is coupled to the state $k + \pi$. So it is convenient to write the Hamiltonian in the reduced zone $-\pi/2$ to $\pi/2$ and label the states by band indices l and u. In this representation the Hamiltonian is a two-band Hamiltonian where the bands l and u are coupled to each k

$$\begin{aligned} H_{eff} = {} & \sum_k \alpha_k^l d_k^{l\dagger} d_k^l + \sum_k \alpha_k^u d_k^{u\dagger} d_k^u + \sum_k \beta_k d_k^{l\dagger} d_k^u + \sum_k \beta_k^* d_k^{u\dagger} d_k^l \\ & - 4g'^2(\frac{1}{4} - m^2 - 2\gamma^2)N + \mathrm{O}\left(\frac{\lambda^4}{\omega^4}\right) \end{aligned} \tag{20}$$

where

$$\alpha_k^l = J\left(1 - \frac{3\lambda^2}{4\omega^2}\right)\cos(k) + \frac{2J\lambda^2}{8\omega^2}\cos(3k) \tag{21}$$

$$\alpha_k^u = -J\left(1 - \frac{3\lambda^2}{4\omega^2}\right)\cos(k) - \frac{2J\lambda^2}{8\omega^2}\cos(3k) \tag{22}$$

$$\beta_k = -8g'^2(m - 2\mathrm{i}\gamma\sin(k)). \tag{23}$$

We diagonalize this Hamiltonian by a Bogoliubov–Valatin transformation and obtain

$$\frac{H_{eff}}{\omega} = \sum_k E_k^l a_k^\dagger a_k + \sum_k E_k^u b_k^\dagger b_k - 4g'^2(\frac{1}{4} - m^2 - 2\gamma^2)N \tag{24}$$

with upper and lower band

$$E_k^{u/l} = \pm\sqrt{\frac{\alpha_k^{l2}}{\omega^2} + 64\frac{g'^4m^2}{\omega^2} + \frac{256g'^4\gamma^2\sin(k)^2}{\omega^2}}. \tag{25}$$

From equation (25) it is clear that the energy spectrum has been split into two separate bands (for non-zero m or γ) characterized by the Bogoliubov transformed creation (annihilation) operators $a_k^\dagger(a_k)$ and $b_k^\dagger(b_k)$. For half-filling ($S_z = 0$) the lower band is completely filled in the ground state. We will take the expectation value of equations (14) and (15) over the ground state to obtain a set of self-consistent equations

$$1 = 8\frac{g'^2}{\omega N}\sum_{k=-\pi/2}^{k=\pi/2}\frac{1}{|E_k^l|} \qquad \text{or } m = 0 \tag{26}$$

and

$$1 = 16\frac{g'^2}{\omega N}\sum_{k=-\pi/2}^{k=\pi/2}\frac{\sin(k)^2}{|E_k^l|} \qquad \text{or } \gamma = 0. \tag{27}$$

If we retain terms up to the order of g^2/ω^2 the integrals involving equations (26) and (27) can be expressed in terms of elliptic functions of the first kind ($K(\nu)$) and the second kind ($E(\nu)$) to give

$$1 = \frac{8g'^2\sqrt{\nu}}{\pi J(1 - \frac{3\lambda^2}{2\omega^2})}K(\nu) \qquad \text{or } m = 0 \tag{28}$$

with

$$\begin{aligned}
&\nu = [1 + \frac{64g'^4m^2}{J^2(1 - 3\lambda^2/(2\omega^2))}]^{-1} \\
&1 = -\frac{32g'^2}{\pi J(1 - \frac{3\lambda^2}{2\omega^2})}\frac{\mathrm{d}}{\mathrm{d}\nu'}E(\nu') \qquad \text{or } \gamma = 0. \\
&\nu' = 1 - \frac{256g'^4\gamma^2}{J^2(1 - 3\lambda^2/(2\omega^2))}.
\end{aligned} \tag{29}$$

