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Thermodynamics of 1D soliton-bearing Hamiltonians: Transfer integral structure and correlation functions

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Abstract. Static correlation functions for the sine–Gordon chain and related one-dimensional models are described in terms of the transfer integral operator formalism. The characteristic signatures of kink-solitons within this formalism are discussed and classes of 'kink-sensitive' and 'kink-insensitive' correlations are emphasised. Special attention is given to the integrated structure factor $\int S(q, \omega)\, d\omega$ and the consistency of several calculations and models of $S(q, \omega)$ is addressed. Possible applications to the interpretation of scattering experiments in quasi-one-dimensional ferro- and antiferromagnetic materials such as $CsNiF_3$ and $(CD_3)_4NMnCl_3$ are discussed.

1. Introduction

There has recently been renewed discussion of the thermodynamics of the classical (e.g. Mikeska 1978, 1980, Bishop 1979, Stoll *et al* 1979, Schneider *et al* 1979, Jôsé and Sahni 1979, Leung *et al* 1980, Maki 1981) and quantum (Maki and Takayama 1979, 1980) sine–Gordon (hereafter SG) chain, primarily stimulated by interest in certain quasi-one-dimensional ferro- and antiferromagnetic easy-plane Heisenberg systems such as $CsNiF_3$ (Kjems and Steiner 1978) or $(CD_3)_4NMnCl_3$ (TMMC hereafter) (Boucher *et al* 1980), for which intriguing neutron scattering data have been obtained. The SG Hamiltonian is

$$H = \sum_{i=1}^{N} hl\left[\tfrac{1}{2}\dot{\phi}_i^2 + \tfrac{1}{2}\frac{c_0^2}{l^2}(\phi_{i+1} - \phi_i)^2 + \omega_0^2(1 - \cos\phi_i)\right] \tag{1}$$

where h sets the energy scale, l is the lattice spacing with lattice index i, and c_0 and ω_0 are the characteristic velocity and frequency respectively. The equation of motion for the field variable $\phi(x, t)$, in the continuum limit $c_0/\omega_0 \gg l$, is the SG equation

$$\ddot{\phi} - c_0^2\phi_{xx} + \omega_0^2 \sin\phi = 0. \tag{2}$$

It is still too early to know, experimentally or theoretically, how useful a continuous classical spin–field SG description is for the actual magnetic materials. Theoretically, questions remain about the quantum effects (Mikeska and Patzak 1977, Bishop 1980a) associated with the finite spin, especially in $CsNiF_3$ where $S = 1$; the crossover to strong spin motions out of the easy plane as the temperature is raised must be considered more carefully (Bishop 1980b); other central peak contributions (besides those attributed to non-linear excitations (Mikeska 1978, 1980, Stoll *et al* 1979, Schneider *et al* 1979) (see § 3)) must be examined (e.g. Malinowski and Kocinski 1972); the effect on e.g.

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domain-wall dynamics of demagnetising fields has yet to be assessed in anisotropic materials†, etc. Traditionally (e.g. Loveluck *et al* 1975) classical statistical mechanics for e.g. $CsNiF_3$ has introduced the *discrete* chain explicitly and the full (classical) coupling $\boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1}$. The reduction to continuum SG recently emphasised (Mikeska 1978) assumes a slowly-varying spin direction from site to site, and is only valid at low T (where topological constraints are weak (José and Sahni 1979) (cf lessons from 2D spin systems (José *et al* 1977)) and domain walls wide compared with a lattice spacing), and at long wavelengths. These questions have been examined in some generality in 1D by Patkós and Ruján (1979) (see also Schneider *et al* 1979, José and Sahni 1979, Riseborough and Trullinger 1980).

In view of such open questions, the present contribution is not placed in the detailed context of a particular magnetic chain. Rather we shall (in common with most current literature) *assume* the basic validity of the SG description and discuss deductions which then follow. The greatest theoretical and experimental interest certainly lies in the structure observed (Kjems and Steiner 1978, Boucher *et al* 1980) in the *dynamic* structure factor $S(q, \omega)$, and in particular mechanisms for the 'central peak' (i.e. weight in $S(q, \omega)$ at frequencies $\omega \approx 0$). Attention has been focused on scattering from 'gases' of 'particle-like' solutions to the SG equation (1), and both 'kink-solitons' (domain walls) (Mikeska 1978) and 'breathers' (soliton–antisoliton or multi-magnon bound states) (Stoll *et al* 1979, Schneider *et al* 1979) have been suggested for this role. All present calculations for $S(q, \omega)$ (e.g. Krumhansl and Schrieffer 1975, Aubry 1976, Kawasaki 1976, Varma 1976, Mikeska 1978, Stoll *et al* 1979, Sahni and Mazenko 1979, Theodorakopoulos 1979, Bennett *et al* 1980) (see also § 3) have limitations on their validity or applicability in strongly non-linear systems such as SG. Accurate molecular dynamics simulations are undoubtedly the most useful guides (Stoll *et al* 1979, Schneider *et al* 1979, Kerr *et al* 1980), although these still have to be interpreted if we wish to think in terms of contributions from 'elementary' modes.

The only truly *exact* information on the statistical mechanics of the SG chain is available for *static* (including q-dependent) properties. Here the transfer integral operator technique (e.g. Scalapino *et al* 1972) can be employed to yield exact expressions (see below), which must then be evaluated numerically in general: at low T some analytic expansions are possible (see below) as they are at high T. Such accurate static data (e.g. for $CsNiF_3$) as have been carefully compared with transfer integral operator results (e.g. magnetisation (Schneider *et al* 1979)) suggest that linearisation in motions out of the easy plane might be reasonable at *low enough T* for typical experimental parameter ranges (Kjems and Steiner 1978, Kakurai *et al* 1980), and indeed that the simple SG description (1), (2) is itself then quite reasonably valid (see also Patkós and Ruján 1979 and § 2.1) if trivial discrete-lattice corrections are included for short wavelengths.

Many more comparisons of static properties (e.g. of specific heat or $\int d\omega S(q, \omega)$) are needed to clarify the limitations of the SG description in real materials, but evidence for quasi-elementary excitations is anyway difficult to disentangle. Carefully chosen dynamic properties are much more important in this respect but one interim static property which can provide more information than most is $\int d\omega S(q, \omega; T)$, to be studied as a function of T (and q where this is experimentally possible) (e.g. Kakurai *et al* 1980). These correlation functions *cannot* yield any information on how weight is distributed in frequency. Nevertheless, they are weak constraints on theoretical proposals for

† Conventionally, for *isotropic* magnets, these only modify the effective mass of (low-velocity) walls (e.g. Winter 1961).

$S(q, \omega)$ and also some degree of elementary mode interpretation has been developed (Currie *et al* 1980) (at least for $k_B T \lesssim 0{\cdot}15 E_K$ (Bishop 1979), where E_K is the kink-soliton creation energy). Various suggestions for $S(q, \omega)$ are summarised in § 3.

It is the quantity $F(q; T) \equiv \int d\omega S(q, \omega; T)$ which we wish to emphasise in this work. The points made below are intentionally slightly technical, because these do not seem to have been fully appreciated in the literature and yet they do contain lessons for the interpretation of $S(q, \omega)$ (cf Bishop 1978). Technical details are presented in the Appendix. In § 2 we draw together salient results from existing literature, add a few new ones, and suggest interpretations emphasising the sensitivity on *which* function of the field is being examined for correlations. Concentrating on SG, we use correlations for $\cos \frac{1}{2}\phi$ and $\cos \phi$ to illustrate the two most important classes—where, respectively, kink-solitons are and are not dominant. In the first class there is an unambiguous correlation length given by the inverse mean kink *separation* and modes other than kinks have a weak effect even though they are more populated thermally. In the second class correlations occur on the scale of a kink *width* ($\approx 2c_0/\omega_0$) and 'anharmonic phonon' modes (including breathers (Stoll *et al* 1979)) are much more important than kinks. Correlations of other SG field (ϕ) functions ($\phi, \sin \phi, \sin \frac{1}{2}\phi$) are mentioned briefly as appropriate, and contrasting applications to the magnetic chains $CsNiF_3$ and TMMC are also noted as topical illustrations (§ 3).

