Equilibrium dynamics of the sine-Gordon chain: A molecular-dynamics study

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Results of a molecular-dynamics study of the discrete sine-Gordon (SG) chain are reported, emphasizing $\phi$-$\phi$, $\sin\phi$-$\sin\phi$, and $\cos\phi$-$\cos\phi$ dynamic correlation functions ($\phi$ is the SG field variable). Correlations at the temperature $k_B T \approx 0.29 E_K$ ($E_K$ is the continuum SG kink-soliton energy) are interpreted in terms of elementary linear and nonlinear modes—kinks, breathers, single-, and multiphonons. The validity of "ideal-gas" approximations is assessed and corrections from lattice discreteness and mode-mode interactions are discussed. Finally, the relevance of our results to planar ferromagnetic chains (e.g., CsNiF$_3$) in an easy-plane applied magnetic field is assessed.

I. INTRODUCTION

In this paper we describe and interpret results from our molecular dynamics (MD) simulation of the sine-Gordon (SG) chain. This is a one-dimensional system where each particle interacts with its neighbors through harmonic forces and also moves in an externally imposed sinusoidal potential which can be thought of as arising from a rigid background lattice. The equations of motion for the system are

$$M \ddot{U}_n = C(U_{n+1} - 2U_n + U_{n-1}) - \frac{2\pi}{a} A \sin \left( \frac{2\pi}{a} U_n \right),$$

$$n = 1, \ldots, N.$$  \hfill (1)

The total number of particles is $N$ each with mass $M$, the displacement of the $n$th particle from its equilibrium position is $U_n$, and the lattice constant is $a$. $C$ and $A$ are constants giving the strengths of the linear and nonlinear forces, respectively.

These equations of motion are integrated by an algorithm due to Beeman,$^1$ which has previously been used in a study of structural phase transitions.$^2$ The total energy is a constant of the motion in this integration scheme. This technique should be contrasted with the coupled Langevin equation scheme of Schneider and Stoll,$^3$ which keeps the temperature constant, and our results for the SG chain may be considered complementary to theirs. The results reported here are limited to a single temperature $T$ (see below).

Our primary aim is to understand the dynamic structure factors

$$S_{XX}(q,\omega) = N^{-1} \int_{-\infty}^{\infty} dt e^{i\omega t} \langle X(q,t)X(-q,0) \rangle,$$  \hfill (2)

where the wave-vector-dependent fluctuation is defined by

$$X(q,t) = \sum_{n=1}^{N} e^{-iq(n-1)a}X_n(t).$$  \hfill (3)

The three local variables for which we present results are (i) the displacement ($U$), or more precisely its phase ($\phi$) relative to the periodic potential

$$X_n(t) \rightarrow \phi_n(t) = \frac{2\pi}{a} U_n(t),$$  \hfill (4)

(ii) the sine ($s$) of this phase variable

$$X_n(t) \rightarrow s_n(t) = \sin \left( \frac{2\pi}{a} U_n(t) \right),$$  \hfill (5)

and (iii), the fluctuation of the cosine ($c$) of the phase variable

$$X_n(t) \rightarrow c_n(t) = \cos \left( \frac{2\pi}{a} U_n(t) \right) - \left( \cos \left( \frac{2\pi}{a} U_n(t) \right) \right),$$  \hfill (6)
The wave vectors \( q \) are determined from the periodic boundary conditions in the usual way:
\[
q = 2\pi m / (N a),
\]
where \( m \) is an integer. We will frequently use the dimensionless wave vector
\[
\tilde{q} \equiv qa / \pi = 2m / N.
\]
We try to interpret results in terms of the natural elementary modes of the SG equation (1), namely kinks, breathers, and phonons (magnons).\(^3\)\(^6\)

Appealing, but intrinsically simplistic “ideal gas” approximations have been widely used in the literature\(^4\)\(^5\) and it is now important to begin to quantify these. An important advantage of the MD simulation is that the integrated weight \( \int S(q, \omega) d\omega \) can be examined separately for “high”- and “low”-frequency regimes, and we will present results for each of these two regimes. This information is not available from transfer integral schemes\(^6\) without phenomenological approximations, and as we shall see, the total and partial integrated weights can have rather different \( q \) dependence. Since “central peaks” (i.e., low-frequency components) have frequently\(^4\) been attributed to kinks, it is important to understand this probe of nonlinear modes more quantitatively. In particular, interpretation of neutron scattering data in easy-plane Heisenberg magnetic chains [e.g., CsNiF\(_3\) or \((\text{CD}_{3})_{3}\text{NMeCl}_{3}\text{(TMMMC)}\)] has so far depended heavily on simple kink theories to explain anomalous central peaks.\(^5\)\(^6\)\(^7\) Although serious questions remain about the validity of a pure SG description (particularly regarding quantum effects,\(^9\) damping, and the importance of nonlinear out-of-plane spin motions\(^10\)\(^12\), we will see that some qualitative trends may help to explain the notable partial successes of ideal kink-gas theory data fits. Having in mind CsNiF\(_3\) in the presence of a 5-kG in-plane magnetic field,\(^6\)\(^7\) we have chosen the following parameters for Eq. (1): \( M = 1 \), \( A = 1 \), \( a = 2\pi \), and \( C = 29.22 \) (see also Ref. 3).

