# Nonadiabatical approach to the Dzyaloshinsky-Moriya interaction in the *XY* spin chain coupled with quantum phonons

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Using the model of the DM interaction in *XY* antiferromagnetic spin chain with spin-phonon coupling, the nonadiabatic effects on the DM interaction have been studied by developing a nonadiabatic analytical approach. The results show that in the nonadiabatic case, to a certain finite phonon frequency, there exists a finite critical value of spin-phonon coupling. As the spin-phonon coupling decreases to the critical value, the system becomes gapless and the spin dimerization is destroyed. The DM interaction leads the system to have a finite critical value of spin-phonon coupling even in the adiabatic limit. The increase in staggered DM interaction will decrease the critical value of spin-phonon coupling, but increase that of phonon frequency, therefore, favors the dimerization. The nonadiabaticity plays an important role in suppressing the enhancement effects of the DM interaction to the dimerization. The dimerized ground state when DM interaction is present can be destroyed by the quantum lattice fluctuations. The threshold value of $\beta$ changing the effect of the DM interaction on the dimerization from suppression to promotion is not simply a constant but a crossover. For appropriate fixed values of spin-phonon coupling, phonon frequency and $\beta$, as $D$ increases, the system undergoes a reentry of phase between spin-dimer state and gapless state.

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## I. INTRODUCTION

Recently, the revealment of the existence of Dzyaloshinsky-Moriya (DM) interaction[1,2] in a variety of quasi-one-dimensional magnets[3–5] has stimulated extensive investigations on the physical properties of DM interaction in these materials. The experiments such as high field neutron-scattering measurements on Cu benzoate[6] and electron paramagnetic resonance investigations in $CuGeO_3$ (Refs. 7–9) manifest that in these materials the DM interaction plays an important role[10–14] and a study of one-dimensional DM Hamiltonians seems to be of great importance.[15] The DM interaction has been used to interpret an anomalous magnetic behaviors in $BaCu_2M_2O_7$ ($M$=Si, Ge),[16,17] $La_2CuO_4$,[18] $Yb_4As_3$,[10] and $YVO_3$-$SrVO_3$ systems.[19] The DM interaction is an antisymmetric spin exchange interaction between two nearest spins and in a magnetic chain the DM vector may spatially vary in both direction and magnitude. However, the symmetry arguments usually rule out most of the possibilities and the theoretical discussions focus mainly on two principal cases, the uniform[20,21] and the staggered DM interactions.[15,21,22] For the spin-Peierls system, using numerical calculation, Derzhko and his co-workers[23] analyzed the ground-state energy of the dimerized spin-$\frac{1}{2}$ transverse *XX* and Heisenberg chains with DM interaction to study the influence of the latter interaction on the spin-Peierls instability. They found that uniform DM interaction may act against the dimerization but staggered DM interaction may act in favor of the dimerization. However, whether the staggered DM interaction always enhances the dimerization or the uniform DM interaction always acts against the dimerization has not been clearly answered. Up to now, all of the theoretical studies on DM interaction in spin-chain systems have used the static model (so called adiabatic approximation or frozen phonon approximation) with the static dimerization parameter $\delta$, and treated the problem in adiabatic limit. By considering the static model, several attempts have been performed to treat the spin-phonon coupling.[23,24] The validity of this static model is based on the assumption that the frequencies of the phonons associated with the dimerization are much smaller than the dimerization gap and the exchange integral. However, this is questionable, and the amplitude of the dimerization is substantially underestimated when compared with estimates from structural data in the spin-Peierls phase.[25] It has been shown that the quantum lattice fluctuations must be taken into account to satisfactorily describe some physical properties of quasi-one-dimensional spin-Peierls system.[26–29] An interesting and still controversial problem is how the DM interaction on the dimerized ground state is modified when quantum lattice fluctuations are taken into account. Furthermore the effect of quantum fluctuations in quasi-one-dimensional systems is more significant than in higher-dimensional systems, resulting in many interesting phenomena. However, with the coupling of spin systems to quantum phonons, this problem is rather difficult to handle analytically, which has brought much uncertainty in the interpretation of experimental data and has limited our understanding of many interesting quantum phenomena of low-dimensional magnetic materials. An analytical and nonadiabatic study of the DM interaction in spin-Peierls system will make it possible to have an insight into the intrinsical properties of the spin chain materials.

In this paper, we focus on the properties of the dimerization order parameter and the Peierls instability of a spin-Peierls chain system with the view of understanding the effects of quantum lattice fluctuations on the DM interaction in the system. A nonadiabatic analytical approach is developed to study the phonon-staggered ordering parameter, the spin dimerization gap and the phase diagram of the system. We find that the threshold value of $\beta$ is not simply a constant but

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a crossover and for appropriate fixed values of $\lambda^2 J/K$, $\omega_\pi/J$, and $\beta$, there exists a reentry of the system into spin-dimer state as $D/J$ increases. The nonadiabaticity plays an important role in suppressing the Peierls dimerization. The paper is organized as follows. In Sec. II, by mapping the Hamiltonian into the Jordan-Wigner fermions and using unitary transformations, we obtain an effective Hamiltonian from the one-dimensional spin-Peierls-Heisenberg *XY* spin chain coupled with phonons. In Sec. III we use the Green's function method to implement perturbation treatment and get the renormalized band function, the renormalized gap function, and self-consistent equation determining the dimerized lattice displacement ordering parameter. The phonon-staggered ordering parameter is calculated. In Sec. IV we study the spin dimerization gap and the phase diagrams. Finally, a brief summary will conclude our presentation in Sec. V.