2. Transfer integral results for static correlations

2.1. *Formalism*

The transfer integral operator formalism is well documented as a means of studying the equilibrium statistical mechanics of 1D Hamiltonians such as (1) (e.g. Scalapino *et al* 1972, Krumhansl and Schrieffer 1975, Currie *et al* 1980). The central component in this approach is the 'transfer integral operator' (TIO) eigenvalue problem:

$$\sum_{-\infty}^{+\infty} d\phi_i \exp[-\beta l h \omega_0^2 f(\phi_{i+1}, \phi_i)]\phi_n(\phi_i) = \exp(-\beta l h \omega_0^2 \epsilon_n)\phi_n(\phi_{i+1}) \tag{3}$$

with the symmetrised function

$$f(\phi_{i+1}, \phi_i) = \tfrac{1}{2}(c_0^2/\omega_0^2 l^2)(\phi_{i+1} - \phi_i)^2 + 1 - \tfrac{1}{2}(\cos \phi_{i+1} + \cos \phi_i).$$

Our remarks below are qualitatively quite general, but much attention has been focused quantitatively on the continuum (or 'displacive') limit of slowly varying fields ($d \equiv c_0/\omega_0 \gg l$). In this case a differential approximation is valid (to $O(l/d)$) in place of equation (3):

$$[-(1/2m^*)(d^2/d\phi^2) + 1 - \cos \phi + V_0]\psi_n(\phi) = \epsilon_n \psi_n(\phi) \tag{4}$$

where

$$\psi_n(\phi) = \exp[-(l/16d)\beta E_K(1 - \cos \phi)]\phi_n(\phi)$$
$$m^* = h^2 \omega_0^2 c_0^2 \beta^2 = (\tfrac{1}{8}\beta E_K)^2$$
$$V_0 = (2\beta\omega_0^2 l h)^{-1} \ln(h c_0^2 \beta / 2\pi l).$$

In this limit, we see that we have to study a pseudo-Schrödinger equation (4) for a particle of 'mass' m^* moving in the periodic potential $(1 - \cos \phi)$. In fact this eigenvalue problem is easily mapped into the Mathieu equation (e.g. Currie *et al* 1980; Appendix) whose eigenstructure has been studied in detail (Abramowitz and Stegun 1970, see also Appendix). In view of the SG potential's periodicity (or the equivalent Mathieu equation) equation (4) poses a 1D 'band-structure' problem. We can label eigenvalues (in a reduced zone scheme) by $\epsilon_{n,k}$ with band index $n(=0, 1, 2, \ldots)$ and a wavevector k in the first Brillouin zone $(-\frac{1}{2}<k\leq\frac{1}{2})$. From Floquet's theorem the corresponding eigenfunctions will then have Bloch form $\psi_{n,k}(\phi)=\exp(ik\phi)u_{n,k}(\phi)$ with $u_{n,k}(\phi+2\pi)=u_{n,k}(\phi)$. The eigenstructure comprises a sequence of continuous bands. At low T (i.e. $m^*\gg 1$) the bands are narrow compared with the band gaps (i.e. 'tight-binding') whereas high T corresponds to the opposite 'free electron' situation. The 'characteristic' eigenfunctions at the top or bottom of bands form sequences of 2π- and 4π-periodic even and odd functions.

Note that the eigenfunctions $\{\phi_n\}$ in equation (3) form a complete orthogonal set on the interval $(-\infty, +\infty)$, for which *all* the 'band structure' functions are necessary. This is appropriate when the SG variable ϕ can physically range over $(-\infty, \infty)$, as when it describes a generalised position variable for instance (e.g. in a generalised dislocation context, cf Rice *et al* 1976). We should contrast this with spin problems where physically indistinct states are recovered by $\{\phi_i\}\to\{\phi_i+2\pi\}$. This periodicity is explicit in the spin coupling $\cos(\phi_{i+1}-\phi_i)$, to which the gradient coupling of literal SG (1) is only an approximation. The 2π-periodic spin coupling form is still only nearest-neighbour, so that the TIO approach remains available (e.g. Loveluck *et al* 1975). Reduction to the literal SG form (4) has been analysed in detail by Pátkos and Ruján (1979) (see also Riseborough and Trullinger 1980). This reduction requires slowly-varying spins $(c_0/\omega_0\gg l$ in the SG approximation) *and* low T $(\ll JS^2$, with J the exchange coupling constant and S the spin magnitude). Most important, however, is the necessary restriction of the TIO (3) or (4) to the range $(-\pi, \pi)$ rather than $(-\infty, \infty)$. This means that when we are allowed to use the SG approximation (with thermal renormalisation of J if necessary (Riseborough and Trullinger 1980)) we must *only* use 2π-periodic Mathieu functions and not the whole band structure. While we frame our remarks below in terms of the more generally useful literal SG equation, we have in mind the above restrictions for applications to e.g. spin chains such as $CsNiF_3$ (Mikeska 1978) or TMMC (Mikeska 1980). (It may be helpful to note that similar remarks apply to 2D *XY* spin models. There also, derivative approximation of the exchange spin coupling is reasonable at low T. However, full treatment of the periodicity at higher T is not merely a quantitative correction (as in 1D) but essential to the description of vortex configurations leading to the qualitatively new feature of a topological phase transition (Kosterlitz and Thouless 1973, José *et al* 1977)).

The transfer operator formalism allows us to evaluate any static correlation function. In particular for any function $A(\phi(x, t))$ the intermediate scattering function $F^A(q, t)$ can be evaluated at $t=0$:

$$F^A(q,0)\equiv F^A(q)=\int \mathrm{d}\omega S^A(q,\omega)=|M_0^A(T)|^2\delta(q)+\sum_{n=1}^{\infty}|M_n^A(T)|^2\frac{\lambda_n^A(T)}{(q\lambda_n^A)^2+1}. \tag{5}$$

Equivalently, the self-correlation function $C^A(x)$ is expressed as

$$\begin{aligned}C^A(x)=\langle A[\phi(x,0)]A^*[\phi(0,0)]\rangle&=\int_{-\infty}^{+\infty}\exp(-\mathrm{i}qx)F^A(q)\,\mathrm{d}x\\&=|M_0^A|^2+\sum_{n=1}^{\infty}|M_n^A|^2\exp(-x/\lambda_n).\end{aligned} \tag{6}$$

We frequently consider instead the correlation function $\tilde{C}^A(x)$ restricted to fluctuations:

$$\tilde{C}^A(x) = \langle[A(x) - \langle A\rangle][A(0) - \langle A\rangle]\rangle = C^A(x) - |M_0^A|^2. \qquad (7)$$

In these expressions M_n denotes the matrix element

$$M_n = (0|A(\phi)|n), \qquad (8)$$

where $|m)$ is an *eigenfunction* of the transfer integral operator (3). The corresponding λ_n's, on the other hand, are determined by the *eigenvalues*:

$$\lambda_n^{-1}(T) = h\beta\omega_0^2(\epsilon_n - \epsilon_0). \qquad (9)$$

$|n = 0)$ is the lowest energy eigenfunction, and $|n)$ $(n = 1, 2, 3, \ldots)$ is the sequence of eigenfunctions for which the corresponding matrix element M_n is *non-zero*: this sequence depends, of course, on the particular function A. We also note a simple sum rule on matrix elements:

$$C^A(x = 0) = M_0^{A^2}(T) = \sum_{n=0}^{\infty} |M^A(T)|^2. \qquad (10)$$

Here $M_0^{A^2} \equiv (0|A^2(\phi)|0)$.

2.2. Examples

We now wish to consider the implications of the formalism of § 2.1 for the particular cases of SG with $A(\phi) = \cos \frac{1}{2}\phi$ and $A = \cos \phi$. These are quite different for transparent physical reasons and this is also evident from the above formalism.