For these parameter values the kink width is approximately \( 10a \). For many, but not all (see below) properties this validates a continuum SG approximation to (1), as is frequently assumed\(^4\)\(^8\): Equation (1) then becomes
\[
c_{0}^{2} \phi_{xx} - \phi_{tt} = \omega_{0}^{2} \sin \phi,
\]
where
\[
c_{0}^{2} = Ca^2 / M
\]
and
\[
\omega_{0}^{2} = 4\pi^2 A / (M a^2).
\]

For the numerical integration of Eq. (1), the dimensionless variable \( \omega_{0} \) was used, and these equations were integrated for 50,000 time steps using a step size of \( \Delta(\omega_{0}) = 0.08 \).

## II. Predictions of Ideal Gas Phenomenology

The structure factor predicted from an ideal relativistic [cf. Eq. (7)] gas of SG kinks, \( S_{K}^{X}(q, \omega) \), is by now well documented\(^3\)\(^4\)\(^13\):
\[
S_{K}^{X}(q, \omega) = \frac{n_{K}(T)}{2\pi q} P \left( \frac{\omega}{q} \right) \gamma^{-1} \left| \frac{\omega}{q} \right| \left| f_{K}^{X}(q, \omega) \right|^2
\]
with \( \gamma(v) = (1 - v^2 / c_{0}^{2})^{-1/2} \), \( n_{K} \) the kink (plus antikink) density, and \( P(v) \) the ideal relativistic gas velocity \( (v) \) distribution,
\[
P(v) = [2c_{0} K_{1}(\alpha)]^{-1} \gamma(v) \exp[-\alpha \gamma(v)],
\]
\( \alpha = E_{K}^{(0)}/k_{B} T \).

(\( K_{1} \) is a modified Bessel function.)

The functions \( f_{K}^{X} \) are “form factors” reflecting the kink shape: they decay on a scale proportional to the inverse kink width, which is given by \( 2d \equiv 2c_{0} / \omega_{0} \). Relevant examples are given in Table I. Result (8) omits all kink diffusion or lifetime effects and is derived in a Hamiltonian framework.

Corresponding ideal gas results\(^3\)\(^13\) for relativistic breather “particles” suggest central- and high-frequency components: for \( X = c \) (c \( \equiv \cos \))
\[
S_{c}^{B}(q, \omega; \omega_{B}; \text{central}) = \frac{n_{B}(T; \omega_{B})}{2\pi q} \left( \frac{\omega}{\omega_{B}} \right)^{2} \left( \frac{\omega_{0}}{\omega_{B}^{2}} \right)^{-1} - 1 \right) \times P \left( \frac{\omega}{q} \right) \gamma^{-1} \left| \frac{\omega}{q} \right| \left| f_{c}^{B}(q, \omega, \omega_{B}) \right|^2.
\]

This central structure derives from the particle-like envelope of a breather of internal frequency \( \omega_{B} \). The internal oscillation itself yields the high-frequency response centered at\(^13\)
\[
\omega_{B}^{m}(q) \equiv \pm 2\omega_{B} (1 - v_{m}^2 / c_{0}^2)^{1/2} \pm v_{m} q,
\]
where \( v_{m} \) is the velocity at which \( \gamma^{-1}(v) P(v) \) is maximum; i.e., \( v_{m} \) also controls the central peak.
TABLE I. Form factors.

| $\chi(\phi)$ | $|f_1^B(Q)|$ |
|-------------|-------------|
| $\phi$      | $2\pi Q^{-1}[\cosh(\frac{1}{2} \pi Qd)]^{-1}$ |
| $\sin\phi$  | $4d (\frac{1}{2} \pi Qd) [\cosh(\frac{1}{2} \pi Qd)]^{-1}$ |
| $\cos\phi$  | $4d (\frac{1}{2} \pi Qd) [\sinh(\frac{1}{2} \pi Qd)]^{-1}$ |

splitting [Eq. (10)]. $\omega_B$ is restricted (classically) to the continuous range $0 \leq \omega_B \leq \omega_0$, but the upper frequency is limited by system size effects since breathers become arbitrarily extended as $\omega_B \to \omega_0$. The breather form factor (see Ref. 13) $f_2^B \to 0$ as $\omega_B \to 0$ or $\omega_0$ and maximizes at $\omega_B = \frac{\omega_0}{2}$. The breather densities are denoted by $n_B(\omega_B; T)$. The total response is the sum of contributions from all allowed breathers and is a competition of form factors, densities, and lifetimes. This competition is not well understood. We have argued previously for a "preferred" breather with frequency $\omega_B \approx \omega_0/\sqrt{2}$, as suggested by the structure of the breather form factor. We expect that this is appropriate at high enough $T$. At low $T$, however, density effects may be expected to strongly favor low-energy (small amplitude, spatially extended) breathers. Contributions from such breathers can be described within conventional perturbation theory, as asserted elsewhere. The corresponding power-series contributions from these anharmonic processes will compete with harmonic multiphonon expansion terms, although these are interrelated and clear separation will be difficult unless large amplitude (nonperturbative) breathers dominate.

In Sec. III we demonstrate signatures of kinks, breathers, and phonons (including multiphonons). Our MD simulation is at the single temperature $k_B T = 0.293 E_K^{(0)}$, which is chosen because central peak splitting is apparent at this $T$ but kink density is still low enough for a qualitative elementary mode interpretation. Splitting is not found at $k_B T < 0.25 E_K^{(0)}$, and correspondingly we know that asymptotic perturbation theories are valid in this $T$ range for power series and exponential (kink) thermodynamic contributions. Concerning applications of SG to magnetic chains, we should emphasize that this mapping is restricted (among other things) to low-velocity particelike excitations. Thus the onset of SG splitting is expected to coincide with the breakdown of the mapping—larger out-of-plane spin motions are energetically preferred. This is consistent with recent classical Heisenberg chain MD results, although damping and quantum effects have yet to be assessed for real magnetic materials. It should be noted that the onset of splitting does not occur at the same $T$ and $q$ for all correlations and is strongly influenced by discreteness (Sec. III), so that the breakdown of a SG mapping may be similarly sensitive.