## II. EFFECTIVE HAMILTONIAN

We start from the one-dimensional spin-Peierls-Heisenberg *XY* spin chain model with a coupling between spins and phonons[15,23,30,31]

$$H = \sum_l J_l \mathbf{S}_l \cdot \mathbf{S}_{l+1} + \sum_l \mathbf{D}_l \cdot (\mathbf{S}_l \times \mathbf{S}_{l+1}) + H_{\mathrm{ph}}, \tag{1}$$

where the phonon energy, the exchange energy and the module of the DM vector are, respectively,

$$H_{\mathrm{ph}} = \sum_l \left( \frac{1}{2M} P_l^2 + \frac{1}{2} K u_l^2 \right), \tag{2}$$

$$J_l = J[1 + \lambda(u_l - u_{l+1})], \tag{3}$$

$$D_l = D[1 + \lambda\beta(u_l - u_{l+1})]. \tag{4}$$

In the model, $\mathbf{S}_l$ is the spin-$\frac{1}{2}$ operator on site $l$, $J>0$ is the usual antiferromagnetic exchange energy, $u_l$ (with conjugated momentum $P_l$) is the displacement of the $l$ ion which modulates the exchange integral $J$ and the module of the DM vector, $\lambda$ is the magnetoelastic (spin-phonon) coupling constant, $K$ is the elastic constant, and $M$ the mass of ions. In this model, the spin couples to the difference between the phonon amplitudes on the two neighboring sites and the form of the lattice vibration energy leads the phonons to be dispersionless.

It has been argued that the directions of $\mathbf{D}_l$ are not changed by the dimerization,[9] however, the dependence of the isotropic exchange interaction and the DM interaction on the intersite distance may be different.[2] Therefore, two kinds of DM interaction, i.e., uniform and staggered interaction will be studied. The parameter $\beta$ is introduced to describe the effect of different DM interaction dependence on the intersite distance. If $\beta=0$ the DM interaction does not depend on the lattice distortion, i.e., DM interaction is uniform, whereas for $\beta=1$ the dependence of DM interaction on the lattice distortion is the same as that for the isotropic exchange interaction $J_l$. Although it was estimated that the DM vector had two components[15] from the specific heat, neutron scattering, and ESR measurement data of copper benzoate, the numerical study by density matrix renormalization group found that a DM vector with only one component gave the best fit to the experimental observations.[32] In view of this as well as for simplification, we choose the vector $\mathbf{D}_l$ to be directed along the *z*-axis, $\mathbf{D}_l = D_l \mathbf{k}$. Thus,

$$\begin{aligned} H = {} & J \sum_l [1 + \lambda(u_l - u_{l+1})](S_l^x S_{l+1}^x + S_l^y S_{l+1}^y) \\ & + D \sum_l [1 + \lambda\beta(u_l - u_{l+1})](S_l^x S_{l+1}^y - S_l^y S_{l+1}^x) \\ & + \sum_l \left( \frac{1}{2M} P_l^2 + \frac{1}{2} K u_l^2 \right). \end{aligned} \tag{5}$$

After the expansion of the operators of lattice modes, $u_l$ and $P_l$, by the phonon creation and annihilation operators $b_q^\dagger$ and $b_q$, and by means of mapping the Hamiltonian into the Jordan-Wigner spinless fermions and the Fourier transformation to momentum space, the Hamiltonian (5) becomes

$$\begin{aligned} H = {} & \sum_q \omega_\pi \left( b_q^\dagger b_q + \frac{1}{2} \right) + \sum_k \epsilon_k c_k^\dagger c_k \\ & + \frac{1}{\sqrt{N}} \sum_{k,q} g(k, k+q)(b_{-q}^\dagger + b_q) c_{k+q}^\dagger c_k, \end{aligned} \tag{6}$$

where $N$ is the total number of sites. The bare band function of the fermions, the phonon frequency and the coupling function are

$$\epsilon_k = J \cos k - D \sin k, \tag{7}$$

$$\omega_\pi = \sqrt{\frac{K}{M}}, \tag{8}$$

$$\begin{aligned} g(k, k+q) = {} & i\lambda \sqrt{\frac{1}{2M\omega_\pi}} \{ J[\sin k - \sin(k+q)] \\ & + D\beta[\cos k - \cos(k+q)] \}. \end{aligned} \tag{9}$$

Within the static assumption and adiabatic limit approximation, this model can be solved exactly,[31] while for realistic case, when the quantum phonons are taken into account, the theoretical analysis becomes much more difficult. In following, we will treat the Hamiltonian (6) nonadiabatically.

Since $\epsilon_k$ can be rewritten as

$$\epsilon_k = J\eta \cos(k + \alpha), \tag{10}$$

with $\alpha = \arctan(D/J)$ and $\eta = \sqrt{1 + (D/J)^2}$, the Fermi level is given by the condition $\epsilon_{k_F} = 0$, and therefore the Fermi wave vector $k_F = \pm \pi/2 - \alpha$. In momentum space, compared with the spin-Peierls system without the DM interaction, the Fermi surface $k_F$ shifts by $\alpha$ as $D$ varies, but the size of the Fermi sea is unchanging. Accordingly, the filling situation of fermions of this system is also unchanging.

