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1981 J. Phys. A: Math. Gen. 14 1417

(http://iopscience.iop.org/0305-4470/14/6/018)

J. Phys. A: Math. Gen. 14 (1981) 1417–1430. Printed in Great Britain

Nonlinear mode phenomenology for sine-Gordon breather excitations

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Received 25 July 1980, in final form 15 October 1980

Abstract. Hamiltonians in one space dimension of the ϕ-four and sine-Gordon classes are considered, emphasising kink- and breather-like excitations. A calculation of classical dynamic structure factors based on a kink ideal gas phenomenology is reviewed in terms of the 'central peaks' predicted. This phenomenological scheme is extended to include *breather* excitations. It is suggested that, for correlations of *appropriate* functions, the breather excitations can give rise to a low-frequency ('central') response from their particle-like envelope and a high-frequency response from their internal oscillatory motions, in qualitative accord with molecular dynamics simulations.

1. Introduction

The statistical mechanics of soliton-bearing systems have become a fashionable subject in recent years (see Currie *et al* 1980, Bishop 1980b).

This is partly because it has been appreciated rather generally that nonlinear excitations can contribute specifically and distinctively to appropriate thermodynamic properties, particularly in low dimensions. Additionally, however, realistic material applications have been suggested for some of the more precisely understood nonlinear equations. These have been mostly in quasi-one and quasi-two dimensions.

Here we will be predominantly concerned with two prototype nonlinear wave equations in *one* space dimension: the 'sine-Gordon' (SG) and 'ϕ-four' Hamiltonians and equations of motion are (cf Currie *et al* 1980)

$$\begin{aligned} H(\mathrm{SG}) &= ha \sum_n \left(\tfrac{1}{2}\phi_{nt}^2 + \frac{c_0^2}{2a^2}(\phi_{n+1}-\phi_n)^2 + \omega_0^2(1-\cos\phi_n) \right), \\ 0 &= \phi_{tt} - c_0^2\phi_{xx} + \omega_0^2 \sin\phi \qquad (c_0/\omega_0 \gg a), \end{aligned} \tag{1.1a}$$

$$\begin{aligned} H(\phi\text{-four}) &= ha \sum_n \left(\tfrac{1}{2}\phi_{nt}^2 + \frac{c_0^2}{2a^2}(\phi_{n+1}-\phi_n)^2 + \tfrac{1}{8}\omega_0^2(\phi^2-1)^2 \right), \\ 0 &= \phi_{tt} - c_0^2\phi_{xx} + \tfrac{1}{2}\omega_0^2\phi(\phi^2-1) \qquad (c_0/\omega_0 \gg a). \end{aligned} \tag{1.1b}$$

Here h sets the energy scale, a is a lattice spacing with lattice index n, and c_0, ω_0 are the characteristic velocity and the frequency respectively. Time and space are denoted by t and x respectively. The SG equation in particular is a useful first model for many systems (see Bishop 1978). Most recently it has been advocated (e.g. Mikeska 1978, 1980) to explain the excitation spectrum in an easy-plane classical ferromagnetic or

0305-4470/81/061417+14\$01.50

anti-ferromagnetic spin chain with easy-plane applied magnetic field (e.g. $CsNiF_3$ or $(CH_3)_4NMnCl_3$(TMMC)). Equilibrium statistical properties of Hamiltonians (1.1) are now well understood (Currie *et al* 1980) *at low temperatures* in terms of contributions from an exponentially small density of spatially limited kink excitations (velocity v)

$$\phi_K(x, t)(\text{SG}) = 4 \tan^{-1}\left[\exp \pm \left(\frac{x - vt}{d(1 - v^2/c_0^2)^{1/2}}\right)\right], \tag{1.2a}$$

$$\phi_K(x, t)(\phi\text{-four}) = \tanh \pm \left(\frac{x - vt}{2d(1 - v^2/c_0^2)^{1/2}}\right), \qquad d = c_0/\omega_0, \tag{1.2b}$$

and from extended, small-amplitude modes ('phonons', 'magnons', etc.). Although a complete numerical solution is available for equilibrium properties from the transfer integral technique (Currie *et al* 1980), normal mode decomposition as above is not rigorously possible except at low temperatures (Bishop 1980b). Thus, although molecular dynamics simulations (Koehler *et al* 1975, Schneider and Stoll 1976, Kerr *et al* 1980) clearly reveal a central role for kinks at higher temperatures, systematic inclusion of kink–kink interactions and of anharmonic phonons has not been possible (with some partial exceptions—see below). *Approximate* thermal renormalisation (Bishop 1979, Sahni and Mazenko 1979) of the kink creation energy has been reasonably successful in treating the main effects on the *kink* gas. However, long-lived *coherent anharmonic* excitations have proven difficult to accommodate so far even in equilibrium properties (see Currie *et al* 1980, Bishop 1980b). In the ideal SG system such coherent motions are known (e.g. Bullough and Dodd 1978) to be strict soliton modes (frequently termed 'breathers'), to be treated on an equal footing with the kinks and phonons, and indeed these three modes are sufficient to specify an arbitrary solution, enjoying all the remarkable strict soliton properties. These properties will be lost in any real SG system because of boundary conditions, lattice discreteness and other perturbations. In other Hamiltonians we can expect that breather modes will be the most unstable against these perturbations, lacking for example the strong topological stability of kinks. Nevertheless, large-amplitude breathing modes are very evident in deterministic and molecular dynamics studies of a *class* of non-integrable Hamiltonians such as ϕ-four (see § 3). Understanding breather contributions is partly academic for static, equilibrium properties—at low temperatures a conventional anharmonic phonon perturbation theory is equally able to reproduce the exact perturbation expansion results deduced from the transfer integral procedure (Bishop *et al* 1980). However, if the coherence of the anharmonic motions gives rise to distinctive features in the *dynamics* (as we have claimed for certain functions (Stoll *et al* 1979); see § 3) then it is important to take account of this (finite lifetime) coherence in building a physically appealing mode phenomenology.