III. MOLECULAR DYNAMICS RESULTS AND INTERPRETATION

In this section we present our MD results for the dynamic correlation functions $S_{q\phi}$, $S_{qx}$, and $S_{qx}$, and interpret them in terms of linear phonon and multiphonon processes and kink and breather elementary modes. Kinks and breathers are both very evident in our data: in Fig. 1 we have shown examples of kink and large-amplitude breather dynamics projected from our data by a technique (see Fig. 1 caption) which suppresses all small-amplitude fluctuations.

Breathers will not contribute to odd $\phi$ correlations such as in $S_{q\phi}$ and $S_{qx}$ $(s = \sin)$, and kink theory (8) is indeed rather successful qualitatively. For $S_{q\phi}$, Eq. (8) and Table I imply a split central peak with maximum at $Q = \bar{Q}_{m}(\alpha/q)$, where $\bar{Q}(\alpha)$ is the maximum of $P(\nu)$ itself:

$$\bar{Q}(\alpha) = \begin{cases} 0, & \alpha > 3 \\ c_0 (1 - \alpha^2 / q)^{1/2}, & \alpha < 3. \end{cases}$$

MD results for the central structure in $S_{q\phi}(q, \omega)/S_{\phi}(q) [S_{\phi}(q) \equiv \int (d\omega / 2\pi) S_{\phi}(q, \omega)]$ are shown in Fig. 2 and compared with the ideal gas prediction. We see that the orders of magnitude of intensities are consistent. However, with $\alpha = (0.293)^{-1} = 3.41$ no splitting is predicted, whereas it is strongly evident (Fig. 2) in MD. Indeed a nonzero mean kink velocity $\bar{v}_m$ is apparent in Fig. 1 and consistent with the frequency location of the splitting. We propose that the basic kink mechanism is supported but that details depend strongly on both mode interactions and discrete lattice effects. Unfortunately, neither of these effects have been precisely assessed beyond linear perturbation order, which is generally insufficient for our purposes. Near-quantitative success in predicting the kink density can be achieved by renormalizing $E_K^{(0)}$: At $k_B T = 0.293 E_K^{(0)}$ we use.
We consider discrete lattice corrections to be equally serious. *Discreteness* becomes important for rapidly moving kinks where the continuous Lorentz symmetry breaks down, including the associated cutoff at $\omega = c_0q$ [Eq. (8)]. The qualitative correction is to *increase* the effective continuum kink width $d$ with increasing $\nu/c_0$ (or $\omega/c_0q$). A consequence is the appearance of some weight for $\omega > c_0q$, as observed by MD (Fig. 2). More importantly, the tendency to enhance weight at smaller $\omega/q$ (giving stronger and lower frequency splitting; Fig. 2) compared with the continuum theory can also be understood qualitatively from the enhancing effects of discreteness on $P$ and $f_K$. In a future publication we will analyze these corrections more fully by including numerical estimates of true kink widths and energies for arbitrary discreteness.

We note that there are no severe central peak broadening mechanisms evident (from mode interactions beyond $\alpha$ renormalization).

$S_{\alpha}(q, \omega)$ is also well-described qualitatively by kink theory as far as its central peak structure is concerned. This can be expected since $S_{\phi\phi}$ and $S_{s\phi}$ are directly related from the field equation of motion (in a Hamiltonian framework):
\[
\frac{S_{\omega}(q, \omega)}{S_{\phi\phi}(q, \omega)} = \left( \frac{\omega}{\omega_0} \right)^2 - 2 \left( \frac{d}{a} \right)^2 \left[ 1 - \cos(qa) \right]^2
\]

(13a)

\[
\lim_{q\gamma \to 0} \left[ g d \gamma^{-1} \left( \frac{\omega}{q} \right) \right]^4.
\]

(13b)

The continuum-limit result (13b) is exactly preserved within kink theory\(^1\) but (13a) extends to all frequencies and predicts that at small \(q\), the central intensity in \(S_{\omega}\) is strongly depressed compared with \(S_{\phi\phi}\), whereas a high-frequency component (from self-consistent phonon modes) is enhanced. Our MD results confirm this (see Fig. 3). A new feature should be emphasized—splitting of the central peak is observed, but only for sufficiently large \(q\) (> \(q^*\)). At \(k_B T / E_0^{(1)} = 0.293\), \(q^*\approx 0.008\), and splitting then develops strongly (Fig. 3). We can understand the appearance of \(q^*\) within kink phenomenology from (8) and Table I. In contrast to \(S_{\phi\phi}\), no splitting is predicted from