For small m or γ the equations provide asymptotic expressions for (i) the antiferromagnetic and (ii) the dimerized phase:

(i) the antiferromagnetic phase ($\gamma = 0; m \neq 0$)

$$\begin{aligned}
&\gamma = 0; \\
&m = p_j \exp\left[-\pi p_j\left(1 - \frac{1.38629}{p_j}\right)\right]
\end{aligned} \tag{30}$$

(ii) the dimerized phase ($m = 0$; $\gamma \neq 0$)

$$m = 0;$$
$$\gamma = \frac{p_j}{2} \exp\left[-\frac{\pi p_j}{2}\left(1 - \frac{0.773\,08}{p_j}\right)\right] \tag{31}$$

where

$$p_j = J\frac{1 - 3\lambda^2/(2\omega^2)}{8g'^2}.$$

When m or γ is large we solve equation (26) or (27) numerically to get the antiferromagnetic or dimerized order parameter.

Finally we minimize the ground-state energy ($E_G(\lambda)$) of the Hamiltonian H_{eff} with respect to λ to get λ and the ground-state energy of the system.

3. Results and discussion of the mean-field study

We have computed the ground-state energy, the lattice distortion and the energy gap for the XY system in the presence of the spin–phonon interaction when the phonon frequency is certainly fast. The results of our calculation show some distinguishing features in the phase diagram which are absent when phonons are treated adiabatically. In the adiabatic approach the spin–phonon coupling to the XY spin system always gives rise to a dimerized phase, whereas our non-adiabatic approach predicts dimerized and antiferromagnetic phases depending on the values of g/ω and J/ω. Here we present the result for two values of the exchange interaction $J/\omega = 0.2$ and 0.4. In our calculation we have neglected terms of the order λ^4/ω^4 or higher. So we do not extend our calculation to large spin–phonon coupling g/ω and confine ourselves to $g/\omega \leqslant 0.5$. In figure 1 we have shown the variation of the lowest energy in the antiferromagnetic as well as the dimerized phase to determine the ground state of the system. For $J/\omega = 0.2$ we find that the dimerized phase represents the ground state when $g/\omega < 0.46$ and the antiferromagnetic phase becomes the ground

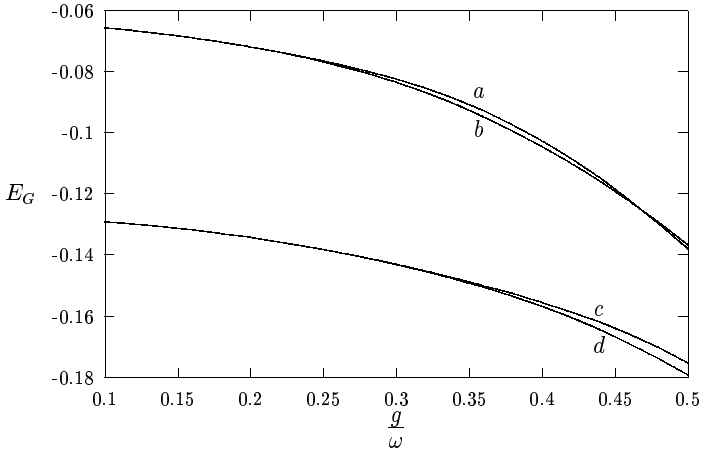

Figure 1. Variation of the minimum energy (in units of the energy of the phonon) with respect to the spin–phonon coupling (g/ω) in the antiferromagnetic phase for $J/\omega = 0.2$ (curve a) and $J/\omega = 0.4$ (curve c) and in the dimerized phase for $J/\omega = 0.2$ (curve b) and $J/\omega = 0.4$ (curve d).

state when $g/\omega > 0.46$. The critical value for the dimerized to antiferromagnetic phase transition increases with the increase of J/ω. For $J = 0.4$ the above-mentioned critical value of g/ω is higher than 0.5 and it is not shown in our plot because we have confined our investigations to $g/\omega = 0.5$.