Unlike the case of equilibrium properties, no exact results are possible for dynamic response functions, $S(q, \omega)$. Conventional finite-order Mori expansions or mode–mode coupling theories fail (e.g. Aubry 1976) precisely in the regions of (q, ω, T) space where kink solutions become important. Mode–mode coupling theories have been devised (Sahni and Mazenko 1979) which introduce by hand a plausible low-temperature kink distribution, but here also the results are prejudiced by the assumption of a distribution only of kinks, whereas breather modes are observed in molecular dynamics to modify kink dynamics seriously. Ultimately 'justification' lies in comparison with 'exact' molecular dynamics (MD) calculations. (Alternative approximate theories have been proposed (e.g. Imada 1979, 1980, private communication, Bennett *et al* 1980) based on a Fokker–Planck approach rather than a Hamiltonian one.) The situation is particularly unclear with regard to the role of coherent 'breather-like' modes: such anharmonic contributions can probably be represented at low T in infinite-order Mori schemes (envelope solitons of the one-dimensional classical Heisenberg chain (Bishop 1980c) versus Mori schemes (Reiter and Sjölander 1977, 1980)), but physical breather signatures are then quite obscure.

In view of the above circumstances, the notion of a 'phenomenology' based on the recognition of nonlinear elementary modes with distinct physical signatures has much appeal. In the absence of exact results it has become fashionable to place a great deal of faith in the simplest form of phenomenology, i.e. using *ideal* gases of elementary modes identified from the deterministic equations of motion (see §§ 2, 3). We expect that such an approach can recover gross general features, although quantitative assessment of mode interactions, finite lifetime effects, diffusive behaviour of particle-like excitations, etc, must be left to comparisons with careful MD simulations (Schneider and Stoll, in preparation, Kerr *et al* 1980). This is not the intention of the present work. Rather, we wish to develop an ideal gas phenomenology for *breather* excitations (§ 3) on the same level as has been developed for kinks previously (§ 2).

Our motivation is to substantiate a novel suggestion made by us earlier (Stoll *et al* 1979), on the basis of molecular dynamics simulations, that for *appropriate* (see § 3) static and dynamic correlation functions, breathers and not kinks should make dominant contributions. Breather modes have a much richer structure than single kinks. The two basic characteristics (see § 3) are (i) a particle-like envelope (translating with velocity v_B ($v_B < c_0$)) and (ii) an internal (for SG, harmonic) oscillation of frequency ω_B ($0 < \omega_B < \omega_0$). SG is considered in detail in § 3 (since breather forms are known analytically there) and we find that these two characteristics give rise to distinct response components in S_{cc} ($S_{cc} \equiv S_{\cos\phi\,\cos\phi}(q, \omega)$): (i) a central peak ($\omega \sim 0$) *in addition* to one from kinks (§ 2) and (ii) a high-frequency ($\omega \sim 2\omega_B$) response. The results are potentially interesting because S_{cc} is suggested (Mikeska 1978) to be relevant for correlations measured (Kjems and Steiner 1978) in the quasi-one-dimensional magnet $CsNiF_3$ (see also § 4).

We begin in § 2 by briefly summarising salient results of ideal gas phenomenologies for *kinks*, which we will need to compare with the breather structure factors obtained in § 3.

2. Kink phenomenology

The idea of using an ideal 'relativistic' (see below) or non-relativistic gas of kinks to construct an approximate dynamic structure factor from these configurations has been employed by several authors (e.g. Krumhansl and Schrieffer 1975, Varma 1976, Kawasaki 1976, Bishop and Krumhansl 1976 unpublished, Mikeska 1978, 1980, Theodorakopoulos 1979, Maki 1981) in the ϕ-four and SG systems.

Three types of phenomenology need to be very carefully distinguished, depending on the system's topology and the type of functions being correlated. It is not appropriate to describe these at length here: we refer the reader to Bishop *et al* (1980) for a fuller review. Very briefly the classes are for: (i) functions globally sensitive to a kink presence, but with restrictions on kink–anti-kink ordering or function values—e.g. ϕ correlations in ϕ-four or $\cos\frac{1}{2}\phi$ correlations in SG exhibit a predominantly Ising character (cf Krumhansl and Schrieffer 1975); (ii) functions globally sensitive to kinks and without restrictions on kink–anti-kink ordering—e.g. ϕ correlations in periodic potentials such as SG (see Bennett *et al* (1980) for a low-T hydrodynamic central mode theory from kinks in a Smoluchowski regime); (iii) functions that are *locally* kink-sensitive, i.e. changed by the presence of a kink only in its vicinity. Examples are ϕ^2 for ϕ-four or $\cos\phi$ for SG (see table 1). Here the phenomenology amounts to the results of a classical ideal particle gas with 'particles' of the kink mass, except for an extra 'form-factor' q-dependence, reflecting the kink's structure and the particular correlation function. *Central peaks* are found which are Gaussian except when damping or diffusion is included, in which cases they typically acquire a diffusive Lorentzian character (Theodorakopoulos 1979, Bishop *et al* 1980). It is class (iii) which is directly relevant to us here and which we now summarise for comparison with breather results in § 3.

Table 1. *Kink* form factors $f_K^F(Q)$ for SG and ϕ-four models (equations (1)) for various functions F of the field ϕ (see § 2). $d\equiv c_0/\omega_0$, $Q\equiv q\gamma^{-1}$. All form-factor integrals (equation (2.4)) can be evaluated directly, but any δ functions have been omitted.

(*a*) *Sine-Gordon*: $\phi_K = 4\tan^{-1}\exp(\pm x/d)$.

$F(\phi)$	$\lvert f_K^F(Q)\rvert$
ϕ	$2\pi Q^{-1}[\cosh(\frac{1}{2}\pi Qd)]^{-1}$
ϕ_x	$Q\gamma\lvert f_K^\phi(Q)\rvert$
ϕ_t	$\omega\lvert f_K^\phi(Q)\rvert$
$\cos\phi$	$4d(\frac{1}{2}\pi Qd)\lvert\sinh(\frac{1}{2}\pi Qd)\rvert^{-1}$
$\sin\phi$	$4d(\frac{1}{2}\pi Qd)[\cosh(\frac{1}{2}\pi Qd)]^{-1}$

(*b*) *ϕ-four*: $\phi_K = \tanh(\pm\frac{1}{2}x/d)$

$F(\phi)$	$\lvert f_K^F(Q)\rvert$
ϕ	$2\pi d\lvert\sinh(\pi Qd)\rvert^{-1}$
ϕ_x	$Q\gamma\lvert f_K^\phi(Q)\rvert$
ϕ_t	$\omega\lvert f_K^\phi(Q)\rvert$
ϕ^2	$4d(\pi Qd)\lvert\sinh(\pi Qd)\rvert^{-1}$