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**FIG. 3.** Frequency spectra of the sine-sine correlation function [cf. Eq. (5)]. Each curve is labeled with the value of its wave vector \(\vec{q}\), and each is normalized by the initial value of its corresponding correlation function. (a) Low-frequency part of the frequency spectra. The arrows locate \(c_{\omega q}\). (b) A typical comparison of MD results with ideal relativistic kink gas theory at \(\vec{q} = 0.02\). The theory curve is calculated from Eqs. (8), (9), and Table I with \(\alpha = 1.61\). (c) High-frequency part of the frequency spectrum. The upward pointing arrows locate the self-consistent-harmonic phonon frequency. At \(\vec{q} = 0.060\) the low-frequency part of the spectrum is also shown [continuing from part (a)], and the downward pointing arrow locates \(c_{\omega q}\).
$P(v)$ and accompanying $\gamma$ factors because these appear in the combination $\gamma^{-4}P(v)$. This predicts a monotonous decrease with $\omega/q$ for all $\alpha$, but there is a competition with the structure factor which produces splitting for $q > q_0^\star(\alpha)$ (the structure factor effect is weak for $S_{\alpha\alpha}$): a little algebra gives

$$\pi q_d^2 \tan(\frac{1}{2} \pi q_d^2 d) = 1 + \alpha.$$  

We find easily that $q_0^\star$ is always larger than the value $q^\star$ observed in MD. Indeed, even with $\alpha = 0$ ($T = \infty$), $q_0^\star$ is only 0.029. To be consistent with $S_{\alpha\alpha}$ we use $\alpha = 1.61$ in Fig. 3(b) for comparison with MD; then $q_0^\star = 0.054$ to be compared with $q^\star \approx 0.008$ from MD. Again we can understand this discrepancy qualitatively as a discrete lattice effect enhancing the competing terms in (8) more strongly as $\omega/q$ increases. Similarly a tail beyond $\omega = \omega_0 q$ is expected and observed $^{13}$ [Figs. 3(a) and 3(b)]. Notice [Fig. 3(a)] that resolvable splitting for $S_{\gamma\alpha}$ is observed in MD for $\bar{q} \leq 0.06$.

The more delicate nature of the splitting in $S_{\gamma\alpha}$ makes it a better candidate for exposing the importance of corrections to ideal gas theory from both mode interactions (e.g., through $\alpha$ renormalization) and discreteness. To emphasize this we show in Fig. 3(b) a comparison of $S_{\alpha\alpha}(q,\omega) / \int S_{\alpha\alpha}(q,\omega; \text{central/}d\omega/2\pi)$ evaluated from MD and kink theory with $\alpha$ renormalized to 1.61. We use $q = 0.02$, which we believe [see Fig. 6(a)] is in a region of quantitative validity for $\alpha$-renormalized kink theory as far as $\int S_{\gamma\alpha}(\text{central}) d\omega$ is concerned. Despite this successful description of the integrated weight, its distribution in frequency is poorly described [Fig. 3(b)]. We ascribe this to the greater role of form factors in determining splitting for $S_{\gamma\alpha}$ (these are unaffected by $\alpha$ renormalization) than for $S_{\alpha\alpha}$. Note that any tendency towards relativistic splitting is beyond linear phonon-kink interaction theory $^{18}$ which also predicts a much too severe reduction in intensity at our $T$.

In Fig. 3(c) we have also shown the strongly weighted high-frequency structure in $S_{\gamma\alpha}$, whose location is quite well described by single-phonon response theory: self-consistent harmonic phonon theory $^{3}$ suggests a response at

$$\tilde{q}(q) = \{\omega_0^2 \langle \cos \phi \rangle + (2C/M)(1 - \cos qa)\}^{1/2},$$

where $\langle \cos \phi \rangle$ is determined self-consistently, or (as we use here) evaluated from MD which gives $\langle \cos \phi \rangle = 0.346$ at our $T$. The locations of $\tilde{q}(q)$ are shown in Fig. 3(c); they are always slight underestimates. Higher-order multiphonon (see below) and anharmonic broadening mechanisms (including soliton-phonon interactions$^{16}$) necessarily also contribute to $S_{\gamma\alpha}$. The asymmetry with additional weight on the high-frequency side of the single-phonon peaks [see Fig. 3(c)] is expected from these mechanisms. Similarly, we find evidence for such contributions to the low-frequency structure in $S_{\gamma\alpha}$ at large $q$ (see below).

We conclude that the structure in $S_{\gamma\alpha}$ and $S_{\gamma\alpha}$ is basically well-described by kinks and phonons, although refined theories of discrete lattice effects and nonlinear mode interactions are still needed.

No such simple conclusions seem to be possible for $S_{\gamma\varepsilon}$, either for its central- or high-frequency structure observed in MD (see Fig. 4, and also Ref. 3). As we have explained elsewhere $^{13,15}$ (see also above), breather modes are expected to contribute strongly in both frequency ranges, whereas they cannot in $S_{\alpha\alpha}$ or $S_{\gamma\gamma}$. However, familiar multiphonon processes$^{3,12,16,19}$ are also clearly relevant and contributing in the same frequency regimes (there is no single-phonon response as in $S_{\alpha\alpha}$ and $S_{\gamma\gamma}$).