Consider first the simplest case of $A(\phi) = \cos \frac{1}{2}\phi$, which is in fact very similar to the often-quoted results of Krumhansl and Schrieffer (1975) or Aubry (1974, 76). These authors considered the 1D 'ϕ-four' model rather than SG. In that case $1 - \cos \phi$ in equation (1) is replaced by $(\phi^2 - 1)^2$, and Krumhansl and Schrieffer (1975) only considered correlations of the order parameter ϕ itself. Returning to $A(\phi) = \cos \frac{1}{2}\phi$ for SG we see on simple symmetry grounds (equivalent to Bragg selection rules using band structure terminology (Currie *et al* 1980)) that despite the continuous eigenspectrum (for literal SG (2)) of the TIO only a discrete set of eigenstates are coupled to the ground state ($n = 0$). Most importantly, the first coupled state ($n = 1$) is at the top of the first band. Thus λ_1 is dominated by tunnel splitting which determines the band *width* whereas $\lambda_n (n \geq 2)$ are controlled by band *gaps*. At low T, asymptotic expansions are available (see Abramowitz and Stegun 1970), both for eigenvalues and eigenfunctions of the Mathieu equation. We give examples of the less familiar matrix element evaluations in the Appendix. The relevant conclusions are

$$M_0^{\cos 1/2} = 0 \qquad (11a)$$

$$M_1^{\cos 1/2} = 1 - O(k_B T/E_K) \qquad (11b)$$

$$\lambda_1 \xrightarrow{T \to 0^+} \tfrac{1}{4}(\pi/2)^{1/2} d (k_B T/E_K)^{1/2} \exp(E_K/k_B T) \qquad (11c)$$

$$\lambda_1 \gg \lambda_{n \geq 2} = (d/n)[1 + O(\exp(-E_K/k_B T), (k_B T/E_K))]. \qquad (11d)$$

Considering equations (6) and (11*c*, *d*) we see that at sufficiently large x ($\gg \lambda_1(T)$), or $q \ll \lambda_1^{-1}(T)$, the first term in the expansion is dominant. Thus the kink-soliton creation energy E_K enters directly through the eigen*values* and $\lambda_1(T)$ defines an unambiguous correlation length. Indeed (11*c*) can be re-expressed as (e.g. Koehler *et al* 1975)

$$\lambda_1(T)=\frac{1}{2\langle n_K(T)\rangle}, \tag{12}$$

where $\langle n_K(T)\rangle$ is the mean density of kinks (plus anti-kinks). Result (12) is exact at low T but probably extends accurately to much higher T (Koehler *et al* 1975, Bishop 1979). It has a simple physical interpretation analogous to correlations in the 1D Ising model (Aubry 1974, 1976, Krumhansl and Schrieffer 1975): The function $A(\phi)=\cos\frac{1}{2}\phi$ changes value asymptotically from $\pm a(T)$ to $\mp a(T)$ as a kink passes (with $a(T)\to 1$, as $T\to 0^+$). We consider a gas of independent kinks with a Poisson distribution for separations (see also Bennett *et al* 1980). Then if $N_K(x)$ is the number of kinks in the interval x, a simple calculation shows

$$C(x)=a^2(T)\langle(-1)^{N_K(x)}\rangle=a^2(T)\exp(-x/\lambda_K) \tag{13}$$

with

$$\lambda_K(T)\equiv(2\langle n_K(T)\rangle)^{-1}. \tag{14}$$

λ_K thus agrees with λ_1 (equation (12)). In this case harmonic and anharmonic modes play quite weak roles (at low T and large x). They act to dress the kinks and thereby affect the kink energy and the correlation length; otherwise they only describe the field oscillations around the SG potential degenerate minima ($\phi=0, 2\pi, \ldots$) and thereby *reduce* the *magnitude* of correlations (not the correlation length).

Turning to $A(\phi)=\cos\phi$, we note immediately that kink-solitons cannot play any Ising-like role, since the asymptotic value of $A(\phi)$ is now *unchanged* by the passage of a kink. Kink effects can thus only occur on the local scale of a kink *width* $2d=2c_0/\omega_0$ (and a Bragg peak from the ordered regions is expected). However, the kink density is exponentially small (at low T) so that correlations from smaller amplitude but more highly populated phonon (and anharmonic phonon) modes become essential. This behaviour follows in the TIO because now the lowest different state ($n=1$) coupled to the ground state ($n=0$) is not in the lowest band. Thus exponential tunnel splitting, i.e. *bandwidths* (which carry the kink density information in the *eigenvalues*), is masked by the band gaps ($\propto k_BT/E_K$). Using asymptotic low-T expansions for Mathieu eigenfunctions and eigenvalues (Abramowitz and Stegun 1970; see Appendix) we find

$$\lambda_n(T)=d/n+\mathrm{O}(dk_BT/E_K),\ \mathrm{O}(d\exp(-\beta E_K)) \tag{15}$$

$$|M_0^{\cos}(T)|^2=1-4k_BT/E_K+\mathrm{O}(k_BT/E_K)^2-4dn_K(T)+\mathrm{O}(dn_K(T)k_BT/E_K) \tag{16a}$$

$$|M_1^{\cos}(T)|^2=\mathrm{O}(k_BT/E_K)^2+\mathrm{O}(dn_K(T)E_K/k_BT),\ \mathrm{O}(dn_K(T)) \tag{16b}$$

$$|M_{n\geq 2}^{\cos}(T)|^2=\mathrm{O}(k_BT/E_K)^2+\mathrm{O}(dn_K(T)E_K/k_BT),\ \mathrm{O}(dn_K(T)). \tag{16c}$$

In addition

$$M_0^{\cos^2}=1-4k_BT/E_K+\mathrm{O}(k_BT/E_K)^2+2dn_K(T)+\mathrm{O}(dn_K(T)k_BT/E_K). \tag{17}$$

Not all coefficients in equations (16) and (17) and similar matrix expressions should be considered exact (see Appendix)—our main point here is to emphasise orders in k_BT/E_K and n_Kd. In particular, where orders have been indicated in equations (15), (16) and (17), numerical coefficients can only be estimated crudely with the usual Mathieu function expansion techniques (cf Appendix), and we have therefore omitted these.

The terms in (16*a*) correspond to the anticipated Bragg peak (see equation (5)) with weight depleted due to both phonon (and anharmonic phonon) and soliton excitations. Notice from equations (16*a*) and (17) that the sum rule (10) is satisfied to the orders reported. Although the Bragg peak loses weight of linear phonon order (k_BT/E_K) the 'phonon' contributions to $S(q \neq 0)$ are $O(k_BT/E_K)^2$—the absence of terms of linear order (see Appendix) is physically important (see below). In addition there are terms of the order of the soliton density whose contribution is very weak compared with those of the anharmonic phonons, especially for $k_BT \ll E_K$. It is important to realise that the soliton activation energy does *not* occur through the eigen*values* as for $A = \cos\frac{1}{2}\phi$ (above), but instead through the eigen*functions* (matrix elements). Furthermore, although one term in the sum (5) is sufficient for $A = \cos\frac{1}{2}\phi$, this is quite inadequate for $A = \cos\phi$. In the latter case the series (5) are probably asymptotic and at best slowly convergent: *many* correlation lengths $\sim d$ (equation (15)) need to be included *both* for the anharmonic phonon and soliton order contributions—depending on the quantitative accuracy desired (cf Scalapino *et al* 1972). These sums are *not* practicable using conventional Mathieu expansions (Appendix), and low-order terminations are generally inadequate. One very elegant procedure for summing the *infinite* series has been introduced by Apel *et al* (1979) generalising techniques of Edwards and Lenard (1962). In conjunction with equations (5), (15) and (16), we can interpret these works to imply that the series of terms of $O(dn_KE_K/k_BT)$ (equation (16)) exactly cancel. The terms of $O(dn_K(T))$ therefore dominate the soliton order terms. When multiplied by their corresponding Lorentzians (equation (5)), the terms in this infinite series *sum* to produce a q dependence specifically characterising the soliton profile. In fact at low T ($\beta E_K \gtrsim 6$) this *portion* of the integrated intensity is entirely consistent (Apel *et al* 1979) with a simple ideal soliton gas phenomenology (e.g. Mikeska 1978) (see equation (24) below), although that cannot itself be considered strong support for specific dynamics.