In a Hamiltonian approach, we suppose that an arbitrary field configuration $\phi(x,t)$, can be decomposed in a 'nonlinear normal mode' representation with an independent kink sector $\phi_K(x,t)$, where

$$\phi_K(x,t)=\sum_n \phi_{Kn}[\gamma_n(x-x_{0n}-v_nt)]. \tag{2.1}$$

Here x_{0n} and v_n are the initial position and velocity of the nth kink, and $\gamma_n\equiv(1-v_n^2/c_0^2)^{-1/2}$. Considering the kink contribution to the dynamic structure factor $S_K(q,\omega)$ for a function $F(\phi)$:

$$S_K(q,\omega)\equiv L^{-1}(2\pi)^{-2}\int dx\int dt\ e^{i(\omega t-qx)}\langle F^*[\phi_K(x,t)]F[\phi_K(0,0)]\rangle \tag{2.2}$$

($\langle\ldots\rangle$ indicates thermodynamic averaging), we make the further ansatz that

$$F[\phi_K(x,t)]\simeq\sum_n F\{\phi_{Kn}[\gamma_n(x-x_{0n}-v_nt)]\}. \tag{2.3}$$

Assertion (2.3) is only an assumption beyond (2.1) if F is not a linear function of ϕ (or ϕ_x, ϕ_t, etc). $\langle\ldots\rangle$ now implies averaging with respect to the kinks' initial positions and velocities. There may be correlations between these which can be included at the expense of numerical labour. As is usual (e.g. Mikeska 1978, Theodorakopoulos 1979), however, we consider incoherent scattering from independent kinks. Introducing the kink 'form factor' $f_K^F(q)$ by

$$f_K^F(q)\equiv\int_{-\infty}^{\infty} d\xi\ e^{-iq\xi}F[\phi_K(\xi)], \tag{2.4}$$

we find easily that

$$S_K(q, \omega) = \frac{n_K(T)}{(2\pi)^2} \int_{-\infty}^{\infty} dt\, e^{i\omega t} \langle |f_K^F(q\gamma^{-1})|^2 \gamma^{-2} e^{-iqvt} \rangle \tag{2.5}$$

where $n_K(T)$ is the density of kinks (and anti-kinks) (see below). Assuming initial positions to be uniformly distributed and the velocity distribution $P(v)$ to be that of an ideal 'relativistic' (cf equation (1)) classical gas (particle mass $M_K \equiv E_K/c_0^2$), equation (2.5) becomes

$$S_K(q, \omega) = \frac{n_K(T)}{(2\pi)^2} \int_{-\infty}^{\infty} dt \int_{-c_0}^{c_0} dv\, e^{i(\omega t - qx)} P(v) \gamma^{-2}(v) |f_K^F(q\gamma^{-1})|^2, \tag{2.6}$$

with

$$P(v) = [2c_0 K_1(\alpha)]^{-1} \gamma^3 e^{-\alpha\gamma}, \tag{2.7}$$

where $\alpha \equiv E_K/k_B T$ and K_1 is a modified Bessel function.

In general we should include kink lifetime, damping or diffusion terms in (2.6) (especially for non-integrable systems). We do not make use of these refinements here, and refer the reader to e.g. Theodorakopoulos (1979), Bishop *et al* (1980). In the diffusionless regime, (2.6) becomes

$$S_K(q, \omega) = \frac{n_K(T)}{2\pi q} P\left(\frac{\omega}{q}\right) \gamma^{-2}\left(\frac{\omega}{q}\right) \left| f_K^F\left[q\gamma^{-1}\left(\frac{\omega}{q}\right)\right] \right|^2 \tag{2.8}$$

or explicitly

$$S_K(q, \omega) = \frac{n_K(\alpha)}{4\pi c_0 K_1(\alpha)} \frac{|f_K^F[q\gamma^{-1}(\omega/q)]|^2}{q} \frac{\exp[-\alpha(1 - \omega^2/c_0^2 q^2)^{-1/2}]}{(1 - \omega^2/c_0^2 q^2)^{1/2}}. \tag{2.9}$$

At low T ($\alpha \gg 1$), equation (2.9) becomes

$$S_K^{NR}(q, \omega) = \frac{n_K(\alpha)\alpha^{1/2}}{c_0(2\pi)^{3/2}} \frac{|f_K^F(q)|^2}{q} \exp(-\alpha\omega^2/2c_0^2 q^2), \tag{2.10}$$

i.e. the non-relativistic limit in which (2.7) is replaced by the Maxwellian distribution

$$P^{NR}(v) = c_0^{-1}(\alpha/2\pi)^{1/2} \exp(-\alpha v^2/2c_0^2). \tag{2.11}$$

Both (2.9) and (2.10) predict a central mode from kinks which may be split in the relativistic case (2.9) (see below). $f_K(q)$ decays characteristically on the scale of an inverse kink width, with Lorentz contraction in the relativistic regime. The effect of the form factor on the frequency structure of the central component depends (especially in the relativistic regime) on the particular function F of kink coordinates. We list some examples in table 1. In particular, note for comparison in § 3 that with $F = \cos$ in SG

$$f_K^{\cos}(Q) = -4d(\tfrac{1}{2}\pi Qd)/\sinh(\tfrac{1}{2}\pi Qd) \tag{2.12}$$

(omitting a trivial δ function, reflecting the long-range order in $\cos\phi$). We re-emphasise that for some functions in table 1 it will not be possible to assume purely incoherent scattering as above, and information about kink separations and kink–anti-kink sequencing must be introduced: see the beginning of this section and Bishop *et al* (1980).

It useful to note (Schneider *et al* 1979, Bishop *et al* 1980) that evolutions of appropriate functions of the order parameter are directly related through the governing equations of motion (1). For instance, it is easily shown that for SG, S_{ss} ($s \equiv \sin\phi$) and $S_{\phi\phi}$ are related by

$$S_{ss}(q,\omega)/S_{\phi\phi}(q,\omega)=\{(\omega/\omega_0)^2-2(d/a)^2[1-\cos(qa)]\}^2. \qquad (2.13)$$

This relationship is completely general and allows us to argue (consistently with molecular dynamics simulations (Schneider *et al* 1979, Kerr *et al* 1980)) that the magnon response in $S_{\phi\phi}$ is strongly enhanced in S_{ss}, whereas the central component in $S_{\phi\phi}$ is strongly depressed in S_{ss} (at small q and ω). Interestingly, this continuum limit of the ratio (2.13) is *precisely* reproduced by the simplest incoherent kink phenomenology, as will be seen from (2.12) and table 1. (Equation (2.13) applies also to the magnon sectors.) No such simple constraints are possible for S_{cc}—it is most closely related to energy density correlations (Bishop *et al* 1980). This is satisfactory because we will argue in § 3 that breathers can contribute strongly to S_{cc} but not to $S_{\phi\phi}$ or S_{ss}.

