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LETTER TO THE EDITOR

On the statistical mechanics of a discrete ϕ^4 chain

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Abstract. The configurational phenomenology of kinks and phonons is examined in the case of a discrete ϕ^4 chain in the displacive limit. Due to the existence of a lattice, an exact description of phonons in the whole Brillouin zone in terms of asymptotic phase shifts is not possible; it can be shown, however, by means of a simple numerical calculation that the change in the phonon density of states due to the presence of a kink obeys two simple sum rules. This enables us to justify a configurational phenomenology for the discrete lattice, which is in full agreement with the exact (transfer integral) results.

The relevance of nonlinear excitations within the context of statistical mechanics has been demonstrated in the pioneering work of Krumhansl and Schrieffer (1975). Their exact calculation of the partition function of a one-dimensional ϕ^4 chain in the displacive limit enabled them to identify a part of the free energy with the gas of phonons and associate the rest with kinks which move, more or less freely, within the lattice. As recently pointed out by Bishop (1978) this rest can be described by (kink) configurational phenomenology, provided one includes the self-energy of the kink; the latter manifests itself partly in terms of a modified phonon density of states which can, *in the continuum limit*, be directly related to the asymptotic phase shifts suffered by phonon modes as they pass through the kink. However, the crucial step, namely the comparison between configurational phenomenology and exact (transfer integral) evaluation of the partition function, has only been performed in the continuum approximation, rather than in the physically relevant case of the *displacive* limit of a discrete system.

The distinction between the two limits (Guyer and Miller 1978), of fundamental importance in itself, can be very simply demonstrated in practice. Thus, numerical simulations show that the kink will partly reflect phonons which are near the Brillouin zone edge. Moreover, even when the kink–phonon interaction is adequately described in terms of a phase shift, the latter's magnitude turns out to be different from that predicted by continuum theory—except in the long-wavelength limit. Similar discrete lattice effects are observed in the space shift suffered by a kink when it collides with a phonon wave packet (Hasenfratz and Klein 1977, Theodorakopoulos 1979, Theodorakopoulos *et al* 1979).

It is the purpose of this Letter to show by means of a simple numerical calculation that it is still possible, by an appropriate generalisation, to define and evaluate the kink's self-energy for a discrete system in the displacive limit. The conclusions of configurational phenomenology remain valid without resort to the continuum limit.

We consider the Hamiltonian (Krumhansl and Schrieffer 1975)

$$H = mu_0^2\omega_0^2 \sum_{i=1}^{N} [\tfrac{1}{2}\dot{\phi}_1^2 + \tfrac{1}{2}\bar{C}(\phi_{i+1} - \phi_i)^2 + V(\phi_i)] \tag{1}$$

of a linear chain of lattice constant l, consisting of N atoms of mass m, coupled by harmonic springs and sitting on on-site double-well potentials $V(\phi) = (\phi^2 - 1)^2/4$. The displacement of the ith atom is given by $u_0\phi_i$, where $\pm u_0$ define the minima of the double-well potential and ω_0 their energy scale; time is measured in units of ω_0^{-1} and $\bar{C} > 1$ is the displacive parameter. Using the transfer integral technique, the free energy per unit length was found to be†

$$F/L = F_0/L - (1/\beta l)[(12/\pi)(1/\bar{C})\beta E_\kappa^0]^{1/2} \exp(-\beta E_\kappa^0) \tag{2}$$

where $\beta = 1/k_B T$, $L = Nl$, and

$$E_\kappa^0 = \tfrac{2}{3}(2\bar{C})^{1/2} mu_0^2\omega_0^2 \tag{3}$$

can be identified with the rest energy of a kink (see below) and F_0 is the free energy of the gas of harmonic phonons of the *discrete* system (1) with $V = 0$.

