

Adiabatic-antiadiabatic crossover in a spin-Peierls chain

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We consider an XXZ spin-1/2 chain coupled to optical phonons with nonzero frequency ω_0 . In the adiabatic limit (small ω_0), the chain is expected to spontaneously dimerize and open a spin gap, while the phonons become static. In the antiadiabatic limit (large ω_0), phonons are expected to give rise to frustration, so that dimerization and formation of spin gap are obtained only when the spin-phonon interaction is large enough. We study this crossover using bosonization technique. The effective action is solved both by the self-consistent harmonic approximation (SCHA) and by renormalization group (RG) approach starting from a bosonized description. The SCHA allows to analyze the low-frequency regime and determine the coupling constant associated with the spin-Peierls transition. However, it fails to describe the SU(2) invariant limit. This limit is tackled by the RG. Three regimes are found. For $\omega_0 \ll \Delta_s$, where Δ_s is the gap in the static limit $\omega_0 \rightarrow 0$, the system is in the adiabatic regime, and the gap remains of order Δ_s . For $\omega_0 > \Delta_s$, the system enters the antiadiabatic regime, and the gap decreases rapidly as ω_0 increases. Finally, for $\omega_0 > \omega_{BKT}$, where ω_{BKT} is an increasing function of the spin-phonon coupling, the spin gap vanishes via a Berezinskii-Kosterlitz-Thouless transition. Our results are discussed in relation with numerical and experimental studies of spin-Peierls systems.

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I. INTRODUCTION

The properties of the spin-Peierls (SP) state in quasi-one-dimensional materials has attracted considerable attention over the last decades since its discovery in the organic compounds of the TTF and TCNQ series,¹⁻³ and more recently in the inorganic compound CuGeO₃.^{4,5} In analogy to the Peierls instability in quasi-one-dimensional metals,⁶ a spin chain undergoes a SP transition by dimerizing into an alternating pattern of weak and strong bonds,⁷⁻⁹ with the magnetic energy gain compensating the energy loss from the lattice deformation. Although this physical picture gives a good qualitative understanding of the SP phenomenon, the real SP transition is in fact much more complicated to describe. In particular, the above picture of SP transition is only valid in the adiabatic regime, in which the frequency of the phonons is negligible compared to the magnetic energy scales in the system, such as the spin gap or the exchange interaction J . The validity of this approximation is clearly dependent on the system at hand. Recently, it was pointed out that the difference between CuGeO₃ and the other SP compounds consists in the high energy of the optical phonons involved in the transition, which is of the order of the exchange integral J .¹⁰⁻¹² Another feature that distinguishes CuGeO₃ from the other organic SP compounds is that no softening of the phonon modes is observed near the transition. All these findings stem from the fact that an adiabatic treatment of the phonon subsystem^{8,9} is inadequate to describe the SP transition in CuGeO₃, and an appropriate treatment of phonons in the antiadiabatic regime is required.^{13,14}

Unfortunately, not many analytical methods to study the system of coupled spin and phonons in the full frequency range are available. The main difficulty relies in the fact that when the phonon frequency becomes comparable to the energy gap in the spin-excitation spectrum, one is entering a quantum regime in which quantum fluctuations completely impregnate the ground state. This is why many of the known studies involving dynamical phonons rely on numerical methods such as exact diagonalization (ED),¹⁵⁻¹⁸ strong coupling expansions,¹⁹ density matrix renormalization group²⁰⁻²³ (DMRG), or quantum Monte Carlo simulations.²⁴⁻²⁸ From the analytical point of view, various approaches have been developed, but they work well either in adiabatic or in the antiadiabatic regime. In the former case, most approaches are based on the mean-field approximation.^{9,29,30} In the latter case, various perturbation studies were performed to derive an effective spin Hamiltonian.^{31,32} Another approach was developed, based on integrating out the phonon modes,³³ in order to map the model onto the Gross-Neveu model,³⁴ for which various exact results are available.^{35,36} Other approaches are based on the flow-equation method¹³ that works well in the antiadiabatic regime, or on the unitary transformation method for the XY spin chain.³⁷ Since various compounds are rather close to the border between the two regimes,¹² it would be thus highly desirable to have a good method to tackle the adiabatic-antiadiabatic crossover. In this paper we provide such a method. We combine the renormalization group (RG) method and the self-consistent harmonic approximation

(SCHA) to study the adiabatic-antiadiabatic crossover in a spin-1/2 Heisenberg chain coupled to dynamical phonons. A previous attempt to use the RG to study this adiabatic-antiadiabatic crossover has been published.³⁸ We will comment on the differences of the two approaches.

The plan of the paper is as follows. In Sec. II we introduce the model of spin chain coupled to dynamical phonons, and write it in the continuum limit using the bosonization representation. In Sec. III we describe a variational approach, inspired from the self-consistent harmonic approximation, and use it to describe the crossover. In the adiabatic regime we find an expression for the spin-Peierls gap consistent with the mean-field treatment of Cross and Fisher.⁹ In the antiadiabatic regime, the gap is essentially described by a sine-Gordon model. In Sec. IV we study the crossover using a renormalization group method. The RG is specially well adapted around the Heisenberg isotropic point. This allows one to extract the phase diagram as a function of the strength of the electron-phonon coupling and the phonon frequency. In Sec. V we discuss the findings of the two methods, both relative to each other and in connection with experiments. Conclusions can be found in Sec. VI, and some technical details have been put in the appendices.

II. MODEL AND CONTINUUM LIMIT

As a simple model which describes a SP system in the following we consider an antiferromagnetic spin-1/2 chain coupled to a set of Einstein oscillators, given by

$$H = H_s + H_p + H_{sp}, \quad (1)$$

with

$$H_s = J \sum_n \mathbf{S}_n \cdot \mathbf{S}_{n+1}, \quad (2)$$

$$H_p = \sum_n \left[\frac{p_n^2}{2m} + \frac{m}{2} \omega_0^2 q_n^2 \right], \quad (3)$$

where \mathbf{S}_n are spin-1/2 operators, $J > 0$, $[q_n, p_{n'}] = i \delta_{n,n'}$. The quantity $m\omega_0^2 = k_e$ is the stiffness of the Einstein phonon. The interaction of spins with phonons can be modeled by

$$H_{sp} = g \sum_n q_n \mathbf{S}_n \cdot \mathbf{S}_{n+1}. \quad (4)$$

The coupling to optical phonons described by (4) is adequate for the CuGeO₃ since it would correspond to a side group effect by Germanium atoms as discussed in Refs. 39 and 40. Acoustic phonons could of course be treated in a very similar way, but one would have to replace q_n with $(q_{n+1} - q_n)$. Note that some authors^{13,18} prefer to diagonalize the phonon Hamiltonian in (2) using the boson operator $b = \sqrt{m\omega_0/2} q + ip/\sqrt{2m\omega_0}$, and write the interaction $\tilde{g} \sum_n (b_n^\dagger + b_n) \mathbf{S}_n \cdot \mathbf{S}_{n+1}$. It is obvious that one has $\tilde{g} = g/\sqrt{2m\omega_0}$. This remark will be useful when we will compare the results of the different approaches. The adiabatic limit is $\omega_0 \rightarrow 0$, $m \rightarrow \infty$ with k_e fixed. In that limit, the phonons become classical, i.e., the q_n 's commute with the Hamiltonian (1), and one can simply mini-

mize the ground state energy with respect to their expectation value. In that limit, the results of Ref. 9 are recovered. The opposite antiadiabatic limit is $\omega_0 \rightarrow \infty$. In that limit, one can integrate out the phonons, and one is left with the Hamiltonian of a frustrated spin-1/2 chain.³¹ For a frustration large enough,⁴¹⁻⁴³ i.e., for large enough spin-phonon coupling, a spontaneous dimerization of the spins takes place, and the system presents a spin gap. Our purpose is to provide a unified treatment of these two limits.

To solve the spin-phonon problem, we use first the well-known Jordan-Wigner transformation to express the spin operators in terms of spinless fermions. Thus, the Hamiltonian H_s becomes

$$H_f = -t \sum_n [c_{n+1}^\dagger c_n + \text{H.c.}] + V \sum_n \left(c_{n+1}^\dagger c_{n+1} - \frac{1}{2} \right) \left(c_n^\dagger c_n - \frac{1}{2} \right), \quad (5)$$

with $t = J/2$ and $V = J$. The spin-phonon Hamiltonian H_{sp} is transformed into

$$H_{fp} = g \sum_n q_n \left[\frac{1}{2} (c_{n+1}^\dagger c_n + c_n^\dagger c_{n+1}) + \left(c_{n+1}^\dagger c_{n+1} - \frac{1}{2} \right) \left(c_n^\dagger c_n - \frac{1}{2} \right) \right]. \quad (6)$$

We now proceed in the standard way to take the continuum limit (see, e.g., Ref. 44, Chap. 6). In the continuous approximation, (6) generates a coupling between the lattice deformation (phonon mode) and the $q = 2k_F = \pi$ component of the charge density, $\rho(2k_F, x)$.

In order to get a continuous description we separate fast and slow components of the phonon field and similarly for the fermion fields, and we get the interaction⁴⁵

$$H_{fp} = i \int dx [q(x) \rho(2k_F, x) - \text{H.c.}]. \quad (7)$$

We now use the boson representation of one dimensional fermion operators. In this representation the Hamiltonian H_f becomes

$$H_f = \frac{1}{2\pi} \int dx uK [\pi \Pi(x)]^2 + \frac{u}{K} [\nabla \phi(x)]^2, \quad (8)$$

where the field $\phi(x)$ is related to the density of fermions⁴⁴ and $[\phi(x), \Pi(x')] = i \delta(x-x')$. We have $u = (\pi/2)J\alpha$, with α the lattice spacing, $K = 1/2$, $q_n = q(x = n\alpha)$ and we have kept only the most relevant terms. Changing the parameter K allows one to explore the more general case of XXZ spin chains with an easy plane anisotropy.⁴⁴ The long-wavelength part of the fermion density is $\rho_{q=0}(x) = -(1/\pi) \nabla \phi(x)$, whereas the higher Fourier components are⁴⁶⁻⁴⁸

$$\rho_{2k_F}(x) = \frac{3}{\pi^2 \alpha} \left(\frac{\pi}{2} \right)^{1/4} \cos[2\phi(x)], \quad (9)$$

where we have specialized to an isotropic spin chain. The prefactor in Eq. (9) has been shown in Ref. 48 to yield a good agreement of the gap calculated within bosonization

and numerical calculations.⁴⁹ The Matsubara action for the phonon field has a standard quadratic form

$$S_p = \frac{\rho}{2} \int dx \int_0^\beta d\tau [(\partial_x q)^2 + \omega_0^2 q^2], \quad (10)$$

where $\rho = m/\alpha$ is the mass density of the optical phonon mode, and $q(x = n\alpha) = q_n$ is the lattice deformation field. In the first approximation (2), we have neglected the fact that the phonon disperses. It can be shown that the dispersion along the chain leads to insignificant corrections. On the contrary, if the phonons are three-dimensional; i.e., if ω disperses with the transverse momentum, then significant changes can occur. Indeed in that case, since the phonons are three-dimensional they couple the different spin chains and can induce a three-dimensional transition at low temperatures. We will come back to the case of three-dimensional phonons in Sec. V.

Since the total action is quadratic in the phonon fields, we can integrate them out to obtain the following bosonized action with a retarded interaction between the electronic densities:

$$\begin{aligned} S = & \int dx \int_0^\beta \frac{d\tau}{2\pi K} \left[u(\partial_x \phi)^2 + \frac{1}{u}(\partial_\tau \phi)^2 \right] \\ & - \frac{g^2}{2(\pi\alpha)^2 \rho \omega_0^2} \int dx \int_0^\beta d\tau \int_0^\beta d\tau' \cos 2\phi(x, \tau) \\ & \times \mathcal{D}_{\omega_0, \beta}(\tau - \tau') \cos 2\phi(x, \tau'), \end{aligned} \quad (11)$$

where $\mathcal{D}_{\omega_0, \beta}(\tau)$ is the propagator of an Einstein phonon of frequency ω_0 corresponding to the action (10):

$$\begin{aligned} \mathcal{D}_{\omega_0, \beta}(\tau - \tau') &= \langle q(\tau)q(\tau') \rangle \\ &= \frac{\omega_0}{2} \left[e^{-\omega_0|\tau - \tau'|} + \frac{2 \cosh(\omega_0(\tau - \tau'))}{e^{\beta\omega_0} - 1} \right]. \end{aligned} \quad (12)$$

The action (11) fully describes a one-dimensional spin chain coupled to phonons, and does not rely on adiabatic or antiadiabatic limit. However, one has to note that because of the cutoff, the action (11) is valid only for $\omega_0 \ll u/\alpha$. For higher values of the phonon frequency ω_0 , the phonon propagator (12) must be replaced with $\delta(\tau - \tau')$. In that case the action (11) is simply the continuum action of a frustrated spin chain,⁴¹ in agreement with the canonical transformation approach.^{13,31}

The action (11) is of course impossible to solve exactly. In order to obtain the physical properties of the system, we will analyze it using two different techniques in the next sections. The first technique is a self-consistent approximation. Such an approximation will be very useful to define the various phases of the system as well as the relevant parameters. As any variational approximation, although it can be very efficient in describing the various phases, it can only describe the transitions between these phases approximately. Therefore, in order to study the critical points we use a renormalization group method, building on the knowledge of the relevant parameters extracted from the SCHA.

III. SELF-CONSISTENT HARMONIC APPROXIMATION

To study the action (11), we apply first the self-consistent harmonic approximation or Gaussian variational method.⁵⁰⁻⁵³ The idea is that the action (11) would be classically minimized by $\phi=0$. One can thus expect that the physics will be dominated by small deviations around this minimum and approximate the action (11) by a quadratic action. We thus consider as a trial action

$$S_0 = \frac{1}{2\beta\Omega} \sum_{q, \omega} G^{-1}(q, \omega_n) \phi^*(q, \omega_n) \phi(q, \omega_n). \quad (13)$$

We have to find the propagator $G(q, \omega_n)$ so that (13) is the best approximation for (11). For that we define the variational free energy

$$F_{var} = F_0 + \langle S - S_0 \rangle_0, \quad (14)$$

where

$$F_0 = -\frac{1}{\beta L} \ln Z_0 = -\frac{1}{\beta} \sum_{q, \omega_n} \ln G(\omega_n), \quad (15)$$

$$Z_0 = \int D\phi e^{-S_0[\phi]}, \quad (16)$$

and $\langle \cdots \rangle_0$ represents an average with respect to the action S_0 .

The second term in the action (11) can be rewritten as

$$\begin{aligned} & - \frac{g^2}{2(\pi\alpha)^2 \rho \omega_0^2} \int dx \int_0^\beta d\tau \int_0^\beta d\tau' \mathcal{D}_{\omega_0, \beta}(\tau - \tau') \\ & \times \{ \cos[2\phi(x, \tau) + 2\phi(x, \tau')] + \cos[2\phi(x, \tau) - 2\phi(x, \tau')] \}. \end{aligned} \quad (17)$$

Given that the phonon propagator (12) decays for a large time difference ($\tau - \tau'$), one can see from (17) that the cosine of the sum is roughly equivalent to $\sim \cos[4\phi(x, \tau)]$ and can be responsible for the opening of a gap in the spectrum, while the cosine of the difference is $\sim (\tau - \tau')^2 [\nabla_\tau \phi(x, \tau)]^2$ and thus will modify the quadratic part of the action.