In figure 2 we show the variation of the dimerized order parameter γ with g/ω for $J/\omega = 0.2$ and 0.4. The figure shows that when g/ω is less than 0.1 the dimerized order parameter is almost zero. From equation (31) we obtain $\gamma \sim 10^{-20}$ at $g/\omega = 0.1$. In the mean-field calculation we neglect quantum fluctuations and always find a non-zero value of the order parameter. However, the quantum fluctuation due to spin excitation would have drastic repercussions on the value of γ and could destroy this small value of γ to give a spin liquid phase. So one may expect a critical spin–phonon coupling (g_c/ω) for the onset of dimerization. Caron and Moukouri [14] have shown the existence of critical spin–phonon coupling (g_c/ω) through the density matrix renormalization group calculation where quantum fluctuations are taken into account rigorously. It is also evident from our figure 2 that the dimerization order parameter decreases with the increase of J/ω which means that we expect a larger g_c/ω for $J/\omega = 0.4$.

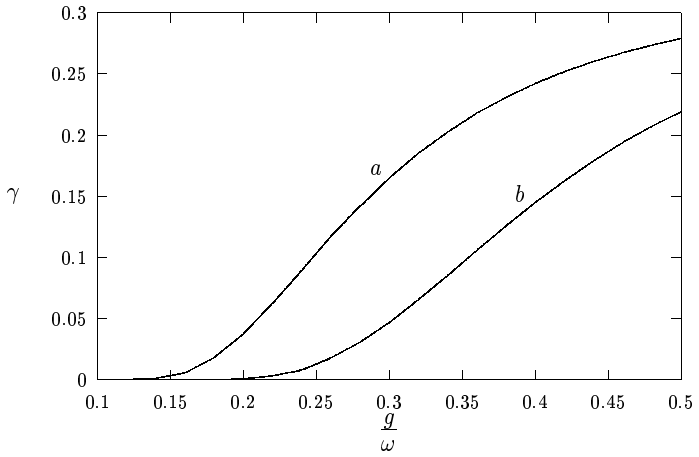

Figure 2. Variation of the dimerized order parameter γ with respect to g/ω for $J/\omega = 0.2$ (curve a) and $J/\omega = 0.4$ (curve b) in the dimerized phase.

Due to the Peierls instability we have two types of bond length, one is greater than the unperturbed lattice constant and the other is less than the unperturbed lattice constant. We represent this lattice deformation by $\langle b_l^\dagger + b_l - b_{l+1}^\dagger - b_{l+1}\rangle = (-1)^l\delta$. In figure 3 we plot the variation of $\delta = 2\lambda\gamma$ with respect to g/ω for $J/\omega = 0.2$ and 0.4 in the dimerized phase. It is seen from the figure that for a small g/ω ratio the lattice distortion is almost zero and it increases with an increase of g/ω or with a decrease of J/ω.

We have also investigated the excitation energy gap (Δ) which is obtained by calculating the lowest excited state energy (i.e. lowest energy of the upper band). In figure 4 we plot the variation of Δ with respect to g/ω for $J/\omega = 0.2$ and 0.4. Like the dimerization order parameter, Δ is also very small for small spin–phonon coupling. The result also points to the possibility of gapless spectra for $g/\omega < g_c/\omega$ and 'gap-full' spectra for $g/\omega > g_c/\omega$.

