Spin-Peierls Transition in the Heisenberg Chain with Finite-Frequency Phonons

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We study the spin-Peierls transition in a Heisenberg spin chain coupled to optical bond phonons. Quantum Monte Carlo results for systems with up to $N = 256$ spins show unambiguously that the transition occurs only when the spin-phonon coupling α exceeds a critical value α_c. Using sum rules, we show that the phonon spectral function has divergent (for $N \to \infty$) weight extending to zero frequency for $\alpha < \alpha_c$. The phonon correlations decay with distance r as $1/r$. This behavior is characteristic for all $0 < \alpha < \alpha_c$ and the $q = \pi$ phonon does not soften (to zero frequency) at $\alpha = \alpha_c$.

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The $S = 1/2$ Heisenberg spin chain is unstable towards dimerization (the spin-Peierls transition) when coupled to an elastic lattice [1]. For phonons in the adiabatic limit, this transition has been predicted to occur for arbitrarily weak spin-lattice coupling [1]. On the other hand, recent work in the antiadiabatic (high-frequency) limit suggests a transition only above a critical coupling [2]. The mechanism of the transition in this limit was suggested to be qualitatively different, with no softening of the $q = \pi$ phonon [2]. A way to reconcile these results has been proposed within an improved mean-field (RPA) theory [3], with the result that a complete phonon softening occurs only for bare phonon frequencies ω_0 less than a critical value. For higher ω_0, a central peak appears in the phonon spectral function and the phonon branch remains gapped. Considering the manifestly uncontrolled nature of mean-field calculations in one dimension, nonperturbative results in the regime of phonon frequencies comparable to the magnetic exchange energy J are required to test this novel scenario.

In this Letter, we address the issues of a critical spin-phonon coupling and the mechanism of the zero temperature dimerization transition in the strictly one-dimensional case, using quantum Monte Carlo (QMC) simulations to obtain numerically exact results for relatively large systems. The model we study is defined by the Hamiltonian

$$H = J \sum_{i=1}^{N} (1 + \alpha x_i) \mathbf{S}_i \cdot \mathbf{S}_{i+1} + \omega_0 \sum_{i=1}^{N} n_i , \qquad (1)$$

where $x_i = (a_i^+ + a_i)/\sqrt{2}$ is the phonon coordinate and $n_i = a_i^+ a_i$ is the phonon occupation number at bond i. We use a recently developed QMC method based on sampling the perturbation expansion in the interaction representation [4]. For a finite lattice at finite inverse temperature β, the expansion converges for any decomposition of $H = H_0 + V$ into diagonal (H_0) and perturbing (V) terms and can be used [5] as a basis for a "world line" Monte Carlo algorithm in continuous imaginary time (i.e., without invoking the Trotter decomposition [6]). We include only the bare phonons in the diagonal term; $H_0 = \omega_0 \sum_i n_i$. The updating of the spin degrees of freedom can then be carried out using a new efficient "operator-loop" algorithm [7], which, in particular, allows for sampling of all winding number sectors and hence direct evaluation of the spin stiffness [8].

We consider an energy $\omega_0 = J/4$ for the bare phonons and study the behavior for values of the spin-phonon coupling in the range $0 \le \alpha/J \le 0.5$. We have studied systems with N up to 256 at inverse temperatures $\beta = J/T$ sufficiently high to give ground state results. Typically, for the system sizes we have considered, β as high as $\approx 2N$ is required to achieve convergence to the $T = 0$ limit of all the quantities of interest. We have used at least $\beta = 4N$ for all calculations presented here.

Note that in the model, Eq. (1), for $\alpha > 0$ there is an energy gain associated with an average uniform phonon displacement $\langle x \rangle = (1/N) \sum_i \langle x_i \rangle > 0$, which leads to an increased average effective spin-spin coupling $J_{\text{eff}} = J + \alpha \langle x \rangle > J$. For $\omega_0/J = 0.25$ at $T = 0$, we find $J_{\text{eff}}/J = 1.018$, 1.071, 1.158, 1.278, and 1.430 for $\alpha = 0.1$, 0.2, 0.3, 0.4, and 0.5, respectively. We will in some cases measure energies in units of J_{eff} instead of the bare exchange J.