In the following, we consider the gapless ($\Delta=0$) and the gapful ($\Delta \neq 0$) case separately, at zero temperature. The gapless case is interesting in connection with systems of electrons at an incommensurate filling interacting with phonons.⁵⁴⁻⁵⁶ In these systems, the term $\cos[2\phi(x, \tau) + 2\phi(x, \tau')]$ does not appear in (17), leading to $\Delta=0$. The spin-Peierls problem corresponds to the half-filling case for the fermions.

A. Incommensurate case

Using (13), the variational free energy is given by

$$\begin{aligned} F_{var} = & \frac{1}{2} \int \frac{dq}{2\pi} \int \frac{d\omega}{2\pi} \{ [G_0^{-1}(q, \omega) - G^{-1}(q, \omega)] G(q, \omega) \\ & - \ln G(q, \omega) \} - \frac{g^2}{2(\pi\alpha)^2 \rho \omega_0^2} \int_{-\infty}^{\infty} d\tau \frac{\omega_0}{2} e^{-\omega_0|\tau|} \\ & \times \langle \cos[2\phi(0, \tau) - \phi(0, 0)] \rangle, \end{aligned} \quad (18)$$

where $G_0^{-1}(q, \omega) = (1/\pi K)(uq^2 + \omega^2/u)$ and we used (12) for $\beta = \infty$. Introducing the propagator for the field ϕ , $G(x, \tau) = \langle \phi(x, \tau) \phi(0, 0) \rangle$, we can rewrite

$$\begin{aligned} & \langle \cos 2\phi(0, \tau) \cos 2\phi(0, 0) \rangle \\ &= \frac{1}{2} \exp \left\{ -4 \int \frac{dq}{2\pi} \int \frac{d\omega}{2\pi} G(q, \omega) [1 - \cos(\omega\tau)] \right\}. \end{aligned} \quad (19)$$

Using this expression, we obtain

$$\begin{aligned} F_{var} &= \frac{1}{2} \int \frac{dq}{2\pi} \int \frac{d\omega}{2\pi} [G_0^{-1}(q, \omega) G(q, \omega) - \ln G(q, \omega)] \\ & - \frac{g^2}{4(\pi\alpha)^2 \rho \omega_0^2} \int_{-\infty}^{\infty} d\tau \frac{\omega_0}{2} e^{-\omega_0|\tau|} \\ & \times \exp \left\{ -4 \int \frac{dq}{2\pi} \int \frac{d\omega}{2\pi} G(q, \omega) [1 - \cos(\omega\tau)] \right\}. \end{aligned} \quad (20)$$

Minimizing the action (20) with respect to $G(q, \omega)$ and using the fact that $G^{-1}(q, \omega) = G_0^{-1}(q, \omega) - \Sigma(q, \omega)$, where Σ is the self-energy, we get

$$\begin{aligned} \frac{\delta F_{var}}{\delta G(q, \omega)} &= 0 = \frac{1}{2} \int \frac{dq}{2\pi} \int \frac{d\omega}{2\pi} \left(\Sigma(q, \omega) + \frac{g^2}{(\pi\alpha)^2 \rho \omega_0^2} \right. \\ & \times \int_{-\infty}^{\infty} d\tau \frac{\omega_0}{2} e^{-\omega_0|\tau|} [1 - \cos(\omega\tau)] \exp \left\{ -4 \int \frac{dq}{2\pi} \right. \\ & \left. \left. \times \int \frac{d\omega}{2\pi} G(q, \omega) [1 - \cos(\omega\tau)] \right\} \right). \end{aligned} \quad (21)$$

As is obvious from the above equation, the low-frequency behavior of $G^{-1}(q, \omega) = G_0^{-1}(q, \omega)$ is similar to the one of $G_0^{-1}(q, \omega)$, and corresponds to a variational action of the form

$$S_0 = \int dx \int_0^\beta \frac{d\tau}{2\pi\bar{K}} \left[\bar{u}(\partial_x \phi)^2 + \frac{1}{\bar{u}}(\partial_\tau \phi)^2 \right]; \quad (22)$$

thus, $G^{-1}(q, \omega) = (1/\pi K)(\bar{u}q^2 + \omega^2/\bar{u})$. In the equation above we thus have

$$\begin{aligned} & \int \frac{dq}{2\pi} \int \frac{d\omega}{2\pi} G(q, \omega) [1 - \cos(\omega\tau)] \\ &= \pi \bar{K} \int \frac{dq}{2\pi} \int \frac{d\omega}{2\pi} \frac{[1 - \cos(\omega\tau)]}{(\bar{u}q^2 + \omega^2/\bar{u})} = \frac{\bar{K}}{2} \ln(\omega_c \tau), \end{aligned} \quad (23)$$

where $\omega_c = u/\alpha$, is a frequency cutoff. Using (23) we can write our variational equation as

$$\Sigma(q, \omega) + \frac{g^2}{(\pi\alpha)^2 \rho \omega_0^2} \int_{-\infty}^{\infty} d\tau \frac{(\omega_0 \tau)}{2} e^{-\omega_0|\tau|} \frac{[1 - \cos(\omega\tau)]}{(\omega_c \tau)^{2\bar{K}}} = 0. \quad (24)$$

If we confine to an expansion up to order ω^2 in $[1 - \cos(\omega\tau)]$, as requested by the analytical behavior of the Green's function for $\omega \rightarrow 0$, we obtain

$$\begin{aligned} \Sigma(q, \omega) &= - \frac{g^2}{(\pi\alpha)^2 \rho \omega_0^2} \int_{-\infty}^{\infty} d\tau \frac{(\omega_0 \tau)}{2} e^{-\omega_0|\tau|} \frac{\omega^2 \tau^2}{(\omega_c \tau)^{2\bar{K}}} \\ &= - \frac{g^2}{(\pi\alpha)^2 \rho \omega_0^2} \left(\frac{\omega_0}{\omega_c} \right)^{2\bar{K}} \frac{\Gamma(3 - 2\bar{K})}{\omega_0^2} \omega^2, \end{aligned} \quad (25)$$

where Γ is the gamma function. As we see the integral is convergent when $K < 3/2$. Going back to the definition of the self-energy, we have

$$\Sigma(q, \omega) = (G_0^{-1} - G^{-1})(q, \omega) = \left(\frac{1}{2\pi u K} - \frac{1}{2\pi \bar{u} \bar{K}} \right) \omega^2. \quad (26)$$

Equating (25) with (26), and using the fact that $u/K = \bar{u}/\bar{K}$, we obtain the following value of the parameter K :

$$K^2 = \bar{K}^2 \left[1 + \frac{2Kg^2}{\pi u \rho \omega_0^2} \left(\frac{u}{\alpha \omega_0} \right)^{2-2\bar{K}} \Gamma(3 - 2\bar{K}) \right]. \quad (27)$$

Expanding around K , we obtain the renormalized value of \bar{K} :

$$\bar{K}^2 \simeq K^2 \left[1 - \frac{2Kg^2}{\pi u \rho \omega_0^2} \left(\frac{u}{\alpha \omega_0} \right)^{2-2K} \Gamma(3 - 2K) \right]. \quad (28)$$

One thus recovers a Luttinger liquid but with a renormalized value of the Luttinger parameter K . Equation (28) implies that $\bar{K} < K$. A similar result can be obtained via the renormalization group analysis (see the next section). In a RG analysis, the result (28) would correspond to integrating the RG equation for the coupling constant g , assuming that K is not renormalized and then computing the lowest-order correction to K with the renormalized coupling constant. Our method thus reproduces in a crude way the renormalization of K downwards. As in Refs. 55–57, we find that the tendency of the system to form charge density waves is increased.

B. Commensurate case

In the commensurate case the derivation of the variational free energy from (14)–(21) remains the same. Let us rewrite (20) in slightly different way:

$$\begin{aligned} F_{var} &= \frac{1}{2} \int \frac{dq}{2\pi} \int \frac{d\omega}{2\pi} [G_0^{-1}(q, \omega) G(q, \omega) - \ln G(q, \omega)] \\ & - \frac{g^2}{4(\pi\alpha)^2 \rho \omega_0^2} \int_{-\infty}^{\infty} d\tau \frac{\omega_0}{2} e^{-\omega_0|\tau|} \left(\frac{1}{2} \exp \left\{ -4 \int \frac{dq}{2\pi} \right. \right. \\ & \left. \left. \times \int \frac{d\omega}{2\pi} G(q, \omega) [1 - \cos(\omega\tau)] \right\} \right. \\ & \left. + \frac{1}{2} \exp \left\{ -4 \int \frac{dq}{2\pi} \int \frac{d\omega}{2\pi} G(q, \omega) [1 + \cos(\omega\tau)] \right\} \right). \end{aligned} \quad (29)$$

Minimizing this action with respect to $G(q, \omega)$, we obtain the following expression for the self-energy:

$$\begin{aligned} \Sigma(q, \omega) = & -\frac{g^2}{(\pi\alpha)^2 \rho \omega_0^2} \int_{-\infty}^{\infty} d\tau \frac{\omega_0}{2} e^{-\omega_0|\tau|} \left([1 - \cos(\omega\tau)] \right. \\ & \times \exp \left\{ -4 \int \frac{dq}{2\pi} \int \frac{d\omega}{2\pi} G(q, \omega) [1 - \cos(\omega\tau)] \right\} \\ & + [1 + \cos(\omega\tau)] \\ & \left. \times \exp \left\{ -4 \int \frac{dq}{2\pi} \int \frac{d\omega}{2\pi} G(q, \omega) [1 + \cos(\omega\tau)] \right\} \right). \end{aligned} \quad (30)$$

As is obvious from Eq. (30), $\Sigma(q, \omega)$ is in fact independent of q . Moreover, we can use the following expansion for the self-energy:

$$\Sigma(q, \omega) = -\frac{1}{\pi \bar{u} \bar{K}} (\Delta^2 + \gamma \omega^2). \quad (31)$$

In Eq. (31), the variational parameter Δ stands for the gap caused by the commensurability, and the variational parameter γ stands for the renormalization of the bare Luttinger exponent K . Such a restricted ansatz is justified by the fact that higher powers of ω in $\Sigma(\omega)$ are associated with irrelevant operators in the action, whereas Δ and γ correspond, respectively, to a relevant and a marginal operator. Keeping only Δ amounts to neglect any renormalization of K by the spin-phonon interaction.

The self-energy (31) leads to a Green's function $G(q, \omega)$:

$$G(q, \omega) = \frac{\pi \bar{K}}{\bar{u} q^2 + \omega^2 / \bar{u} + \bar{u} \Delta^2}, \quad (32)$$

where Δ is the mass term. The integral of the Green's function is:

$$\int \frac{dq}{2\pi} \int \frac{d\omega}{2\pi} G(q, \omega) e^{i\omega\tau} = \frac{\bar{K}}{2} K_0(\Delta \bar{u} \tau), \quad (33)$$

where K_0 is the Bessel function. The corresponding variational action is

$$S_0 = \int dx \int_0^\beta \frac{d\tau}{2\pi \bar{K}} \left[\bar{u} (\partial_x \phi)^2 + \frac{1}{\bar{u}} (\partial_\tau \phi)^2 + \frac{\bar{u}}{\xi^2} \phi^2 \right], \quad (34)$$

where $u/\xi = \Delta$ is the gap and $u/K = \bar{u}/\bar{K}$ as no term $(\partial_x \phi)^2$ is generated from (17).

Equating the coefficient of (31) with that coming from the expansion for small ω of (30), we obtain the following two equations:

$$\begin{aligned} \frac{\bar{u} \Delta^2}{\pi \bar{K}} = & \frac{2g^2}{(\pi\alpha)^2 \rho \omega_0^2} \int_{-\infty}^{\infty} d\tau \frac{\omega_0}{2} e^{-\omega_0|\tau|} \exp \left\{ -4 \int \frac{dq}{2\pi} \right. \\ & \left. \times \int \frac{d\omega}{2\pi} G(q, \omega) (1 + \cos \omega\tau) \right\}, \end{aligned} \quad (35)$$

$$\begin{aligned} \frac{\gamma}{\pi \bar{u} \bar{K}} = & \frac{2g^2}{(\pi\alpha)^2 \rho \omega_0^2} \int_{-\infty}^{\infty} d\tau \frac{\omega_0}{2} e^{-\omega_0|\tau|} \\ & \times \frac{\tau^2}{2} [e^{-4\int (dq/2\pi) \int (d\omega/2\pi) G(q, \omega) [1 - \cos(\omega\tau)]} \\ & - e^{-4\int (dq/2\pi) \int (d\omega/2\pi) G(q, \omega) [1 + \cos(\omega\tau)]}]. \end{aligned} \quad (36)$$

Using that $u/K = \bar{u}/\bar{K}$, the left-hand side (l.h.s.) of (36) can also be rewritten as

$$\frac{\gamma}{\pi \bar{u} \bar{K}} = -\frac{1}{2\pi u K} + \frac{1}{2\pi \bar{u} \bar{K}}. \quad (37)$$

The two self-consistent equations (35) and (36) can be solved analytically in the antiadiabatic limit ($\omega_0 \gg \Delta$). Using (33), and after a straightforward but lengthy calculation, we obtain

$$\bar{K}^2 \simeq K^2 \left[1 - \frac{Kg^2}{\pi u \rho \omega_0^2} \left(\frac{u}{\alpha \omega_0} \right)^{2-2K} \Gamma(3-2K) \right] \quad (38)$$

which is the same change of K than in (28). The system also develops a gap given by

$$\Delta = \frac{u}{\alpha} \left[\frac{Kg^2}{\pi u \rho \omega_0^2} \left(\frac{u}{\alpha \omega_0} \right)^{2K} \Gamma(1+2K) \right]^{1/(2-4\bar{K})}. \quad (39)$$

As we can see from (38), for $K > 1/2$, we can have $\bar{K} < 1/2$, so that (39) can still lead to a gap provided that g is large enough. Combining the two Eqs. (38) and (39), we finally have

$$\bar{K}^2 \simeq K^2 \left[1 - (\Delta \alpha)^{2-4\bar{K}} \frac{\Gamma(3-2K)}{\Gamma(1+2K)} \right]. \quad (40)$$

The SCHA thus correctly describes the formation of a gap in the antiadiabatic limit. As for the incommensurate case, the SCHA captures part of the effects of the renormalization of the parameters. Note that the SCHA, as any variational method, is efficient in capturing the nature of the ordered phases, but in order to determine the nature of transition one needs the full RG analysis. Such an analysis will be discussed in Sec. IV.

