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Discreteness effects in a Φ^4 chain with long-range interactions

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Abstract. We study the influence of discreteness on kink motion in a one-dimensional Φ^4 chain with long-range atomic interactions of Kac–Baker type. We use a discretized Hamiltonian formalism in which the kink appears as a canonical degree of freedom. It is shown that the kink oscillatory motion and lattice trapping processes depend strongly on the range of interaction.

1. Introduction

A number of computer simulations and theoretical studies have been made on the importance of the discreteness effects on the structural and dynamical properties of Sine–Gordon (Kerr *et al* 1981, Peyrard and Kruskal 1984, Willis *et al* 1986, Stancioff *et al* 1986, Boesch *et al* 1989) and Φ^4 (Schmidt 1979, Combs and Yip 1983, 1984, Kunz and Combs 1985) chains. Soliton energy loss to phonons and pinning effects were found in these initial studies. The Φ^4 chain generalized to include non-linear nearest-neighbour interactions and linear second-neighbour interactions along the chain has been studied. The effect of energy radiation due to discreteness effects under an external field has been studied with and without other extrinsic dissipation mechanisms (Pnevmatikos *et al* 1987). A model of a non-linear 1D lattice with a long-range coupling of the Lennard-Jones type has been studied previously (Ishimori 1982).

Another long-range potential is the Kac–Baker type; this potential has been studied extensively in connection with the Ising model (Kac and Helfand 1973, Helfand 1964, Baker 1961) and the Pott models (Viswanathan and Meyer 1977). It has also been used to discuss, in the continuum limit, the effects of solitons on the thermodynamic properties of a chain (Sarker and Krumhansl 1981). The case of an anharmonic non-magnetic chain with long-range interactions was studied (Remoissenet and Flytzanis 1985), and recently the same potential was used in an anharmonic magnetic Heisenberg chain (Ferrer 1989). Also, by using the kernel operator, the influence of long-range interactions between particles, on the commensurate–incommensurate phase transition has been investigated (Pokrovsky and Virosztek 1983).

In this paper, we apply, in the non-relativistic limit, an extension of the field theoretical technique to the discrete kink problem to evaluate the weight of the force range interaction parameter on kink motion in a one dimensional discrete lattice. The formalism has recently been exposed and used (Willis *et al* 1986) in the Sine-Gordon lattice. The organization of the paper is as follows. In section 2, we present the model Hamiltonian and the formalism. In section 3 we derive the equations of motion for soliton coordinate and dressing, and their properties are analysed in terms of the range of interactions, while the last section is devoted to a summary.

2. The model Hamiltonian and formalism

We consider an infinite one-dimensional lattice of ions lying on the bistable Φ^4 potential. These ions are assumed to interact via the Kac–Baker potential. In this long-range interaction potential, the interactions between particles fall off exponentially as the distance between them increases. The Hamiltonian of such a system is:

$$H = \tfrac{1}{2}\Sigma(\mathrm{d}y_i/\mathrm{d}t)^2 + \tfrac{1}{2}\Sigma V_{ij}(y_i - y_j)^2 + \tfrac{1}{4}\Sigma(y_i^2 - 1)^2 \tag{1a}$$

where y_i is the displacement of the ith atom from its equilibrium site $x_i = ib$, b is the lattice constant which has been set equal to the unity.

$$V_{ij} = [J(1-r)/2r]r^m \tag{1b}$$

is the Kac–Baker potential $(0 < r < 1)$; $m = \mathrm{abs}(i - j)$ is the distance between atoms on different sites i and j. V_{ij} is chosen so that the total potential experienced by one atom due to all others is finite in the thermodynamic limit (the number of atoms is infinite); it is equal to the constant J. For $r = 0$, the model reduces to a nearest-neighbour interaction problem. The limit $r = 1$, which should be taken only when the number of particles is infinite, corresponds to the infinite range problem, also called the Van der Waals model since the behaviour of the system in this limit is identical to a Van der Waals model (Baker 1961).

In the continuum limits, the Hamiltonian system (1) exhibits solitons or kinks solutions given implicitly by the equation (Sarker and Krumhansl 1981):

$$(x - vt)/\sqrt{2}\xi = -3(\sigma/2)^{1/2}\sinh^{-1}[2\sigma/(1+\sigma)]^{1/2}y + (1+3\sigma)^{1/2}\tanh^{-1}[(1+3\sigma)/(1+\sigma+2\sigma y^2)]^{1/2}y \tag{2}$$

where $\xi^2 = [J(1+r) - r - v^2(1-r)^2]/(1-r)^2$ and $\sigma = r/(1-r)^2\xi^2$. v defines the velocity at the kink's point of steepest gradient. The parameter ξ has the dimension of length and gives a measure of the soliton width. For mathematical simplicity, the implicit solution (2) has been reduced to the analytic expression

$$y_k(x,t) = \tanh[K(x - vt)] \tag{3}$$

$$K^2 = (1-r)^2/2[J(1+r) - r] \tag{4}$$

where (4) is considered to be the pseudo-kink width. The soliton profiles given by (2) suffer slightly because of the approximation (3). Equation (4) shows that the physical applications of our model belong to the non-relativistic regime. Since K^{-1} should be greater than one lattice spacing, we require $J > \tfrac{1}{2}$.