The most direct signal of the dimerization that can be measured in our simulations is the approach of the staggered phonon correlation function $(-1)^r \langle x_i x_{i+r} \rangle$ to a nonzero value at long distances r. Our results for this quantity indicate a critical coupling $0.1 < \alpha_c/J < 0.35$ for $\omega_0/J = 0.25$ [9]. In order to improve on the accuracy of this rough estimate, and to circumvent potential problems with detecting a very small dimerization (as would be the case for very weak coupling if the mean-field result $\alpha_c = 0$ would be correct), we have also considered several other quantities. It is particularly useful to study the effects of the dynamic phonons in the spin sector (in general, our simulation results for spin quantities have smaller statistical fluctuations than the phonon correlations). Thus we discuss here results for the spin stiffness and the staggered spin susceptibility.

If the dimerization transition occurs at some critical coupling $\alpha_c > 0$, it is expected to be of the Kosterlitz-Thouless (KT) type [10]. The spin stiffness ρ_s, i.e., the ground state energy curvature with respect to a uniform twist ϕ in the spin-spin interaction [11],

$$\rho_s = \frac{1}{N} \frac{\partial^2 E_0(\phi)}{\partial \phi^2}, \tag{2}$$

is then expected to exhibit a discontinuous jump from a finite value for $\alpha \leq \alpha_c$ to zero for $\alpha > \alpha_c$ (reflecting the opening of a spin gap). For a finite system the jump will be smoothed. In Fig. 1 we show results for the stiffness versus α/J for several system sizes. The behavior expected for a KT transition is seen clearly—ρ_s rapidly approaches zero for $\alpha/J \gtrsim 0.4$ but appears to converge to a finite value for $\alpha/J \lesssim 0.2$, indicating a critical coupling between these values, in agreement with our previous results for the dimerization. It is, however, not easy to extract an accurate value for α_c using these results. The scaling behavior is complicated by logarithmic corrections, which we expect to be present for all $\alpha \leq \alpha_c$ as in the case of the Heisenberg chain [i.e., $\alpha = 0$ in Eq. (1)]. This is in contrast to the finite temperature KT transition in the two-dimensional XY model, where ρ_s approaches its asymptotic value algebraically for $T < T_c$ and logarithmically only exactly at T_c [12,13]. An indication of the difficulties associated with the log corrections in the spin-phonon chain can be seen in our stiffness data for $\alpha = 0$, for which the exact infinite-size value is known to be (in our units) [11] $\rho_s = 1/4$; about 8% lower than what we find for $N = 128$.

Although the log corrections complicate the extraction of α_c from the stiffness data, their presence in other quantities can in fact be useful in numerical calculations. The asymptotic behavior of the spin correlation function of the Heisenberg chain is known from bosonization and conformal field theory [14,15]

$$\langle S_i^z S_{i+r}^z \rangle \sim \frac{(-1)^r}{r} \ln^{1/2}(r/r_0). \tag{3}$$

We expect this form to apply for all $\alpha < \alpha_c$. The logarithmic correction should vanish at the critical point α_c, as it is known to do, e.g., at the critical point of the frustrated $J_1 - J_2$ chain [16]. We have calculated the staggered spin susceptibility

$$\chi_s(\pi) = \frac{1}{N} \sum_{m,n} (-1)^{n-m} \int_0^\beta d\tau \, \langle S_n^z(\tau) S_m^z(0) \rangle, \tag{4}$$

for which Eq. (3) and conformal invariance imply the finite-size scaling form [15]

$$\chi_s(\pi) \sim N \ln^{1/2}(N/N_0). \tag{5}$$

In Fig. 2 we graph $[\chi_s(\pi)/N]^2$ vs $\ln(N)$ for α/J in the range 0.1–0.3. For $\alpha/J = 0.1$ and 0.2 the linear behavior for the larger system sizes is consistent with the form (5) expected in the gapless phase, whereas for $\alpha/J = 0.25$ and 0.3 there is a decrease with increasing N, corresponding to a finite asymptotic value for $\chi_s(\pi)$ and therefore the presence of a spin gap. For $\alpha/J = 0.23$ the curve is almost flat within statistical errors for $N \geq 32$, implying that $\chi_s(\pi)$ diverges linearly with N without log correction. Based on these results we conclude that $\alpha_c/J = 0.225 \pm 0.015$.