C. Adiabatic-antiadiabatic crossover in the SCHA

Using the SCHA we are now in a position to describe the crossover from adiabatic to antiadiabatic regime. We will assume that we are far from the point $K = 1/2$ and in fact that we have $K < 1/2$. For the spin chain this would correspond in being in the Ising limit. In that regime, we can neglect the renormalization of K and take $K = \bar{K}$ in our variational action. The variational free energy (29) can be written

$$\begin{aligned} F = F_0 - & \frac{u}{2\pi K \xi^2} G(0, 0) - \frac{g^2}{4(\pi\alpha)^2 \rho \omega_0^2} \left(\frac{e^\gamma \alpha}{2\xi} \right)^{2K} \int_0^\infty d\tau \mathcal{D}(\tau) \\ & \times [e^{-4G(0, \tau)} + e^{4G(0, \tau)}], \end{aligned} \quad (41)$$

where $G(0, \tau)$ is given by Eq. (33). Using the expansion for

the Bessel function we obtain the following approximate expression:

$$G(0, \tau) = -\frac{K}{2} \ln \left(\frac{\sqrt{(u\tau)^2 + \alpha^2} e^\gamma}{\xi} \right), \quad \text{if } u\tau \ll 2e^{-\gamma}\xi,$$

$$G(0, \tau) = 0, \quad \text{if } u\tau \gg 2e^{-\gamma}\xi, \quad (42)$$

where γ is the Euler-Mascheroni constant.⁵⁸ Using the above expression for the Green's function, we are able to calculate the variational free energy (41), and minimizing it with respect to ξ we obtain the following variational equation:

$$\frac{u}{4\pi K \xi^2} = \frac{g^2}{(\pi\alpha)^2 \rho \omega_0^2} \left[\left(\frac{e^\gamma \alpha}{2\xi} \right)^{2K} e^{-2e^{-\gamma}\omega_0 \xi / u} + \left(\frac{e^\gamma \alpha}{2\xi} \right)^{4K} \left(\frac{u}{\alpha \omega_0} \right)^{2K} \gamma \left(1 + 2K, \frac{\omega_0 \xi}{u} \right) \right], \quad (43)$$

where $\gamma(\cdot, \cdot)$ is the incomplete gamma function.⁵⁸

Two interesting limits in Eq. (43) must be discussed. If $\omega_0 \xi / u \rightarrow 0$, one is in the adiabatic limit, whereas the antiadiabatic one corresponds to $\omega_0 \xi / u \rightarrow \infty$. In the adiabatic limit, one sees that the term on the right hand side of (43) reduces to a contribution $\sim (a/\xi)^{2K}$, the term depending on the incomplete Gamma function being zero in that limit. As a result, the Cross-Fisher prediction for the gap,⁹

$$\Delta = \frac{u}{\alpha} \left(\frac{g^2}{2k_e} \right)^{1/(2-2K)} \quad (44)$$

is recovered. In the antiadiabatic limit, the exponential term in (43) disappears, and the incomplete Gamma function can be replaced by a gamma function, leading to the result for the gap we have found in Sec. III B, in (39). In this limit, the gap can be understood as resulting from a $\cos 4\phi$ interaction induced by integrating out the phonon modes.

To perform a general study for any $\omega_0 \xi / u$, we rewrite (43) for ξ as

$$\frac{\left(\frac{\alpha}{\xi} \right)^{2-2K}}{e^{-2e^{-\gamma}(\omega_0 \xi / u)} + (u e^\gamma / 2 \omega_0 \xi)^{2K} \gamma \left(1 + 2K, 2e^{-\gamma} \frac{\omega_0 \xi}{u} \right)} = \frac{4Kg^2}{\pi u \rho \omega_0^2} \left(\frac{e^\gamma}{2} \right)^{2K}. \quad (45)$$

In terms of the gap, this equation reads

$$f\left(\frac{\Delta}{\omega_0}\right) = \frac{4Kg^2}{\pi u \rho \omega_0^2} \left(\frac{u}{\omega_0 \alpha} \right)^{2-2K} \left(\frac{e^\gamma}{2} \right)^{2K}, \quad (46)$$

where

$$f(x) = \frac{x^{2-2K}}{e^{-2(e^{-\gamma})/x} + \left(x \frac{e^\gamma}{2} \right)^{2K} \gamma \left(1 + 2K, 2 \frac{e^{-\gamma}}{x} \right)}. \quad (47)$$

The graph of the function $f(x)$ is represented on Fig. 1. In this figure, the crossover from the adiabatic to the antiadiabatic regime is easily observed, with the two limiting forms

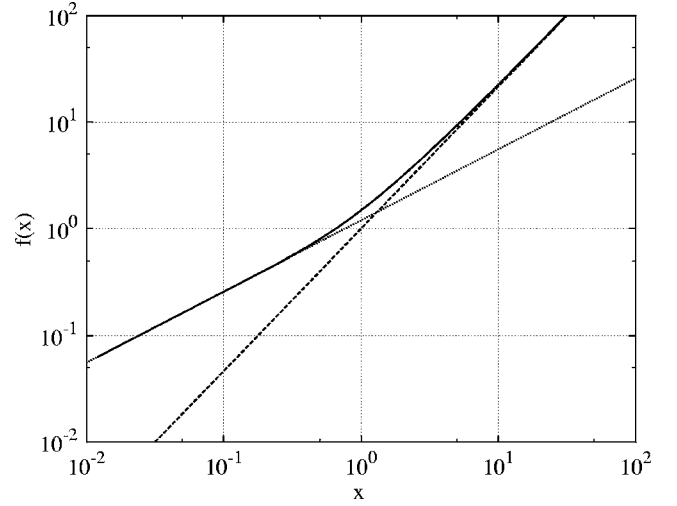


FIG. 1. The graph of the function $f(x)$ (solid line) defined in Eq. (47) with $K=1/3$. Two regimes are visible. For $\Delta \gg \omega_0$, $f(x) \sim x^{2-2K}$ (dashed curve). In that regime, the gap is given by the adiabatic formula Eq. (44). For $\Delta \ll \omega_0$, $f(x) \sim x^{2-4K}$ (dotted curve) and the gap is given by the antiadiabatic formula Eq. (39). The crossover regime is observed for $0.3 < \Delta/\omega_0 < 3$.

of the gap given, respectively, by Eqs. (44) and (39). The SCHA allows one to obtain the full interpolating function between the two regimes, and thus to obtain precisely the crossover scale. We obtain that the limit between the adiabatic and the antiadiabatic regime is given by $\omega_0 \sim \Delta$ and not by $\omega_0 \sim J$. This point will be further discussed in the forthcoming Sec. IV.

The SCHA also yields the expectation value of the nearest-neighbor correlations $S_n \cdot S_{n+1}$, as it is proportional to $(-1)^n \langle \cos 2\phi \rangle$. One finds

$$\langle S_n \cdot S_{n+1} \rangle \sim \left(\frac{\alpha}{\xi} \right)^K. \quad (48)$$

For $\omega_0 \ll \Delta$, i.e., in the adiabatic regime, one has

$$\langle S_n \cdot S_{n+1} \rangle \sim \left(\frac{g^2}{\pi \rho u \omega_0^2} \right)^{K/(2-K)}. \quad (49)$$

In the antiadiabatic regime, for $K < 1/2$, we find

$$\langle S_n \cdot S_{n+1} \rangle \sim \left[\frac{g^2}{\pi \rho u \omega_0^2} \left(\frac{u}{\alpha \omega_0} \right)^{2K} \right]^{K/(2-4K)}. \quad (50)$$

IV. RG ANALYSIS

As we have discussed in the previous section, the SCHA describes only approximately the renormalization of the quadratic part by the phonon coupling term. Such a renormalization of the parameter K is of course especially crucial to take into account precisely close to the isotropic Heisenberg point $K=1/2$. In this section, we thus apply an RG method to analyze the adiabatic-antiadiabatic crossover.

Attempts to an RG analysis of such a problem or of directly related fermionic problems have been described in the literature. In particular, an RG analysis was performed¹⁸ at

$T=0$ based on a previous work on spinful fermions coupled to phonons.^{59–61} In this work, the interaction of the spinful fermions with the electrons is viewed as a retarded back-scattering interaction. However, although this description is appropriate for fermions, in the case of the spin chain it neglects the fact that the staggered dimer operator gives rise to more relevant interactions than current-current ones. As a result, this fermionic description underestimates the size of the dimerization gap. Our analysis, directly based on the boson representation of the spin chain does not suffer from such a limitation. In addition to providing us with a better description of the dimerization gap, the use of the boson representation also allows us to tackle the case of a finite frequency ω_0 and nonzero temperature.

Another closely related problem is the one of fermions in a random potential,⁶² which has an action quite similar to (11) but with a constant \mathcal{D} . One could be tempted to simply reuse the RG equations derived for this system. However, here, the situation is more subtle. In (12), for $\omega_0/T \rightarrow 0$, $\mathcal{D}(\tau) \rightarrow T$. Therefore, we see that the rescaling of the temperature is going to modify the RG equations with respect to the case of disordered fermions. Moreover, for $\omega_0/T \rightarrow \infty$, $\mathcal{D}(\tau) = (\omega_0/2)e^{-\omega_0|\tau|}$. As a result, the limit of $T \rightarrow 0$ is delicate to handle properly. In particular, the definition of the spin-phonon coupling constant becomes ambiguous in this limit.

However the variational analysis performed in the previous section allows us to build the correct RG procedure. First, the variational approach shows that in order to obtain the correct results, it is important to first perform the calculation of the ground state free energy for $0 < T \ll \Delta$, where Δ is the spin-Peierls gap, and then take the limit of $T \rightarrow 0$. Second, it gives us that the proper dimensionless coupling constant measuring the strength of the electron-phonon interaction is

$$G = \frac{g^2}{\pi u \rho \omega_0^2}. \quad (51)$$

We now proceed with the RG. We start from the following action:

$$\begin{aligned} S = & \int dx \int_0^\beta \frac{d\tau}{2\pi K} \left[u(\partial_x \phi)^2 + \frac{1}{u}(\partial_\tau \phi)^2 \right] \\ & - \frac{1}{2\rho\omega_0^2} \left(\frac{g}{\pi a} \right)^2 \int dx \int_0^\beta d\tau \int_0^\beta d\tau' \cos 2\phi(x, \tau) \\ & \times \mathcal{D}_{\omega_0, \beta}(\tau - \tau') \cos 2\phi(x, \tau') \\ & - \frac{2g_\perp}{(2\pi a)^2} \int dx \int_0^\beta d\tau \cos 4\phi. \end{aligned} \quad (52)$$

The $\cos(4\phi)$ operator is the marginal operator needed to describe an spin-isotropic spin chain. The derivation of the equations is given in Appendix C. They read

$$\frac{d}{dl} \left(\frac{1}{K} \right) = \left(\frac{g_\perp}{\pi u} \right)^2 + \frac{g^2}{\pi u \rho \omega_0^2} \frac{\alpha}{u} \mathcal{D}_{\omega_0(l)} \left(\frac{\alpha}{u} \right), \quad (53a)$$

$$\frac{d}{dl} \left(\frac{g_\perp}{\pi u} \right) = (2 - 4K) \frac{g_\perp}{\pi u} + \frac{g^2}{\pi u \rho \omega_0^2} \frac{\alpha}{u} \mathcal{D}_{\omega_0(l)} \left(\frac{\alpha}{u} \right), \quad (53b)$$

$$\frac{d}{dl} \left(\frac{g^2}{\pi u \rho \omega_0^2} \right) = \left[2(1 - K) + \frac{g_\perp}{\pi u} \right] \frac{g^2}{\pi u \rho \omega_0^2}, \quad (53c)$$

$$\frac{d\omega_0}{dl} = \omega_0. \quad (53d)$$

These RG equations are conveniently expressed using the coupling constant G defined in Eq. (51). At this one-loop order, we find no corrections to the phonon frequency as can be seen in (53d). However, we expect such corrections to be obtained in a higher-loop-order calculation.

A. Anisotropic case

Since the action (11) also describes spinless fermions coupled to phonons, our equations have similarities with the RG equations that have been derived for the electron-phonon problem.^{55–57,60,63} There are however important differences. First, for a spin chain the equivalent fermionic band is automatically half-filled (in the absence of an external magnetic field). Thus, in addition to the standard terms that were considered for the electron-phonon problem with incommensurate filling, one has here to take into account the marginal umklapp operator $\cos(4\phi)$ as in Ref. 63. Second, in the electron-phonon problem a different coupling constant is used,^{55–57} namely, $Y_{sp}^2 = G[\omega_0(l)\alpha/u]$. Such a definition appears natural when looking at the RG Eqs. (53a) and (53b), since Y_{sp} seems to be the amount by which K is renormalized in the limit $T=0$. However, such definition would be at odds with the calculations performed with the SCHA. In fact, the integral $\int_0^\infty dl (\alpha/u) \mathcal{D}_{\omega_0 e^l}(\alpha/u) = 1$ for all ω_0 . As a result, if we neglect g_\perp in (53a), and the renormalization of K in (53c), we find the following approximate RG equations for G and K :

$$G(l) = G(0)e^{(2-2K)l}, \quad (54)$$

$$\frac{d}{dl}(K^{-1}) = G(0)e^{(2-2K)l} \frac{\omega_0 \alpha}{u} e^l \exp\left(-\frac{\omega_0 \alpha}{u} e^l\right), \quad (55)$$

and by a variable change to $V = (\omega_0 \alpha / u) e^l$, we easily obtain that

$$K^{-1}(\infty) - K^{-1}(0) = G(0) \left(\frac{u}{\omega_0 \alpha} \right)^{2-2K} \Gamma(3-2K). \quad (56)$$

This equation is easily understood: ω_0 gives an energy cutoff that stops the RG flow of K induced by G at an energy scale of order $\omega_0 = u/\alpha e^{-l^*}$. We note that it is identical to the SCHA result (28). We thus see that at that scale, K is renormalized by an amount proportional to $G(l^*)$ and not $G(l) \times [\omega_0(l)\alpha/u]$ as a result of the exponential factor in (55). This confirms that the right coupling constant in this theory is G and not $G\omega_0(l)\alpha/u$. In Ref. 63, the same prescription was used to define the coupling constant, whereas in Ref. 38, the incorrect rescaling of Ref. 55 was used. As a result, we

expect the conclusions of Ref. 38 to be incorrect in the adiabatic regime.

Until now, we have assumed that at the scale $l^* = \ln[u/(\alpha\omega_0)]$, the coupling constant $G(l^*) \ll 1$. If this assumption breaks down, since the coupling constant $G(l) = e^{(2-2K)l}G(0)$, one finds a gap

$$\Delta = \frac{u}{\alpha}G(0)^{1/(2-2K)} > \omega_0. \quad (57)$$

This gap is in agreement with the SCHA result and with the mean-field theory treatment of Cross and Fisher.⁹ For $K < 1/2$, in the antiadiabatic limit $\omega_0 \gg u/\alpha$, we know from the SCHA that the phonons can generate a relevant perturbation $\cos 4\phi$ and thus induce a gap.³³ This effect is also captured in the RG by (53b). This can be seen by a two step renormalization procedure. In the first step, for $l < l^* = \ln(u/\alpha\omega_0)$, a term g_\perp is induced by the RG flow. This term is found to be of order

$$y(l^*) = \frac{g_\perp(l^*)}{\pi u} = G(0) \left(\frac{u}{\alpha\omega_0} \right)^{2-2K} \left[\gamma(2K+1, 1) - \gamma \left(2K+1, \frac{\alpha\omega_0}{u} \right) \right]. \quad (58)$$

Since $\omega_0 \ll u/\alpha$, we can actually neglect $\gamma(2K+1, \alpha\omega_0/u)$ in Eq. (58). For $l > l^*$, $\mathcal{D}_{\omega_0(l)}(\alpha/u) \rightarrow 0$, and we can drop G from the RG equations. We then have a simple Kosterlitz-Thouless RG flow, which leads to a gap of the form

$$\Delta = \frac{u}{\alpha} \left[G(0) \left(\frac{u}{\alpha\omega_0} \right)^{2K} \gamma(2K+1, 1) \right]^{1/(2-4K)}. \quad (59)$$

This gap is in agreement with the SCHA prediction in the antiadiabatic limit (38). Therefore, we see that SCHA and RG methods agree perfectly, far from the isotropic point, once the proper coupling constant is used in the RG.

Using our RG equations, we can now study the SU(2) invariant limit for which the SCHA cannot be used, due to importance at that point of the marginally irrelevant operator $\cos(4\phi)$.

B. SU(2) invariant case

In the isotropic limit, we have

$$K = \frac{1}{2} \left(1 - \frac{g_\perp}{2\pi u} \right). \quad (60)$$

This ensures that, in the absence of spin-phonon coupling, the flow will renormalize to the fixed point $K^* = 1/2$ and $g_\perp^* = 0$. It is then easily seen that the Eqs. (53a) and (53b) reduce to a single equation for $y = g_\perp / \pi u$. This leads to the following RG flow:

$$\frac{dy}{dl} = y^2 + G(l) \frac{\omega_0 \alpha}{2u} e^l e^{-(\omega_0 \alpha / u) e^l}, \quad (61)$$

$$\frac{dG}{dl} = \left(1 + \frac{3}{2}y \right) G. \quad (62)$$

These RG equations allow for the full interpolation between the adiabatic and antiadiabatic limit.