In figure 5 we show the variation of the critical value g_c'/ω for the dimerized to antiferromagnetic phase transition with respect to J/ω. We observe a decrease of g_c'/ω with the decrease of J/ω and in the limit $J/\omega \to 0$ the system shows an antiferromagnetic

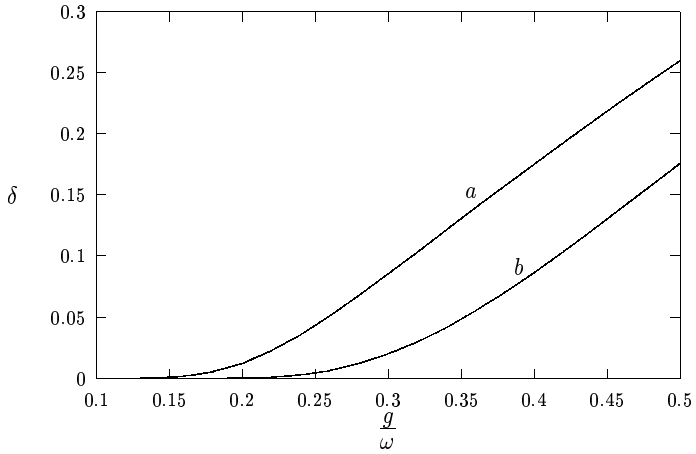

Figure 3. Variation of the lattice distortion δ with respect to g/ω in the dimerized phase for $J/\omega = 0.2$ (curve a) and $J/\omega = 0.4$ (curve b).

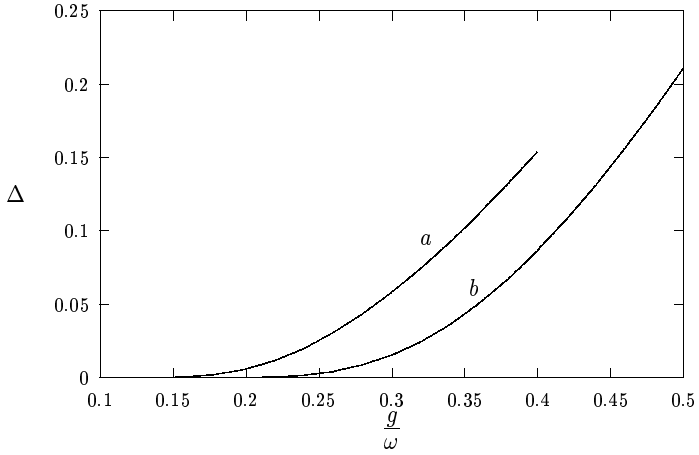

Figure 4. The excitation energy gap Δ as a function of g/ω in the dimerized phase for $J/\omega = 0.2$ (curve a) and $J/\omega = 0.4$ (curve b).

order for any finite spin–phonon coupling. This feature is significantly different if the spin–phonon coupling is treated adiabatically where the ground state of the XY model with spin–lattice interaction always represents the dimerized phase. Our results signify that the quantum correction may play a very important role in determining the phases of the ground state of the spin-Peierls systems.

4. The bond operator method

In the last section we observed the dimerized ground state in the intermediate range of the spin–phonon coupling parameter. A useful approach to describe the dimerized phase is the bond operator technique introduced by Chubukov [26] and Sachdev and Bhatt [27]. Recently the bond operator method has been used successfully to study the frustrated Heisenberg chain

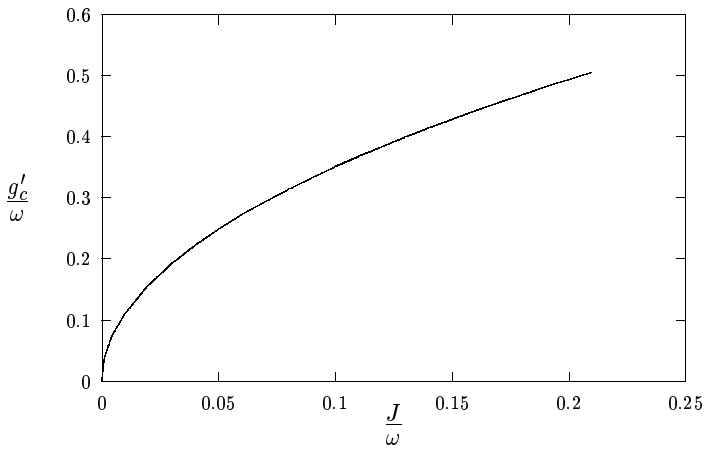

Figure 5. Variation of the critical value g_c'/ω for the dimerized to antiferromagnetic phase transition with respect to J/ω.