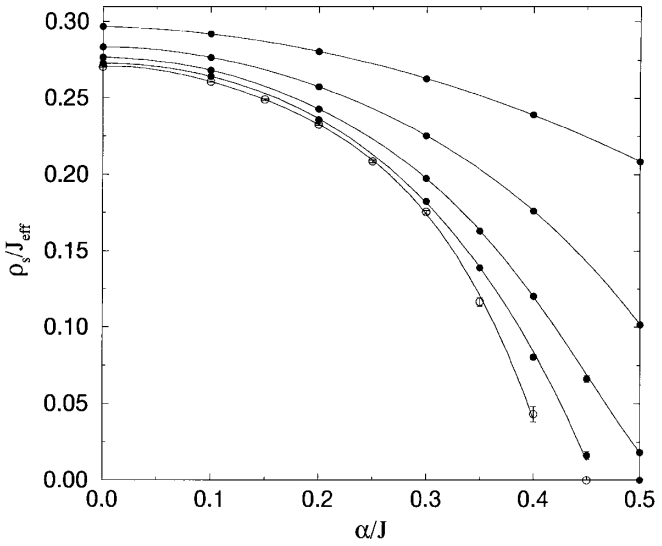

FIG. 1. Spin stiffness vs spin-phonon coupling for system sizes $N = 8$, 16, 32, 64, and 128 (ρ_s decreases with increasing N). Where not shown, statistical errors are smaller than the symbols. The curves are high-order polynomial fits to the data points.

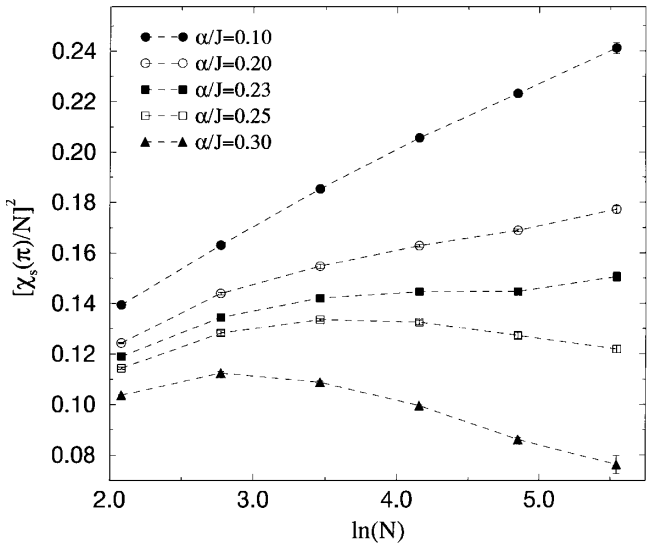

FIG. 2. Size dependence of the staggered spin susceptibility for different values of the spin-phonon coupling. A linear behavior of $[\chi_s(\pi)/N]^2$ vs $\ln(N)$ is expected in the gapless phase, with slope zero at the critical point. A decrease with increasing N indicates the presence of a spin gap.

Having established a KT transition and the critical coupling, we now turn to the question of the behavior of the $q = \pi$ phonons at the transition. We consider the phonon spectral function

$$A(q,\omega) = \sum_{m,n} e^{-\beta E_n} |\langle m|x_q|n\rangle|^2 \delta(\omega - [E_m - E_n]), \tag{6}$$

where $x_q = (1/\sqrt{N}) \sum_{j=1}^{N} \exp(-iqj) x_j$. This real-frequency dynamic quantity cannot be obtained directly in our simulations. In order to avoid the problems associated with numerically continuing imaginary time data to real frequency, we here study sum rules that relate $A(q,\omega)$ to quantities that can be directly calculated. Two useful integrals that can be easily obtained from Eq. (6) are

$$S_x(q) = \int_0^\infty d\omega\, A(q,\omega)(1 + e^{-\beta\omega}), \tag{7a}$$

$$\chi_x(q) = 2\int_0^\infty d\omega\, A(q,\omega)\omega^{-1}(1 - e^{-\beta\omega}), \tag{7b}$$