The simple analysis of the previous section showed that the gap should behave as $\Delta = (u/\alpha)G(0)$ in the adiabatic limit. For the isotropic case, using (61) and (62), we obtain logarithmic corrections to the gap $\Delta = (u/\alpha)G|\ln G|^{-3/2}$ resulting from the marginal flow of $y(l)$. These logarithmic corrections (for details see the Appendix D) are identical to those obtained by incorporating the logarithmic corrections to the gap of the dimerized spin-1/2 chain^{42,49,64} into the Cross-Fisher mean-field theory. This confirms that G is the right coupling constant to study the formation of the spin-Peierls gap in the adiabatic limit. On the other hand, as discussed in the previous section, in the antiadiabatic limit, it is the flow of $y(l)$ that determines whether or not the gap is formed. To analyze the flow in the antiadiabatic regime, we can use the approximation $G(l) = G(0)e^l$; i.e., we neglect the logarithmic corrections to the flow of G . We have checked that this approximation leads to a good agreement with the numerical study of the RG flow using the fourth-order Runge-Kutta algorithm. Using the previous approximation, the RG flow [(61) and (62)] can be reduced to a Riccati differential equation (cf. Appendix E) leading to the following dependence of the gap on G :

$$\Delta = \omega_0 e^{\gamma-1} \exp \left[-\frac{2\omega_0 \alpha}{uG(0)} \right], \quad (63)$$

for the case of $y(0) = 0$. When $y(0) < 0$, it is found that a gap exists only if

$$\frac{uG(0)}{2\omega_0 \alpha} > \frac{|y(0)|}{1 + |y(0)| \ln(ue^{1-\gamma}/\alpha\omega_0)}. \quad (64)$$

The physical content of this equation is transparent. At the scale l^* such that $\omega_0 e^{l^*} = u/\alpha$, $G(l^*)$ is equal to the l.h.s. of the inequality, whereas $|y(l^*)|$ is equal to the right-hand side of the inequality. The gap can form only if the renormalized spin-phonon interaction is stronger than the renormalized marginal coupling at the energy scale ω_0 . This is in agreement with the two-step RG approach⁶⁰ of the preceding section. When the condition (64) is satisfied, the gap behaves as

$$\Delta = \omega_0 e^{-(1-\gamma)} \exp \left[\frac{-1}{\frac{uG(0)}{2\omega_0 \alpha} + \frac{y(0)}{1 - y(0) \ln \left(\frac{ue^{1-\gamma}}{\omega_0 \alpha} \right)}} \right]. \quad (65)$$

This expression shows that the gap vanishes as $\exp[-Ct/(G(0)-G^c)]$ when the spin-phonon coupling constant goes to the critical value, indicating that the phase transition between the gapped phase and the gapless phase in the antiadiabatic regime is in the Berezinskii-Kosterlitz-Thouless (BKT) universality class. For fixed $G(0)$, Eq. (65) also indicates that there exists ω_{BKT} such that for $\omega_0 > \omega_{BKT}$ the gap vanishes via a BKT transition. The implicit equation giving ω_{BKT} reads

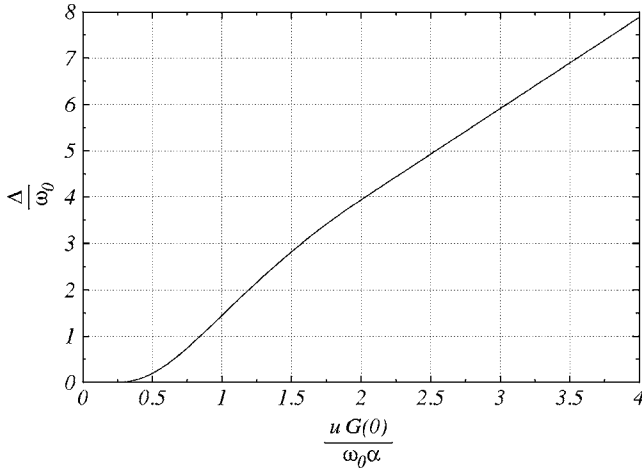


FIG. 2. The behavior of the gap Δ as a function of the spin-phonon coupling constant G in the case $y(0)=0$. When $G \gg \alpha\omega_0/u$, the system is in the adiabatic regime, and the gap Δ varies linearly with G . When $G \ll \alpha\omega_0/u$, the gap decreases very rapidly with an essential singularity for $G(0)=0$ described by Eq. (65).

$$\frac{uG(0)}{2\alpha} = \omega_{BKT} \frac{|y(0)|}{1 + |y(0)| \ln \left(\frac{ue^{1-\gamma}}{\alpha\omega_{BKT}} \right)}, \quad (66)$$

which shows that ω_{BKT} is an increasing function of the spin-phonon coupling constant.

The functional dependence of the gap on the spin-phonon coupling constant (65) is similar to the one obtained in the case of a frustrated spin chain. This result is roughly in agreement with the results of canonical transformations that eliminate the phonons from the spin Hamiltonian.^{13,31} Upon closer inspection however, one finds that the factor of $u/\alpha\omega_0$ does not appear in the formulas giving the spin gap in that case. The reason is that the canonical transformations of Refs. 13 and 31 are valid in the limit $\omega_0 \gg J$ and only the instantaneous interactions are present, whereas in our theory one needs to renormalize until the scale ω_0 reaches J before the interactions can be considered instantaneous. Thus, we find that there is an intermediate regime $\Delta < \omega_0 < J$, in which

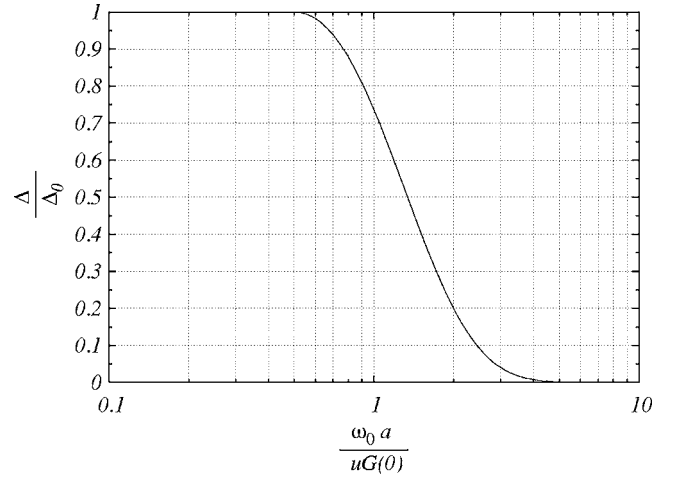


FIG. 3. The behavior of the gap Δ as a function of phonon frequency ω_0 for a fixed value of $G(0)$ and $y(0)=0$. In the adiabatic regime $\omega_0 \ll uG(0)/\alpha$, the gap is independent of ω_0 and is equal to $\Delta_0 = uG(0)/\alpha$. In the antiadiabatic regime, the gap is a rapidly decreasing function of phonon frequency given by Eq. (65).

the gap is still larger than in the frustrated chain limit. The frustrated chain results are recovered only when $\omega_0 \rightarrow J$. In the case of the Heisenberg spin chain, the value of $y(0)$ has been estimated to be of the order of -0.25 ,⁴² which is rather large. For this reason, we cannot make quantitative predictions on the value of the gap. However, we can expect from this large value of the marginal interaction that the critical value of the spin-phonon interaction needed to obtain the spin gap in the antiadiabatic regime will be rather large. The behavior of the gap as a function of the strength of the coupling constant for the case $y(0)=0$ as given by Eq. (E20) is represented in Fig. 2. The behavior of the gap as a function of frequency is represented in Fig. 3. Concerning the expectation value of $\mathbf{S}_n \cdot \mathbf{S}_{n+1}$, we have that $\langle \cos 2\phi \rangle \sim e^{-Kl_0}$. In the adiabatic regime, we find

$$\langle \cos 2\phi \rangle \sim \left(\frac{g^2}{2\pi u \rho \omega_0^2} \right)^{1/3}, \quad (67)$$

whereas, in the antiadiabatic regime, we have

$$\langle \cos 2\phi \rangle \sim \left(\frac{\omega_0 \alpha}{u} \right)^{1/2} \exp \left[- \frac{1}{2 \left[\frac{u}{\alpha \omega_0} \frac{g^2}{2\pi u \rho \omega_0^2} - \frac{|y(0)|}{1 + |y(0)| \ln \left(\frac{ue^{1-\gamma}}{\omega_0 \alpha} \right)} \right]} \right]. \quad (68)$$

An ansatz can be made to describe the crossover between the adiabatic and the antiadiabatic regime. In the adiabatic regime, $G(l) \sim 1$ for l such that $\omega_0 e^l \ll u/\alpha$ and $y(l) \ll 1$. We can analyze the crossover from the adiabatic to the antiadiabatic regime by matching the expressions obtained in the two

cases. This matching procedure (see Appendix E) predicts that the crossover of the two regimes is obtained when $uG(0)/\alpha = 2\omega_0$ [for the case of $y(0)=0$]. The resulting phase diagram is shown in Fig. 4, where three regimes are visible. As ω_0 increases, we go from the gapped adiabatic regime to

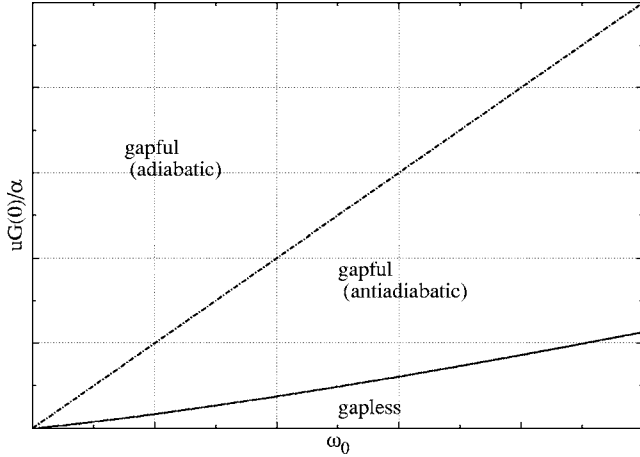


FIG. 4. The phase diagram in the (G, ω_0) plane, where G is the spin-Peierls coupling constant and ω_0 the phonon frequency. The solid line corresponds to the BKT transition between the gapped and the gapless phase described by Eq. (64). The dash-dotted line is a crossover line between the antiadiabatic regime $uG(0)/\alpha \ll \omega_0$, and the adiabatic regime $uG(0)/\alpha \gg \omega_0$.

the gapped antiadiabatic regime and finally to the gapless regime. As is shown, the strength of spin-phonon interaction increases the size of the gapped regime.

V. DISCUSSION

We shall here discuss our results for the spin-Peierls model and compare with the ones present in the literature. The main purpose is to give an overview of the informations that can be extracted using the SCHA and the RG analysis. We stress that our results are also applicable to strongly interacting fermionic systems via the Jordan-Wigner transformation. Moreover, for fermionic systems, both the case of on-site (Holstein) phonons and on-bond phonons can be dealt with as they correspond, respectively, to a term $\cos 2\phi$ or $\sin 2\phi$ in the action.

A. Comparison with numerical calculations

The first result, obtained within SCHA, is the criterion for the crossover from the adiabatic to the antiadiabatic regime, which is $\omega_0 \sim \Delta_s$, where Δ_s is the static gap, and not $\omega_0 \sim J$, as could have been naively been expected. This criterion was obtained previously by a two-cutoff renormalization group analysis in Ref. 60 in the case of interacting fermions. Such result is in agreement with a DMRG study of the XY spin chain coupled to dispersionless phonons of frequency ω_0 , where the crossover is observed when $\Delta_s \sim \omega_0$.⁶⁵ Another DMRG study in Ref. 21 also showed that in the case of spinless fermions interacting with Holstein phonons, the phase transition between the gapful Peierls state (adiabatic) to the gapless Luttinger liquid state (antiadiabatic) was also obtained when $\omega_0 \sim \Delta_s$.

The second result, obtained using the RG for the $SU(2)$ invariant case concerns the behavior of the spin gap in the adiabatic and antiadiabatic cases. We have found that for low frequency ($\omega_0 \ll \Delta_s$), one is in the adiabatic regime with a

spin gap given by the mean-field approximation⁹ $\Delta \sim \Delta_s \sim g^2/m\omega_0^2$, but for $\omega_0 \gg \Delta_s$, in the antiadiabatic regime, the spin gap starts to decrease rapidly with the frequency. This result is in agreement with the DMRG study of Ref. 65. In fact, in this regime the RG analysis yields

$$\Delta = \omega_0 e^{-(1-\gamma)} \exp \left[\frac{-1}{\frac{uG(0)}{2\omega_0\alpha} + \frac{y(0)}{1 - y(0)\ln\left(\frac{ue^{1-\gamma}}{\omega_0\alpha}\right)}} \right], \quad (69)$$

for $g^2/2\pi^2 m\omega_0^3 > |y(0)|/[1 + |y(0)|\ln[ue^{1-\gamma}/(\omega_0\alpha)]]$; otherwise the gap vanishes. In (69), we have assumed that $y(0) < 0$; i.e., that we are dealing with an unfrustrated spin chain that would not dimerize spontaneously if $g=0$. The three different regimes are illustrated in Fig. 4. An immediate consequence of (69) is that for a sufficiently high frequency ω_0 , or for sufficiently weak spin-phonon coupling constant, a BKT transition to a gapless state is obtained. This transition is analogous to the one that takes place in the frustrated Heisenberg chain when $J_2 < 0.24J_1$.⁶⁶⁻⁶⁹

Our findings for the behavior of the gap, both in the adiabatic and in the antiadiabatic regime, are in qualitative agreement with the quantum Monte Carlo results of Ref. 28 on the one-dimensional $S=1/2$ Heisenberg model. There, it was obtained that for heavy phonon (i.e., low frequency), a static gap was present, while in the case of a light phonon (i.e., high frequency), no spin gap was observed at the lowest temperature accessible in the simulation. It is not obvious whether the absence of a dimerization gap was because the temperature was still above the zero temperature gap or because of the true absence of a gap above the ground state. In either case, these results indicate that the spin gap is very strongly decreased with respect to the static result when the phonon frequency is increased. References 24 and 70, using stochastic series expansion methods, also found that for small spin-phonon coupling and $\omega_0/J=1/4$ no spin gap was obtained, but that increasing the spin-phonon coupling above a critical $\alpha_c=0.225J$ caused a phase transition from the uniform gapless phase to the dimerized gapped phase, in agreement with our results. In Ref. 26, the existence of dimerization and spin gap was analyzed by quantum Monte Carlo simulations of the Heisenberg model for various spin-phonon couplings and phonon frequencies. A phase diagram (Fig. 9 of Ref. 26) was plotted. In agreement with (69), it was shown that the critical spin-phonon coupling to induce dimerization was an increasing function of the phonon frequency. ED studies^{17,18} also show unambiguously the existence of a threshold in the spin-phonon interaction to induce a spin gap when the phonon frequency is nonzero. A constant spin gap is obtained when \tilde{g} behaves roughly as $\omega_0^{1/2}$ which seems in agreement with the predictions of (69). Finally, a similar qualitative agreement is found in the one-dimensional Holstein model for spin-1/2 electrons by DMRG study.²² The system undergoes a quantum phase transition between the metallic phase and the Peierls insulating phase at a finite critical value of the electron-phonon interaction. Concerning the BKT universality class of the transition predicted by (69), in the DMRG study of Ref. 23 it was indeed found that as a

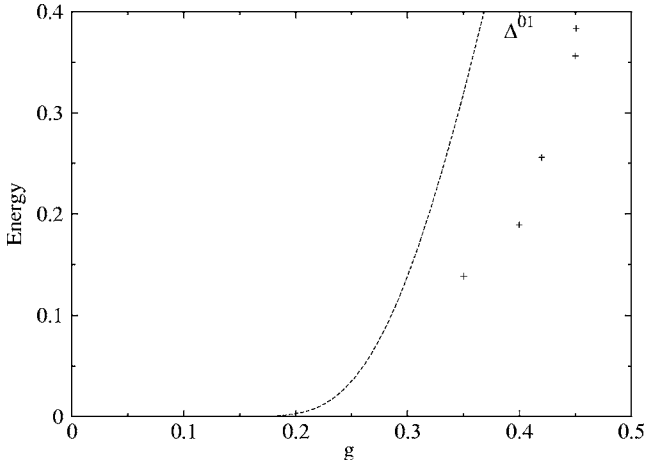


FIG. 5. Comparison of our prediction for Δ^{01} with the results of exact diagonalization (Ref. 18). In both cases, the gap is an increasing function of the spin-phonon coupling constant. Our results are roughly twice the exact diagonalization result.

function of the coupling constant the quantum phase transition from the gapless to the gapped state is a BKT transition. A BKT transition was also found in the related fermionic case in Refs. 21 and 65. Another result of Ref. 23 regards the evaluation, by finite-size scaling, of Luttinger exponent K_ρ of the spinless fermions. It was found that approaching the transition at a critical value of g_c , K_ρ has small deviation from $1/2$ from 0.59 to 0.42. Such finding is in agreement with a BKT transition driven by the operator $\cos 4\phi$ since the value of the Luttinger exponent at the transition is then $K=1/2$.