All of the above remarks for $A = \cos\phi$ generalise equally well (with changes of coefficients only) to e.g. $A = \phi^2$ in the ϕ-four model, and all similar 'kink-insensitive' correlations in a general class of models (e.g. Currie *et al* 1980).

It may help to reinforce the fundamental differences between the correlations of $A(\phi) = \cos\phi$ and $\cos\frac{1}{2}\phi$ by considering the different ways that the same Bragg peak evolves in the two cases as $T \to 0^+$. This is summarised schematically in figure 1. In the 'kink-insensitive' case $A(\phi) = \cos\phi$ there is an incomplete Bragg peak plus a distribution of weight in q space characterised by the squared Fourier transform of the kink profile, that is $(2\pi qd^2/\sinh(\pi qd/2))^2$ (Mikeska 1978; Bishop 1981; see also equation (21)). The weight in the latter component approaches zero $\sim(k_BT/E_K)^2$ as $T \to 0^+$, and all weight transfers to the Bragg peak in this limit. (NB If we consider the fluctuation correlation function $\tilde{C}$ (equation (9)) then there is no Bragg peak and $\tilde{F} \to 0$ as $T \to 0$). The kink-sensitive case $A(\phi) = \cos\frac{1}{2}\phi$ is quite different. Here there is no Bragg peak for $T \neq 0$, but rather a narrow (width $\sim d^{-1}(E_K/k_BT)^{1/2} \times \exp(-E_K/k_BT)$) and large amplitude ($\sim d(k_BT/E_K)^{1/2}\exp(-E_K/k_BT)$) structure at small q, which merges with the $A(\phi) = \cos\phi$ result at larger q. Of course the *same* Bragg peak emerges in both cases as $T \to 0^+$.

3. Dynamic correlations and easy-plane magnetic chains

We now comment on the consistency of various theories for *dynamic* correlation functions $S(q, \omega)$. Integrated intensities $\int d\omega S(q, \omega)$ contain limited information and

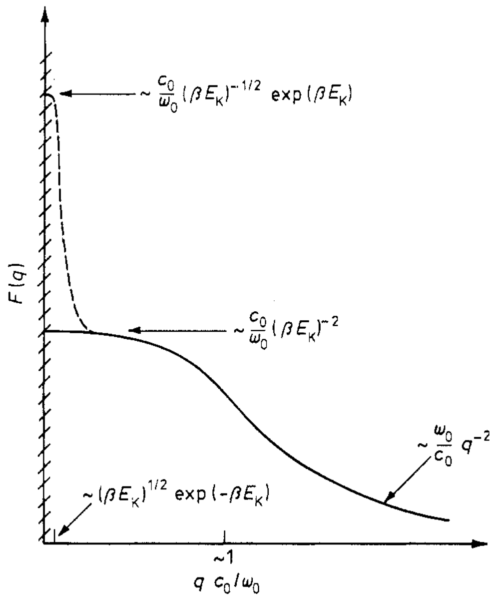

Figure 1. The integrated structure factors (schematic), $F(q) \equiv \int d\omega S(q, \omega)$, for self correlations of $\cos\phi$ (full curve) and $\cos\frac{1}{2}\phi$ (broken curve), illustrating the contrasting ways in which a complete Bragg peak (/ / / / /) emerges as $T \to 0^+$ (see § 2).

have to be interpreted carefully, as we suggest below. Nevertheless, the transfer integral results are constraints which need to be satisfied. The case $A(\phi) = \cos\frac{1}{2}\phi$ for a 2π-periodic SG model is essentially equivalent at low T to ϕ correlations in the ϕ-four model. The latter example has been considered approximately in a Hamiltonian framework† by e.g. Krumhansl and Schrieffer (1975), and in a non-linear mode–mode coupling theory by Sahni and Mazenko (1979). These theories can always be constructed to yield a non-diffusive low-frequency ('central') mode from *kinks* with integrated weight agreeing with equations (5) and (11): one interpolation form suggested (Krumhansl and Schrieffer 1975, Sahni and Mazenko 1979, Mikeska 1980) is

$$S(q, \omega) \sim \frac{2\tau}{\omega^2\tau^2 + 1} \frac{4\langle n_K\rangle}{q^2 + 4\langle n_K\rangle^2}, \tag{18a}$$

i.e.

$$\int_0^\infty S(q, \omega)\, d\omega \sim 4\pi \frac{\langle n_K\rangle}{q^2 + 4\langle n_K\rangle^2}.$$

The characteristic decay time τ is $\propto (M_K/k_B T)^{1/2}\langle n_K\rangle^{-1}$, with M_K the kink 'rest' mass ($E_K = M_K c_0^2$); i.e. $\tau \propto$ mean *kink collision* time. In addition to (18*a*) there is weight at higher frequency from (anharmonic) phonon modes. These are described self consistently in the approach of Sahni and Mazenko (1979). In the transfer integral scheme we need to keep many orders $n \geq 2$ in equation (5) to describe this integrated high-frequency response and the central (kink) weight (from $n = 1$) is large at small $q \lesssim \langle n_K(T)\rangle$: from equations (5) and (16) we can suppose (as is observed in molecular

† Corresponding structure factors have also been studied approximately in a Langevin approach with intermediate and large (extrinsic) damping (e.g. Imada 1979).

dynamic simulations) that the central weight becomes small with respect to the phonon weight for $q \gtrsim \langle n_K(T) \rangle$. It is appropriate to emphasise that the form (18*a*) is one of several interpolation formulae for the dynamic structure factor where kinks control the order parameter profile over long distances ('kink-sensitive functions'). Other interpolation forms are possible within the same general phenomenological picture. For instance, Maki (1981) has proposed instead of (18*a*) the form

$$S(q, \omega) \sim \langle n_K \rangle \frac{\langle n_K \rangle \tau}{[4\langle n_K \rangle^2 + q^2 + (\omega\tau\langle n_K \rangle)^2]^{3/2}}. \tag{18b}$$

Integrating (18*b*) on ω agrees with (18*a*) and the TIO result. This example illustrates the relative weakness of the static constraint of the TIO—the q dependence of the central kink peaks in (18*a*) and (18*b*) are quite different for moderate q.

Correlations of $A(\phi) = \phi$ are special for bounded potentials such as in literal SG since ϕ can vary over $(-\infty, +\infty)$, so we anticipate a divergence as $T \to 0^+$. These correlations are quite different from order parameter–order parameter correlations in the ϕ-four model which are most akin to $A(\phi) = \cos \frac{1}{2}\phi$ as remarked above. In particular one can show (see also Schneider *et al* (1979))

$$\int d\omega \, S^{\phi\phi}(q, \omega) \propto \frac{\exp(-\beta E_K)}{q^2 d}. \tag{19}$$

The direct kink activation energy dependence arises in the TIO procedure because eigen*states* within the first Mathieu band are coupled to the ground state. The calculation is slightly more subtle, however, because all states couple within the first band and must be included (for the literal SG model; see § 2.1). Note the hydrodynamic-like divergence as $q \to 0$. Conventional hydrodynamic theory (e.g. Forster 1975) would suggest

$$S^{\phi\phi}(q, \omega) \propto \frac{Dd^{-1} \exp(-\beta E_K)}{\omega^2 + (Dq^2)^2}, \tag{20}$$

with D a (T-dependent) diffusion coefficient. Expression (20) is consistent with expression (19) up to possible pre-exponential factors. Recently Bennett *et al* (1980) have made the attractive proposal that a hydrodynamic mode does indeed dominate long time scales for SG-like systems, and derives from the simple *topological* conservation of the *difference* between the number of kinks and anti-kinks. The consistency of expressions (19) and (20) is again not a severe test of specific dynamics. In particular the form (e.g. T dependence) of D is not constrained by (19). Bennett *et al* (1980) limit their derivation of the diffusion coefficient to an overdamped low-T regime with $D \propto T$. The situation in the small damping or Hamiltonian limit, where (19) strictly applies, is less certain, depending on the particular intrinsic (mode–mode coupling) damping mechanisms.