At present it is not clear to what extent these various anharmonic effects are related (i.e., anharmonically broadened multiphonon processes versus extended breathers), although there are MD indications (below) that they can be distinguished as separate contributions at our temperature. No useful relationships can be learned from the equations of motion, as was the case for $S_{\gamma\alpha}$. Kinks should certainly make a central peak contribution to $S_{\gamma\varepsilon}$. According to ideal kink phenomenology [Eq. (8) and Table I],

$$\frac{S_{\gamma\varepsilon}(q,\omega)}{S_{\gamma\gamma}(q,\omega)} = \tanh^{-2}[\frac{1}{2} \pi q \gamma^{-1}(\omega/q)].$$

Pure multiphonon theory$^{3,16,19}$ (i.e., without anharmonic broadening) yields a power series in ($k_B T / E_k^{(0)}$). The two-phonon term $O(k_B T / E_k^{(0)} \delta)$ comprises (i) a low-frequency continuous (difference) component which is essentially flat for $0 \leq \omega \leq c_0 q$ with a square-root singularity at $\omega = c_0 q$. There is then a gap before the onset of a continuous high-frequency (sum) component again with a square-root singularity typical of one dimension (see below). The $q$ dependences of breather, multiphonon, and kink contributions are distinguishable. From their form factors (Table I), kink structure-factor contributions decay characteristically for $\frac{1}{2} \pi q \gamma \geq 1$, i.e., $\bar{q} \leq 0.05$ with our parameter values. Breather contributions represent longer-ranged correlations—breathers all have at least twice a kink’s spatial extent so that their form factors$^{13}$ [in (10)] generally produce decay at smaller $q$ than for kinks. On the other hand, multipho-
non processes decay at larger characteristic $q$’s (e.g., at $q d \sim 2$ for two-phonon terms) and with a Lorentzian rather than Gaussian dependence.

In Fig. 4 we have shown the MD data for low- and high-frequency structures in $S_{cc}$. At high frequency the noise level is high for small $\vec{q}$ ($\leq 0.005$), but the broad two-peaked structures shown are within the numerical resolution. For $\vec{q} \geq 0.05$, weight in the lower-frequency structure is lost (or masked by weight in the higher-frequency structure).

**FIG. 4.** Frequency spectra of the cosine-cosine correlation function [cf. Eq. (6)]. Each curve is labeled by the value of its wave vector $\vec{q}$, and each is normalized by the initial value of its corresponding correlation function. (a) Low-frequency part of the frequency spectrum. The downward pointing arrows locate $c(q)$. (b) The high-frequency part of the frequency spectrum. The downward pointing arrows locate $\omega_{\mu}(q)$. The upward pointing solid arrows locate $\omega_{\nu}(q)$ as given by Eq. (15), with $\langle \cos \phi \rangle$ determined from the long-wavelength limit of $S_{\nu}(q, \omega)$. If $\omega_{\nu}(\cos \phi)$ is fit to the high-frequency peak of $S_{\nu}(q, \omega)$ at $\vec{q} = 0.002$ and that value used to compute $\omega_{\nu}(q)$ at other $q$ values, the result is located at the upward pointing dashed arrow.
structure). For this q regime the two-phonon sum process fits increasingly well as q increases with a little smearing upon the predicted\textsuperscript{15,16,19} square-root singularity at
\[
\omega_2(q) = \left[4\omega_0^2 + c_0^2 q^2\right]^{1/2} = 2\omega_0 \left(\cos\phi\right)^{1/2} \left[1 + \left(\frac{1}{2}q\phi\right)^2 / \left(\cos\phi\right)\right]^{1/2}.
\]
(15)

In writing (15) we have used the self-consistent phonon frequency as a reasonable approximation. An incipient square-root singularity becomes very plausible as q increases [see Fig. 4(ii)]. Supposing that breather contributions are being comparatively lost with increasing q, it is also consistent that weight should be taken from lower frequencies first, since this is contributed from the more extended breathers whose form factors decay most rapidly with increasing q. The quadratic prediction for \(\omega_2(q)\) [Eq. (15)] should be contrasted with the linear one for \(\omega_0^m(q)/\omega_0\) from breather phenomenology [Eq. (11)]. It is hard to be definitive about the identification of the high-frequency peaks with our present data, and we do not believe that our understanding of breather or multiphonon structure-factor contributions and interrelations is sufficient to attempt an absolute comparison at this time. However, qualitatively, one interpretation is that the lower peak should be associated with a "dominant" breather,\textsuperscript{13,15} i.e., dominant frequency \(\overline{\omega}_B\) (and corresponding breather extent\textsuperscript{13}). The selection of \(\overline{\omega}_B\) is a combination of form factor [see below (11)], lifetime, and density effects which is not precisely known. Nevertheless we can impose a consistency requirement if we suppose that the location of the split central peak [Fig. 4(a)] is determined by the same breather type. In view of the anticipated discreteness and interaction effects (cf. discussions of \(S_{\text{eff}}\) and \(S_{ph}\)), we do not fit to the bare theory, Eq. (10), but rather take \(v_m\) directly from the MD data which gives \(v_m / c_0 = \omega_m / c_0 q \approx 0.59\), where we have taken an average \(\omega_m\) for \(q < 0.06\). Fitting the lower high-frequency peak to (11) for \(\overline{q} = 0.002\) suggests \(\overline{\omega}_B \approx 0.7\omega_0\). This agrees surprisingly well with earlier expectations.\textsuperscript{13,15} Note, however, that \(\overline{\omega}_B\) is quite weakly preferred (see below). In Fig. 4 we have indicated the location of \(\omega_0^m(q)\) and \(\omega_2(q)\) according to the above prescriptions. We observe that these coincide closely for much of our q range, and resolution of two distinct contributions in the MD data is not possible for intermediate q. Instead of \(\left(\cos\phi\right)^{1/2}\) in (15) we have used the actual long-wavelength phonon frequency observed in \(S_m\) (Fig. 3). Even so, \(\omega_2(q)\) is a slight underestimate of the observed peaks for all q. This could be a result of the broadening of (harmonic) two-phonon sum processes from the intrinsic anharmonicity in our system, and of higher-order multiphonon contributions which are also important (especially at our high \(T\)).