[28, 29] and two spin ladder models [30, 31]. In this section we will study the instability of the dimerized phase of our effective Hamiltonian (equation (12)) with the help of a quite different approach, namely the bond operator technique. For this purpose we transform our effective fermionic Hamiltonian to the corresponding effective spin Hamiltonian by the well known Jordon–Wigner transformation [23]. In spin language the effective Hamiltonian can be written as

$$H_{eff} = \frac{J}{2}\left(1-\frac{3\lambda^2}{4\omega}\right)\sum_l (S_{l+1}^+ S_l^- + S_l^+ S_{l+1}^-) + g'^2 \sum_l (S_l^+ S_{l+2}^- + S_{l+2}^+ S_l^-)$$
$$+4g'^2 \sum_l S_l^z S_{l+1}^z + \frac{J\lambda^2}{8\omega^2}\sum_l (S_{l+1}^z S_{l+2}^z S_l^+ S_{l+3}^- + S_{l+1}^z S_{l+2}^z S_{l+3}^+ S_l^-) - g'^2 N \quad (32)$$

where $S_l^+ = S_l^x + \mathrm{i}S_l^y$ and $S_l^- = S_l^x - \mathrm{i}S_l^y$ and S_l^x, S_l^y, S_l^z are the x, y, z components of a spin-$\frac{1}{2}$ operator at the site l. In our mean-field calculation we found that the term involving the the third nearest-neighbour fermionic interaction does not play a significant role in determining the phases of the system. So for our present calculation we shall neglect the last term in our effective spin Hamiltonian. In the bond operator method, the Hilbert space of spin degrees of freedom is represented in terms of singlets and triplets on local bonds (nearest-neighbour sites). The corresponding one-singlet $|s_i\rangle$ and three-triplet $|t_{\alpha i}\rangle$ (where $\alpha = x, y, z$) states are created out of the vacuum by applying the operators

$$\begin{aligned}
|s_i\rangle &= s_i^\dagger|0\rangle = \frac{1}{\sqrt{2}}(|\uparrow_{2i}\downarrow_{2i+1}\rangle - |\downarrow_{2i}\uparrow_{2i+1}\rangle)\\
|t_{xl}\rangle &= t_{xl}^\dagger|0\rangle = -\frac{1}{\sqrt{2}}(|\uparrow_{2l}\uparrow_{2l+1}\rangle - |\downarrow_{2l}\downarrow_{2l+1}\rangle)\\
|t_{yi}\rangle &= t_{yl}^\dagger|0\rangle = \frac{\mathrm{i}}{\sqrt{2}}(|\uparrow_{2l}\uparrow_{2l+1}\rangle + |\downarrow_{2l}\downarrow_{2l+1}\rangle)\\
|t_{zl}\rangle &= t_{zl}^\dagger|0\rangle = \frac{1}{\sqrt{2}}(|\uparrow_{2l}\downarrow_{2l+1}\rangle + |\downarrow_{2l}\uparrow_{2l+1}\rangle).
\end{aligned} \quad (33)$$

The operators $s_l^\dagger$ (s_l), $t_{\alpha l}^\dagger$ ($t_{\alpha l}$) where $\alpha = x, y, z$, are chosen to satisfy the bosonic commutation relations

$$[s_l, s_m^\dagger] = \delta_{l,m} \qquad [s_l^\dagger, t_{\alpha,l}^\dagger] = 0 \qquad [t_{\alpha,l}, t_{\beta,m}^\dagger] = \delta_{\alpha,\beta}\delta_{l,m}. \tag{34}$$