In view of recent concerns with the 1D easy-plane ferromagnet $CsNiF_3$ in an easy-plane magnetic field, the case $A(\phi) = \cos \phi$† is especially interesting. Since 2π kinks have only a *local* ('kink-insensitive') effect in this case and $\langle \cos \phi \rangle$ is finite, the approach of Krumhansl, Schrieffer and others (e.g. Aubry 1976) for calculating dynamic correlations is considerably modified. An ideal (renormalised mass) kink gas approximation can nevertheless be employed (e.g. Kawasaki 1976, Mikeska 1978,

† $A(\phi) = \sin \phi$ follows from $A(\phi) = \phi$ in view of the equation of motion (2) (Schneider *et al* 1979)—for the literal SG model (1), (2): the situation is different for the periodic coupling problem, cf § 2.1 and Appendix.

Bishop 1981) with the result that for low $k_B T$ ($<0{\cdot}15$–$0{\cdot}2\, E_K$)

$$S^{\cos\cos}(q,\omega) \approx \left(\frac{4}{\pi}\right)^2 \frac{\beta E_K}{\omega_0 q} \exp\{-\beta E_K[1+\tfrac{1}{2}(\omega/c_0 q)^2]\} \left(\frac{(\pi/2)qc_0/\omega_0}{\sinh[(\pi/2)qc_0/\omega_0]}\right)^2 \tag{21a}$$

$$\int S^{\cos\cos}(q,\omega)\,\mathrm{d}\omega = \frac{4}{\pi}\langle n_K\rangle \frac{c_0}{\omega_0}\left[\frac{(\pi/2)qd}{\sinh[(\pi/2)qd]}\right]^2 \xrightarrow{q\to 0} (4/\pi)d^2\langle n_K\rangle \qquad (d \equiv c_0/\omega_0). \tag{21b}$$

We emphasise that this result is due only to *kink* (and anti-kink) excitations. It predicts a 'central peak' but with different form than for $A(\phi)=\cos\frac{1}{2}\phi$ (equation (18)). The result (21*a*) is no more than that expected from an ideal gas of particles of finite extent. Comparing equation (21*b*) with the *infinite* sum of kink contributions (5), Apel *et al* (1979) find that the (low T) kink statics is reproduced exactly. The success of an ideal kink gas approach in this sense probably has the same origin as the kink theory of Bennett *et al* (1980) for $S^{\phi\phi}$—namely all distributions of kink positions have equal probability and we have made a low-T assumption. In deriving (21*a*) we have omitted all lifetime or diffusion effects. This is reasonable at low T and q, although these corrections can be included (Bishop, unpublished; Theodorakopoulos 1979), giving a Lorentzian character to the low-T central structure rather than the pure gaussian form (21*a*). Comparisons with molecular dynamics (Stoll *et al* 1979, Kerr *et al* 1980) support the view that a renormalised effective kink energy $E_K(T)$ must be used. This is particularly true at higher $k_B T(\gtrsim\frac{1}{4}E_K(0))$ where the pseudo-relativistic velocity dependence implicit in equation (2) plays a role and (together with discreteness effects) can lead to a splitting of the central peak (Stoll *et al* 1979, Kerr *et al* 1980) (for the nearly-integrable discrete SG model).

The kink contributions to a central peak were emphasised by Mikeska (1978). However, note from the TIO result that (for $A=\cos\phi$) the kink contributions to $\int S(q,\omega)\,\mathrm{d}\omega$ are exponentially weak. Indeed the central peak weight alone observed in MD and experimentally is greater than can be predicted in terms of these kink effects (Kerr *et al* 1980). As we noted, the remaining integrated weight is $\mathrm{O}(T/E_K)^2$ and dominates the exponential contribution—in fact the power series expansion is at best slowly convergent and higher-order powers should be included for quantitative accuracy—numerical evaluations are best (cf Scalapino *et al* 1972). A mode interpretation of MD simulation results *can* be made which is consistent with these features (Stoll *et al* 1979, Kerr *et al* 1980, T Schneider and E Stoll 1980 unpublished). It is suggested that both multi-magnon (e.g. two-magnon) processes (D Baeriswyl 1978, G Reiter 1979, private communications; see also Allroth and Mikeska 1980) and anharmonic magnon processes corresponding to bound magnon (i.e. breather; cf Dashen *et al* 1975) responses (Maki 1981, Bishop 1981) can both give central peak as well as high frequency response components of $\mathrm{O}(k_B T/E_K)^2$ and higher. It is important to emphasise that 'anharmonic spin-wave effects' are not merely broadening mechanisms for other responses (e.g. linear multi-magnon mechanisms) but also include highly (space and time) coherent non-linear excitations (breathers) with both particle and oscillatory degrees of freedom. These observations apply equally well to ϕ^2 correlations in the ϕ-four and similar models. We have already noted the conceptual and TIO similarity with $A(\phi)=\cos(\phi)$ in SG. Correspondingly, two-phonon processes are very similar, and numerical evidence for long-lived classical breather-like modes in ϕ-four is strong (e.g. Aubry 1974, Kudryavtsev 1975, Klein *et al* 1979, C Wingate and D Campbell 1979 unpublished) even in MD simulations (e.g. T R Koehler 1975 unpublished). Similarly, multi-phonon bound states viewed as quantum breather analogues are convincingly documented in the ϕ-four model (e.g. Dashen *et al* 1975).

At elevated temperatures contributions from kinks can become substantial. (For instance, compare the contributions of exponential and $O(T/E_K)^2$ in (16), (21*b*).) However, elementary mode (kink, breather) interpretation then becomes less well defined and should not be represented in analytic form (such as $\sim(k_BT/E_K)^2$ or $\sim\exp(-E_K/k_BT)$), even if quantum effects are neglected. This observation is very relevant for recent experimental studies of $CsNiF_3$ (Kjems and Steiner 1978, Kakurai *et al* 1980). Bearing in mind the periodicity of spin coupling $\cos(\phi_i-\phi_{i+1})$ (Patkós and Rujān 1979, Riseborough and Trullinger 1980, § 2.1) the *effective* continuum SG creation energy is reduced and T-dependent. Most of the experiments have been at $T=10$–12 K with $k_BT/E_K^{(\text{eff})}=0{\cdot}3$–$0{\cdot}4$. This is too high (Bishop 1979) for useful mode interpretation or simple analytic representations (e.g. Mikeska 1978). $T<9$ K would be far more interesting theoretically from this point of view. (Higher and lower temperatures are certainly interesting but for different reasons, namely the approach to 3D ordering ($T\sim2{\cdot}65$ K) and effects of a crossover to 1D isotropic Heisenberg behaviour (Bishop 1980b).)