Within the above breather interpretation, we must conclude from Fig. 4 that \(\overline{\omega}_B\) is only weakly preferred—significant weight is contributed from a wide range of frequencies around \(\overline{\omega}_B\). We certainly expect that \(\overline{\omega}_B \approx \omega_0\), as \(T \to 0\) because of breather density effects dominating form factor considerations (cf. Sec. III). In that case, the important breathers will be included in low-order anharmonic perturbation theories.\textsuperscript{16} This approach has been advocated by Maki et al.,\textsuperscript{20} emphasizing two-phonon bound states (low-energy breathers) as an alternative mechanism for the lower high-frequency peak in \(S_{\text{eff}}\). Additional low-\(T\) (\(\lesssim 0.2\)K) MD simulations are highly desirable to understand relative breather contributions unambiguously.

Considering the central peak in \(S_{\text{eff}}\), we recall that kinks [Eq. (3)], breathers [Eq. (10)], and two-phonon difference processes\textsuperscript{3,12,16,19} all yield broad central peaks with cutoff \(\omega = c_0 q\) in the continuum limit. This agrees with the MD results (Fig. 4) except for the familiar tail for \(\omega > c_0 q\) from discreteness. For \(\overline{q} < 0.05\) there appear to be two central components—one with maximum at \(\omega = 0\) and one split to \(\pm \omega_m \approx 0.59c_0 q\). One proposal (above) associated the latter primarily with breathers. For \(\overline{q} \geq 0.05\) the \(\omega \approx 0\) structure is lost and \(\omega_m / c_0 q\) increases with q (e.g., \(\omega_m / c_0 q \approx 0.87\) for \(\overline{q} = 0.18\)). We argue below that kinks alone can substantially account for the integrated central intensity in \(S_{\text{eff}}\) for \(\overline{q} < 0.05\), so that a quite plausible alternative possibility at our \(T\) is that \(\omega_m\) corresponds to the splitting appropriate to the kink central peak. Note, however, that bare kink theory [Eq. (8) and Table I] only predicts splitting for \(k_B T > E_k^{(0)}\), a substantially higher \(T\) than for \(S_{ph}\) [Eq. (12)]. Thus discrete lattice enhancement would have to be even more severe, dominating continuum form-factor influences and \(\alpha\) renormalizations. Two-phonon difference processes yield a peak at \(\omega_m \leq c_0 q\) as stated earlier, the pure two-phonon difference process predicts a square-root singularity at \(\omega = c_0 q\) which is softened here by higher-order multiphonon effects, anharmonicity, and discreteness. For \(\overline{q} > 0.05\), this last mechanism fits neatly with our understanding (above) of the high-
frequency weight in $S_{cc}$ in the same large $q$ regime, where kinks (or breathers) contribute significantly less.

More detailed comments on the integrated weights $S_{cc}(q)$ and $S_{ss}(q)$ are in order. These contain less information than the detailed frequency structure but do support and quantify the interpretations we have made already. Results are shown in Fig. 5, where we contrast the total and partial (central) weights. Note that their $q$ dependencies are quite distinct and we emphasize again that only the total intensities are rigorously available from transfer integral calculations. In particular, the total intensities all decrease monotonically with increasing $q$ (and agree with transfer integral results). By contrast, the central component of $S_{ss}(q)$ has a maximum at $q \approx 0.07$ and is approximately proportional to $q^2$ as $q \to 0$, in qualitative agreement with kink theory predictions, even at our relatively elevated $T$. We also show in Fig. 6(a) the absolute prediction of kink theory [Eq. (8)] with $\alpha = 1.61$. There is quantitative agreement for $q \leq 0.05$, where kink contributions are expected to be strongest, but there is significant additional weight at larger $q$ [see Fig. 6(a)]. This may be due to third (and higher)-order multiphonon contributions which should dominate those from kinks at large $q$. In addition, diffusive effects which are omitted in our ballistic kink theory become more important with increasing $q$, and discrete lattice effects will certainly move the location of the maximum in $S_{ss}(q)$. If $\alpha$ is not renormalized (i.e., $\alpha = 3.41$ is used), $S_{ss}(q)$ is overestimated by $\sim 50\%$ at small $q$.

To compare with MD results for $S_{cc}(q)$ we have computed [Figs. 6(b) and 6(c)] isolated contributions from kinks [integrating Eq. (8)] and from two-phonon difference processes:

$$
\int_{0}^{E_1} S_2(q, \omega) d\omega = \frac{d}{\pi} \left( \frac{k_B T}{E_k^{(0)}} \right)^2 \left[ 1 + (\frac{1}{2} q d)^2 \right]^{-1}.
$$

(16)

Evidently, a very high proportion of the observed central weight in $S_{cc}$ can be accounted for in this way. Kinks dominate for $q < 0.075$ and two-phonon processes for $q > 0.075$. The small additional weight at large $q$ can be attributed to higher-order multiphonon processes (which decay more slowly with $q$) and anharmonicity. There appears little room for strong breather contributions at small $q$ (where they should be expected). This may be misleading: we should be wary of separating modes more than qualitatively at our $T$, especially where several nonlinearly-related contributions are competing and particularly for kinks and large-amplitude breathers. Certainly, the structure observed in $S_{cc}(q)$ at small $q$ (Fig. 5) is quite outside of isolated kink or two-phonon theory and in the anticipated breather regime. All of this points
to the need for a better understanding of how these various processes are interrelated in a strongly non-linear system. The separation will be much clearer (classically or quantum mechanically) at low $T$, where kinks and large-amplitude breathers will contribute much less weight because of their higher activation energies.