Our aim is to analyse some dynamical and static properties of kink motion in our system. For this purpose, we consider the decomposition of the discrete displacement y_i in the manner:

$$y_i = y_k^i(X(t)) + \psi_i \tag{5a}$$

which yields

$$\mathrm{d}y_i/\mathrm{d}t = \mathrm{d}\psi_i/\mathrm{d}t + y_k^{i(1)}\,\mathrm{d}X/\mathrm{d}t \tag{5b}$$

with $y_k^i(X(t)) = \tanh[K(i-X)]$ defining the continuum kink at the discrete lattice i; $y_k^{i(1)} = \mathrm{d}y_k^i/\mathrm{d}X$ and ψ_i is the correction or dressing on the continuum kink (3) because of the discreteness of the lattice. The dynamical variable $X(t)$ is the position coordinate for the kink. In order to derive the equation of motion for $X(t)$, we need to reformulate the Hamiltonian description. This will be achieved by introducing in (1) the above coordinates and their canonically conjugate momenta. We also need two constraint conditions on the discrete variables and a new formulation of the canonical bracket. The constraints are

$$C_1 = \Sigma y_k^{i(1)}\psi_i = 0 \qquad C_2 = \Sigma y_k^{i(1)} p_i = 0 \tag{6}$$

where p_i is the conjugate momentum of the dressing ψ_i. These constraints have already been used in Φ^4-field theory (Tomboulis 1975, Willis *et al* 1986). The first one tends to minimize the correction in the domain-wall region and the second means that the kinetic energy of the new Hamiltonian must not have cross terms between the soliton kinetic energy and the particles kinetic energies. The new canonical brackets are defined as follows (Dirac 1964, Willis *et al* 1986):

$$\{\psi_i, p_j\} = \delta_{ij} - M^{-1} y_k^{i(1)} y_k^{j(1)} \tag{7}$$

where δ is the kronecker delta and $M = \Sigma(y_k^{i(1)})^2$. The equation (7) is defined in the manner that $\{C_1, C_2\} = 0$, as it must be if the constraint $C_1 = C_2 = 0$ is to be satisfied. One must note that the conventional Poisson bracket yields $\{C_1, C_2\} = M$ not equal to zero. This violates the requirement that $C_1 = C_2 = 0$. As a consequence of the above, the new Hamiltonian of our system is:

$$H = P^2/2M + \tfrac{1}{2}\Sigma(\mathrm{d}\psi_i/\mathrm{d}t)^2 + \Sigma V(\psi_i + y_k^i(X), r) \tag{8a}$$

which can be rewritten as:

$$H = P^2/2M + \tfrac{1}{2}\Sigma(\mathrm{d}\psi_i/\mathrm{d}t)^2 + U(X, \psi_i, r) \tag{8b}$$

M, defined previously, is the dimensionless mass of the soliton and $P = M(\mathrm{d}X/\mathrm{d}t)$ is the conjugate momentum of the dynamical variable X.

$$V(\psi_i + y_k^i(X), r) = \tfrac{1}{4}[(\psi_i + y_k^i)^2 - 1]^2 + \Sigma V_{ij}[(\psi_i + y_k^i) - (\psi_j + y_k^j)]^2 \tag{8c}$$

$$U(X, \psi_i, r) = \Sigma V(\psi_i + y_k^i(X), r) \tag{8d}$$

where $U(X, \psi_i, r)$ is the generalized potential of the Hamiltonian system.