In the antiadiabatic regime we predict a power-law relationship between the critical spin-phonon coupling g_c and the frequency ω_0 . We note that a power-law relation between the critical spin-phonon coupling was found in Ref. 20. However, the results of Ref. 20 are obtained in the limit of XY anisotropy, so that a direct comparison of the exponents is not possible. We can make a more direct comparison with the data of Ref. 18. If we call g_{DA} the spin-phonon coupling constant used in Ref. 18, it is related to our spin-phonon coupling constant by

$$\frac{g^2}{m\omega_0} = 4J^2 g_{DA}^2, \quad (70)$$

yielding for the dimensionless spin-Peierls coupling constant

$$G = \frac{4g_{DA}^2}{\pi^2\omega_0}. \quad (71)$$

The exact diagonalizations in Ref. 18 were performed for $\omega_0=0.3J$. The dimensionless parameter $u/(\alpha\omega_0)=\pi/(2 \times 0.3) \approx 5.2$, indicating that a continuum description such as ours should be still applicable. The values given in Ref. 18, Fig. 1, lead to a dimensionless coupling constant in the range $[0.17, 0.27]$, which is at the limit of the perturbative regime. Since $\pi G/2 < .429 < 2\omega_0/J=0.6$, we are in the antiadiabatic regime, not far from the crossover. The gap we are calculating is Δ^{01} since our RG approach does not take solitons into account. The result of the comparison is shown in Fig. 5,

where we have replotted the data of Ref. 18 for the gap Δ^{01} , along with the formula (E20) in which logarithmic corrections are neglected. Obviously, the overall behaviors of the gap with the coupling constant are very similar. On a more quantitative level, there is a discrepancy between our results and those of Ref. 18 by roughly a factor of 2. Such difference is clearly not due to the logarithmic corrections. Because our coupling constant is already rather large, the logarithmic corrections should be rather small. Moreover, if the discrepancy was caused by logarithmic corrections, it would diminish as the coupling constant increases, which is not the case here. This leaves us with three possible explanations of the quantitative difference between our results and those of Ref. 18. The most likely explanation is that a coupling constant G in the range $[0.17, 0.27]$ is already a rather large value of the coupling constant, and a one-loop RG such as ours is not sufficient to obtain the gap quantitatively in this regime. A two-loop or higher-order calculation may reduce the scale of the gap with respect to one loop and lead to better agreement. However, since the usual techniques for deriving renormalization group equations^{71–73} are restricted to one loop, one needs to develop a field theoretic RG approach⁷⁴ to check this. Such an approach is beyond the scope of the present paper. Alternatively numerical data for a smaller coupling constant would be interesting to compare to. The second possible explanation is that our procedure to match the results of the RG in the adiabatic and the antiadiabatic is introducing an incorrect scale factor in the antiadiabatic limit. This is possible, if for instance, when we are in still the adiabatic regime but near the crossover, the interaction with the phonons is causing a reduction of the gap. Such an effect is ignored in the Eq. (E20). A possible last explanation is that because the ratio of the phonon frequency to the exchange coupling is still not very small, the continuum treatment is not sufficiently accurate. Note, however, that despite the relatively extreme case of this numerical data (large coupling constant and phonon frequency) with respect to a continuum approach and first-order RG analysis, the quantitative agreement is still reasonably good.

In addition to providing an analytical framework to describe the behavior of the spin-Peierls gap as a function of coupling constant or frequency, our analysis allows us to extract other physical quantities. In particular a quantity that can be deduced from our calculations to describe the Peierls ordering structure of the ground state is the dimerization $\delta = \langle q_n \rangle$. We can calculate it from the magnetic order parameter through the relation, $\delta = (-)^n (g/k_e) \langle \mathbf{S}_i \cdot \mathbf{S}_{i+1} \rangle = (-)^n (g/k_e) \times \langle \cos(2\phi) \rangle$. In the adiabatic regime, the results of the RG analysis gives

$$\delta \sim (-)^n \frac{g}{k_e} \left(\frac{g^2}{2\pi u \rho \omega_0^2} \right)^{1/3}, \quad (72)$$

whereas in the antiadiabatic regime we obtain

$$\delta \sim (-)^n \frac{g}{k_e} \left(\frac{\omega_0 \alpha}{u} \right)^{1/2} \exp \left[- \frac{1}{2 \left[\frac{u}{\alpha \omega_0} \frac{g^2}{2 \pi u \rho \omega_0^2} - |y(0)| \right]} \right]. \quad (73)$$

Since by scaling, the expectation value of $\langle \cos(2\phi) \rangle$ is related to the spin-Peierls gap by the relation $\langle \cos 2\phi \rangle \sim (\Delta/J)^K$, we immediately obtain the scaling relation for the dimerization order parameter: $\delta \sim (g/k_e)(\Delta/J)^K$. It was found in ED studies¹⁸ (Fig. 1 of Ref. 18) that the alternation δ in the exchange integral and the spin gap were increasing functions of the spin-phonon coupling constant with a threshold. The correlation of displacement and dimerization predicted by (72) and (73) are also neatly illustrated on Fig. 8 of Ref. 26.

From the behavior of $\langle \cos(2\phi) \rangle$ in the adiabatic and antiadiabatic regime we can also immediately infer some features of the spin-spin correlations function. In the antiadiabatic regime, from (68), we deduce that for a fixed frequency, the correlations decrease at increasing the spin-phonon coupling [Fig. 15 of Ref. 26]. At a fixed spin-phonon coupling and increasing ω_0 , the spin-spin correlation functions become instead less and less affected by g . These findings are again in agreement with the results obtained in Ref. 26. We thus see that our derivation provides a unified framework explaining and generalizing the previous studies.

B. Relation to experiments

Let us now turn to experimental systems. Our results clearly show that nonadiabatic phonon dynamics strongly renormalizes the magnetic correlations and the dependence of the gap.

A well known example of a material where such strong renormalizations are observed is the spin-Peierls material¹² CuGeO_3 . In this material, the phonon frequency is rather high compared to the actual spin gap ($\omega_0 \sim 310$ K). Interestingly, the thermodynamics of this material can be fitted with a frustrated spin chain model,⁷⁵ with $J_2/J_1=0.36$, i.e., well into the spin gap regime. As was pointed out,^{12,13} such a dimerization is not intrinsic but due to the spin-phonon coupling itself. Indeed, our RG analysis shows that the low-energy properties of a spin chain coupled to dynamical phonons are similar at low energy to those of a frustrated spin chain provided that the phonon frequency is *above* the zero temperature spin gap, which is the case in CuGeO_3 . In such a system one can expect a very strong reduction of the gap due to the finite phonon frequency as shown in Fig. 3, and was noted before for CuGeO_3 . As a point of comparison of the interplay between the phonon frequency and the phonon coupling constant, we have reported in Fig. 6 the various compounds listed in Table 1 of Ref. 12. From Eq. (44), we expect $\Delta_{MF} \sim (u/\alpha)G(0)$, and therefore using Eq. (E20), $\Delta = \omega_0 e^{-3.93\omega_0/\Delta_{MF}}$. Note that the values of the gap taken here are only indicative, in connection with our one-dimensional analysis. Indeed, they are dependent (i) on the measurement method and differ slightly depending on which quantity is measured and (ii) in part of the interchain couplings, which

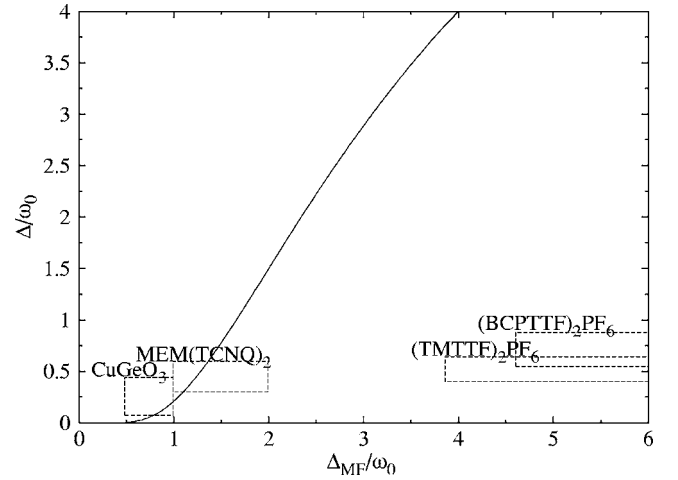


FIG. 6. Various compounds exhibiting a spin-Peierls transition plotted on a gap Δ/ω_0 vs Cross-Fisher gap Δ_{MF}/ω_0 . The data for the gap Δ , the phonon frequency ω_0 and the Cross-Fisher gap Δ_{MF} are extracted from Table 1 of Ref. 12. Note that the experimental determination of the gap is to be taken with a grain of salt given the differences between the various determinations from various measurements (neutrons, thermodynamics, etc.) The full line is Eq. (E20), which is the dependence of the gap on frequency that we expect when logarithmic corrections to scaling is neglected.

we have not treated in the present theory. We nevertheless see in Fig. 6 that the agreement between our calculated values of the spin-Peierls gap and the observed one for various systems both in the antiadiabatic regimes is quite decent. Although CuGeO_3 is the material for which the effects of the phonon frequency are the stronger, another material for which the present study could be relevant is MEM(TCNQ)_2 . For this material the phonon frequency is of the same order as the spin-Peierls gap $\Delta \sim 30\text{--}60$ K, and one can thus still expect effects of the finite phonon frequency on the spin-Peierls gap. The other two compounds $(\text{TMTTF})_2\text{PF}_6$ and $(\text{BCPTTF})_2\text{PF}_6$ are closer to the adiabatic regime (since they have $\Delta_{MF}^{\sigma} > \omega_0$) and thus are expected to have a gap less dependent of the phonon frequency than CuGeO_3 or MEM(TCNQ)_2 . We note that for these two compounds, the agreement with our formula is not good. For $(\text{TMTTF})_2\text{PF}_6$, this might result from the fact that the charge localization temperature $T\rho \approx 200$ K is relatively low compared to the spin-Peierls transition temperature and charge fluctuations can still influence the transition. Indeed, a description based on adiabatic phonons interacting with both charge and spin fluctuations can account for both the magnetic susceptibility and the NMR relaxation rate in this material.⁶¹ A related explanation of the discrepancy could be the existence of a charge ordering transition^{76,77} in $(\text{TMTTF})_2\text{PF}_6$. Such a transition can affect the mean-field spin-Peierls transition temperature of the material^{78,79} and can thus invalidate our simplistic estimate of the spin-Peierls coupling constant. Finally, in both TTF materials, antiferromagnetic interchain coupling could be relatively important, and may diminish the spin-Peierls ordering, resulting in a smaller spin-Peierls gap.⁸⁰

In order to further test the above determination of the gap, it would be interesting to be able to vary continuously the

phonon frequency. Pressure could be an interesting way to address this question. Since when applying pressure, both the exchange constant and the phonon frequency are to be affected, one has to compute the net effect on the gap, which our theory allows us to do. Such measurements could allow to follow the behavior of the gap such as described in Fig. 3.

VI. CONCLUSIONS

In the present paper, we have analyzed spin-Peierls problem for a single spin-1/2 chain coupled to an optical phonon of frequency ω_0 using bosonization techniques. The bosonized action was approximately solved by using the self-consistent harmonic approximation.^{51,52} In the low-frequency limit, we have reproduced the result obtained by Cross and Fisher by the mean-field approximation.⁹ In the high-frequency limit, we have shown that the retarded interaction was giving rise to a term that was local in time and was identical to the bosonized form of a frustrating next-nearest-neighbor interaction, in agreement with the canonical transformation approach.³¹ The self-consistent approximation also allowed us to describe entirely the crossover between the two regimes. In the regime that we have considered, the crossover frequency was given by the spin-Peierls gap Δ_s calculated for a static phonon ($\omega \rightarrow 0$ with $k_e = m\omega_0^2$ fixed). The adiabatic regime extends in the region $\omega_0 \ll \Delta_s$, and the antiadiabatic regime extends in the region $\omega_0 \gg \Delta_s$. All the previous findings can be recovered by the renormalization group by using a two-step approximation as in Ref. 60. We stress that although we use the same two-step approximation as Ref. 60, the behavior of the spin gap that we obtain in the low-frequency limit in our renormalization group is different from the one that one would deduce from the renormalization group applied to spinful fermions at half-filling coupled to optical phonons, as in Ref. 60. The reason for this is that in our problem the charge mode is absent, making the spin-phonon interaction more relevant than in Ref. 60. The advantage of the renormalization group approach over the self-consistent approximation is that the former is applicable in the SU(2) invariant case, where the induced nonretarded approximation becomes marginal. For the SU(2) invariant case, the crossover frequency between the adiabatic and the antiadiabatic limit remains $\omega_0 \sim \Delta_s$. However, due to the marginality of the induced term, a BKT transition in the antiadiabatic limit between the gapped state and the gapless state becomes possible. Near the transition, the spin gap Δ drops very rapidly with the phonon frequency as $\Delta \sim e^{-C\omega_0/(\omega_{BKT}-\omega_0)}$ and vanishes for $\omega_0 > \omega_{BKT}$. These results are in qualitative agreement with numerical studies²³ and with the canonical transformation method.³¹ As the frequency ω_{BKT} is a increasing function of the spin-phonon coupling, for fixed ω_0 there exists a critical spin-phonon coupling below which the spin gap disappears. We have also examined in the light of the present theory the existing experimental compounds exhibiting a spin-Peierls transition, as summarized, for example, in Ref. 12. We find a good qualitative agreement with the dependence of the gap predicted by our theory.

Our analysis thus provides a unified analytical framework in which to analyze the spin-Peierls transition. It leads the

way to interesting extensions. In particular one could expect to tackle with similar methods the effects of the interchain couplings, or the effect of impurities on the spin-Peierls transition (see, e.g., Ref. 81 and references therein).