Fig. 6(c) compares the integrated high-frequency MD weight with the prediction of two-phonon sum processes—these give the same weight as Eq. (16). The agreement is good for large $q$ except for small additional weight from higher-order multiphonon contributions. However, as $\bar{q}$ decreases below $\approx 0.1$ there is an increasing additional weight [Fig. 6(c)] which must be accounted for, consistent with our discussion of frequency distributions. Indeed, pure two-phonon theory supplies less than 50% of the observed weight for $\bar{q} \leq 0.05$. Although some anharmonic broadening will occur for multiphonon processes, it is tempting to attribute the additional weight to breather excitations as implied in Fig. 6(c)—dominated by preferred large-amplitude breathers or by extended, perturbative, two-bound-phonon breathers (see above). It is interesting to note that isolated ideal breather theory predicts comparable high- and low-frequency weights in $S_{\infty}(q)$. Clearly the large weight attributed to breathers at high frequency is not matched at low frequency according to our earlier discussion. This probably reemphasized the dangers of separating mode contributions too simplistically (since they are competing for central weight), but may also indicate the greater stability of breather internal degrees of freedom (responsible for high-frequency responses) compared with breather translation.

In Fig. 7 we have compared the percentages of component central- and high-frequency weights in $S_{\infty}(q)+S_{\infty}(q)$. Note the comparable contributions from both $S_{\infty}$ components at all $q$, and also large central contribution from $S_{\infty}$ for $\bar{q} \geq 0.05$.

FIG. 7. Spectral weight in central peak and high-frequency components of $S_{\infty}(q,\omega)$ and $S_{\infty}(q,\omega)$ as a percentage of total weight in $S_{\infty}+S_{\infty}$.

IV. CONCLUDING COMMENTS

Our intention in Sec. III was to seek evidence for elementary contributions to correlation functions in the SG chain. In summary, our conclusions are the following.

(i) Central weight in $S_{\infty}$ is due to kinks for $\frac{1}{2} \pi q d \leq 1$. At larger $q$ additional contributions from third (and higher)-order multiphonon processes seem likely.

(ii) The high-frequency weight in $S_{\infty}$ is predominately a one-phonon response, with anharmonic broadening as well as contributions from higher-order multiphonon processes (especially important at larger $q$).

(iii) $S_{\infty}$ and $S_{\infty}$ are exactly related [Eq. (13)] so that basic mechanisms and relative scales are understood. However, the origin of central-peak splitting within ideal kink theory is quite different. Also harmonic multiphonon contributions are not applicable to $S_{\infty}$; thus the relationship (13) implies connections between anharmonic and multiphonon contributions.

(iv) The central- and high-frequency weight in $S_{\infty}$ at large $q (qd \geq 2)$ is predominantly the result of two-phonon processes, with small contributions from higher-order multiphonon processes.

(v) For $qd \leq 2$ other mechanisms become increasingly important to $S_{\infty}$ in addition to two-phonon (and higher-order) terms. At our $T (\approx 0.3E_{K}/k_{B})$, kinks give a very large contribution to the central weight. The size of this contribution according to elementary kink gas theory may be misleading because of contributions anticipated from particlelike breather modes: at low $qd \lesssim 2/\pi$ anomalies do appear in the $q$ dependence of the central weight (Fig. 5). In the same $q$ range considerable additional weight (beyond two-phonon difference contributions) occurs at high frequency. This additional weight occurs over a broad frequency range but has a weak maximum at a frequency that scales with $q$ differently from the two-phonon sum-onset frequency. The additional weight is probably due to anharmonicity in the form of bound phonons (breathers).

(vi) Comparable data at other (particularly lower) temperatures are needed for convincing identification of competing processes—kinks versus breathers in $S_{\infty}$ (central weight); intermediate-amplitude breathers [from structure-factor effects (3)] versus low-amplitude (low-order perturbational) breathers [supported by density enhancement (20)].

(vii) Ideal kink theory requires strong corrections due to mode-mode interactions and discrete lattice
effects. Neither of these are understood rigorously beyond low-order perturbation theory which is inadequate for $k_B T \geq 0.2 E_K$ or moderate velocity kinks. Nevertheless, qualitative expectations are supported by MD results (see discussions of $S_{\phi\phi}$ and $S_{\omega}$).

We conclude with a few remarks concerning application of SG theory to CsNiF$_3$.\textsuperscript{5,7} We noted earlier that this application should be viewed very cautiously until more complete theoretical studies are available. Indeed it has been suggested\textsuperscript{11} that a literal SG description does not apply at our $T$, a view with which we agree for the classical anisotropic Heisenberg model without external damping. Nevertheless, several features observed\textsuperscript{7} in experiments on CsNiF$_3$ are in surprisingly good agreement with our results. Some general remarks are, therefore, in order.

(i) It is not expected\textsuperscript{5,10,11} that resolvable central peak splitting would survive the perturbations on SG of real materials [damping, large out-of-plane fluctuations, or the discrete spin (all of which will affect kink, breather, and multiphonon processes differently)], but if it did, at small $q$, then ideal-gas fits would require distinct renormalizations as we have discussed.

(ii) Applications of kink-only theory may be quite good [especially for low and intermediate $\tilde{q} \leq 0.05$ (Ref. 22)] at moderately high $T$ (where they have been mostly applied\textsuperscript{7}). Contributions to $S_{\omega}$ (central) from multiphonon contributions only dominate at large $q$. Contributions to the high-frequency weight in $S_{ss} + S_{\omega}$ from $S_{\omega}$ (i.e., in addition to the phonon contribution) are significant for all $q$ (Fig. 7). These should be looked for even though they appear as a low-amplitude extended background. They should certainly appear at sufficiently low $T$ (or high magnetic field)—corresponding responses have been observed\textsuperscript{25} in TMMC.