The equations of motion derived from equation (1) are

$$\ddot{\phi}_n = \bar{C}(\phi_{n-1} + \phi_{n-1} - 2\phi_n) + \phi_n - \phi_n^3. \tag{4}$$

The nonlinear system (4) admits propagating kink solutions as long as the velocity does not become too large (Currie *et al* 1977). In fact, the form of the static solution is well approximated by

$$\phi_\kappa(n) \cong \tanh[n/(2\bar{C})^{1/2}] \tag{5}$$

as long as $\bar{C} > 1$ (Koehler *et al* 1975). Here we should perhaps point out that in general there will be two types of discrete lattice effects: those which arise as a result of a decrease in the displacive parameter $\bar{C}$ (such as deviations of the kink form from equation (5) or pinning effects) and those inherent to discrete systems (such as the fact that a kink, no matter how extended, will still not be transparent to phonons with wave vector $Q \leqslant \pi/l$). We shall only be concerned with the second type of effect, so that equations (5) and (3) are, for our purposes, sufficiently good approximations for the kink's form and energy respectively.

It is possible to perform linear stability analysis for the discrete system defined by equations (4) and (5). The *ansatz*

$$\phi_n(\tau) = \phi_\kappa(n) + u_n^{(j)} \exp(-\mathrm{i}\Omega_j\tau) \tag{6}$$

leads to

$$\mathscr{L}u_n^{(j)} \equiv u_{n+1}^{(j)} + q_n u_n^{(j)} + u_{n-1}^{(j)} = \lambda_j u_n^{(j)}; \qquad n = 1, 2 \ldots N \tag{7}$$

where

$$q_n = -2 + (3/\bar{C})[1 - \phi_\kappa^2(n)] \tag{8}$$

$$\lambda_j = (2 - \Omega_j^2)/\bar{C} \tag{9}$$

and $u_0 = u_{N+1} = 0$. Our objective is to follow the change in the eigenvalue spectrum of

† Our transfer integral result corresponds to equation (30) of Bishop (1978), including the correction by a factor $(\pi/e)^{1/2}$ (see footnote 34 of Bishop 1978).

equation (7) brought about by the presence of the kink. In the absence of the kink we have $\mathscr{L} \to \mathscr{L}^{(0)}$ with

$$q_n^{(0)} = -2. \tag{8'}$$

We may now form the Sturm sequence $\{D_n(\lambda)\}$ for $n = 0, 1 \ldots N$, defined by $D_0(\lambda) = 1$, $D_1(\lambda) = a_1 - \lambda$

$$D_n(\lambda) = (q_n - \lambda)D_{n-1}(\lambda) - D_{n-2}(\lambda) \qquad n = 2, 3 \ldots N \tag{10}$$

and determine the eigenvalue spectrum of either $\mathscr{L}$ or $\mathscr{L}^{(0)}$ by making use of the fact that the number of zeros $\delta R(\lambda)$ of the polynomial $D_N(\lambda)$ in the interval $(\lambda - \delta\lambda, \lambda)$ equals the increase in the number of sign changes in the sequence $\{D_n(\lambda)\}$ as λ increases from $\lambda - \delta\lambda$ to λ (Polozhii 1965).

If this procedure is performed for both $\mathscr{L}$ and $\mathscr{L}^{(0)}$ (in our case the spectrum of $\mathscr{L}^{(0)}$ is known exactly) the resulting difference $\delta\Delta R(\lambda_m) = \delta R(\lambda_m) - \delta R^{(0)}(\lambda_m)$ between the number of eigenvalues of $\mathscr{L}$ and $\mathscr{L}^{(0)}$ respectively in a given interval $(\lambda_m - \delta\lambda_m, \lambda_m)$ can be evaluated. For the calculation of the kink's self-energy we shall need

$$\sum_m{}' \, \delta\Delta R(\lambda_m) = -a \tag{11}$$

and

$$\lim_{\delta\lambda_m \to 0} \sum_m{}' \, \delta\Delta R(\lambda_m) \ln(2 - \bar{C}\lambda_m) = -2 \ln b \tag{12}$$

where the prime denotes that summation is restricted to $-4 < \lambda_m < 0$ ('phonon' modes). In the continuum approximation it was possible to set $\delta\Delta R(\lambda) = \Delta\rho(\lambda)\delta\lambda$ and relate the change in the phonon density of states $\Delta\rho$ directly to the phonon phase shift. Such a connection does not appear to be possible in the discrete system. Thus, the main point of this letter is in fact to argue that, only because $a(\bar{C})$ and $b(\bar{C})$ exist and are well behaved in the displacive limit $\bar{C} \gg 1$, is configurational phenomenology justifiable for the physically relevant case of a discrete lattice.