ACKNOWLEDGMENTS

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APPENDIX A: EXPRESSION OF THE PROPAGATOR IN THE SCHA

We need to obtain an expression for the propagator G . We have

$$G(x, \tau) = \frac{\pi K u}{\beta} \sum_{\omega_n = 2\pi n/\beta} \int \frac{dq}{2\pi} \frac{e^{i(qx - \omega_n \tau)}}{\omega_n^2 + u^2(q^2 + \xi^{-2})} = \frac{\pi K}{u} \mathcal{G}(x, \tau). \quad (\text{A1})$$

The reduced propagator \mathcal{G} satisfies the partial differential equation (PDE)

$$\left[u^2 \partial_\tau^2 + \partial_x^2 - \frac{1}{\xi^2} \right] \mathcal{G}(x, \tau) = -\delta(x) \sum_{n=-\infty}^{\infty} \delta(\tau - n\beta), \quad (\text{A2})$$

and the following properties:

$$\begin{aligned} \mathcal{G}(x, \tau + \beta) &= \mathcal{G}(x, \tau), \\ \mathcal{G}(\pm x, \pm \tau) &= \mathcal{G}(x, \tau). \end{aligned} \quad (\text{A3})$$

To solve the partial differential equation (A2), we consider first the auxiliary partial differential equation

$$\left[u^2 \partial_\tau^2 + \partial_x^2 - \frac{1}{\xi^2} \right] \mathcal{G}_0(x, \tau) = -\delta(x) \delta(\tau). \quad (\text{A4})$$

Clearly, if we have a solution of (A4), we can easily deduce from it a solution of (A2):

$$\mathcal{G}(x, \tau) = \sum_{n=-\infty}^{\infty} \mathcal{G}_0(x, \tau - n\beta). \quad (\text{A5})$$

An explicit solution of the PDE (A4) is readily found by Fourier transformation, and application of Eq. 9.6.21 of Ref. 58. One has

$$\mathcal{G}_0(x, \tau) = \frac{u}{2\pi} K_0 \left(\frac{\sqrt{x^2 + u^2 \tau^2}}{\xi} \right), \quad (\text{A6})$$

and thus

$$\mathcal{G}(x, \tau) = \frac{u}{2\pi} \sum_{n=-\infty}^{\infty} K_0 \left(\frac{\sqrt{x^2 + u^2(\tau - n\beta)^2}}{\xi} \right). \quad (\text{A7})$$

It is easily seen that the series in (A7) is convergent, and that the function defined by (A7) satisfies all the conditions (A3). The result (A7) could also have been obtained by using the Fourier transform of the Dirac comb. We note that in reality we have cheated slightly. Because of the cutoff on the momentum integral in (A1), the function $\delta(x)$ is in fact smeared out into a function $\delta_\Lambda(x)$, which goes to the delta function only for $\Lambda \rightarrow \infty$. Consequently, the true propagator \mathcal{G}_Λ is in fact the convolution of $\delta_\Lambda(x)$ with the function defined by Eq. (A7). A simple way to incorporate the cutoff in (A7) is to perform the replacement $x^2 \rightarrow x^2 + \alpha^2$, with $\alpha \sim \lambda^{-1}$. This substitution has the advantage of preserving the symmetries (A3). Finally, we have

$$G(x, \tau) = \frac{K}{2} \sum_{n=-\infty}^{\infty} K_0 \left(\frac{\sqrt{x^2 + u^2(\tau - n\beta)^2 + \alpha^2}}{\xi} \right). \quad (\text{A8})$$

APPENDIX B: SOLUTION OF THE VARIATIONAL EQUATIONS

In the present section, we study the solution of the variational equations derived from minimization of the free energy (41) with respect to ξ . The contribution of the region $\tau \ll \xi/u$ can be written as

$$\begin{aligned} & \frac{g^2}{4(\pi\alpha)^2 \rho \omega_0^2} \left(\frac{e^\gamma \alpha}{2\xi} \right)^{2K} \int_0^{2e^{-\gamma} \omega_0 \xi / u} dv e^{-v} \left[\left(\frac{e^\gamma u}{2\xi \omega_0} \right)^{2K} v^{2K} \right. \\ & \quad \left. + \left(\frac{e^\gamma u}{2\xi \omega_0} \right)^{-2K} v^{-2K} \right] \\ & = \frac{g^2}{4(\pi\alpha)^2 \rho \omega_0^2} \left(\frac{e^\gamma \alpha}{2\xi} \right)^{2K} \left[\left(\frac{e^\gamma u}{2\xi \omega_0} \right)^{2K} \gamma \left(1 + 2K, 2e^{-\gamma} \frac{\omega_0 \xi}{u} \right) \right. \\ & \quad \left. + \left(\frac{e^\gamma u}{2\xi \omega_0} \right)^{-2K} \gamma \left(1 - 2K, 2e^{-\gamma} \frac{\omega_0 \xi}{u} \right) \right], \quad (\text{B1}) \end{aligned}$$

where γ is the incomplete gamma function (see Ref. 58, Chap. 6, p. 260). Using the identity

$$\begin{aligned} & \left(\frac{\alpha}{\xi} \right)^{2K} \left(\frac{u}{\xi \omega_0} \right)^{-2K} \gamma \left(1 - 2K, 2e^{-\gamma} \frac{\omega_0 \xi}{u} \right) \\ & = \left(\frac{\alpha \omega_0}{u} \right)^{2K} \left[\Gamma(1 - 2K) - \Gamma \left(1 - 2K, 2e^{-\gamma} \frac{\omega_0 \xi}{u} \right) \right] \quad (\text{B2}) \end{aligned}$$

and noting that the first term in the right-hand side is independent of ξ , we can rewrite up to a renormalization the short-distance contribution to the variational free energy as

$$\begin{aligned} & \left(\frac{u \alpha e^\gamma}{2\xi^2 \omega_0} \right)^{2K} \gamma \left(1 + 2K, 2e^{-\gamma} \frac{\omega_0 \xi}{u} \right) \\ & - \left(\frac{\alpha \omega_0}{u} \right)^{2K} \Gamma \left(1 - 2K, 2e^{-\gamma} \frac{\omega_0 \xi}{u} \right). \quad (\text{B3}) \end{aligned}$$

The contribution of the region $\tau \gg \xi/u$ can be rewritten as:

$$\begin{aligned} & 2 \frac{g^2}{4(\pi\alpha)^2 \rho \omega_0^2} \left(\frac{\alpha e^\gamma}{2\xi} \right)^{2K} \int_{2e^{-\gamma} \omega_0 \xi / u}^{\infty} dv e^{-v} \\ & = \frac{g^2}{2(\pi\alpha)^2 m \omega_0^2} \left(\frac{\alpha e^\gamma}{2\xi} \right)^{2K} e^{-2e^{-\gamma} \omega_0 \xi / u}. \quad (\text{B4}) \end{aligned}$$

Thus, the variational free energy to use reads

$$\begin{aligned} F = F_0 & - \frac{u}{2\pi K \xi^2} \langle \phi^2 \rangle - \frac{g^2}{4(\pi\alpha)^2 \rho \omega_0^2} \left[2 \left(\frac{\alpha e^\gamma}{2\xi} \right)^{2K} e^{-2e^{-\gamma} \omega_0 \xi / u} \right. \\ & + \left(\frac{\alpha e^\gamma}{2\xi} \right)^{4K} \left(\frac{u}{\alpha \omega_0} \right)^{2K} \gamma \left(1 + 2K, 2e^{-\gamma} \frac{\omega_0 \xi}{u} \right) \\ & \left. - \left(\frac{\alpha \omega_0}{u} \right)^{2K} \Gamma \left(1 - 2K, 2e^{-\gamma} \frac{\omega_0 \xi}{u} \right) \right]. \quad (\text{B5}) \end{aligned}$$

APPENDIX C: DERIVATION OF THE RENORMALIZATION GROUP EQUATIONS

To derive the renormalization group equations, we start from the action (52), where the function $\mathcal{D}_{\omega_0, \beta}(\tau)$ is defined in (12) and satisfies

$$\int_{-\beta/2}^{\beta/2} \mathcal{D}_{\omega_0, \beta}(\tau) d\tau = 1. \quad (\text{C1})$$

Renormalization group equations are obtained from operator product expansion techniques (OPE).^{72,82} The following OPEs are needed:

$$\begin{aligned} \cos 2\phi(x, \tau) \cos 2\phi(x', \tau') & \sim \frac{1}{2} \left\{ 1 - \frac{1}{2} [2(x - x') \partial_x \phi(x, \tau) \right. \\ & \quad + 2(\tau - \tau') \partial_\tau \phi(x, \tau)]^2 \\ & \quad \left. + \cos 4\phi(x, \tau) \right\}, \quad (\text{C2}) \end{aligned}$$

$$\cos 2\phi(x, \tau) \cos 4\phi(x', \tau') \sim \frac{1}{2} \cos 2\phi(x, \tau), \quad (\text{C3})$$

$$\begin{aligned} \cos 4\phi(x, \tau) \cos 4\phi(x', \tau') & \sim \frac{1}{2} \left\{ 1 - \frac{1}{2} [4(x - x') \partial_x \phi(x, \tau) \right. \\ & \quad \left. + 4(\tau - \tau') \partial_\tau \phi(x, \tau)]^2 \right\}. \quad (\text{C4}) \end{aligned}$$

To find the renormalization group equations, we write the partition function, and expand to second order around the Gaussian fixed point. The important contributions are of first order in g^2 [due to the nonlocality of the action (52)], and of second order in g_\perp^2 and g_\parallel^2 . Then, we change the cutoff by $\alpha \rightarrow \alpha e^{dl}$. We then apply the OPEs (C2) to obtain the short-distance contributions of the terms with $\alpha^2 < (x - x')^2 + u^2(\tau - \tau')^2 < \alpha^2 e^{2dl}$ to the renormalization of the coupling constants. Proceeding in that way, we obtain the following corrections $O(dl)$ to the action:

$$\begin{aligned}
 & -\frac{1}{2\rho\omega_0^2}\left(\frac{g}{\pi\alpha}\right)^2\mathcal{D}_{\omega_0(l)}\left(\frac{\alpha}{u}\right) \\
 & \times\int_{\alpha<u|\tau-\tau'|<\alpha e^{dl}}dx d\tau d\tau'\left[-(\tau-\tau')^2(\partial_\tau\phi)^2+\frac{1}{2}\cos 4\phi\right],
 \end{aligned} \tag{C5}$$

coming from the g^2 term

$$\begin{aligned}
 & -\frac{1}{2u}\left(\frac{2g_\perp}{(2\pi\alpha)^2}\right)^2\int_{\alpha<r<\alpha e^{dl}}rdr d\theta\frac{1}{2}\left[1-8r^2\cos^2\theta(\partial_x\phi)^2\right. \\
 & \left.-8\frac{r^2}{u^2}\sin^2\theta(\partial_\tau\phi)^2\right],
 \end{aligned} \tag{C6}$$

coming from the g_\perp^2 term, and

$$\begin{aligned}
 & -\frac{2g_\perp}{(2\pi\alpha)^2}\times-\frac{1}{2\rho\omega_0^2}\left(\frac{g}{\pi\alpha}\right)^2\int dx d\tau d\tau'\cos 2\phi(x,\tau) \\
 & \times\mathcal{D}_{\omega_0(l)}(\tau-\tau')\times 2\int_{\alpha<|r-r'|<\alpha e^{dl}}dx'' d\tau''\frac{1}{2}\cos 2\phi(x,\tau)
 \end{aligned} \tag{C7}$$

coming from the $g_\perp g^2$ term. The term (C5) contributes to the renormalization of K, u, g_\perp . The term (C6) contributes to the renormalization of u, K . Finally, the term (C7) contributes to the renormalization of g^2 . After having performed the mode integration, we have to restore the original cutoff.⁷² An operator O of scaling dimension d_O is rescaled as $O\rightarrow Oe^{-d_O l}$, whereas coordinates are rescaled as $x\rightarrow xe^{dl}$ and $\tau\rightarrow\tau e^{dl}$. One also finds $\beta\rightarrow\beta e^{-dl}$, i.e., $T\rightarrow Te^{dl}$. As a result of this operation, we obtain $g_\perp\rightarrow g_\perp e^{(2-4K)dl}$. The rescaling of g^2 is a bit more subtle. First, we notice that the rescaling of $\alpha\rightarrow\alpha e^{dl}$ amounts to a rescaling of ω_0, β inside the function \mathcal{D} . Hence, the rescaling acts on \mathcal{D} as

$$\mathcal{D}_{\omega_0, \beta}\rightarrow\mathcal{D}_{\omega_0(l)e^{dl}, \beta e^{-dl}e^{dl}}, \tag{C8}$$

and this way of rescaling \mathcal{D}_{ω_0} guarantees that the constraint (C1) remains satisfied. The rescaling of \mathcal{D} absorbs the opposite rescaling of one of the components x, τ, τ' . As a result, the rescaling of g^2 is given by $g^2\rightarrow e^{(2-2K)dl}g^2$. We notice that this result is in contrast with the case of a disordered system,⁶² in which the disorder D is rescaled as $D\rightarrow De^{(3-2K)dl}$. Mathematically, the difference arises because in the case of phonons, we want to keep the weight in the function \mathcal{D} constant under the RG flow. This constraint means that physically we are converting the non-local interaction that exists at high energy into a local one represented by the g_\perp term by integrating out successively its short-distance contributions. The remaining weight is then given by $2\int_\alpha^{\beta/2e^{-l}}\mathcal{D}_{\omega e^l, \beta e^{-l}}(\tau)d\tau$ and goes to zero as l is increased. Adding all the $O(dl)$ contributions, both from integration of short-distance terms and from rescaling, we finally obtain the renormalization group equations as

$$\frac{d}{dl}\left(\frac{1}{2\pi u K}\right)=\frac{\alpha}{u}\left(\frac{g}{\pi u}\right)^2\frac{1}{\rho\omega_0^2}\mathcal{D}_{\omega_0}(\alpha/u)+\frac{g_\perp^2}{2\pi^3 u^3}$$

$$\frac{d}{dl}\left(\frac{u}{2\pi K}\right)=\frac{g_\perp^2}{2\pi^3 u},$$

$$\frac{d}{dl}\left(\frac{g_\perp}{\pi u}\right)=(2-4K)\frac{g_\perp}{\pi u}+\alpha\left(\frac{g}{\pi u}\right)^2\frac{1}{\rho\omega_0^2}\mathcal{D}_{\omega_0}(\alpha/u),$$

$$\frac{d}{dl}\left(\frac{g^2}{\pi u\rho\omega_0^2}\right)=\left(2-2K+\frac{g_\perp}{\pi u}\right)\frac{g^2}{\pi u\rho\omega_0^2},$$

$$\frac{d\omega_0}{dl}=\omega_0,$$

$$\frac{dT}{dl}=T. \tag{C9}$$

We note that for $g=0$ these equations reduce to the usual RG equations of the sine-Gordon model.⁷³ If we neglect the contribution of g_\perp to the renormalization of g^2 , we see that the gap obtained for $g^2/(u\rho\omega_0^2)\sim 1$ coincides with the gap predicted by Cross and Fisher.⁹ Taking g_\perp into account for $K\sim 1/2$ leads to logarithmic corrections in the dependence of the gap on G . These corrections are discussed in Appendix D.