The spin-phonon coupling and the Peierls dimerization are two main respects in this model. In order to take into account the spin-phonon correlation and the static phonon-staggered ordering induced by the move of the neighboring ions in opposite directions in the dimerized state to form a

dimer pattern, the unitary transformation is applied to $H$,[33,34] $\tilde{H}=\exp(S)H\exp(-S)$. After averaging the transformed Hamiltonian over the phonon vacuum state we get an effective Hamiltonian for the fermions

$$H_{\text{eff}}=\frac{1}{2}KNu_0^2+\sum_k E_0(k)c_k^\dagger c_k+\sum_k i\Delta_0(k)c_{k-\pi}^\dagger c_k - \frac{1}{N}\sum_{q,k,k'}\frac{g(k,k+q)g(k',k'-q)}{\omega_\pi} \times\delta(k+q,k)[2-\delta(k'-q,k')]c_{k+q}^\dagger c_k c_{k'-q}^\dagger c_{k'}, \quad (11)$$

where

$$E_0(k)=\epsilon_k-\frac{1}{N}\sum_{k'}\frac{g(k',k)g(k,k')}{\omega_\pi^2}\delta(k',k)\delta(k,k')(\epsilon_k-\epsilon_{k'}), \quad (12)$$

$$\Delta_0(k)=2\lambda u_0[J\sin k+D\beta\cos k][1-\delta(k-\pi,k)], \quad (13)$$

and

$$\delta(k+q,k)=(1+|\epsilon_{k+q}-\epsilon_k|/\omega_\pi)^{-1} \quad (14)$$

is a function of the energies of the incoming and outgoing fermions in the fermion-phonon scattering process. The dimerized lattice displacement ordering parameter $u_0$ can be determined by the variational principle to minimize the ground state energy.

Note that in the adiabatic limit, where $\omega_\pi=0$, one has $\delta(k',k)=0$ and $H_{\text{eff}}$ goes back to the adiabatic mean-field Hamiltonian

$$H_{\text{eff}}(\omega_\pi=0)=\frac{1}{2}KNu_0^2+\sum_k\epsilon_k c_k^\dagger c_k + \sum_k i2\lambda u_0[J\sin k+D\beta\cos k]c_{k-\pi}^\dagger c_k. \quad (15)$$

By means of the Bogoliubov transformation (15) can be diagonalized exactly. Thus, our effective Hamiltonian works well in the adiabatic limit $\omega_\pi=0$. In fact, if we take the static assumption and adiabatic limit (neglect the kinetic energy), i.e., let $\lambda(u_l-u_{l+1})=(-1)^l\delta$, after the Jordan-Wigner and the Fourier transformations, the Hamiltonian (5) becomes

$$H=\frac{1}{2}KN\left(\frac{\delta}{2\lambda}\right)^2+\sum_k(J\cos k-D\sin k)c_k^\dagger c_k + \sum_k i\delta(J\sin k+D\beta\cos k)c_{k-\pi}^\dagger c_k. \quad (16)$$

If we let $\delta=2\lambda u_0$, this model is same as that of our effective Hamiltonian in the adiabatic limit (15). This model can be solved exactly and the ground state energy is

$$E_g=\frac{1}{2}KN\left(\frac{\delta}{2\lambda}\right)^2 - \sum_{k>0}\sqrt{(J\cos k-D\sin k)^2+\delta^2(J\sin k+D\beta\cos k)^2}. \quad (17)$$

By means of the variational principle, the equation to determine $\delta$ can be obtained,

$$1=\frac{1}{N}\sum_{k>0}\frac{4\lambda^2}{K}\frac{(J\sin k+D\beta\cos k)^2}{\sqrt{(J\cos k-D\sin k)^2+\delta^2(J\sin k+D\beta\cos k)^2}}. \quad (18)$$

The last term in $H_{\text{eff}}$ is a four-fermion interaction. As we are dealing with a one-dimensional system in nonadiabatic circumstances due to finite phonon frequency $\omega_\pi$, how to treat this four-fermion interaction is a difficult problem.

## III. ANALYTIC APPROACH

Note that the four-fermion term in Eq. (11) goes to zero when $\omega_\pi\to 0$ [see Eq. (15)], therefore, in this case, the four-fermion term can be treated as a perturbation $H'_{\text{eff}}$ and the others as unperturbed Hamiltonian $H^0_{\text{eff}}$. We use the Green's function method to implement the perturbation treatment. The unperturbed Green's function is

$$G_0(k,\omega_n)=\{i\omega_n-E_0(k)\sigma_z-\Delta_0(k)\sigma_x\}^{-1}.$$

The self-energy $\Sigma^*(k,\omega_n)$ can be calculated by the perturbation theory[35]

$$\begin{aligned}\Sigma^*(k,\omega_n)=&-\frac{T}{N}\sum_{k'>0}\sum_m\frac{g(k,k)g(k',k')}{\omega_\pi}T_r[\sigma_z G_0(k',\omega_m)]\sigma_z\\ &+\frac{T}{N}\sum_{k'>0}\sum_m\frac{g(k,k')g(k',k)}{\omega_\pi}\delta(k',k)[2-\delta(k,k')][G_0(k',\omega_m)+\sigma_z G_0(k',\omega_m)\sigma_z]\\ &+\frac{T}{N}\sum_{k'>0}\sum_m\frac{g(k-\pi,k')g(k'-\pi,k)}{\omega_\pi}\delta(k',k-\pi)[2-\delta(k,k'-\pi)][i\sigma_y G_0(k',\omega_m)i\sigma_y-\sigma_x G_0(k',\omega_m)\sigma_x]\\ &-\frac{T}{N}\sum_{k'>0}\sum_m\frac{g(k-\pi,k)g(k'-\pi,k')}{\omega_\pi}[\delta(k,k-\pi)+\delta(k',k'-\pi)\\ &-\delta(k,k-\pi)\delta(k',k'-\pi)]\{T_r[i\sigma_y G_0(k',\omega_m)]i\sigma_y+T_r[\sigma_x G_0(k',\omega_m)]\sigma_x\}. \quad (19)\end{aligned}$$