3. Equations of motion and influence of the long-range parameter

The Poisson brackets formalism, equations (7) and (8) yield these equations of motion for soliton coordinate $X(t)$ and the dressing ψ_i:

$$\mathrm{d}^2X/\mathrm{d}t^2 + \tfrac{1}{2}(\mathrm{d}X/\mathrm{d}t)^2\,\mathrm{d}\ln M/\mathrm{d}X = (-1/M)\,\mathrm{d}U/\mathrm{d}X \tag{9}$$

$$\mathrm{d}^2\psi_i/\mathrm{d}t^2 = -(\psi_i + y_k^i(X))^3 + (1-2J)(\psi_i + y_k^i(X)) + [J(1-r)/r]\Sigma r^m(y_k^j + \psi_j) - y_k^{i(1)}[\mathrm{d}^2X/\mathrm{d}t^2 + \tfrac{1}{2})(\mathrm{d}X/\mathrm{d}t)^2\,\mathrm{d}\ln M/\mathrm{d}X]. \tag{10a}$$

Equation (10a) shows that the corrections ψ_i are coupled to the kink motion. Similar equations have been obtained in the sine–Gordon lattice with first-neighbour interactions (Willis *et al* 1986). The difference between these equations and ours is that the generalized potential depends not only on X and ψ_i, but also on the parameter r which characterized the range of interactions between particles. As we will show below, the r dependence has a strong influence on the generalized potential, thus on the kink motion.

If $r = 0$, equation (10a) is reduced to:

$$\mathrm{d}^2\psi_i/\mathrm{d}t^2 - J(\psi_{i+1} + \psi_{i-1} - 2\psi_i) + [3(y_k^i)^2 - 1]\psi_i = (J/12)(y_k^{i(4)}) - y_k^{i(1)}[\mathrm{d}^2X/\mathrm{d}t^2 + \tfrac{1}{2}(\mathrm{d}X/\mathrm{d}t)^2\ \mathrm{d}\ln M/\mathrm{d}X] \tag{10b}$$

in which we have neglected the derivatives of order greater than four, $y_k^{i(n)}$ is the X derivative of y_k^i of the nth order. The first term of the right-hand side arises from the kink structure and the second one from the kink acceleration.

To evaluate the X potential derivative with a good accuracy, we need to determine the dynamical variable ψ_i by equation (10). But, since the contribution of ψ_i does not modify the shape of the generalized potential (Combs and Yip 1983, 1984, Willis *et al* 1986) (it modifies the size), we shall, in this paper, discuss the case where ψ_i approaches zero (e.g. the continuum limit). Our restriction is somewhat justified since for all values of J greater than $\frac{1}{2}$, the pseudo-kink width is larger than the unity: e.g. than the lattice spacing which has been taken equal to unity ($b = 1$). In this case, the X derivative of the potential is:

$$\mathrm{d}U/\mathrm{d}X = \Sigma y_k^{i(1)}[(y_k^i)^3 - (1-2J)y_k^i - L_i] \tag{11a}$$

where the auxilliary quantity L_i (Sarker and Krumhansl 1981) is:

$$L_i = [J(1-r)/r]\Sigma(r^m y_k^j) = \mathrm{d}^2y_k^i/\mathrm{d}t^2 - (1-2J)y_k^i + (y_k^i)^3. \tag{11b}$$

Following the recursive formula

$$(r + 1/r)L_i = L_{i+1} + L_{i-1} + [J(1-r)/r](y_k^{i+1} + y_k^{i-1} - 2ry_k^i) \tag{11c}$$

and using Taylor expansion formula in which the derivatives order greater than four are neglected, one obtains

$$\mathrm{d}U/\mathrm{d}X = -[r/12(1-r)^2]\Sigma y_k^{i(1)}[\![[(y_k^i)^3]^{(4)} + \{[J(1+r)-r]/r\}(y_k^i)^{(4)}]\!]. \tag{11d}$$

This is an odd periodic function (with period 1) which is reduced to the Fourier series:

$$\mathrm{d}U/\mathrm{d}X = \Sigma E_n \sin(2\pi nX) \cong E_1 \sin(2\pi X) \tag{12a}$$

where

$$E_n = -(r/6(1-r)^2)(\{[J(1+r)-r]/r\}I_n + J_n) \tag{12b}$$

with

$$I_n = -8n^2\pi^3K^2\sinh^{-1}(n\pi^2/K)[2(q+1)/3 - 4(q+1)(q+4)/15] \tag{12c}$$

$$J_n = 24K^4\pi\sinh^{-1}(n\pi^2/K)[-54(q+1)(q+4)(q+9)(q+16)/567 + 788(q+1)(q+4)(q+9)/315 - 142(q+1)(q+4)/15 + 8(q+1)/3] \tag{12d}$$