APPENDIX D: LOGARITHMIC CORRECTIONS TO SCALING

Let us consider a spin-1/2 chain with a static dimerization, described by the Hamiltonian

$$H=J\sum_n(1+\delta(-)^n)\mathbf{S}_n\cdot\mathbf{S}_{n+1}. \tag{D1}$$

Bosonization and scaling arguments^{9,41} lead to the prediction of a gap $\Delta\sim\delta^{2/3}$. However, the presence of a marginally irrelevant operator induces corrections to scaling^{42,48,64,83,84} and the gap behaves in fact as

$$\Delta=\left[\frac{1.723\delta^{2/3}}{\left(1+\frac{2}{3}|y(0)|\ln\frac{|y(0)|}{1.3612\delta}\right)}\right]^{1/2}. \tag{D2}$$

As a result of logarithmic corrections, the ground state energy of the dimerized spin chain behaves as

$$\frac{E_0}{J}=-\frac{0.2728\delta^{4/3}}{1+\frac{2}{3}|y_2(0)|\ln\frac{|y(0)|}{1.3612\delta}}. \tag{D3}$$

If we now consider that the chain (D1) is coupled to adiabatic phonons, one needs to minimize the total energy $k_e/g^2\delta^2-B\delta^{4/3}|\ln\delta|^{-1}$ with respect to δ yielding $\delta^{2/3}|\ln\delta|\sim g^2/k_e$. The gap thus behaves as

$$\Delta=6.07\frac{g^2}{m\omega_0^2}\left|\ln\frac{g^2}{m\omega_0^2}\right|^{-3/2}, \tag{D4}$$

where we have used the factors quoted in Eqs. (D2) and (D3) and Ref. 48. We know show how the expression (D4) can be

recovered within our RG approach. Using the initial conditions with SU(2) symmetry, the RG equations are given by the Eqs. (61) and (62).

If we now assume that $G(0) \ll y(0)$, in Eq. (61) we can take $G=0$, so that the previous equations reduce to the single BKT equation

$$\frac{dy}{dl} = y^2. \quad (\text{D5})$$

For $y < 0$, this equation flows to a fixed point $y^* = 0$ with the flow given by

$$y(l) = \frac{y(0)}{1 - y(0)l}. \quad (\text{D6})$$

Using (D6) in Eq. (62), we can easily integrate it and obtain

$$G(l) = G(0) \frac{e^l}{[1 + |y(0)l|]^{3/2}}. \quad (\text{D7})$$

This equation should break down for $G(l_0) \approx |y(l_0)|$, and after that an exponential flow of G is expected. Using Eq. (D7), the strong coupling behavior is obtained when

$$e^{l^*} = \frac{1}{G(l_0)e^{-l_0}} = \frac{(1 + |y(0)l_0|)^{3/2}}{G(0)}, \quad (\text{D8})$$

where l_0 is given by

$$G(0)e^{l_0} = |y(0)|[1 + |y(0)l_0|]^{1/2}. \quad (\text{D9})$$

Solving Eq. (D9) by iteration and using the first iteration, one finds the following scaling for the spin-Peierls gap valid for small G :

$$\Delta_{sp} \approx e^{-l^*} = \frac{G(0)}{\left[1 + |y(0)l_0| \ln \left(\frac{|y(0)l_0|}{G(0)} \right) \right]^{3/2}}. \quad (\text{D10})$$

This behavior is in agreement with the behavior obtained in Eq. (D4) by considering logarithmic corrections to the energy of the dimerized chain.

APPENDIX E: STUDY OF THE SU(2) INVARIANT RG EQUATIONS

We consider the system of two coupled first-order differential equations (61) and (62). A convenient approach in the antiadiabatic regime is to recast this differential system as a single differential equation. It is also convenient to make the approximation $G(l) = G(0)e^l$ as to render the second-order equation linear. Introducing⁸⁵

$$Y(l) = \exp \left[- \int_0^l y(l') dl' \right], \quad (\text{E1})$$

we obtain the following second-order differential equation:

$$\frac{d^2 Y}{dl^2} = - \frac{\omega_0 G(0) \alpha}{2u} e^{2l} e^{-(\omega_0 \alpha / u) e^l} Y(l), \quad (\text{E2})$$

$$= - \frac{uG(0)}{2\omega_0 \alpha} \left(\frac{\omega_0 \alpha e^l}{u} \right)^2 e^{-(\omega_0 \alpha / u) e^l} Y(l), \quad (\text{E3})$$

with the initial conditions for $Y(0) = 1$ and $Y'(0) = -y(0)$.

It is possible to simplify the second-order differential equation (E2) by a variable change to $s = (\omega_0 \alpha / u) e^l$. Writing $Y(l) = Z[(\omega_0 \alpha / u) e^l]$, one finds that $Z(s)$ satisfies the differential equation

$$\frac{d^2 Z}{ds^2} + \frac{1}{s} \frac{dZ}{ds} + \frac{uG(0)}{2\omega_0 \alpha} e^{-s} Z(s) = 0, \quad (\text{E4})$$

with initial conditions

$$Z \left(\frac{\omega_0 \alpha}{u} \right) = 1, \quad (\text{E5})$$

$$\frac{\omega_0 \alpha}{u} \frac{dZ}{ds} \left(\frac{\omega_0 \alpha}{u} \right) = -y(0). \quad (\text{E6})$$

Equation (E4) can be recast in the form of an integral equation which reads

$$Z(s) = 1 - y(0) \ln \left(\frac{su}{\omega_0 \alpha} \right) - \frac{uG(0)}{2\omega_0 \alpha} \int_{\omega_0 \alpha / u}^s \frac{ds'}{s'} \int_{\omega_0 \alpha / u}^{s'} s'' e^{-s''} Z(s'') ds''. \quad (\text{E7})$$

We study first the antiadiabatic limit, $uG(0)/\alpha \ll \omega_0$. Let us begin with the case $y(0) = 0$. By iterating Eq. (E7) once, we obtain

$$Z(s) = 1 - \frac{uG(0)}{2\omega_0} \left[\left(1 + \frac{\omega_0 \alpha}{u} \right) \ln \left(\frac{su}{\omega_0 \alpha} \right) + e^{-s} - e^{-\omega_0 \alpha / u} + E_1(s) - E_1 \left(\frac{\omega_0 \alpha}{u} \right) \right] + o \left(\frac{uG(0)}{2\omega_0} \right), \quad (\text{E8})$$

where E_1 is defined in Ref. 58. Using the fact that $-\omega_0 \alpha / u \ll 1$, and $\omega_0 \alpha / u e^l \gg 1$, we can rewrite this equation as

$$Y(l) = 1 - \frac{uG(0)}{2\omega_0} \left[l - \ln \left(\frac{u}{\omega_0 \alpha} \right) + \gamma - 1 \right], \quad (\text{E9})$$

where $\gamma = 0.577\dots$ is Euler-Mascheroni's constant.⁵⁸ The gap is obtained when $Y(l^*) = 0$, i.e.,

$$l^* = \ln \left(\frac{u}{\alpha \omega_0} \right) + \frac{2\omega_0 \alpha}{uG(0)} + 1 - \gamma. \quad (\text{E10})$$

The differential equation (E4) can also give some indication on the crossover scale to the adiabatic regime. Assuming that $uG(0)/2\omega_0 \alpha \gg 1$, it is reasonable to replace the term e^{-s} with 1 in (E4), yielding the approximate equation

$$\frac{d^2 Z}{ds^2} + \frac{1}{s} \frac{dZ}{ds} + \frac{uG(0)}{2\omega_0 \alpha} Z(s) = 0. \quad (\text{E11})$$

The solution of the above differential equation is easily found⁵⁸ in terms of Bessel functions. One has

$$Z(s) = AJ_0 \left(\left(\frac{uG(0)}{2\omega_0\alpha} \right)^{1/2} s \right) + BY_0 \left(\left(\frac{uG(0)}{2\omega_0\alpha} \right)^{1/2} s \right). \quad (\text{E12})$$

The initial conditions yield the following linear system for A, B :

$$\begin{aligned} AJ_0 \left(\left(\frac{\omega_0\alpha G(0)}{2u} \right)^{1/2} \right) + BY_0 \left(\left(\frac{\omega_0\alpha G(0)}{2u} \right)^{1/2} \right) &= 1, \\ AJ_1 \left(\left(\frac{\omega_0\alpha G(0)}{2u} \right)^{1/2} \right) + BY_1 \left(\left(\frac{\omega_0\alpha G(0)}{2u} \right)^{1/2} \right) &= y(0) \\ &\times \sqrt{\frac{2u}{\omega_0\alpha G(0)}}. \end{aligned} \quad (\text{E13})$$

If we consider the case of $y(0)=0$, we find

$$A = -\frac{\pi}{2} \left(\frac{\omega_0\alpha G(0)}{2u} \right)^{1/2} Y_1 \left(\left(\frac{\omega_0\alpha G(0)}{2u} \right)^{1/2} \right), \quad (\text{E14})$$

$$B = \frac{\pi}{2} \left(\frac{\omega_0\alpha G(0)}{2u} \right)^{1/2} J_1 \left(\left(\frac{\omega_0\alpha G(0)}{2u} \right)^{1/2} \right). \quad (\text{E15})$$

For $\omega_0\alpha G(0)/u \ll 1$, an approximate solution is $Z(s) = J_0[uG(0)/(2\omega_0\alpha)]^{1/2}s$. We obtain $Z(s)=0$ for $[uG(0)/(2\omega_0\alpha)]^{1/2}s = j_{0,1} \approx 2.40482$ (cf. Ref. 58). The resulting strong coupling scale would be given by

$$l^* = \ln \left[\frac{j_{0,1}}{G(0)} \left(\frac{2u}{\omega_0\alpha} \right) \right]. \quad (\text{E16})$$

We note that at this scale $G(l^*) \gg 1$, but $(\omega_0\alpha/u)e^{l^*} \ll 1$. This indicates that $G(l)$ is reaching strong coupling before the scale l^* is reached, and in this regime, the gap is produced by G directly. The true strong coupling scale in this adiabatic regime is then $l_{ad}^* = \ln[1/G(0)]$. The above calculation thus allows to determine when the crossover from adiabatic to antiadiabatic regime is obtained.

Comparing l_{ad}^* with l_{antiad}^* we find that their difference is minimal when $uG(0)/\omega_0\alpha = 2$. Thus, for $uG(0) \ll \omega_0\alpha$, we are in the antiadiabatic regime, and

$$\Delta = \omega_0 e^{-(1-\gamma)e^{-2\omega_0\alpha/u}G(0)}. \quad (\text{E17})$$

For $uG(0) \gg \omega_0\alpha$, the gap behaves as $\Delta = CuG(0)$. We need to match the two results. To do this, we require that the two expressions of the gap are equal and have the same derivative with respect to $G(0)$ when $uG(0)/\alpha = 2\omega_0$. This yields the following ansatz for the gap:

$$\Delta = \frac{C}{2e} \frac{u}{\alpha} G(0), \quad \frac{u}{\alpha} G(0) \gg \omega_0, \quad (\text{E18})$$

$$\Delta = C\omega_0 e^{-2\omega_0\alpha/u} G(0), \quad \frac{u}{\alpha} G(0) \ll \omega_0. \quad (\text{E19})$$

The constant C can be obtained using results for the adiabatic limit. Using Eq. (8) of Ref. 86, we find that $C/(2\pi e) = 0.627$, leading to $C = 10.7$. This leads us to the following ansatz for the gap:

$$\Delta = 0.627 \frac{g^2}{m\omega_0^2} \text{ for } 2\omega_0 < \frac{u}{\alpha} G(0), \quad (\text{E20})$$

$$\Delta = 10.7\omega_0 e^{-2\pi m\omega_0^3/g^2} \text{ for } 2\omega_0 > \frac{u}{\alpha} G(0). \quad (\text{E21})$$

The above ansatz Eq. (E20) tends to overestimate the gap in the adiabatic regime as it neglects completely the effect of the nonzero frequency on the gap. However, the lack of a precise criterion to decide when the RG flow has reached the strong coupling regime prevents us from finding a better answer.

We now turn to the case of $y(0) \neq 0$. We first look at the antiadiabatic limit. We obtain by iterating the equation (E7) that

$$\begin{aligned} Z(s) &= 1 - y(0) \ln \left(\frac{us}{\omega_0\alpha} \right) - \frac{uG(0)}{2\omega_0\alpha} \left\{ \left(1 + \frac{\omega_0\alpha}{u} \right) e^{-\omega_0\alpha/u} - y(0) \right. \\ &\times \left[e^{-\omega_0\alpha/u} + E_1 \left(\frac{\omega_0\alpha}{u} \right) \right] \left. \right\} \ln \left(\frac{us}{\omega_0\alpha} \right) + \frac{uG(0)}{2\omega_0\alpha} \left[1 \right. \\ &- y(0) \ln \left(\frac{u}{\omega_0\alpha} \right) \left. \right] \left[E_1 \left(\frac{\omega_0\alpha}{u} \right) + e^{-\omega_0\alpha/u} - E_1(s) - e^{-s} \right] \\ &- \frac{uG(0)}{2\omega_0\alpha} y(0) \left[2E_1 \left(\frac{\omega_0\alpha}{u} \right) + 2G \left(\frac{\omega_0\alpha}{u} \right) \right. \\ &+ e^{-\omega_0\alpha/u} \ln \left(\frac{\omega_0\alpha}{u} \right) - E_1 \left(\frac{\omega_0\alpha}{u} \right) \ln \left(\frac{\omega_0\alpha}{u} \right) E_1(s) \ln s \\ &\left. - 2E_1(s) - 2G(s) - e^{-s} \ln s \right]. \end{aligned} \quad (\text{E22})$$

Using the expansions of E_1 and G for small argument,

$$E_1(s) = -\gamma - \ln s + o(1), \quad (\text{E23})$$

$$G(s) = -\frac{1}{2}(\ln s)^2 + \frac{\Gamma''(1)}{2} + o(1). \quad (\text{E24})$$

We find the following expression for $Y(l)$ at small $uG(0)/(\omega_0\alpha)$:

$$\begin{aligned} Y(l) &= 1 + \frac{uG(0)}{2\omega_0\alpha} \left[1 - \gamma + \ln \left(\frac{u}{\omega_0\alpha} \right) \right] - \epsilon y(0) \left[\ln^2 \left(\frac{u}{\omega_0\alpha} \right) \right. \\ &+ 2(1-\gamma) \ln \left(\frac{u}{\omega_0\alpha} \right) + \Gamma''(1) - 2\gamma \left. \right] - \left\{ \frac{uG(0)}{2\omega_0\alpha} + y(0) \right. \\ &\left. - \frac{uG(0)}{2\omega_0\alpha} y(0) \left[1 - \gamma + \ln \left(\frac{u}{\alpha\omega_0} \right) \right] \right\} l. \end{aligned} \quad (\text{E25})$$

For $y(0) < 0$ a solution exists if

$$\frac{uG(0)}{2\omega_0\alpha} > \frac{|y(0)|}{1 + |y(0)| \ln \left(\frac{ue^{1-\gamma}}{\alpha\omega_0} \right)}. \quad (\text{E26})$$

In other words, the existence of the gap is controlled by the ratio of the coupling constant to the marginally irrelevant perturbation measured at the energy scale $\omega_0 e^{1-\gamma}$. We have⁵⁸ $\Gamma''(1) = \gamma^2 + \pi^2/6$. However, for what follows, it is convenient

to make an approximation $\Gamma''(1) \sim \gamma^2 + 1$. One can then rewrite

$$Y(l) = 1 + \frac{uG(0)}{2\omega_0\alpha} \left[1 - y(0) \ln \left(\frac{ue^{1-\gamma}}{\omega_0\alpha} \right) \right] \ln \left(\frac{ue^{1-\gamma}}{\omega_0\alpha} \right) - \left\{ y(0) + \frac{uG(0)}{2\omega_0\alpha} \left[1 - y(0) \ln \left(\frac{ue^{1-\gamma}}{\omega_0\alpha} \right) \right] \right\} l. \quad (\text{E27})$$

The strong coupling scale is obtained for $Y(l^*)=0$ which gives us

$$l^* = 1 - \gamma + \ln \left(\frac{u}{\omega_0\alpha} \right) + \frac{1}{\frac{uG(0)}{2\omega_0\alpha} + \frac{y(0)}{1 - y(0) \ln \left(\frac{ue^{1-\gamma}}{\omega_0\alpha} \right)}}. \quad (\text{E28})$$

We note that making $y(0)=0$ in the above formula gives back the expression (E10).