Analytic expressions for the kink (plus anti-kink) density are limited to low T ($\leqslant 0.2E_K$) where the following results have been found (e.g. Currie *et al* 1980):

$$n_K(T)(\text{SG})=4(2\pi)^{-1/2}d^{-1}(\beta E_K)^{1/2}\exp(-\beta E_K), \qquad (2.14)$$

$$n_K(T)(\phi\text{-four})=(6/\pi)^{1/2}d^{-1}(\beta E_K)^{1/2}\exp(-\beta E_K). \qquad (2.15)$$

At higher temperatures, the 'effective' kink energy is renormalised and only approximate estimates of this and the consequent modified kink density are available (Bishop 1979).

Finally we consider the central peak *splitting* predicted at higher T by (2.9). Notice that low-frequency peaks are predicted centred at $\pm\omega_m(q)$ where $\omega_m=v_m(T)q$ and v_m is the maximum of a function $g(\gamma)$: $\gamma\equiv(1-v^2/c_0^2)^{-1/2}$. From (2.11) and table 1, we see that for $F=\phi$ or ϕ_x, g is simply $P(v)$, the *relativistic* ideal gas velocity distribution (2.9). For other functions F, the kink form factors are such that g differs from P. Of course, whether such central peak splitting will be observed depends sensitively on the corrections to any ideal gas picture—mode–mode interactions of various kinds. Also the strict cut-offs predicted ($v=c_0$) depend on the literal validity of an ideal gas velocity distribution *and* the Lorentz covariance of the continuum SG, ϕ-four, etc models (cf equations (1.1)). The former is mitigated by mode–mode interactions, and the latter by discrete lattice effects which are most severe for kink velocities $\to c_0$ because of Lorentz contraction and (discrete lattice) renormalisation of the kink energy—molecular dynamics simulations do indeed find some weight in central peaks extending beyond the continuum theory cut-off ($\omega=c_0q$) (e.g. Schneider *et al* 1979, Kerr *et al* 1980). Splitting is clearly observed for (nearly integrable) SG but at best marginally for, e.g., ϕ-four where collision effects (including kink–breather) are very evident (T R Koehler 1975 unpublished).

We also remark that at elevated temperatures it is quantitatively misleading to use the bare kink energy $E_K^{(0)}=M_Kc_0^2$. $n_K(T)$ (in equation (2.5), etc) is the kink (and anti-kink) average density at temperature T. Within an ideal gas framework we must use an *effective* excitation energy $E_K^{(T)}<E_K^{(0)}$ even at the lowest T (Koehler *et al* 1975, Bishop 1979). The effective kink energy reduction reflects the interaction between a kink and linear phonons (Currie *et al* 1980) and other modes. It therefore accommodates some of the grosser deficiencies of a strictly ideal gas approach. In a similar way we expect that the effective α in (2.12) is strongly modified. In fact, using $E_K=E_K^{(T)}$ predicts that any central peak splitting will occur at substantially lower temperatures

than would be predicted using $\alpha=\beta E_K^{(0)}$; this is consistent with MD simulations (Schneider and Stoll in preparation, Kerr *et al* 1980). A further refinement (Trullinger and Bishop 1981) is to use $E_K^{(T,v)}$, an effective kink energy which depends on both T and v. In this way, the kink velocity distribution in effect deviates from the ideal gas relativistic form, (2.7).

3. Breather phenomenology

We have proposed elsewhere (Stoll *et al* 1979) that coherent anharmonic phonon excitations of a quasi-breather nature play an essential role in the correlations of cos ϕ for the SG dynamics. Molecular dynamics simulations have revealed (Stoll *et al* 1979, Schneider *et al* 1979, Kerr *et al* 1980) two distinct features in the excitation spectrum, $S_{cc}(q,\omega)$. These can be qualitatively understood (Stoll *et al* 1979) in terms of a low-frequency response from the quasi-breather envelope and a high-frequency component from internal oscillations. Although breathers are shorter-lived than kinks on a realistic SG chain (i.e. discrete with periodic boundary conditions) and the statistical weighting is much less well understood, in view of the novelty of the above suggestion it is worthwhile to assess how much information can be obtained from a breather phenomenology at the same level adopted for kinks in § 2. In addition, we can expect central peak contributions from kinks also (§ 2), and it will be helpful to have a guide to their relative contributions.

The ideal SG breather is (Bullough and Dodd 1978)

$$\phi_B(x,t;\omega_B,v,x_0,\phi_0)=4\tan^{-1}\left(\frac{(\omega_0^2/\omega_B^2-1)^{1/2}\sin\{\gamma\omega_B[t-v(x-x_0)/c_0^2]+\phi_0\}}{\cosh[\gamma d^{-1}(x-x_0-vt)(1-\omega_B^2/\omega_0^2)^{1/2}]}\right) \quad (3.1)$$

where the translation velocity v and initial position x_0 are conjugate; likewise the internal frequency ω_B and phase ϕ_0 are conjugate. v is restricted to $0\leq|v|<c_0$ and ω_B to $0<\omega_B<\omega_0$. Note that the maximum amplitude A_B of the breather motion is

$$A_B=4\tan^{-1}(\omega_0^2/\omega_B^2-1)^{1/2} \quad (3.2)$$

with Lorentz-corrected frequency $\gamma\omega_B$. The breather has a characteristic extension $2d_B$ with

$$d_B=d\gamma^{-1}(1-\omega_B^2/\omega_0^2)^{-1/2}. \quad (3.3)$$

Integrating the SG Hamiltonian (1.1*a*) ($h=1$) with (3.1) gives the breather energy E_B as

$$E_B=16c_0\omega_0\gamma(1-\omega_B^2/\omega_0^2)^{1/2}=2E_K(0)(1-\omega_B^2/\omega_0^2)^{1/2}\gamma. \quad (3.4)$$

We see that, as $\omega_B\to\omega_0$, $E_B\to0$, $A_B\to0$ and $d_B\to\infty$ ('phonon' limit), whereas, as $\omega_B\to0$, the breather approaches a full kink–anti-kink profile ($A_B\to2\pi$, $E_B\to2E_K$, $d_B\to d\gamma^{-1}$).

To set up a breather phenomenology we will suppose that breathers are uncorrelated in x_0, v, ϕ_0, ω_B. This is the same level of approximation adopted for kinks. Similarly we will take no account of finite lifetimes of the breather excitations†.