(iii) Recent experiments\textsuperscript{7} probing the central integrated intensity in the interesting $q$ range $\tilde{q} \leq 0.05$, are consistent with the MD results reported here as we demonstrate in Fig. 8. This is, however, not a very sensitive test except at small $q$—$S_s(q) + S_{\omega}(q)$ has a maximum at $\tilde{q} \leq 0.04$ according to Fig. 5; This is largely driven by $S_{ss}$ and so again is qualitatively within kink theory (and in good agreement with neutron scattering data\textsuperscript{7}). However, consistent frequency distribution of weight would be the most clear-cut diagnostic.

Similarly, regarding the absolute scale in Fig. 8, it is interesting to note that at $\tilde{q}=0.1$ the total central weight in spin-wave units\textsuperscript{21} is 1.1. This compares favorably with the experimental observation\textsuperscript{7} of $\approx 1.0$, despite the possible breakdown of (e.g., frequency-dependent) SG predictions at this $T$\textsuperscript{5,11}. $T$ and $q$ dependence of integrated weights are only weakly sensitive to, e.g., out-of-plane fluctuation perturbations.\textsuperscript{11} It is not clear how sensitive the apparent structure (Fig. 5) in $S_{\omega}(q)$ is to perturbations from SG (it is not a kink property).

(iv) The weight in out-of-easy-plane fluctuations (linear theory\textsuperscript{9}) is much less (factor of $\sim 30$ with our parameters) than in $S_{ss}$, so careful experiments would be needed to distinguish it.

(v) A very serious open question for CsNiF$_3$ is the validity of a SG field theory description for an $S=1$ magnetic chain dynamics. If it is argued that most weight in the classical (or quantum-field theory) SG model correlation functions can be attributed to single-phonon (magnon) or two-phonon sum-difference processes,\textsuperscript{12} then we expect that they can be satisfactorily reconciled with equivalent processes\textsuperscript{12} in the $S=1$ chain simply by rescaling effective Hamiltonian parameters, as is familiar for the linear magnon modes already.\textsuperscript{23} If, however, strongly nonlinear modes also contribute importantly to the SG correlations (as implied here for certain regions of $T$, $\omega$, and $q$ space), then much less clear questions must be faced, especially for dynamics—namely, the nonlinear analogs (if any) in an $S=1$ chain and the importance of out-of-easy-plane fluctuations upon them.

In a future paper we will present corresponding MD results for correlations of $\sin \frac{1}{2} \phi$ and of $\cos \frac{1}{2} \phi$. These are experimentally relevant (although at lower $T$) to the antiferromagnet TMMC (Ref. 8).
and are theoretically interesting as largely kink-sensitive functions\textsuperscript{6,8,24} at small \( q \). The relevant kink phenomenologies must be distinguished, however, from the ones used above, where, e.g., kink densities directly controlled a central peak intensity. In the kink-sensitive function cases, kinks are responsible for a broadened Bragg central peak and their density controls the broadening. Appropriate kink phenomenology is then akin to that required for \( \phi \) correlations in the \( \phi \)-four model\textsuperscript{5,26} but contrasts will be drawn because of the strong role of quasi-breathers in \( \phi^4 \) which affect kink dynamics much more severely than in SG. In particular, central peak splitting in \( \phi^4 \) in lost\textsuperscript{3,27} We have also obtained MD results for a SG chain with a random array of impurities\textsuperscript{19,28} Dynamic responses for this system will be presented elsewhere and compared with the results and mode interpretations for the pure chain.

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\textsuperscript{13}A. R. Bishop, J. Phys. A 14, 1417 (1981). Notice that the right-hand side of Eq. (13a) is zero at \( \omega = 2(d / a) | \sin(qa / 2) |, \) implying that \( S_{\alpha}(q, \omega) \) is zero at this frequency. The MD results for \( S_{\alpha}(q, \omega) \) in Fig. 3(a) show a sharp cutoff near this \( \omega \), but are not precisely zero due to numerical errors. This failure of the data for \( S_{\alpha}(q, \omega) \) to vanish at this point means that Eq. (13a) is not useful for obtaining \( S_{\alpha}(q, \omega) \) directly from the \( S_{\alpha}(q, \omega) \) data.
\textsuperscript{14}Note that upon quantization, the SG breather spectrum becomes discretized such that the lowest energy (most extended) breather coincides with the single "elementary" quantum (the phonon or magnon). Inclusion of this low-energy discretization of the spectrum is essential in the construction of a statistical theory (see, e.g., Ref. 20).
\textsuperscript{17}A. R. Bishop, Solid State Commun. 30, 37 (1979).
\textsuperscript{21}For experimental and theoretical comparison with other works, we use here the absolute units of scattering intensity advocated in Ref. 16, viz., the zero-temperature, long-wavelength one-spin wave intensity which with our parameters becomes \( \approx 0.052 d \), with \( d \approx 5.406a \).
\textsuperscript{22}The characteristic \( q \) values quoted throughout the paper are determined by the scale \( d^{-1} \). Consequently these values are sensitive to the magnetic field strength in, for instance, CsNiF\(_3\). Having this example in mind, we have assumed a field of 5 kG
(cf. Ref. 7).
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