In the perturbation calculation we have taken into account the fact that the forward and backward scattering terms contribute nothing to the "charge" gap.[36,37] From Eq. (19) one can get that $\Sigma^*(k,\omega_n)$ is irrelative to $\omega_n$, therefore the spectrum structure of $G(k,\omega_n)$ should be

$$G(k,\omega_n) = \{i\omega_n - E(k)\sigma_z - \Delta(k)\sigma_x\}^{-1}.$$

From $G(k,\omega_n)$ the renormalized band function and the gap function can be derived

$$E(k) = E_0(k) - \frac{1}{N}\sum_{k'} \frac{g(k,k')g(k',k)}{\omega_\pi} \times \delta(k',k)[2 - \delta(k,k')]\frac{E_0(k')}{\sqrt{E_0^2(k') + \Delta_0^2(k')}}, \quad (20)$$

$$\Delta(k) = 2\lambda u_0(J\sin k + D\beta\cos k)[c - d\delta(k-\pi,k)], \quad (21)$$

where

$$c = 1 + \frac{1}{N}\sum_{k>0} \frac{2\lambda^2}{K}(J\sin k + D\beta\cos k) \times \delta(k-\pi,k)\frac{\Delta_0(k)}{2\lambda u_0\sqrt{E_0^2(k) + \Delta_0^2(k)}}, \quad (22)$$

$$d = c - \frac{1}{N}\sum_{k>0} \frac{2\lambda^2}{K}(J\sin k + D\beta\cos k)\frac{\Delta_0(k)}{2\lambda u_0\sqrt{E_0^2(k) + \Delta_0^2(k)}}. \quad (23)$$

The self-consistent equation to determine $u_0$ is

$$1 = \frac{1}{N}\sum_{k>0} \frac{4\lambda^2}{K}(J\sin k + D\beta\cos k)^2[1 - \delta(k-\pi,k)] \times \frac{c - d\delta(k-\pi,k)}{\sqrt{E^2(k) + \Delta^2(k)}}. \quad (24)$$

If let $\omega_\pi = 0$ and $\delta = 2\lambda u_0$, this equation becomes the same as Eq. (18). This also verifies our effective Hamiltonian works well in the adiabatic limit.

For investigation on the nonadiabatic effect on DM interaction to the dimerization of the system, we calculate the phonon-staggered ordering parameter

$$m_p = \frac{1}{N}\sum_l (-1)^l\langle u_l\rangle = \frac{1}{N}\sum_{k>0}\frac{2\lambda}{K}[J\sin k + D\beta\cos k]\frac{\Delta(k)}{\sqrt{E^2(k) + \Delta^2(k)}}. \quad (25)$$

In the nonadiabatic case, the phonon-staggered ordering parameter $m_p$ is determined by not only $D$ and $\beta$ but also $\lambda$ and $\omega_\pi$. Figure 1(a) shows the dimensionless parameter $\lambda m_p$ as functions of the spin-phonon coupling $\lambda^2 J/K$ in the cases of $D/J=0.6, \omega_\pi/J=0.01$ with different staggered DM interaction parameters, $\beta=0.9$ (dash line), 0.5 (solid line), and 0.1 (dash-dot line). One can see that because of the nonadiabatic effect, for a certain value of $\beta$, there exists a finite critical value of spin-phonon coupling constant. $\lambda m_p$ decreases as the coupling constant or $\beta$ decreases. At the critical value [for example, $(\lambda^2 J/K)_c = 0.114$ for $\beta=0.5$, $D/J=0.6$, and $\omega_\pi/J=0.01$], $\lambda m_p$ disappears. The result of the adiabatic limit ($\omega_\pi=0, \beta=0.5$) is also shown in dot line for comparison. If there is no DM interaction, the system is never really gapless within the adiabatic approach, because $\lambda m_p$ remains nonzero, although it becomes very small for weak spin-phonon coupling, but, as shown in the figure, the finite DM interaction leads the system to have a finite critical value of spin-phonon coupling even in the adiabatic limit. The dependences of $\lambda m_p$ on the phonon frequency $\omega_\pi/J$ in the case of $D/J=0.6, 2\lambda^2 J/K=0.6$ are plotted in Fig. 1(b) for $\beta=0.1$ (dot line), 0.5 (dash line), and 0.9 (solid line). $\lambda m_p$ decreases as the phonon frequency increases or $\beta$ decreases. At the critical value $\omega_{\pi c}$, $\lambda m_p$ goes to zero, which indicates that the quantum lattice fluctuations can destroy the dimerized Peierls state. The increase of the staggered DM interaction $\beta$ will decrease the critical value of spin-phonon coupling, but increase that of phonon frequency, therefore, favors the dimerization.