† In the ideal fully integrable SG system interactions between solitons take place purely through asymptotic phase-shifts in the conjugate variables x_0, ϕ_0, leaving v and ω_B unchanged asymptotically, as well as the soliton energy.

Even this simplest phenomenology is quite complicated in the case of breathers. It will therefore be helpful to present the low-temperature non-relativistic form first to isolate central features. Considering breathers of frequency ω_B and correlations in $F[\phi]$, we write (cf § 2)

$$S_B^{FF}(q, \omega; \omega_B)$$

$$= (2\pi)^{-4} n_B(T; \omega_B) \left\langle \int dx\, dx'\, dt\, dt' \exp[i\omega(t-t') - iq(x-x')] \right.$$

$$\left. \times F[\phi_B(\omega_B; x - vt; t - vx/c_0^2)] F[x \to x'; t \to t'] \right\rangle, \tag{3.5}$$

where we have transformed away x_0 and ϕ_0. Making the transformation of variables $x_1 = x - vt$, $x_2 = x' - vt'$, $t_1 = t - vx/c_0^2$, $t_2 = t' - vx'/c_0^2$ and introducing the low-temperature velocity distribution $P^{NR}(v)$ (equation (2.11)), we find

$$S_B^{FF}(q, \omega; \omega_B)$$

$$= n_B(T; \omega_B)(2\pi)^{-4} \int_{-\infty}^{\infty} dv \int dx_1 \int dx_2 \int dt_1 \int dt_2$$

$$\times \gamma^4 P^{NR}(v) \exp[i\gamma^2(\omega - qv)(t_1 - t_2)] \exp[-i\gamma^2(q - v\omega/c_0^2)(x_1 - x_2)]$$

$$\times F\left[4 \tan^{-1}\left(\frac{(\omega_0^2/\omega_B^2 - 1)^{1/2} \sin(\omega_B t_1)}{\cosh[x_1 d^{-1}(1 - \omega_B^2/\omega_0^2)^{1/2}]}\right)\right] F[x_1 \to x_2, t_1 \to t_2]. \tag{3.6}$$

The example of greatest interest to us is $F = \cos$:

$$\cos\left[4 \tan^{-1}\left(\frac{(\omega_0^2/\omega_B^2 - 1)^{1/2} \sin(\omega_B t)}{\cosh[x d^{-1}(1 - \omega_B^2/\omega_0^2)^{1/2}]}\right)\right]$$

$$= 1 - \frac{2(\omega_0^2/\omega_B^2 - 1)\,\mathrm{sech}^2[x d^{-1}(1 - \omega_B^2/\omega_0^2)^{1/2}] \sin^2(\omega_B t)}{\{1 + (\omega_0^2/\omega_B^2 - 1)\,\mathrm{sech}^2[x d^{-1}(1 - \omega_B^2/\omega_0^2)^{1/2}] \sin^2(\omega_B t)\}^2}. \tag{3.7}$$

The factor of unity in (3.7) reflects the long-range order in cos and is omitted (as for kinks). The remaining structure in (3.7) from the breather profile will be considered in more detail shortly. For the moment we suppose that high-frequency breathers ($\omega_B \lesssim \omega_0$) will be dominant at low temperatures in view of their lower creation energies (equation (3.4)). For these frequencies it is reasonable to neglect the denominator in (3.7), and we define a 'breather envelope form factor' (cf table 1 and (2.12))

$$f_B(Q) \equiv \int_{-\infty}^{\infty} d\xi\, e^{-iQ\xi}\, \mathrm{sech}^2(\xi/d) = 2d(\tfrac{1}{2}\pi Q d)/\sinh(\tfrac{1}{2}\pi Q d). \tag{3.8}$$

With this approximation (3.6) becomes

$$S_B^{cc}(q, \omega; \omega_B)$$

$$= \frac{n_B(T; \omega_B)}{2\pi^3} \frac{\omega_0^2}{\omega_B^2} \left(\frac{\omega_0^2}{\omega_B^2} - 1\right)$$

$$\times \int_{-\infty}^{\infty} dv\, dt_1\, dt_2\, \gamma^4 P^{NR}(v) \left| f_B\left(\frac{q(1 - v\omega/c_0^2 q)\gamma^2}{(1 - \omega_B^2/\omega_0^2)^{1/2}}\right)\right|^2$$

$$\times \exp[i\gamma^2(\omega - qv)(t_1 - t_2)] \sin^2(\omega_B t_1) \sin^2(\omega_B t_2). \tag{3.9}$$

The separation into envelope and internal motion contributions is now evident if we note that

$$\sin^2(\omega_B t) = \tfrac{1}{2}[1 - \cos(2\omega_B t)]. \tag{3.10}$$

For, performing the t_1 integral (say) in (3.9), we have

$$\int dt_1 \exp[i\gamma^2(\omega - qv)t_1] \sin^2(\omega_B t_1)$$
$$= \pi\gamma^{-2}q^{-1}\left[\delta(v - \omega/q) - \tfrac{1}{2}\delta\left(v - \frac{\omega}{q} + \frac{2\omega_B\gamma^{-2}}{q}\right) - \tfrac{1}{2}\delta\left(v - \frac{\omega}{q} - \frac{2\omega_B\gamma^{-2}}{q}\right)\right]. \tag{3.11}$$

Using (3.11), the t_2 and v integrals in (3.9) can be performed. Neglecting all relativistic factors γ (consistent with our low-T assumption), we find

$$S_B^{cc}(q, \omega; \omega_B)$$
$$= \frac{n_B(T; \omega_B)}{2\pi q} \frac{\omega_0^2}{\omega_B^2}\left(\frac{\omega_0^2}{\omega_B^2} - 1\right)\left[\!\left[f_B^2\left[q\left(1 - \frac{\omega_B^2}{\omega_0^2}\right)^{-1/2}\right] P^{NR}\left(\frac{\omega}{q}\right)\right.\right.$$
$$+ \frac{1}{4} f_B^2\left\{\frac{q}{(1 - \omega_B^2/\omega_0^2)^{1/2}}\left[1 - \frac{\omega^2}{c_0^2 q^2}\left(1 - \frac{2\omega_B}{\omega}\right)\right]\right\} P^{NR}\left(\frac{\omega - 2\omega_B}{q}\right)$$
$$\left.\left. + \frac{1}{4} f_B^2\left\{\frac{q}{(1 - \omega_B^2/\omega_0^2)^{1/2}}\left[1 - \frac{\omega^2}{c_0^2 q^2}\left(1 + \frac{2\omega_B}{\omega}\right)\right]\right\} P^{NR}\left(\frac{\omega + 2\omega_B}{q}\right)\right]\!\right]. \tag{3.12}$$

Several implications follow from this low-temperature phenomenology.