where $S_x(q)$ and $\chi_x(q)$ are the static structure factor and susceptibility

$$S_x(q) = \langle x_{-q} x_q \rangle, \tag{8a}$$

$$\chi_x(q) = \int_0^\beta d\tau \langle x_{-q}(\tau) x_q(0)\rangle. \tag{8b}$$

Using Eqs. (7a) and (7b) one can readily verify [17] that the ratio

$$R(q) = 2S_x(q)/\chi_x(q) \tag{9}$$

is an upper bound for the lowest phononic excitation of momentum q. For $\alpha \geq \alpha_c$ we therefore expect $R(\pi) \to 0$ as $N \to \infty$, reflecting the presence of two degenerate ground states with momenta 0 and π (linear combinations of the two possible real-space dimerized states). For $\alpha = 0$, $R(q) = \omega_0$ for all q. A transition caused by a softening of the $q = \pi$ phonon would imply $R(\pi) > 0$ for $\alpha < \alpha_c$ and $R(\pi) \to 0$ as $\alpha \to \alpha_c$. This behavior is not seen in our results. Instead, $R(\pi)$ appears to approach zero as N is increased even for α much smaller than the critical value, as shown in Fig. 3. Hence *the spectral weight extends to zero frequency also in the nondimerized systems.*

We also find that the total spectral weight, given by the structure factor according to Eq. (7a), diverges with N. In Fig. 4 we graph $S_x(\pi)$ versus the logarithm of the system size for values of α both below and above the critical coupling. We find a linear increase for $\alpha < \alpha_c$, indicating a logarithmic divergence and therefore an inverse distance decay of the real-space phonon correlation function. For $\alpha = 0.3 > \alpha_c$ the divergence is faster than logarithmic. The expected linear in N behavior cannot be observed close to α_c for the system sizes we have studied, due to large short-distance contributions to $S_x(\pi)$. For $\alpha \geq 0.4$ we do observe an almost linear divergence with N.

These results show that, in the thermodynamic limit, there is infinite $q = \pi$ phonon spectral weight also for

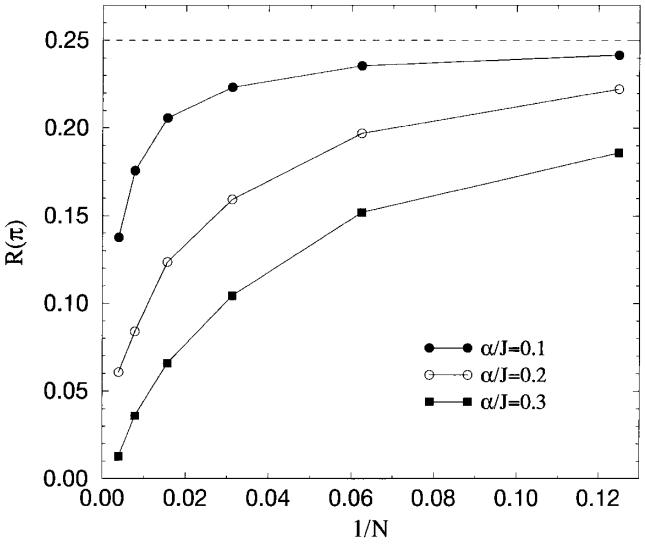

FIG. 3. Upper bound $R(\pi) = 2S_x(\pi)/\chi_x(\pi)$ for the lowest $q = \pi$ phonon excitation energy vs the inverse system size. The dashed line is at the noninteracting ($\alpha = 0$) value ω_0/J.

$\alpha < \alpha_c$. This weight extends to zero frequency. The rate of decay of $R(\pi)$ with increasing N, seen in Fig. 3, shows that the low-frequency weight grows rapidly with N. The only plausible explanation for this is that the phonon spectral function has a central peak with infinite integral. We now elaborate on the reasons for this behavior.