Our numerical results summarised in table 1 indicate that this indeed is the case. Furthermore, the limiting values of a and b are equal within numerical accuracy to the continuum values.

Table 1. Characteristics of the eigenvalue spectrum of the discrete ($N = 200$) ϕ^4 chain for $\bar{C} = 4, 16, 64$. The two eigenvalues for which $\lambda > 0$ are listed separately. Results obtained in the continuum approximation are shown for the sake of comparison; in particular $(\ln b)_{\text{cont}} = -(2\pi)^{-1} \int_{-\infty}^{\infty} (\mathrm{d}q)\delta'(q) \ln \Omega(q)$, where $\delta(q)$ is the asymptotic phase shift for a phonon of wave vector q, and a_{cont} equals the number of bound states. The slightly negative values of Ω_{T}^2 indicate the instability which characterises the approach of equation (5) to the true discrete kink solution (Currie *et al* 1977). The length of the intervals $\delta\lambda_m$ in equation (12) was chosen to satisfy $\delta\lambda_m < 10^{-2}(2/\bar{C} - \lambda_m)/N$. This yields an accuracy of better than 0·5% for b.

	$\bar{C} = 4$	$\bar{C} = 16$	$\bar{C} = 64$	Continuum
Ω_{L}^2	1·4755	1·4942	1·4986	$\frac{3}{2}$
Ω_{T}^2	−0·0122	−0·0030	−0·0008	0
a	2	2	2	2
$b/6$	0·930	0·981	0·995	1

It is now possible to calculate the kink's self-energy Σ_κ in the low-temperature regime $\beta E^0_\kappa \gg 1$ according to the scheme put forward by Bishop (1978). Before doing this, however, we state the basic result of configurational phenomenology for the nonphonon part of the free energy density:

$$(F-F_0)/L = (2E^0_\kappa/B\hbar\omega_0 l)(1/2\pi\beta E^0_\kappa\bar{C})^{1/2}\exp[-\beta(E^0_\kappa+\Sigma_\kappa)]. \tag{13}$$

For the ϕ^4 system, where topology demands that a kink should be followed by an anti-kink and *vice versa*, we obtain $B=2$. This can be seen by a simple counting argument for a system of n_κ kinks and $n_{\bar{\kappa}}$ anti-kinks ($n_{\text{tot}}=n_{\bar{\kappa}}+n_\kappa=\text{const.}$). Of the total number of configurations $2^{n_{\text{tot}}}$, only one survives a given boundary condition; hence $B=2$.

The self-energy appearing in equation (13) is given in the discrete lattice case by

$$\Sigma_\kappa = \Delta F + k_{\text{B}}T\ln(\beta\hbar\omega_0\Omega_{\text{L}}) \tag{14}$$

where

$$\begin{aligned}\Delta F &= k_{\text{B}}T\lim_{\delta\lambda_m\to 0}\sum_m{}'\,\sigma\Delta R_m\ln(\beta\hbar\omega_0\Omega_m)\\ &= k_{\text{B}}T[-a\ln(\beta\hbar\omega_0)+\ln b].\end{aligned} \tag{15}$$

Setting $B=2$, $\Omega^2_{\text{L}}=\frac{3}{2}$, $a=2$ and $b=6$, we may collect the results (13)–(15) and verify that equations (2) and (13) become identical. Configurational phenomenology is thus seen to reproduce the transfer integral result in the displacive limit without resort to the continuum approximation.

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