(i) In view of the Gaussian form of $P^{NR}(v)$, equation (3.12) predicts a Gaussian central peak for each breather frequency plus separate components centred at $\omega = \pm 2\omega_B$. The latter do not have Gaussian form because of the frequency-dependent form factor—weight is displaced to $|\omega| \gtrsim 2\omega_B$ from $|\omega| \lesssim 2\omega_B$.

(ii) Equation (3.12) is only valid for $\omega_B \lesssim \omega_0$. We see therefore that the effective q in the form factors f_B is greatly enhanced so that, from (3.8), f_B is exponentially small. Indeed, if we consider $\omega \sim 0$ or $\pm 2\omega_B$ and q finite, the ω_B dependence in (3.12) is $\sim n_B(T; \omega_B) \exp[-\pi q d(1 - \omega_B^2/\omega_0^2)^{-1}]$. The breather contribution to S_B^{cc} is evidently a competition between the breather density (which will increase with decreasing creation energy, i.e. as ω_B *increases*) and the form factor f_B (which increases as ω_B *decreases*). Furthermore, we can expect lifetimes to be less for extended ($\omega_B \to \omega_0$) breathers, and this will also be part of the competition. Of course the observable structure factor $S_B^{cc}(q, \omega)$ is a sum over all breathers:

$$S_B^{cc}(q, \omega) \equiv \int_0^{\omega_0} d\omega_B \, S_B^{cc}(q, \omega; \omega_B). \tag{3.13}$$

(N.B. for *quantum* SG, the breather spectrum is discrete, depending on the strength of the quantum coupling constant (e.g. Maki and Takayama 1979, Bishop 1980a).)

(iii) The intermediate structure factor $S^{cc}(q, t = 0) \equiv \int d\omega S^{cc}(q, \omega)$ can be calculated exactly using transfer integral techniques (e.g. Bishop 1981), with the result (classically) that

$$S^{cc}(q, t = 0) \propto (\beta E_K)^{-2} \qquad (q, T \to 0). \tag{3.14}$$

This behaviour is partly due to breather excitations (see also § 4), so that (3.14) imposes a constraint on the integrated form of (3.12).

(iv) Without performing detailed integrations, we see from (3.12) that the *integrated* high- and low-frequency components of $S_B^{cc}(q, \omega)$ should have roughly comparable magnitudes with the high-frequency weight ~one half the central peak weight. This is broadly consistent with molecular dynamics simulations (Stoll *et al* 1979, Kerr *et al* 1980).

Within approximation (3.12) we might suppose that the greatest contribution, as far as the form factor f_B is concerned, comes from the lowest-frequency breather. A closer examination of (3.7) shows that this is not the case. The breather profile spends most time at its extremal values. If we consider $\sin^2(\omega_B t) \approx 1$ and examine the *complete* envelope form factor (i.e. the full form (3.7) in (3.8)), it is easy to show that $f_B \to 0$ as $\omega_B \to 0$ or ω_0 and maximises for $\omega_B = \omega_B^m$:

$$\omega_B^m = \omega_0/\sqrt{2}. \tag{3.15}$$

This was already anticipated (Stoll *et al* 1979) from the cosine properties since this 'most favourable' breather has amplitude $A_B = \pi$ (equation (3.2)). It has energy $E_B(\omega_B^m) = \sqrt{2}E_K$ and is thus expected to be even slightly *less* populated than free kinks. However, estimates show that (3.15) is not a very strongly selected frequency, so that many breathers will contribute substantially and in aggregate dominate kinks at low T.

It is appropriate to note here that symmetric oscillatory motions (taking positive and negative values) such as SG breathers only contribute because we are considering an *even* function (cos). Contributions from the breather sector are identically zero for *odd* functions (ϕ, $\sin \phi$, etc). This is evident (at arbitrary T) from (3.6) and is consistent with striking differences observed in molecular dynamics simulations (Schneider *et al* 1979, Kerr *et al* 1980). (This property may not hold exactly for asymmetric potentials such as ϕ-four—cf the end of this section.)

Our present understanding of classical breather densities $n_B(\omega_B; T)$ is unfortunately incomplete. The difficulties are rather technical and we refer the reader to Bishop (1980b) for a discussion. (Reasonable breather densities in a *quantum* framework have been proposed (e.g. Maki and Takayama 1979, Chung 1980), which emphasises the quantum lower limit $\hbar\omega_0$ to a breather energy—in realistic materials, defect-limited chain lengths will also be important limitations on breather extent.) In this situation it is premature to make detailed comparisons of contributions to $S_{cc}(q, \omega)$ from breathers and kinks (see § 7). Similarly, we consider it premature to implement the multiple integrations necessary to include the full structure in (3.7): we have given the ingredients for when $n_B(\omega_B; T)$ are available, but our main aim here is to justify the qualitative proposals made by Stoll *et al* (1979). It *is* essential to examine qualitatively some of the *relativistic* effects on the structure predicted by (3.12), by including some sensitivity to the 'most favourable' breather. Since a breather profile spends most of a cycle near the full envelope, we can, for instance, make the plausible approximation (under-estimate) of neglecting time dependence in the denominator of (3.7), and define a new envelope form factor

$$\bar{f}_B(Q; \omega_B) \equiv \int_{-\infty}^{\infty} d\xi \, e^{-iQ\xi} \frac{\operatorname{sech}^2(\xi/d)}{[1 + (\omega_0^2/\omega_B^2 - 1)\operatorname{sech}^2(\xi/d)]^2}. \tag{3.16}$$