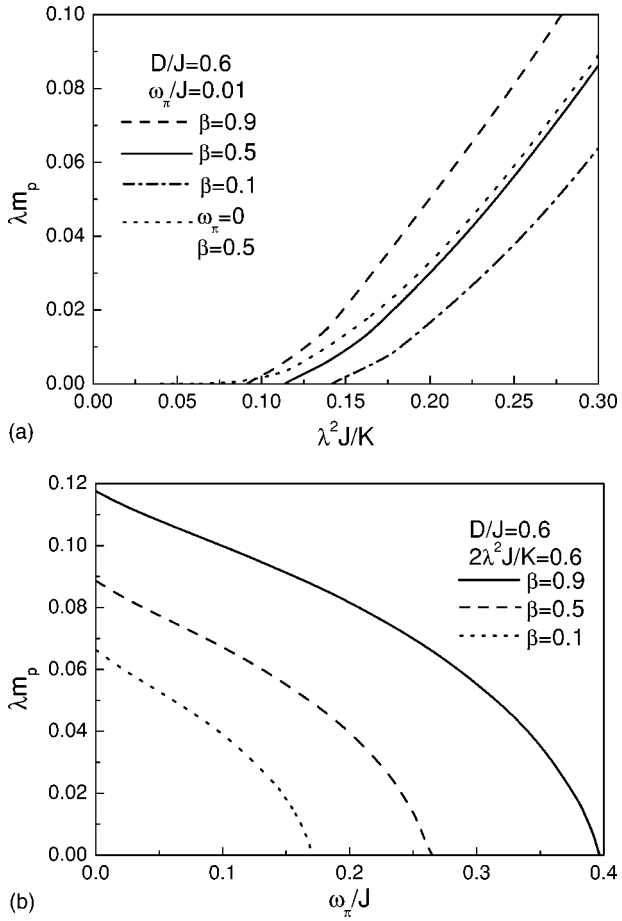


FIG. 1. (a) The dimensionless parameter $\lambda m_p$ as functions of the spin-phonon coupling $\lambda^2 J/K$ in the cases of $D/J=0.6, \omega_\pi/J=0.01$ with different staggered DM interaction parameters, $\beta=0.9$ (dash line), 0.5 (solid line), and 0.1 (dash-dot line). The dot line is the result of the adiabatic limit ($\omega_\pi=0, \beta=0.5$). (b) The dependences of $\lambda m_p$ on the phonon frequency $\omega_\pi/J$ in the cases of $D/J=0.6, 2\lambda^2 J/K=0.6$ for $\beta=0.1$ (dot line), 0.5 (dash line), and 0.9 (solid line).

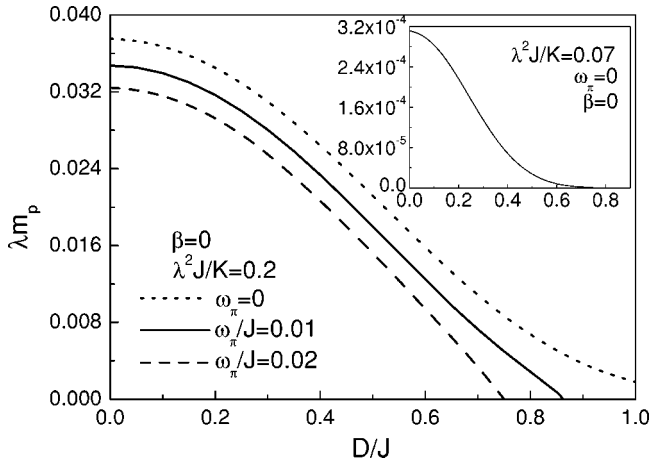


FIG. 2. The phonon-staggered ordering parameter $\lambda m_p$ as functions of the uniform DM interaction $D/J$ for the spin-phonon coupling $\lambda^2 J/K=0.2$ with different phonon frequencies $\omega_\pi/J=0.01$ (solid line) and 0.02 (dash line). The dot line is the adiabatic limit results. Inset: the uniform DM interaction can destroy the dimerization state even in the adiabatic limit. The parameter values used in the inset are $\beta=0, \omega_\pi=0$, and $\lambda^2 J/K=0.07$.

When $\beta=0$ the DM interaction is uniform. The phonon-staggered ordering parameter $\lambda m_p$ as functions of the uniform DM interaction $D/J$ are plotted in Fig. 2 for the spin-phonon coupling $\lambda^2 J/K=0.2$ with different phonon frequencies $\omega_\pi/J=0.01$ (solid line) and 0.02 (dash line). The dot line is the adiabatic limit results. It is evident that the nonadiabaticity plays an important role in suppressing the Peierls dimerization. The uniform DM interaction also acts against the dimerization and can destroy the dimerization state even in the adiabatic limit if the spin-phonon coupling is small, which can be seen clearly in the inset of this figure. The parameter values used in the inset are $\beta=0$, $\omega_\pi=0$, and $\lambda^2 J/K=0.07$.

If $0<\beta\leqslant 1$, the DM interaction includes both the uniform and the staggered components. Figure 3(a) shows the phonon-staggered ordering parameter $\lambda m_p$ as functions of $D/J$ in the cases of $\lambda^2 J/K=0.5$ and $\omega_\pi/J=0.01$ with different staggered DM interaction parameters from $\beta=1.0$ (line 1) to $\beta=0$ (line 6). One can see that for large $\beta$, the effect of the DM interaction is to increase the dimerization, while the nonadiabatic effect is to suppress it. When $\beta$ is small, the effect of the DM interaction on the dimerization is contrary to that of large $\beta$. Obviously, there exists a finite threshold value of $\beta$. When $\beta$ increases to cross this value, the effect of the DM interaction on the dimerization changes from suppression to promotion. In the studying system, the total contribution to the dimerization comes from the result of competitions between the lattice distortion, the spin dimerization, the uniform and the staggered DM interactions, and the change of $\beta$ strongly influences the competition result. The threshold value $\beta_c$ can be obtained by letting the variation $\partial m_p/\partial D=0$ $(D\neq 0)$, and in the nonadiabatic case, $\beta_c$ is determined by a set of values of $D$, $\lambda$, and $\omega_\pi$. If $\beta_c$ was simply a constant as previous works predicted,[23,24] $\lambda m_p$ would not change with $D$ when $\beta=\beta_c$ as is shown in dash line in this figure. However, in view of the determination of $m_p$ by