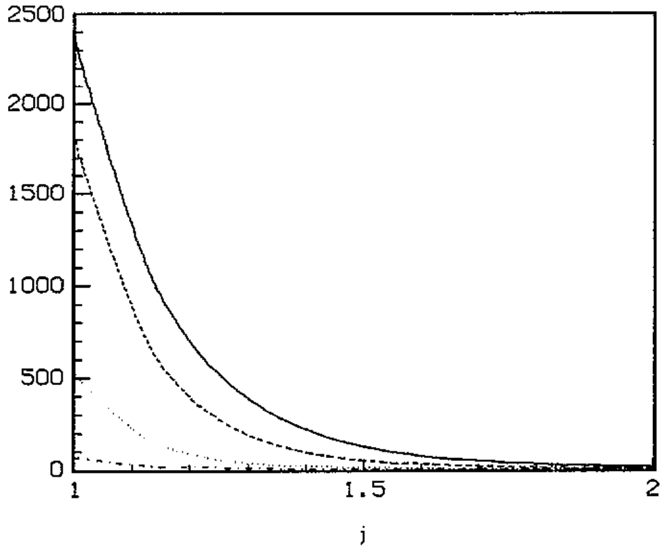

Figure 1. The potential wall E_1 (in millions) plotted as a function of elastic coefficient J for the range interaction parameter r equal to 0.1 (full curve), 0.2 (broken curve), 0.3 (dotted curve) and 0.4 (chain curve).

and $q = (\pi n/K)^2\, \mathrm{d}U/\mathrm{d}X$ can be seen as the Peierls–Nabarro force which is responsible for the pinning of dislocation segments in crystal materials and the quantity $E_{\mathrm{PN}} = E_1/\pi$ is the Peierls–Nabarro barrier (Nabarro 1967, Willis *et al* 1986, Combs and Yip 1983). We also find that the kink dimensionless mass M has the periodic form:

$$M = M_0 + \Sigma M_n \cos(2\pi n X) \cong M_0 + M_1 \cos(2\pi X) \tag{13a}$$

with

$$M_0 = 4K/3 \qquad M_n = (8\pi^2 n/3)(q+1)\sinh^{-1}(n\pi^2/K). \tag{13b}$$

The kink dimensionless mass is related to kink width: as the kink width increases (e.g. the range of the interaction increases), M_0 and M_n tend to zero. This means the disappearance of the kink when the range of interaction is very large. Since the kink width becomes infinite for large values of interaction parameter, it corresponds to the case in which all the particles sit at the top of the double well ($y_k = 0$) and have high energy. A situation energetically less favourable for the system to support and inappropriate for long-range order at finite temperature.

As the consequence of the periodic structure of the potential, kink can be trapped while propagating along the chain and can emit phonons while oscillating in the potential depth. The potential wall E_1 is plotted as a function of elastic coefficient J for various values of the range interaction parameter r (figure 1).

From this figure we see that E_1 vanishes exponentially as r and J increase. It is also seen that the maximum value of the potential wall decreases as the range of interaction increases. This means that for a large range of interaction, the pinning and the trapping effects are absent from the lattice. Since $U \cong cte$ in this limit, the discrete lattice effects are insignificant: the kink travels freely in the chain.

When r is equal to zero, E_1 is reduced to

$$E_1 = 2\pi^3\{3\sinh[(2J\pi^4)^{1/2}]\}^{-1}[2(q_0+1)/3 - 4(q_0+1)(q_0+4)/15] \qquad (14)$$

where $q_0 = 2\pi^2 J$.

The expression (14), different from the one obtained numerically by Combs and Yip (1983), gives the rigorous expression of the energy barrier height in the Φ^4 lattice with first-neighbour interactions. As r tends to one, E_1 vanishes, the width of the soliton becomes infinite and the discreteness effect theory cannot be applied. The constant mass M_0 decreases as r increases and the X dependence of the kink mass is unimportant since $M_1 \ll M_0$. This leads to:

$$V(t) = V_0 - (E_1/M_0)\int_0^t \sin(2\pi X)\,dt \qquad (15)$$

where V_0 is the kink initial velocity.

4. Summary

We have studied the effect of long-range interactions on kink motion in a Φ^4 discrete lattice. In the model chosen, interaction between displacement fields at different points falls off exponentially with separation, and the range of interaction can be varied continuously.

We have discovered that the lattice generalized potential depends strongly on the long-range interaction parameter r. As the range of the interaction increases, the pinning effects and the trapping process are theoretically absent in the chain (E_1 tends to zero). This means that, when the range of interactions is large, the discreteness effects are weak and the soliton velocity is constant (the soliton moves freely in the chain). This is in accordance with the fact that with large values of r, the soliton recovers many lattice spacings (e.g. the continuum limit).

In a later work, we hope to use a numerical technique to analyse the influence of the correction ψ_i as well as the effects of kink–phonon interactions on the equation of motion. Because of the mathematical complexity, the model has been limited to a free system, but the long-range interaction Hamiltonian system can be generalized to incorporate external field with and without time dependence, and in addition incorporate a Rayleigh dissipative function. This can give a theoretical explanation of damping processes which occur during the kink propagation. It would also be of great interest to look at the influence of thermal processes on energy barrier height.

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