To calculate $S_B^{FF}(q, \omega; \omega_B)$ we follow the same steps starting with (3.5), except that we retain the full 'relativistic' breather form (3.1) and keep account of all γ factors. After transforming away x_0 and ϕ_0, we introduce new (relativistic) variables $x_1 = \gamma(x - vt)$, $x_2 = \gamma(x' - vt')$, $t_1 = \gamma(t - vx/c_0^2)$, $t_2 = \gamma(t' - vx'/c_0^2)$. Using the full relativistic velocity distribution $P(v)$ (equation (2.7)), equation (3.6) is then replaced by

$$S_{\mathrm{B}}^{FF}(q, \omega; \omega_{\mathrm{B}})$$
$$= (2\pi)^{-4} n_{\mathrm{B}}(T; \omega_{\mathrm{B}}) \int_{-c_0}^{c_0} \mathrm{d}v \int \mathrm{d}x_1\, \mathrm{d}x_2\, \mathrm{d}t_1\, \mathrm{d}t_2$$
$$\times P(v) \exp[\mathrm{i}\gamma(\omega - qv)(t_1 - t_2) - \mathrm{i}\gamma(q - v\omega/c_0^2)(x_1 - x_2)]$$
$$\times F\left[4 \tan^{-1}\left(\frac{(\omega_0^2/\omega_{\mathrm{B}}^2 - 1)^{1/2} \sin(\omega_{\mathrm{B}} t_1)}{\cosh[x_1 d^{-1}(1 - \omega_{\mathrm{B}}^2/\omega_0^2)^{1/2}]}\right)\right] F[x_1 \to x_2, t_1 \to t_2]. \tag{3.17}$$

Considering $F = \cos$ and adopting approximation (3.15), expression (3.9) becomes instead

$$S_{\mathrm{B}}^{\mathrm{cc}}(q, \omega; \omega_{\mathrm{B}})$$
$$= \frac{n_{\mathrm{B}}(T; \omega_{\mathrm{B}})}{2\pi^3} \frac{\omega_0^2}{\omega_{\mathrm{B}}^2} \left(\frac{\omega_0^2}{\omega_{\mathrm{B}}^2} - 1\right) \int_{-c_0}^{c_0} \mathrm{d}v \int \mathrm{d}t_1\, \mathrm{d}t_2\, P(v) \bar{f}_{\mathrm{B}}^2 \left(\frac{q(1 - v\omega/c_0^2 q)\gamma}{(1 - \omega_{\mathrm{B}}^2/\omega_0^2)^{1/2}}\right)$$
$$\times \exp[\mathrm{i}\gamma(\omega - qv)(t_1 - t_2)] \sin^2(\omega_{\mathrm{B}} t_1) \sin^2(\omega_{\mathrm{B}} t_2). \tag{3.18}$$

Following the decomposition (3.10), we find, as in (3.11) and (3.12), that the breather *envelope* gives rise to a central component

$$\frac{n_{\mathrm{B}}(T; \omega_{\mathrm{B}})}{2\pi q} \frac{\omega_0^2}{\omega_{\mathrm{B}}^2} \left(\frac{\omega_0^2}{\omega_{\mathrm{B}}^2} - 1\right) \bar{f}_{\mathrm{B}}^2 \left(\frac{q\gamma^{-1}(\omega/q)}{(1 - \omega_{\mathrm{B}}^2/\omega_0^2)^{1/2}}\right) \gamma^{-1}\left(\frac{\omega}{q}\right) P\left(\frac{\omega}{q}\right), \tag{3.19}$$

which should be compared with the contribution from kink particles (equation (2.10)). The contributions from breather *oscillations* now occur through the δ function (cf equation (3.11)):

$$\gamma^{-1} q^{-1} \delta(v - \bar{v}_{\pm}(\omega, q; \omega_{\mathrm{B}})) \tag{3.20}$$

where

$$\bar{v}_{\pm} = \frac{\omega}{q} \pm \frac{2\omega_{\mathrm{B}}}{q} \left(1 - \frac{\omega^2}{c_0^2 q^2} + \frac{4\omega_{\mathrm{B}}^2}{c_0^2 q^2}\right)^{1/2} \Big/ \left(1 + \frac{4\omega_{\mathrm{B}}^2}{c_0^2 q^2}\right). \tag{3.21}$$

We find high-frequency contributions (cf (3.12))

$$\frac{n_{\mathrm{B}}(T; \omega_{\mathrm{B}})}{8\pi q} \frac{\omega_0^2}{\omega_{\mathrm{B}}^2} \left(\frac{\omega_0^2}{\omega_{\mathrm{B}}^2} - 1\right) \left\{ \bar{f}_{\mathrm{B}}^2 \left[\frac{q\gamma(\bar{v}_+)}{(1 - \omega_{\mathrm{B}}^2/\omega_0^2)^{1/2}} \left(1 - \frac{\bar{v}_+ \omega}{c_0^2 q}\right)\right] \gamma^{-1}(\bar{v}_+) P(\bar{v}_+) + (\bar{v}_+ \to \bar{v}_-) \right\}. \tag{3.22}$$

At low temperatures $\gamma^{-1}(v)P(v)$ has its maximum at $v_{\mathrm{m}} = 0$, so that (3.21) predicts a response centred at $\omega_{\mathrm{m}} = \pm 2\omega_{\mathrm{B}}$ as did (3.12). At higher T, however, $\gamma^{-1}P(v)$ is maximal at $v_{\mathrm{m}} \neq 0$. From (3.21) we see then that the high-frequency response is displaced to a frequency which also depends on wavevector q. Specifically, we find after a little algebra that (3.21) predicts a response centred at

$$\frac{\omega_{\mathrm{m}}}{q} = \pm v_{\mathrm{m}} \pm \frac{2\omega_{\mathrm{B}}}{q} \left(1 - \frac{v_{\mathrm{m}}^2}{c_0^2}\right)^{1/2}. \tag{3.23}$$

This conclusion depends somewhat on the behaviour of $\bar{f}_{\mathrm{B}}$, but we do not expect any serious qualitative sensitivity.

We anticipate that the qualitative features suggested above for SG will also be exhibited in other models *if* correlations of appropriately sensitive functions are studied. This is less easy to demonstrate than for SG, since analytic breather expressions are generally not available. Indeed, breathers only enjoy strict stability in the completely integrable SG model. However, *very* long-lived breather-like excitations are observed numerically in a number of similar one-dimensional models (e.g. Aubry 1974, Kudryavtsev 1975, Klein *et al* 1979, Ablowitz *et al* 1979). Very precise recent studies by Wingate (1980) and Negele and Campbell (1980) are especially persuasive for ϕ-four. Amplitude and frequency are related (similarly to SG), except that oscillations are necessarily asymmetric. Breathers are also very evident in molecular dynamics simulations (e.g. T R Koehler 1975, unpublished) of a ϕ-four chain: indeed they play an important role in determining *kink* dynamics (unlike SG). Central peak splitting is unlikely to survive in this non-integrable case, but we do anticipate low- and high-frequency responses in correlations of ϕ^{2n} ($n = 1, 2, \ldots$).