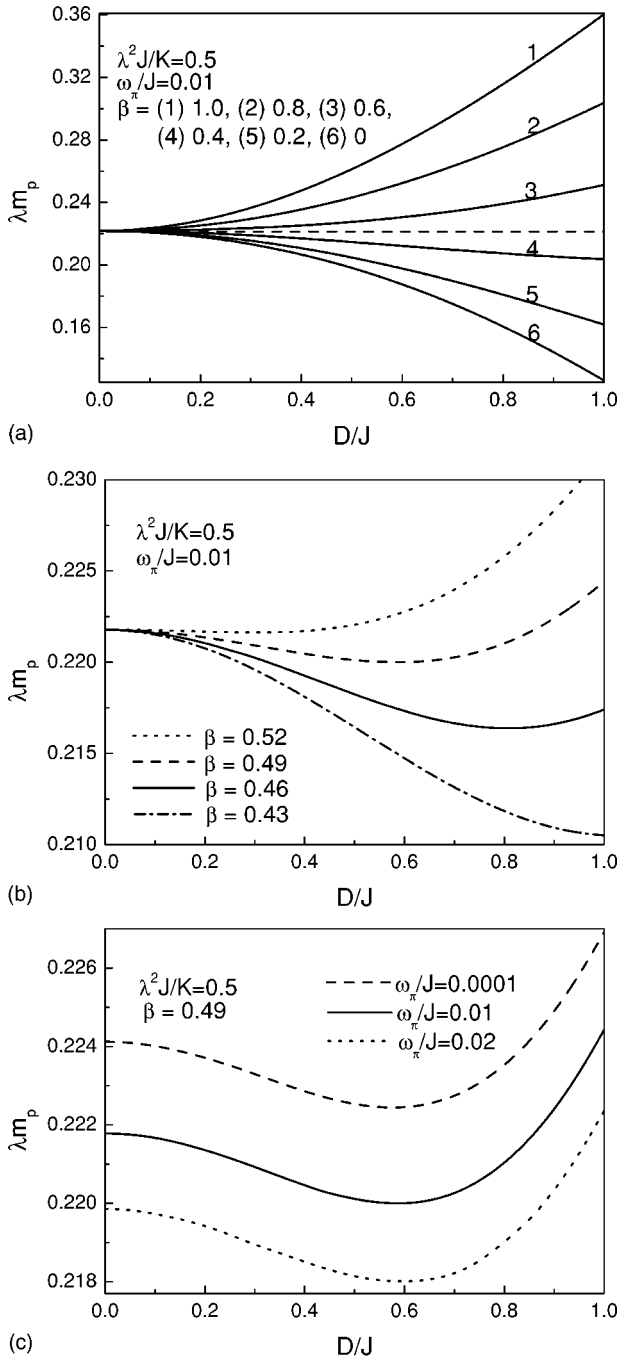


FIG. 3. (a) The phonon-staggered ordering parameter $\lambda m_p$ as functions of $D/J$ in the cases of $\lambda^2 J/K=0.5$ and $\omega_\pi/J=0.01$ with different staggered DM interaction parameters from $\beta=1.0$ (line 1) to $\beta=0$ (line 6). (b) The change of $\lambda m_p$ with $D/J$ in the region of the crossover for different staggered DM interaction parameters $\beta=0.43$ (dash-dot line), 0.46 (solid line), 0.49 (dash line), and 0.52 (dot line) in the case of $\lambda^2 J/K=0.5$ and $\omega_\pi/J=0.01$. (c) The effect of quantum lattice fluctuations on the dimerization parameter in the crossover in the case of $\lambda^2 J/K=0.5$ and $\beta=0.49$ with different phonon frequencies $\omega_\pi/J=0.0001$ (dash line), 0.01 (solid line), and 0.02 (dot line).

$D$, $\beta$, $\lambda$, and $\omega_\pi$, one might wonder why the DM interaction should have no effect on dimerization when $\beta=\beta_c$. Our calculation indicates that $\beta_c$ is not simply a constant but a cross-

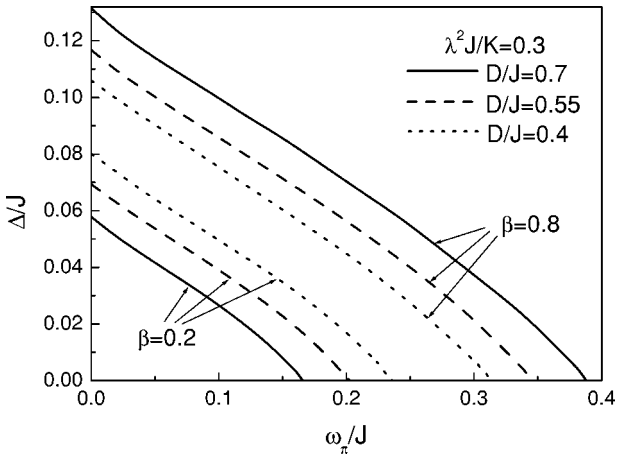


FIG. 4. The dimerization gap as function of the phonon frequency in the cases of $J\lambda^2/K=0.3$ with different DM interaction parameters.

over which makes the behavior of the DM interaction in the region of this crossover to be complicated. The change of $\lambda m_p$ with $D/J$ in the region of this crossover is presented in Fig. 3(b) for different staggered DM interaction parameters $\beta=0.43$ (dash-dot line), 0.46 (solid line), 0.49 (dash line), and 0.52 (dot line) in the case of $\lambda^2 J/K=0.5$ and $\omega_\pi/J=0.01$. We find that for certain $\lambda^2 J/K$ and $\omega_\pi/J$, the crossover has its bottom boundary $\beta_{\mathrm{bot}}$ and top one $\beta_{\mathrm{top}}$. When $\beta$ is smaller (larger) than $\beta_{\mathrm{bot}}$ ($\beta_{\mathrm{top}}$), $\lambda m_p$ decreases (increases) monotonously as $D/J$ increases, while when $\beta_{\mathrm{bot}}<\beta<\beta_{\mathrm{top}}$, as $D/J$ increases $\lambda m_p$ decreases at first until it reaches its minimum at a definite value of $D/J$, and thereafter increases. The definite value of $D/J$ changes from 1 to zero when $\beta$ changes from $\beta_{\mathrm{bot}}$ to $\beta_{\mathrm{top}}$. The effect of quantum lattice fluctuations on the dimerization parameter in the crossover is illustrated in Fig. 3(c) in the cases of $\lambda^2 J/K=0.5$ and $\beta=0.49$ with different phonon frequencies $\omega_\pi/J=0.0001$ (dash line), 0.01 (solid line), and 0.02 (dot line).