Finally we mention essential differences between $CsNiF_3$ and TMMC. These are two quasi-1D magnets for which neutron scattering evidence is quoted in support of SG soliton excitations (Kjems and Steiner 1978, Boucher *et al* 1980). TMMC is an antiferromagnet and solitons correspond only to π (not 2π) rotations of a sub-lattice orientation angle. This leads only to a slightly different SG equation but with very striking physical consequences: $CsNiF_3$ and TMMC are to be interpreted quite differently in terms of solitons (probing kink-insensitive and sensitive correlations respectively). We refer the reader to e.g. Mikeska (1978, 1980) for original details of derivations of the approximate SG description of in-plane motions in these two cases. Here we only emphasise that the correlations presently measured in $CsNiF_3$ (Kjems and Steiner 1978) are for $A(\phi)=\sin\phi$ and $\cos\phi$; and for TMMC (Boucher *et al* 1980) $A(\phi)=\sin\frac{1}{2}\phi$ and $\cos\frac{1}{2}\phi$. Dynamic correlations for $A(\phi)=\sin\phi$ and $\sin\frac{1}{2}\phi$ are quite similar, predominantly contributing to spin-wave modes with weakly-weighted central peaks at low q. More interesting are the contributions from correlations for $A(\phi)=\cos\frac{1}{2}\phi$ and $\cos\phi$. We have carefully stressed the differences for these cases in this work. The implication is that anharmonic excitations play an important role for $CsNiF_3$, masking the kink central peak contributions (at sufficiently low T) and giving an additional *non* spin-wave high-frequency mode. Solitons enter the transfer integral expressions dominantly through eigen*functions*, as we have seen. By contrast, for TMMC the central peak is due predominantly to kinks (with different contributions from $A(\phi)=\sin\frac{1}{2}\phi$ and (mostly) $\cos\frac{1}{2}\phi$), and kinks enter the transfer integral results through eigen*values* directly. Breather contributions for $\cos\frac{1}{2}\phi$ correlations are much weaker because those of amplitude $\leq2\pi$ are most important (rather than $\sim\pi$ for $\cos\phi$ (Stoll *et al* 1979)) but their density is then exponentially smaller than that of kinks. TMMC should therefore be a much more direct probe of *kinks*† but $CsNiF_3$ is even more interesting (and complicated) theoretically since it might allow probing of the conceptually more unfamiliar *breather* excitations and other anharmonicity effects. We must caution again, however, against the use of low-T asymptotic expansions beyond their temperature range of validity (Bishop 1979). Such expansions are useful guides to

† Kinks should dominate correlations in *out* of easy-plane motions even for $CsNiF_3$, since these are determined at sufficiently low T by correlations of $A(\phi)=\phi$, the *in*-plane SG variable (e.g. Schneider *et al* 1979).

mode interpretations as we have seen, but cannot replace numerical implementation of transfer integral procedures for static properties at currently typical experimental temperatures. Experiments at lower temperatures would be very useful, although these must be optimised with respect to consequent loss of scattering intensity.

4. Summary

In § 2 we surveyed the general structure of static correlation functions for the classical SG system (and related systems such as ϕ-four) deduced formally by the transfer integral operator (TIO) technique. We emphasised the striking differences between correlations of 'kink-sensitive' and 'kink-insensitive' functions, and studied how these details arise within the above formalism. For a kink-sensitive function (such as $\cos \frac{1}{2}\phi$ in 2π-periodic SG) an unambiguous correlation length proportional to the mean kink *separation* is easily identified. However, for a kink-insensitive function (such as $\cos \phi$) the natural length scale is $\sim$ kink *width* and we need to sum many terms in the TIO approach for an adequate representation even at low T: anharmonic modes dominate. Thus care must be exercised with analytic implementations of the TIO.

Similarly striking differences between these two types of function were noted in § 3 for corresponding *dynamic* correlation functions. Although fully rigorous theories are not available in general (certainly for Hamiltonian systems), we compared several suggested forms to check for their frequency-integrated consistency with the TIO.

Finally, in § 3 we cited two easy-plane magnetic chain systems as exemplars of these general remarks. Assuming (for purposes of illustration—see § 1) the basic validity of a classical, continuum SG description for in-plane spin dynamics, we noted that the ferromagnet $CsNiF_3$ corresponds to a kink-insensitive case. Here anharmonic modes (breathers, multi-magnons) certainly play an important role, but simple mode interpretations must be cautioned against at currently studied temperatures (Kjems and Steiner 1978, Kakurai *et al* 1980). By contrast the antiferromagnet TMMC belongs to the kink-sensitive class, and at low T a pure kink interpretation of the observed 'central response' (Boucher *et al* 1980) should be adequate (in the absence of other contributing mechanisms). Both of these materials are therefore potentially interesting for studying 'elementary' SG excitations but they must be analysed quite differently, and experimental conditions chosen more carefully.

5. Addendum

Since submitting this work we have received preprints that include some related material by T Schneider and E Stoll, and by K Maki. These works are conveniently summarised by their authors in Schneider and Stoll 1981. Also, Leung and Hone (1980) have independently reached similar conclusions to ourself.

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Appendix

We illustrate a method of derivation for the intermediate structure factors $F(q) \equiv \int d\omega S(q, \omega)$ (§§ 2, 3). We use Goldstein's and Sip's asymptotic expansions (in our problem valid at low $T \ll E_K/k_B$) for Mathieu eigenvalues and eigenfunctions, which are conveniently collated in Abramowitz and Stegun (1970). (See also Guyer and Miller 1978.) We shall want to illustrate the origins of results in the text, but also the limitations of this general approach which were emphasised there. (cf Apel *et al* 1979.)

The transfer integral effective SE (4) is equivalent to the standard Mathieu equation (Abramowitz and Stegun 1970):

$$d^2/dx^2 + a - 2q\cos(2x)\tilde{\psi}(x) = 0, \tag{A1}$$

where V_0 in equation (4) can be omitted and

$$\begin{aligned} q &= -4m^*; \qquad & x &= \tfrac{1}{2}\phi; \\ a &= 8m^*(\epsilon - 1); \qquad & \tilde{\psi}(x) &= \psi(\phi). \end{aligned} \tag{A2}$$

We are concerned with expansions for $q \to -\infty (T \to 0^+)$, and (in the cases below) only with the characteristic eigenfunctions, i.e. $k = 0, \frac{1}{2}$ (cf notation of § 2), corresponding to band tops and bottoms. These are (real) linear combinations of Bloch functions. They can be even (band index n (§ 2) even) or odd (n odd), and π-periodic in x ($k = 0$) or 2π-periodic in x ($k = \frac{1}{2}$):

$$\begin{aligned} & ce_{2r}(x, q) \qquad && \text{(even, } \pi\text{-periodic)} \\ & ce_{2r+1}(x, q) && \text{(even, } 2\pi\text{-periodic)} \\ & se_{2r+1}(x, q) && \text{(odd, } 2\pi\text{-periodic)} \\ & se_{2r+2}(x, q) && \text{(odd, } \pi\text{-periodic)} \end{aligned} \tag{A3}$$

($r = 0, 1, 2, \ldots$). It will also be convenient to use the relationships

$$\begin{aligned} ce_{2r}(x, -q) &= (-1)^r ce_{2r}(\pi/2 - x, q) \\ ce_{2r+1}(x, -q) &= (-1)^r se_{2r+1}(\pi/2 - x, q). \end{aligned} \tag{A4}$$

The normalisation used below is $\int_0^{2\pi} ce^2(x)\,dx = \int_0^{2\pi} se^2(x)\,dx = \pi$, with $\pi^{1/2}\psi(\phi) \to ce(x), se(x)$.

Consider first the ground state $ce_0(x, q < 0) \equiv ce_0(y, |q|)$ ($y \equiv \pi/2 - x$). For $|\cos y| \leqslant 2^{1/4}|q|^{-1/8}$, that is, $y \approx \pi/2$, $x \approx 0$, we can use the expansion due to Sips (Abramowitz and Stegun 1970, §§ 20.9.15–20), from which we find ($|q| \gg 1$)

$$ce(x, q) \simeq (\pi/2)^{1/4}|q|^{1/8}(1 + \tfrac{1}{8}|q|^{-1/2} + \ldots)[D_0 - \tfrac{1}{16}|q|^{-1/2}(D_2 + \tfrac{1}{4}D_4) + \ldots]$$

where $D_n(\alpha) = (-1)^n \exp(\frac{1}{4}\alpha^2)(d^n/d\alpha^n)(\exp(-\frac{1}{2}\alpha^2))$ and $\alpha = 2|q|^{1/4}\cos y$. Thus

$$ce_0(x, q) \simeq (\pi/2)^{1/4}|q|^{1/8}\exp(-|q|^{1/2}\sin^2 x) \tag{A5a}$$

i.e. in (4)

$$ce_0(x, q) \equiv \pi^{1/2}\psi_{00}(\phi, q) \simeq (\pi/2)^{1/4}|q|^{1/8}\exp(-\tfrac{1}{4}|q|^{1/2}\phi^2) \qquad (|\phi| \approx 0). \tag{A5b}$$