In order to ensure that the physical states are either singlet or triplet one has to impose the constraints

$$s_i^\dagger s_i + \sum_{\alpha=x,y,z} t_{\alpha i}^\dagger t_{\alpha i} = 1. \tag{35}$$

Unfortunately, it is a difficult task to satisfy this local constraint and the dimer interactions exactly. In order to perform the calculation of the ground-state energy and the lowest excited states we follow the approximations which are generally used to calculate the triplet dispersions in this method [28]: (i) we treat the local constraint by eliminating the singlet operator via $s_i^\dagger = s_i = (1 - \sum_\alpha t_{\alpha i}^\dagger t_{\alpha i})^{\frac{1}{2}}$, (ii) we restrict ourselves to quadratic terms only. It was previously shown by Gopalon *et al* [32] and Sachdev and Bhatt [27] that the effect of higher-order terms on the ground-state energy or lowest excitations is quite small and therefore we expect that this approximation will not modify our results significantly.

Within the above-mentioned approximations the effective Hamiltonian reduces to

$$\begin{aligned} H_{eff} = &-\frac{J}{4}\left(1 - \frac{3\lambda^2}{4\omega^2}\right)N - \frac{3g'^2}{2}N + \left[\frac{J}{2}\left(1 - 3\frac{\lambda^2}{4\omega^2}\right) + 2g'^2\right]\sum_l (t_{xl}^\dagger t_{xl} + t_{yl}^\dagger t_{yl+1}) \\ &+ \left[-\frac{1}{4}J\left(1 - \frac{3\lambda^2}{4\omega^2}\right) + 2g'^2\right]\sum_l (t_{xl}^\dagger t_{xl+1} + t_{x,l}^\dagger t_{xl}^\dagger + t_{yl}^\dagger t_{yl+1} + t_{yl}^\dagger t_{yl+1}^\dagger + \text{H.C.}) \\ &+ J\left(1 - \frac{3\lambda^2}{4\omega^2}\right)\sum_l t_{zl}^\dagger t_{z,l} - g'^2 \sum_l (t_{zl}^\dagger t_{zl+1} + t_{zl}^\dagger t_{zl+1}^\dagger + \text{H.C.}). \end{aligned} \tag{36}$$

This one-body Hamiltonian can be diagonalized readily to give

$$\begin{aligned} H_{eff} = &-\frac{J}{4}\left(1 - \frac{3\lambda^2}{4\omega^2}\right)N - \frac{3g'^2}{2\omega}N + \sum_{k,\alpha=x,y,z} \sqrt{((A_k^\alpha)^2 - 4(B_k^\alpha)^2)}(a_k^{\alpha\dagger} a_k^\alpha + \tfrac{1}{2}) \\ &- \frac{1}{2}\sum_{k,\alpha=x,y,z} A_k^\alpha \end{aligned} \tag{37}$$

where

$$\begin{aligned} A_k^{x,y} &= \frac{J}{2}\left(1 - \frac{3\lambda^2}{4\omega^2}\right) + 2g'^2 - \frac{1}{2}\left[J\left(1 - \frac{3\lambda^2}{4\omega^2}\right) - 8g'^2\right]\cos(2k) \\ B_k^{x,y} &= -\frac{1}{4}\left[J\left(1 - \frac{3\lambda^2}{4\omega^2}\right) - 8g'^2\right]\cos(2k) \\ A_k^z &= J\left(1 - \frac{3\lambda^2}{4\omega^2}\right) - 2g'^2\cos(2k) \\ B_k^z &= -g'^2\cos(2k). \end{aligned} \tag{38}$$

Finally we minimize the ground-state energy

$$E_G(\lambda) = -\frac{J}{4}\left(1 - \frac{3\lambda^2}{4\omega^2}\right)N - \frac{3g'^2}{2\omega}N + \frac{1}{2}\sum_{k,\alpha=x,y,z} \sqrt{(A_k^\alpha)^2 - 4(B_k^\alpha)^2} - \frac{1}{2}\sum_{k\alpha=x,y,z} A_k^\alpha \tag{39}$$

with respect to λ to obtain λ and the ground-state energy of the system. Here the ground state is dimerized and the excitations are characterized by the two types of dispersion relations