## IV. SPIN DIMERIZATION AND PHASE DIAGRAM

In the spin dimerized state the Peierls distortion opens a gap at the Fermi surface. Substituting the Fermi wave vector $k_F=\pm\pi/2-\alpha$ into the gap function Eq. (21), we get the dimerization gap

$$\Delta=\Delta(k_F)=2\lambda u_0(J\cos\alpha+D\beta\sin\alpha)(c-d). \tag{26}$$

It can be rewritten in dimensionless form as

$$\Delta/J=2\lambda u_0(c-d)\frac{1+\beta(D/J)^2}{\sqrt{1+(D/J)^2}}. \tag{27}$$

Figure 4 shows the dimerization gap as function of the phonon frequency in the cases of $J\lambda^2/K=0.3$ with different DM interaction parameters. The dimerization gap decreases as the phonon frequency increases, and at the critical value of phonon frequency the system becomes gapless. This figure also shows clearly whether the effect of the DM interaction on the dimerization is suppression or promotion depends on the value of staggered DM interaction parameter $\beta$. Calculations from Eqs. (25) and (26) indicate that $m_p$ and $\Delta$ vanish at the same critical value of $\omega_\pi$, which implies that the lattice distortion and the spin dimerization are two inseparable features of the spin-Peierls ground state.

From Eq. (24), let $u_0=0$, we get the self-consistent equation of phase-transition points

$$1=\frac{1}{N}\sum_{k>0}\frac{4\lambda^2}{K}(J\sin k+D\beta\cos k)^2[1-\delta(k-\pi,k)]\times\frac{c-d\,\delta(k-\pi,k)}{|E(k)|}. \tag{28}$$

Figure 5(a) shows the phase diagram of our result in the $\omega_\pi/J\sim 2\lambda^2 J/K$ plane. As shown in the figure, the increase in $D/J$ leads the phase boundary to move to a larger spin-phonon coupling when $\beta$ is small (solid and dash-dot lines), but move to smaller one when $\beta$ is large (dash and dot lines). To a fixed spin-phonon coupling, there exists a finite critical value of the phonon frequency. As the phonon frequency increases to the critical value, the spin dimerization state is destroyed and the system becomes gapless. Figure 5(b) shows the ground-state phase diagram in the $\beta\sim D/J$ plane in the cases of $\omega_\pi/J=0.01$ with different spin-phonon couplings. One can see that to a certain definite phonon frequency, the spin-phonon coupling has a divide-line value which is not dependent on $D/J$ or $\beta$. Along a phase boundary determined by a certain spin-phonon coupling being smaller (much larger) than the divide-line value, $\beta$ decreases (increases) as $D/J$ increases. If the spin-phonon coupling is larger than, but not too much, the divide-line value, along a phase boundary, as $D/J$ increases the staggered DM interaction parameter $\beta$ increases first until it reaches its maximum, and then decreases. This implies that on a phase boundary line, to same $\beta,\lambda^2 J/K$ and $\omega_\pi/J, D/J$ can take two different values, which can be seen clearly in Fig. 5(c). This phase diagram shows the influences of DM interaction on phase transition in the $\lambda^2 J/K\sim\beta$ plane for $\omega_\pi/J=0.01$ with $D/J=0.2$ (dash line) and 0.6 (solid line). In Fig. 5(d), the phase diagram is shown in the $\lambda^2 J/K\sim D/J$ plane for $\omega_\pi/J=0.01$ with $\beta=0.62$ (solid line) and 0.64 (dash line). The inset in this figure illustrates a full view of the phase diagram for hole range of $\beta$ ($\beta=0$, 0.65, and 1). This figure indicates that for appropriate fixed values of $\beta$, $\lambda^2 J/K$, and $\omega_\pi/J$, there exist two critical values of DM interaction $(D/J)_{c1}$ and $(D/J)_{c2}$. As $D/J$ increases from zero to 1, at first, the system is in the spin-dimer state. At the first critical value $(D/J)_{c1}$, the dimerization gap disappears and the system becomes gapless. At the second critical value $(D/J)_{c2}$, the system reenters the spin-dimer state. For example, by using the input parameters $\omega_\pi/J=0.01, 2\lambda^2 J/K=0.212$, and $\beta=0.62$, we obtain $(D/J)_{c1}=0.403$ and $(D/J)_{c2}=0.899$.