Turning to the crossover to the adiabatic regime, we note that again, due to the lack of a precise criterion for cutting the RG flow, we can only propose an ansatz to relate the two regimes. Extending the reasoning made in the previous discussion of the case $y(0)=0$, we expect that the crossover happens when $l_{ad}^* - l_{antiad}^*$ is minimal. The lengthscale l_{ad}^* has been obtained in section D. It reads

$$l_{ad}^* = -\ln G(0) + \frac{3}{2} \ln [1 - |y(0)| \ln G(0)]. \quad (\text{E29})$$

Minimizing the difference of length scales then gives

$$\left[\frac{uG(0)/2\omega_0\alpha}{\frac{uG(0)}{2\omega_0\alpha} - \frac{|y(0)|}{1 + |y(0)| \ln(ue^{1-\gamma}/\omega_0\alpha)}} \right]^2 = 1 + \frac{3}{2} \frac{|y(0)|}{1 - |y(0)| \ln G(0)}. \quad (\text{E30})$$

In the case of $y(0) \ll 1$, one can write $(u/\alpha)G(0) = 2\omega_0(1$

+ ϵ). The quantity ϵ is straightforward to obtain by expanding (E30). Finally, one has

$$\frac{u}{\alpha} G(0) = 2\omega_0 \left[1 + 2 \frac{|y(0)|}{1 + |y(0)| \ln \left(\frac{ue^{1-\gamma}}{\omega_0\alpha} \right)} - \frac{3}{2} \frac{|y(0)|}{1 + |y(0)| \ln \left(\frac{u}{2\omega_0\alpha} \right)} \right]. \quad (\text{E31})$$

Therefore, the crossover scale is only weakly affected by the presence of logarithmic corrections. An ansatz similar to Eq. (E20) can be derived in the case of a spin chain with marginally irrelevant operator. Using the results of Ref. 48, combined with the Appendix D, we obtain the following expression of the gap in the adiabatic regime:

$$\Delta = 1.96886 \frac{u}{\alpha} G(0) \left[\frac{1}{1 + |y(0)| \ln \left(\frac{|y(0)|^{2/3}}{2.1557G(0)} \right)} \right]^{3/2}. \quad (\text{E32})$$

Our calculation of the crossover scale shows that this expression is valid provided $2\omega_0 < uG(0)/\alpha$. For $2\omega_0 > uG(0)/\alpha$, an expression of the gap of the form $\Delta \sim \mathcal{C}e^{-l^*}$ with l^* given by Eq. (E28) is valid. Matching the two expressions for $2\omega_0 = uG(0)/\alpha$ yields

$$\Delta = 10.704\omega_0 \left[\frac{e^{|y(0)|/[1+|y(0)| \ln(ue^{-\gamma}/\omega_0\alpha)]}}{1 + |y(0)| \ln \left(\frac{|y(0)|^{2/3}u}{2 \times 2.1557\omega_0\alpha} \right)} \right]^{3/2} \times \exp \left[\frac{-1}{\frac{uG(0)}{2\omega_0\alpha} - \frac{|y(0)|}{1 + |y(0)| \ln(ue^{-\gamma}/\omega_0\alpha)}} \right] \quad (\text{E33})$$

for $2\omega_0 > uG(0)/\alpha$. Letting $y(0) \rightarrow 0$, in Eqs. (E32) and (E33), we recover the previous formulas (E20).

- ¹J. W. Bray, L. V. Interrante, I. S. Jacobs, and J. C. Bonner, in *Extended Linear Chain Compounds*, edited by J. Miller (Plenum, New York, 1983), Vol. 3.
- ²Q. Liu, S. Ravy, J. P. Pouget, C. Coulon, and C. Bourbonnais, *Synth. Met.* **56**, 1840 (1993).
- ³L. Ducasse *et al.*, *Synth. Met.* **27**, 543 (1988).
- ⁴M. Hase, I. Terasaki, and K. Uchinokura, *Phys. Rev. Lett.* **70**, 3651 (1993).
- ⁵J. P. Boucher and L. P. Regnault, *J. Phys. I* **6**, 1939 (1996).
- ⁶R. Peierls, *Quantum Theory of Solids* (Oxford University Press, Oxford, UK, 1955).
- ⁷P. Pincus, *Solid State Commun.* **4**, 1971 (1971).
- ⁸E. Pytte, *Phys. Rev. B* **10**, 4637 (1974).
- ⁹M. C. Cross and D. S. Fisher, *Phys. Rev. B* **19**, 402 (1979).
- ¹⁰M. Braden, G. Wilkendorf, J. Lorenzana, M. Aïn, G. J. McIntyre,

- M. Behruzi, G. Heger, G. Dhalenne, and A. Revcolevschi, *Phys. Rev. B* **54**, 1105 (1996).
- ¹¹M. Braden, B. Hennion, W. Reichardt, G. Dhalenne, and A. Revcolevschi, *Phys. Rev. Lett.* **80**, 3634 (1998).
- ¹²J.-P. Pouget, *Eur. Phys. J. B* **20**, 321 (2001); **24** 415 (2001).
- ¹³G. S. Uhrig, *Phys. Rev. B* **57**, R14004 (1998).
- ¹⁴C. Gros and R. Werner, *Phys. Rev. B* **58**, R14677 (1998).
- ¹⁵G. Wellein, H. Fehske, and A. P. Kampf, *Phys. Rev. Lett.* **81**, 3956 (1998).
- ¹⁶B. Büchner, H. Fehske, A. Kampf, and G. Wellein, *Physica B* **259–261**, 956 (1999).
- ¹⁷D. Augier and D. Poilblanc, *Eur. Phys. J. B* **1**, 19 (1998).
- ¹⁸D. Augier, S. Poilblanc, E. Sorensen, and I. Affleck, *Phys. Rev. B* **58**, 9110 (1998).

- ¹⁹S. Trebst, N. Elstner, and H. Monien, *Europhys. Lett.* **56**, 268 (2001).
- ²⁰L. G. Caron and S. Moukouri, *Phys. Rev. Lett.* **76**, 4050 (1996).
- ²¹R. Bursill, R. McKenzie, and C. J. Hamer, *Phys. Rev. Lett.* **80**, 5607 (1998).
- ²²E. Jeckelmann, C. Zhang, and S. R. White, *Phys. Rev. B* **60**, 7950 (1999).
- ²³R. J. Bursill, R. H. McKenzie, and C. J. Hamer, *Phys. Rev. Lett.* **83**, 408 (1999).
- ²⁴A. W. Sandvik, R. R. P. Singh, and D. Campbell, *Phys. Rev. B* **56**, 14510 (1997).
- ²⁵R. H. McKenzie, C. J. Hamer, and D. W. Murray, *Phys. Rev. B* **53**, 9676 (1996).
- ²⁶R. W. Kühne and U. Löw, *Phys. Rev. B* **60**, 12125 (1999).
- ²⁷C. Raas, U. Löw, G. S. Uhrig, and R. W. Kühne, *Phys. Rev. B* **65**, 144438 (2002).
- ²⁸H. Onishi and S. Miyashita, *J. Phys. Soc. Jpn.* **72**, 392 (2003).
- ²⁹G. S. Uhrig and H. J. Schulz, *Phys. Rev. B* **54**, R9624 (1996).
- ³⁰A. M. Tsvelik, *Phys. Rev. B* **45**, 486 (1992).
- ³¹K. Kuboki and H. Fukuyama, *J. Phys. Soc. Jpn.* **56**, 3126 (1987).
- ³²A. Weisse, G. Wellein, and H. Fehske, *Phys. Rev. B* **60**, 6566 (1999).
- ³³E. Fradkin and J. E. Hirsch, *Phys. Rev. B* **27**, 1680 (1983).
- ³⁴D. J. Gross and A. Neveu, *Phys. Rev. D* **10**, 3235 (1974).
- ³⁵A. B. Zamolodchikov and A. B. Zamolodchikov, *Ann. Phys. (N.Y.)* **120**, 253 (1979).
- ³⁶M. Karowski and H. J. Thun, *Nucl. Phys. B: Field Theory Stat. Syst.* **190**[FS3], 61 (1981).
- ³⁷H. Zheng, *Phys. Rev. B* **56**, 14414 (1997).
- ³⁸P. Sun, D. Schmeltzer, and A. R. Bishop, *Phys. Rev. B* **62**, 11308 (2000).
- ³⁹W. Geertsma and D. Khomskii, *Phys. Rev. B* **54**, 3011 (1996).
- ⁴⁰R. Werner, C. Gros, and M. Braden, *Phys. Rev. B* **59**, 14356 (1999).
- ⁴¹F. D. M. Haldane, *Phys. Rev. B* **25**, R4925 (1982); *ibid.* **26**, 5257(E) (1982).
- ⁴²I. Affleck, D. Gepner, T. Ziman, and H. J. Schulz, *J. Phys. A* **22**, 511 (1989).
- ⁴³P. Lecheminant, in *Frustrated Spin Systems*, edited by H. T. Diep (World Scientific, Singapore, 2005), and references therein.
- ⁴⁴T. Giamarchi, *Quantum Physics in One Dimension*, International Series of Monographs on Physics Vol. 121 (Oxford University Press, Oxford, UK, 2004).
- ⁴⁵Note that we are neglecting the interaction of the phonons with the $q \rightarrow 0$ component of the energy density. This will lead us to predict a spin gap at high frequency ω_0 . However, strictly speaking, taking the Hamiltonian (2)–(6), and performing the canonical transformation for $\omega_0 \gg J$, no frustration is actually generated due to the local character of the Einstein phonons. This indicates that the current-current interaction terms induced by the $q \rightarrow 0$ component may compensate those induced by the $2k_F$ term for sufficiently high frequency. However, since this effect does not exist for dispersive phonons, we will neglect the $q \rightarrow 0$ contribution in what follows.
- ⁴⁶S. Lukyanov, *Phys. Rev. B* **59**, 11163 (1999).
- ⁴⁷I. Affleck, *J. Phys. A* **31**, 4573 (1998).
- ⁴⁸E. Orignac, *Eur. Phys. J. B* **39**, 335 (2004).
- ⁴⁹T. Papenbrock, T. Barnes, D. J. Dean, M. V. Stoitsov, and M. R. Strayer, *Phys. Rev. B* **68**, 024416 (2003).
- ⁵⁰R. P. Feynman, *Statistical Mechanics* (Benjamin Reading, MA, 1972).
- ⁵¹S. Coleman, *Phys. Rev. D* **11**, 2088 (1975).
- ⁵²Y. Suzumura, *Prog. Theor. Phys.* **61**, 1 (1979).
- ⁵³T. Giamarchi and P. Le Doussal, *Phys. Rev. B* **53**, 15206 (1996).
- ⁵⁴J. Voit and H. J. Schulz, *Phys. Rev. B* **34**, R7429 (1986).
- ⁵⁵J. Voit and H. J. Schulz, *Phys. Rev. B* **37**, 10068 (1988).
- ⁵⁶J. Voit and H. J. Schulz, *Phys. Rev. B* **36**, 968 (1987).
- ⁵⁷J. Voit and H. J. Schulz, *Mol. Cryst. Liq. Cryst.* **119**, 449 (1985).
- ⁵⁸M. Abramowitz and I. Stegun, *Handbook of Mathematical Functions* (Dover, New York, 1972).
- ⁵⁹G. T. Zimanyi, S. A. Kivelson, and A. Luther, *Phys. Rev. Lett.* **60**, 2089 (1988).
- ⁶⁰L. G. Caron and C. Bourbonnais, *Phys. Rev. B* **29**, 4230 (1984).
- ⁶¹C. Bourbonnais and B. Dumoulin, *J. Phys. I* **6**, 1727 (1996).
- ⁶²T. Giamarchi and H. J. Schulz, *Phys. Rev. B* **37**, 325 (1988).
- ⁶³K. Yonemitsu and M. Imada, *Phys. Rev. B* **54**, 2410 (1996).
- ⁶⁴J. L. Black and V. J. Emery, *Phys. Rev. B* **23**, R429 (1981).
- ⁶⁵L. G. Caron and S. Moukouri, *Phys. Rev. Lett.* **76**, 4050 (1996).
- ⁶⁶K. Okamoto and K. Nomura, *Phys. Lett. A* **169**, 433 (1992).
- ⁶⁷R. Chitra, S. Pati, H. R. Krishnamurthy, D. Sen, and S. Ramasesha, *Phys. Rev. B* **52**, 6581 (1995).
- ⁶⁸S. Eggert, *Phys. Rev. B* **54**, R9612 (1996).
- ⁶⁹S. R. White and I. Affleck, *Phys. Rev. B* **54**, 9862 (1996).
- ⁷⁰A. W. Sandvik and D. K. Campbell, *Phys. Rev. Lett.* **83**, 195 (1999).
- ⁷¹J. V. José, L. P. Kadanoff, S. Kirkpatrick, and D. R. Nelson, *Phys. Rev. B* **16**, 1217 (1977).
- ⁷²J. L. Cardy, *Scaling and Renormalization in Statistical Physics*, Cambridge Lecture Notes in Physics (Cambridge University Press, Cambridge, UK, 1996).
- ⁷³H. J. F. Knops and L. W. J. Den Ouden, *Physica A* **103**, 597 (1980).
- ⁷⁴D. J. Amit, Y. Y. Goldschmidt, and G. Grinstein, *J. Phys. A* **13**, 585 (1980).
- ⁷⁵G. Castilla, S. Chakravarty, and V. J. Emery, *Phys. Rev. Lett.* **75**, 1823 (1995).
- ⁷⁶D. S. Chow, F. Zamborszky, B. Alavi, P. J. Tantilillo, A. Baur, C. A. Merlic, and S. E. Brown, *Phys. Rev. Lett.* **85**, 1698 (2000).
- ⁷⁷P. Monceau, F. Y. Nad, and S. Brazovskii, *Phys. Rev. Lett.* **86**, 4080 (2001).
- ⁷⁸J. Riera and D. Poilblanc, *Phys. Rev. B* **62**, R16243 (2000).
- ⁷⁹M. Sugiura, M. Tsuchiizu, and Y. Suzumura, *J. Phys. Soc. Jpn.* **73**, 2487 (2004).
- ⁸⁰S. Inagaki and H. Fukuyama, *J. Phys. Soc. Jpn.* **52**, 3620 (1983).
- ⁸¹J.-P. Pouget, S. Ravy, J. Schoeffel, G. Dhalenne, and A. Revcolevschi, *Eur. Phys. J. B* **38**, 581 (2004).
- ⁸²V. Brunel and T. Jolicœur, *Phys. Rev. B* **58**, 8481 (1998).
- ⁸³L. P. Kadanoff, *Phys. Rev. B* **22**, 1405 (1980).
- ⁸⁴M. Nauenberg and D. J. Scalapino, *Phys. Rev. Lett.* **44**, 837 (1980).
- ⁸⁵E. Ince, *Ordinary Differential Equations* (Dover, New York, 1956).
- ⁸⁶E. Orignac and R. Chitra, *Phys. Rev. B* **70**, 214436 (2004).