$[(A_k^{(x,y)})^2 - 4(B_k^{(x,y)})^2]^{1/2}$ and $[(A_k^{(z)})^2 - 4(B_k^{(z)})^2]^{1/2}$. Now the ground state is stable as long as the excitations are well defined. Therefore, the dimerized ground state becomes unstable when

$$\sqrt{(A_{k=0}^{(x,y)})^2 - 4(B_{k=0}^{(x,y)})^2} = 0 \tag{40}$$

or

$$\sqrt{(A_{k=0}^{(z)})^2 - 4(B_{k=0}^{(z)})^2} = 0. \tag{41}$$

Equations (40) and (41) give two values of the critical spin–phonon coupling constant g'_{c1}/ω and g'_{c2}/ω between which the ground state is dimerized. In figure 6 we have plotted $g'_{c1} = g'_{c1}/\omega$ and $g'_{c2} = \frac{g_{c2}}{\omega}$ as a function of J/ω. From the analysis of the results of the bond operator method and the mean-field approach it is clear that our system undergoes two types of phase transition: (i) one is from the spin liquid phase to the dimerized phase which occurs at $g = g_{c1}$ and (ii) the other is from the dimerized phase to the antiferromagnetic phase which occurs at $g = g_{c2}$ as we vary the spin–phonon coupling parameter (g) from a very low value.

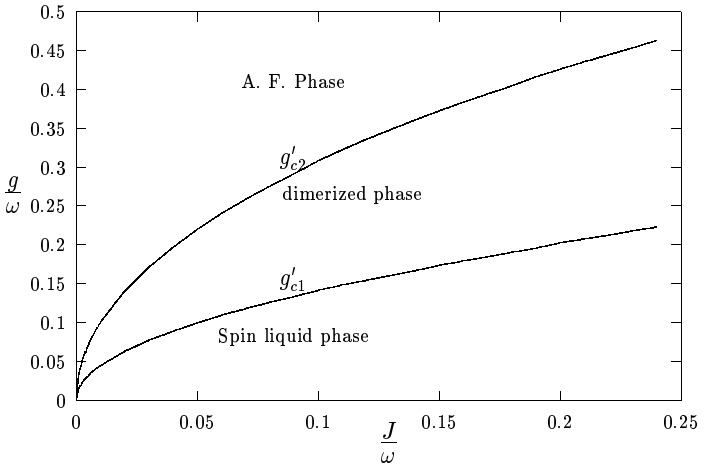

Figure 6. Variation of the critical values g'_{c1} for the spin liquid to dimerized phase transition and g'_{c2} for the dimerized to antiferromagnetic phase transition with respect to J/ω.

5. Conclusion

In summary, we have studied the interacting spin–phonon problem non-adiabatically. We have chosen the Lang–Firsov variational wavefunction to integrate out the phonon degrees of freedom and obtain an effective spinless fermionic Hamiltonian which is solved in the framework of the mean-field approximation and the bond operator technique to calculate the ground-state energy, the minimum excitation energy gap and the lattice distortion developed in the ground state. Our investigation indicates two types of phase transition, one is from the spin liquid phase to the dimerized phase and the other is from the dimerized phase to the antiferromagnetic phase as we vary the spin–phonon coupling from a very low value. However, these phase transitions are absent if we neglect the quantum lattice fluctuations and treat the problem in the adiabatic approximation. So it is evident that the behaviour of a

spin-Peierls system is significantly modified by quantum lattice fluctuations and an intense investigation is required to explore the effect of non-adiabatic corrections to the spin-Peierls systems. For a realistic calculation of an inorganic spin-Peierls system like $CuGeO_3$ one has to study the Heisenberg spin chain with next-nearest-neighbour frustration.

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