## V. CONCLUSIONS

The effects of quantum lattice fluctuations on the DM interaction in the spin-Peierls chain model have been studied through a nonadiabatic analytical approach and the phonon-

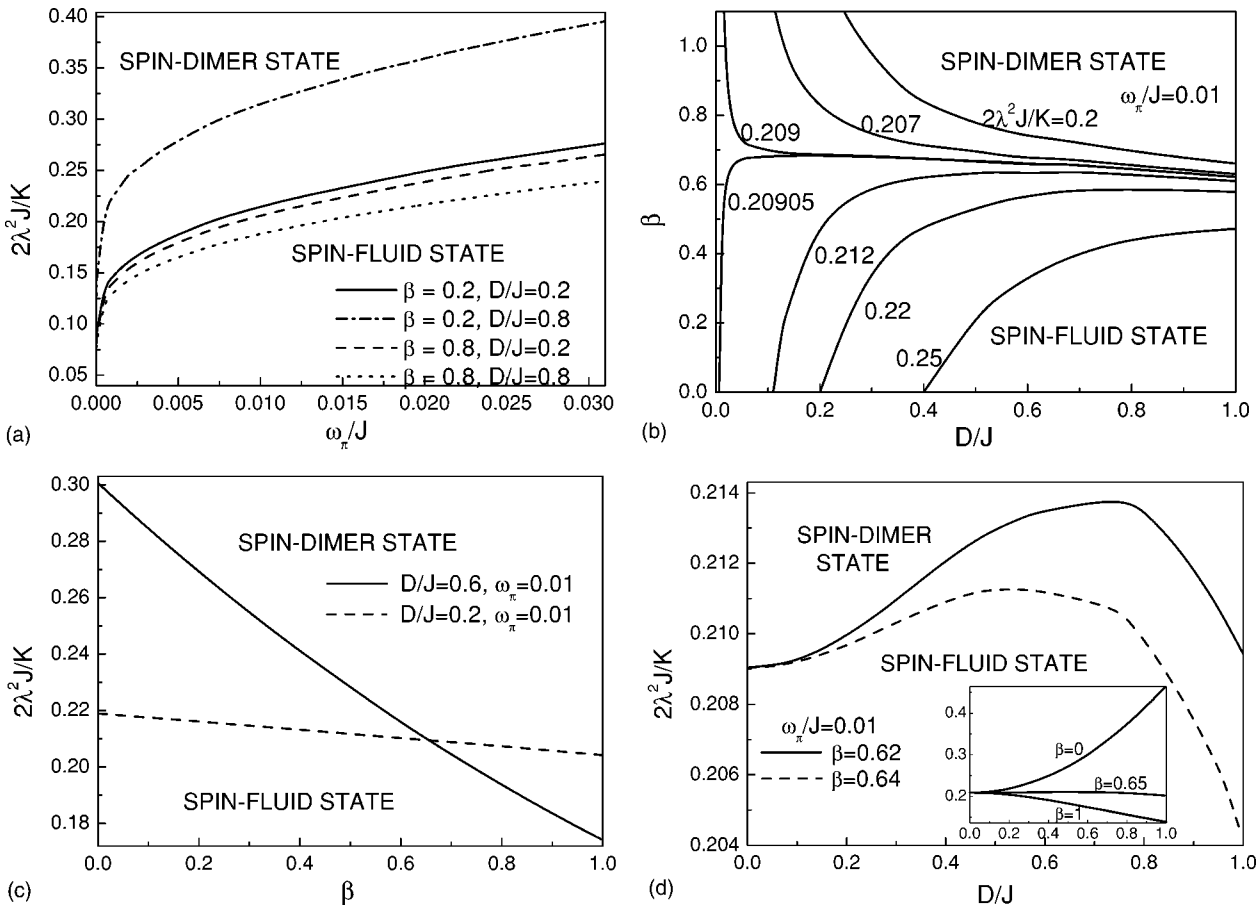


FIG. 5. (a) The phase diagram in the $\omega_\pi/J \sim 2\lambda^2 J/K$ plane. (b) The ground-state phase diagram in the $\beta \sim D/J$ plane in the cases of $\omega_\pi/J=0.01$ with different spin-phonon couplings. (c) The influences of DM interaction on phase transition in the $\lambda^2 J/K \sim \beta$ plane for $\omega_\pi/J=0.01$ with $D/J=0.2$ (dash line) and 0.6 (solid line). (d) The phase diagram in the $\lambda^2 J/K \sim D/J$ plane for $\omega_\pi/J=0.01$ with $\beta=0.62$ (solid line) and 0.64 (dash line). The inset illustrates a full view of the phase diagram for hole range of $\beta$ ($\beta=0$, 0.65, and 1).

staggered ordering parameter, the spin dimerization gap as well as the phase diagram of the system are derived. The results show that in the nonadiabatic case, to a certain finite phonon frequency, there exists a finite critical value of the spin-phonon coupling constant. As the spin-phonon coupling decreases to the critical value, the system becomes gapless and the spin dimerization is destroyed. The DM interaction leads the system to have a finite critical value of spin-phonon coupling even in the adiabatic limit. The increase in staggered DM interaction will decrease the critical value of spin-phonon coupling, but increase that of phonon frequency, therefore, favors the dimerization. The nonadiabaticity plays an important role in suppressing the effects of the uniform DM interaction on the dimerization. For large $\beta$, the effect of the DM interaction is to increase the dimerization, while the nonadiabatic effect is to suppress it. When $\beta$ is small, the effect of the DM interaction on the dimerization is contrary to that of large $\beta$. Obviously, there exists a finite threshold value of $\beta$. When $\beta$ increases to cross this value, the effect of the DM interaction on the dimerization changes from suppression to promotion. Furthermore, our result indicates that the threshold value of $\beta$ is not simply a constant but a crossover which makes the behavior of the DM interaction in the region of this crossover to be complicated. For appropriate fixed values of $\lambda^2 J/K$, $\omega_\pi/J$, and $\beta$ (in the crossover region), as $D/J$ increases from zero to 1, the phase of the system transits from spin-dimer state to gapless state, and, then, enters the spin-dimer state again.

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