In the absence of spin-phonon couplings, the low-lying excitations of the system are the two-spinon singlet and triplet states of the Heisenberg chain. Our results indicate that an arbitrarily weak coupling to the phonons induces an infinite phonon spectral weight into these states at the staggered momentum $q = \pi$. The asymptotic real-space staggered phonon correlation function has the same $1/r$ decay as the spin-spin correlation function (perhaps differing by multiplicative logarithmic corrections that cannot be detected in our results for the phonon correlations). This is not completely surprising, considering that the Heisenberg chain is also characterized by an inverse distance decay of the dimerization correlation function $\langle (S_i \cdot S_{i+1})(S_{i+r} \cdot S_{i+1+r})\rangle$, as also recently noted by Gros and Werner [3]. The corresponding susceptibility is therefore divergent and this leads to the spontaneous dimerization for arbitrarily weak spin-phonon couplings in the adiabatic case $\omega_0 = 0$. What we have shown here is that dynamic ($\omega_0 > 0$) phonons destroy the long-range order for weak spin-phonon couplings but nevertheless the spin and phonon excitations remain coupled in a manifestly nonperturbative fashion.

The most plausible scenario for the mechanism of the spin-Peierls transition is then the following: For weak coupling α, the phonon spectral function at $q = \pi$ has a finite-weight peak close to the bare frequency ω_0, as well as a central peak with divergent frequency integral [$\ln(N)$ divergent as a function of system size]. As α is increased

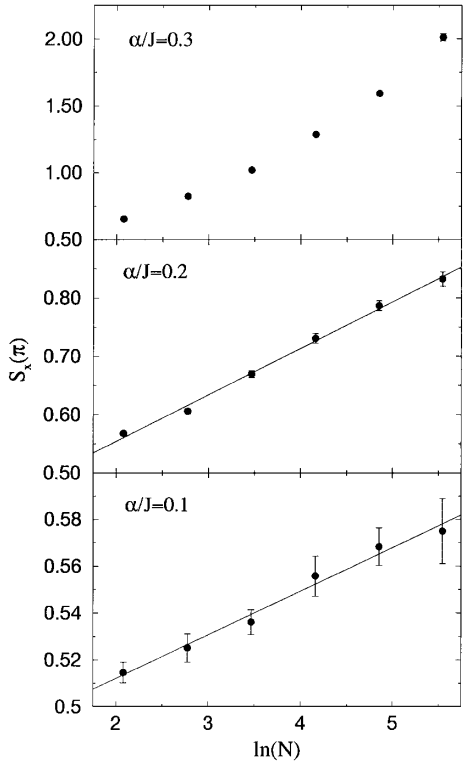

FIG. 4. Staggered phonon structure factor vs the logarithm of the system size. The linear behavior for $\alpha = 0.1$ and 0.2 corresponds to an inverse distance decay of the real-space phonon correlation function. Note that with our definition of the phonon coordinate, the noninteracting structure factor equals $1/2$.

the finite-frequency peak may shift slightly but remains at finite frequency. The central peak sharpens and at $\alpha = \alpha_c$ acquires a δ function component, corresponding to the development of static long-range order. For $\alpha > \alpha_c$ this δ function remains, and a gap develops to the remainder of what was the finite-width central peak for $\alpha \leq \alpha_c$. This gap is the excitation energy of a lattice/magnetic soliton pair.

On general grounds, we find it unlikely that there would be any qualitative changes in the nature of the $T = 0$ transition as ω_0 is varied. A recent density matrix renormalization group study of a model closely related to the one we have studied also finds unambiguously that the critical coupling $\alpha_c > 0$ for any ω_0 [18]. In addition, our results are consistent with the calculations in the antiadiabatic limit [2] (although the infinite low-frequency $q = \pi$ phonon weight for $\alpha < \alpha_c$ was not noted there), even though our $\omega_0 = J/4$ is closer to the adiabatic regime. Our estimated α_c is in good quantitative agreement with a recent calculation within an effective spin model [19].

We have here discussed only the $T = 0$ quantum phase transition in the strictly one-dimensional case. The finite T_c in real materials such as $CuGeO_3$ [20] can be due to three-dimensional phonons, as well as interchain magnetic couplings. The nonsoftening nature of the quantum phase transition that we have found here clearly supports the suggestion [2,3] that the finite-T transition may also be nonsoftening. In the improved RPA theory [3], softening occurs below a critical value of ω_0. In future work, we plan to extend our simulations to two- and three-dimensional systems and hope to address this important issue.

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