Physically we expect the expansion near $\phi = 0$ (modulo 2π) to relate to major 'phonon' order contributions. On the other hand we expect ψ_{00} to be exponentially small (at low T) near $\phi = \pi$ (modulo 2π) and to relate to soliton-order contributions. For $\phi \sim \pi$, that is $y \sim 0$, we can use an expansion valid for $|\cos y| \gtrsim 2^{1/2}|q|^{-1/4}$ (Abramowitz and Stegun 1970, §§ 20.9.11–14):

$$ce_0(y, q) \sim (ce_0(0, q)/2^{1/2}F_0(0))[W_1(P_0 - P_1) + W_2(P_0 + P_1)]$$

with

$$\begin{aligned}
&F_0(0) \sim 1 + \tfrac{1}{8}|q|^{-1/2} + \dots \\
&P_0(y) \sim 1 + \tfrac{1}{8}|q|^{-1/2}(\cos y)^{-2} + \dots \\
&P_1(y) \sim \tfrac{1}{8}(\sin y/\cos^2 y)|q|^{-1/2} + \dots \\
&W_1 = [\cos(\tfrac{1}{2}y + \tfrac{1}{4}\pi)/\cos y]\exp(2|q|^{1/2}\sin y) \\
&W_2 = [\sin(\tfrac{1}{2}y + \tfrac{1}{4}\pi)/\cos y]\exp(-2|q|^{1/2}\sin y).
\end{aligned}$$

Thus

$$\psi_{00}(\phi, q) \simeq 2^{1/2}\pi^{-1/2}ce_0(y = 0, |q|)\cosh[|q|^{1/2}(\pi - \phi)] \qquad (\phi \sim \pi, |q| \gg 1).$$

The term $ce_0(0, |q|)$ has to be determined independently from (Abramowitz and Stegun 1970, § 20.9.23)

$$\frac{ce_0(y = 0, |q|)}{ce_0(y = \pi/2, |q|)} \sim 2^{3/2}\exp(-2|q|^{1/2}), \tag{A6}$$

whence, using (A5b),

$$\psi_{00}(\phi, q) \simeq 4(\pi/2)^{1/4}\pi^{-1/2}|q|^{1/8}\exp(-2|q|^{1/2})\cosh[|q|^{1/2}(\pi - \phi)]. \tag{A7}$$

Using similar expansions we can in principle study ce_{2n} generally. For instance, in equation (4), we find

$$\begin{aligned}
\psi_{20}(\phi, q) &\equiv \pi^{-1/2}ce_2(\tfrac{1}{2}\phi, q) \\
&\underset{\phi\sim 0}{\sim} 2^{-1/2}(\pi/2)^{1/4}|q|^{1/8}(-|q|^{1/2}\phi^2 + 1)\exp(-\tfrac{1}{4}|q|^{1/2}\phi^2)
\end{aligned} \tag{A8}$$

and

$$\psi_{20}(\phi, q) \underset{\phi\sim\pi}{\sim} \pi^{-1/2}ce_2(0, q)\cosh[(\pi - \phi)|q|^{1/2}]$$

with

$$ce_2(y = 0, q)/ce_2(\pi/2, q) \sim -32\sqrt{2}|q|\exp(-2|q|^{1/2}) \tag{A9}$$

so that

$$\psi_{20}(\phi, q) \underset{\phi\sim\pi}{\sim} 32(\pi/2)^{1/4}\pi^{-1/2}q^{9/8}\cosh[|q|^{1/2}(\pi - \phi)]\exp(-2|q|^{1/2}). \tag{A10}$$

Similarly, we find

$$\psi_{40}(\phi, q) \equiv \pi^{-1/2} ce_4(\tfrac{1}{2}\phi, q) \underset{\phi\sim 0}{\sim} (2\sqrt{6})^{-1}(\pi/2)^{1/4}|q|^{1/8} \times \exp(-\tfrac{1}{4}q^{1/2}\phi^2)(3-6q^{1/2}\phi^2+q\phi^4) \tag{A11}$$

and

$$\psi_{40}(\phi, q) \underset{\phi\sim\pi}{\sim} \pi^{-1/2} ce_4(y=0, |q|)\cosh[|q|^{1/2}(\pi-\phi)]. \tag{A12}$$

Problems arise in finding accurate expressions for $ce_4(0, |q|)$ (and $ce_{2n}(0, q)$ with $n > 3$). Only crude estimates are possible using tables and $ce_4(y=0)$ is already rather large even for large $|q|$.

We can also use the same expansions for the 2π-periodic (in x) Mathieu functions. For instance

$$ce_1(x, -q) = se_1(y, |q|) \approx (\pi/2)^{1/4}|q|^{1/8}\cos(x)\exp(-q^{1/2}\sin^2 x) \tag{A13a}$$

$$\approx (\pi/2)^{1/4}|q|^{1/8}\exp(-\tfrac{1}{4}|q|^{1/2}\phi^2). \tag{A13b}$$

$ce_1(x, -q)$ can be expressed for $\phi \sim \pi$ as $\frac{1}{2}|q|^{-1/2} se_0'(0, |q|)\sinh[q^{1/2}(\pi-\phi)]$, but we shall not pursue this further since the function vanishes for $\phi = \pi$: solitons do not arise from the eigenfunctions in such cases, but from the eigenvalues (§ 2). We note that eigenvalue differences for the Mathieu equation follow from § 20.2.31 of Abramowitz and Stegun (1970), taking the forms (11c, d) in the text.

To illustrate uses of the above results† consider correlations of $A = \cos\phi$ (§ 2). As $T \to 0^+$, we approximate

$$\begin{aligned} M_0^{\cos}(T) \equiv \frac{1}{\pi}\int_0^{2\pi} \mathrm{d}\phi\, ce_0^2(\tfrac{1}{2}\phi)\cos\phi &\simeq \left(\frac{1}{2\pi}\right)^{1/2} q^{1/4}\int \cos\phi\,\exp(-\tfrac{1}{2}q^{1/2}\phi^2)\,\mathrm{d}\phi \\ &+16\left(\frac{1}{2\pi}\right)^{1/2} q^{1/4}\exp(-4q^{1/2})\int \cos\phi\,\cosh^2[q^{1/2}(\phi-\pi)]\,\mathrm{d}\phi, \end{aligned} \tag{A14}$$

where we have used (A5) and (A7). The exponentially small-order term is retained even though it is dominated by phonon order terms (at low T), since the former exhibits 'soliton' contributions. The integral ranges in (A14) are not easily prescribed rigorously. However, at large q (low T) we can reasonably extend the first integral range to $(-\infty, \infty)$ and expand $\cos\phi$ (see below also). Then, we obtain 'phonon' order contributions. The second integral in definition (A14) is presumably a better representation of higher-order phonon contributions. However, as in the expansions of eigen*values* (Abramowitz and Stegun 1970, §§ 20.2.30, 31), we can expect in addition non-perturbative pieces of exponentially small weight (at low T) but representing interesting soliton effects (Currie *et al* 1980). Physically these should correspond to the transition regions $\phi \sim \pi$ and noting ((A2)) that $4|q|^{1/2} = \beta E_{\mathrm{K}}$, we will simply evaluate the second integrand in (A14) at $\phi = \pi$. It will be appreciated that handling the 'soliton' piece in the present approach is not at all rigorous, but the result is suggestive. With the above approximations equation (A14) yields

$$M_0^{\cos}(T) \simeq 1 - 2(\beta E_{\mathrm{K}})^{-1} + \mathrm{O}(\beta E_{\mathrm{K}})^{-2} - 8(2\pi)^{-1/2}(\beta E_{\mathrm{K}})^{1/2}\exp(-\beta E_{\mathrm{K}}) \tag{A15}$$

† To simplify presentation we have used ψ functions instead of ϕ functions (see equation (4)) (recall that equation (4) is valid in the limit $d \gg l$), although these corrections are important in typical numerical implementations.

or

$$|M_0^{\cos}|^2 \simeq 1-4(\beta E_{\rm K})^{-1}+{\rm O}(\beta E_{\rm K})^{-2}-4dn_{\rm K}(T)+{\rm O}[d(\beta E_{\rm K})^{-1}n_{\rm K}]$$

where we have used $dn_{\rm K}(T)=4(2\pi)^{-1/2}(\beta E_{\rm K})^{1/2}\exp(-\beta E_{\rm K})$ (Currie *et al* 1980), and $d\equiv c_0/\omega_0$. The coefficient of the soliton-order term is uncertain in the above scheme but result (A15), describing the weight taken out of the Bragg peak (see § 2 and figure 1), actually agrees very well with the form suggested by Mikeska (1978).