4. Summary and discussion

In the preceding sections we surveyed the simplest classical approaches to calculations of dynamic structure factors $S(q, \omega)$, which explicitly recognise quasi-elementary nonlinear modes. We concentrated on one-dimensional models of the sine-Gordon (SG) and ϕ-four classes, although the basic philosophies are considerably more general. In particular, we made use of kink (§ 2) *and* breather (§ 3) excitations. Both of these enjoy a particle-like character leading to 'central peak' structure (i.e. weight for $\omega \simeq 0$ in $S(q, \omega)$). However, the extra internal oscillatory degree of freedom in breathers leads to additional high-frequency structure in correlations of *appropriate* field (ϕ) functions. We demonstrated this (§ 3) in SG for cos ϕ correlations and predicted the extension in, e.g., ϕ-four for, e.g., ϕ^2 correlations (§ 3).

The use of an ideal gas phenomenology was central to our procedure, but we stressed the need for quantitative representation of mode–mode interactions and discrete lattice effects. This is especially true of the possibility of central peak *splitting*, following from the pseudo-relativistic form of the equations of motion (1). Kink–kink and (especially) kink–breather collisions are observed in molecular dynamics to be severe in the non-integrable ϕ-four case, and lifetime corrections to ideal kink gas theories (especially those omitting breathers) are essential: no substantial splitting is observed (T R Koehler 1975 unpublished, Schneider and Stoll 1976). SG (with $d \gg a$) exhibits very clear splitting (Schneider *et al* 1979, Kerr *et al* 1980) because of its near integrability. Even there, however, splitting is observed at substantially lower temperatures than predicted by a purely ideal relativistic gas; renormalisations of the 'particle's' effective energy (Bishop 1979) or of the effective velocity distribution (Trullinger and Bishop 1981) are necessary to partially represent mode interactions. In the absence of exact theories, detailed assessment of renormalised ideal gas theories awaits comparison with careful MD simulations (Schneider and Stoll 1980, in preparation, Kerr *et al* 1980). However, a few further general observations are in order.

The structure factors we have discussed can all be made consistent with rigorous *static* constraints on $\int S(q, \omega)\, d\omega$ (see Bishop (1981)). These constraints are, however, quite weak, and in particular do not give information on the *distribution* of weight in frequency space. Therefore, nonlinear mode interpretations, if their validity can be established, are very useful physical guides. Perhaps the most interesting suggestions from this point of view are those presented for breathers (§ 3). We proposed that SG breathers in correlations of cos ϕ give weight at both low and high frequency. Kinks, on the other hand, contribute only to a low-frequency (central) component. It is difficult to be precise about the relative contributions from kinks and breathers, because information (see § 3) on equilibrium density (and lifetime) of the latter is even poorer than for kinks (which are themselves only understood rigorously at low T). The integrated breather density certainly dominates that of kinks at low T (Bishop 1981), but we argued in § 3 that breathers of intermediate amplitude are most important. The density of breathers of this amplitude should be *comparable* to that of kinks† and their contributions to $S_{cc}(q, \omega)$ should also be comparable (cf equations (2.9) and (3.19)). However, there are many breather amplitudes around π contributing substantially, and for this reason breather contributions should still dominate kink contributions in cos ϕ correlations at small q. (Contrast this with expectations for cos $\frac{1}{2}\phi$ correlations (Bishop 1981).) This prediction is supported by molecular dynamics simulations (Kerr *et al* 1980). These show that pure kink phenomenology (§ 2) predicts the total central weight in $S_{ss}(q, \omega)$ quite well, whereas at *low* q and T, a substantial weight is left unaccounted for by the corresponding (table 1) kink theory for $S_{cc}(q, \omega)$.

It is likely that breather effects can partly be recovered by more conventional anharmonic phonon (magnon) perturbation theories, since breathers indeed represent the (classical *or* quantum) anharmonicity—this is explicit for extended (low-amplitude) classical breathers which may be reached in low-order perturbation theory, or for quantum breathers which are multi-magnon (phonon) bound states (see Bishop 1980a). We prefer, however, to emphasise the *specific* spatial and temporal coherence of breathers, especially if large-amplitude breathers are important. At this time it is not clear to what extent conventional multi-magnon (phonon) sum and difference processes (D Baeriswyl 1979, private communication, Reiter 1981) are to be considered independent of breather contributions, but there is molecular dynamics evidence for separate contributions (Schneider and Stoll, in preparation, Kerr *et al* 1980).

It would be tempting to draw conclusions from our results with regard to easy-plane magnetic chains such as $CsNiF_3$ or TMMC (e.g. Mikeska 1978, 1980). Much recent work has suggested a mapping of these systems onto a continuum SG field. *If* this is valid then we would indeed assert (Bishop 1981) that $CsNiF_3$ is a novel solid state environment in which to study *breathers* (or continuous deformations of these to larger out-of-plane spin motions (Bishop 1980c)), whereas TMMC probes kinks. However, it is our opinion that further work is needed to substantiate the mapping to any simple SG theory, especially for the $S=1$ material $CsNiF_3$. Therefore, implications are premature. Our results are, of course, directly relevant to classical molecular dynamics simulations (e.g. Stoll *et al* 1979, Schneider *et al* 1979, Kerr *et al* 1980, Schneider and Stoll, in preparation).

Acknowledgments

Section 3 of this work was begun at IBM Zürich Research Laboratory during June 1979, when we enjoyed the hospitality of Dr T Schneider, and completed at the Aspen Institute of Physics in July 1979. Helpful discussions with Drs T Schneider and E Stoll are gratefully acknowledged. The work at LASL has been performed under the auspices of the US DOE.

† Although breather densities are not rigorously available, it is certainly reasonable to suppose $n_B(T; \omega_B) \sim \exp(-\beta E_B)$ in the same sense that $n_K \sim \exp(-\beta E_K)$ (equation (2.14)).

Note added. Since completing this work we have received a preprint from Drs T Schneider and E Stoll describing detailed molecular dynamics simulations for the SG chain. As far as our results here are concerned, the data are broadly in agreement with the alternative simulations of Kerr *et al* (1980). Schneider and Stoll also include some discussion of two-magnon processes (§ 4). In addition, we have received a preprint from Drs Takayama and K Maki who describe related ideal gas dynamic structure factor calculations from kinks, breathers and two-magnon processes for a *quantum* SG field theory. Inclusion of the breather density $n_B(T; \omega_B)$ suggested by these authors into our formulae will be reported in a future publication.

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