Calculations of higher-order matrix elements proceed in the same way. (We shall restrict the discussion below to 2π-periodic (in ϕ) Mathieu solutions appropriate to the periodic coupling spin problem (§ 2.1). A further subset of matrix elements are finite if we admit 4π-periodic solutions also, i.e. for the literal SG (1), (2).) From § 2, (A8) and (A10)

$$\begin{aligned}M_1^{\cos}(T) &\equiv \frac{1}{\pi}\int_0^{2\pi} {\rm d}\phi\, ce_0(\tfrac{1}{2}\phi)\cos\phi\, ce_2(\tfrac{1}{2}\phi)\\ &\approx \frac{1}{2}\pi^{-1/2}q^{1/4}\int_{-\infty}^{\infty}\exp(-\tfrac{1}{2}q^{1/2}\phi^2)(q^{1/2}\phi^2-1)(1-\tfrac{1}{2}\phi^2)\,{\rm d}\phi\\ &\quad -128(2\pi)^{-1/2}q^{5/4}\exp(-4q^{1/2})\\ &\approx 2\sqrt{2}(\beta E_{\rm K})^{-1}+{\rm O}(\beta E_{\rm K})^{-2}-(\beta E_{\rm K})^2\,dn_{\rm K}(T).\end{aligned}\tag{A16}$$

Thus,

$$|M_1^{\cos}|^2 \simeq 8(\beta E_{\rm K})^{-2}+{\rm O}(\beta E_{\rm K})^{-3}-4\sqrt{2}\,\beta E_{\rm K}dn_{\rm K}(T)+{\rm O}(dn_{\rm K}(T)).\tag{A17}$$

Notice that, in the first integral in (A16), all terms of ${\rm O}(\beta E_{\rm K})^0$ cancel. This property can be shown to hold for all the matrix elements $M_n^{\cos}$ *if* we expand integrands to sufficient order. Such a situation is expected from the behaviour of (see equation (10))

$$\begin{aligned}M^{\cos^2} &\equiv \frac{1}{\pi}\int_0^{2\pi} ce_0^2(\tfrac{1}{2}\phi)\cos^2\phi\,{\rm d}\phi\\ &\approx 1-4(\beta E_{\rm K})^{-1}+16(\beta E_{\rm K})^{-2}+{\rm O}(\beta E_{\rm K})^{-3}+2dn_{\rm K}+{\rm O}((\beta E_{\rm K})^{-1}dn_{\rm K}).\end{aligned}\tag{A18}$$

In (18) we see that the 'linear phonon' order is already exhausted by $|M_0^{\cos}|^2$. We also note the absence of terms of ${\rm O}(d\beta E_{\rm K}n_{\rm K})$ in (A18), from which we imply that such terms in $\Sigma|M_n^{\cos}|^2$ will sum to zero (cf Apel *et al* 1979).

Calculation of matrix elements for $\cos\frac{1}{2}\phi$ (equations (11)) proceeds similarly. (Here we shall admit coupling to 4π-periodic (in ϕ) Mathieu solutions also, having in mind antiferromagnet applications, such as to TMMC (Mikeska 1980), since the effective periodic SG potential is there $(1-\cos 2\phi)$ (Mikeska 1980) and $\cos\phi$ correlations then correspond to the present calculation.) Since $ce_1(x,-q)$ vanishes at $x=\pi/2$ ($\phi=\pi$), we do not look for soliton contributions. From § 2 and (A13) we estimate

$$M_1^{\cos^{1/2}}(T)\approx(2\pi)^{-1/2}q^{1/4}\int_{-\infty}^{\infty}{\rm d}\phi\,\exp(-\tfrac{1}{2}q^{1/2}\phi^2)(1-\tfrac{1}{8}\phi^2)$$

giving

$$|M_1^{\cos^{1/2}}|^2\approx 1-(\beta E_{\rm K})^{-1}+{\rm O}(\beta E_{\rm K})^{-2}.\tag{A19}$$

In this case soliton evidence appears through the dominant correlation length (from eigenvalue differences)—see equations (9) and (11*d*). The same situation occurs for correlations of $\sin\phi$ (for the literal SG model where we include 4π-periodic Mathieu solutions (in ϕ), cf § 3), but it is essential to recognise the full periodicity of ce_1, cf equation (13*a*):

$$
\begin{aligned}
M_1^{\sin}(T) &= \frac{1}{\pi}\int_0^{2\pi} \mathrm{d}\phi \sin\phi \, ce_0(\tfrac{1}{2}\phi)ce_1(\tfrac{1}{2}\phi) \\
&= \frac{8q^{1/4}}{(2\pi)^{1/2}}\int_0^1 \mathrm{d}z \, z(1-z^2)^{1/2}\exp(-2q^{1/2}z^2) \\
&\overset{|q|\to\infty}{\approx} \frac{8q^{1/4}}{(2\pi)^{1/2}}\int_0^\infty \mathrm{d}z\, z\exp(-2q^{1/2}z^2) \\
&= 2(2/\pi)^{1/2}(\beta E_{\mathrm{K}})^{-1/2}
\end{aligned}
$$

i.e.

$$
|M_1^{\sin}(T)|^2 \overset{T\to 0}{\approx} (8/\pi)(\beta E_{\mathrm{K}})^{-1} + \mathrm{O}(\beta E_{\mathrm{K}})^{-2}. \tag{A20}
$$

Notice that while the correlation lengths for $\cos\frac{1}{2}\phi$ and $\sin\phi$ are the same (and soliton dominated), the amplitude of correlations are very different (compare (A19) and (A20)) as we can expect physically.

Finally we note that alternative approximations can be used to integrals occurring in the various matrix elements above. For example we can retain the $(0, 2\pi)$ integral range and *assume* that the validity of fully-periodic large-q approximations such as (A5*a*) can be extended over the whole range. Then

$$
\begin{aligned}
|M_0^{\cos}| &\approx (2\pi)^{-1/2}q^{1/4}\int_0^{2\pi}\mathrm{d}\phi\cos\phi\exp(-2q^{1/2}\sin^2\tfrac{1}{2}\phi) \\
&= (2\pi)^{1/2}q^{1/4}I_1(q^{1/2})\exp(-q^{1/2}),
\end{aligned}
$$

where I_1 is a modified Bessel function. Thus

$$
|M_0^{\cos}(T)|^2 \overset{|q|\to\infty}{\approx} 1 - 3(\beta E_{\mathrm{K}})^{-1} + \mathrm{O}(\beta E_{\mathrm{K}})^{-2}. \tag{A21}
$$

Similarly

$$
\begin{aligned}
M_0^{\cos^2}(T) &\approx (\pi/2)^{1/2}q^{1/4}\exp(-q^{1/2})[I_0(q^{1/2}) + I_2(q^{1/2})] \\
&\overset{|q|\to\infty}{\approx} 1 - \tfrac{7}{2}(\beta E_{\mathrm{K}})^{-1} + \mathrm{O}(\beta E_{\mathrm{K}})^{-2}.
\end{aligned} \tag{A22}
$$

We see that differences occur only in numerical coefficients (compare equations (A15) and (A18) with (A21) and (A22) respectively), implying the need for consistent expansions for *ce*, *se*. This is evident, for instance, in the manipulations above (A5*a*) if we seek to retain pre-exponential factors of $\mathrm{O}(q^{-1/2})$. Thus *coefficients* in our various matrix element expressions should not all be exact. However, since our main interest is only to establish *orders* of (βE_{K}) we will not pursue these corrections here.

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