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1982 J. Phys. A: Math. Gen. 15 L645

(http://iopscience.iop.org/0305-4470/15/11/013)

J. Phys. A: Math. Gen. **15** (1982) L645–L648. Printed in Great Britain

LETTER TO THE EDITOR

Soliton structures in a discrete chain

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Received 28 June 1982

Abstract. Periodic soliton structures are shown to be energetically favourable in a certain range of parameters of the Frenkel–Kontorova model. These structures form cascades which can be obtained from each other by a scaling transformation.

The problem of the commensurate–incommensurate (CI) phase transition is closely related to the Frenkel–Kontorova model. This model describes a one-dimensional chain of particles connected with strings of length a and placed in an external periodic field $V(x)$. The problem consists in the minimising of the potential energy

$$E = \sum_n [\tfrac{1}{2}(x_{n+1} - x_n - a)^2 + V(x_n)] \tag{1}$$

where x_n is the coordinate of the nth particle. Here we consider the case of a weak potential $|V| \ll 1$ with the period $b = a(1+\delta)$ and the initial misfit $\delta \ll 1$. A crude description of such a system may be given by the continuous approximation (Frank and Van der Merve 1949, Pokrovsky and Talapov 1978), which predicts a continuous transition from a commensurate (C) to an incommensurate (I) phase at a certain value of $\delta = \delta_{c1} \sim \sqrt{V}$. At $\delta < \delta_{c1}$ the C phase with $x_n = nb$ has the lowest energy. At $\delta > \delta_{c1}$ solitons appear spontaneously in a chain. The equilibrium distance between solitons is

$$l \sim l_0 |\ln[(\delta - \delta_{c1})/\delta_{c1}]| \tag{2}$$

where $l_0 \sim V^{-1/2}$ is the width of a single soliton. The principal effect of a discreteness is the pinning of solitons by a lattice. The pinned phase exists in a narrow interval of the misfit

$$\delta_{c1} < \delta < \delta_{c2} \tag{3}$$

where $\delta_{c2} - \delta_{c1} \sim \exp(-\pi^2 V^{-1})$ (Aubry 1979, Pokrovsky 1981). The main purpose of this work is to investigate the soliton structures in the abovementioned range of a misfit (3).

The minimising of the energy (1) leads to a second-order difference equation, which can be reduced to the following system of first-order difference equations:

$$x_{n+1} = x_n + y_n, \qquad y_{n+1} = y_n + V'(x_n + y_n). \tag{4}$$

This system can be treated as a mapping T of the two-dimensional space onto itself. Owing to the periodicity of $V(x)$ this transformation can be considered as a mapping of a two-dimensional torus $0 \leqslant x, y \leqslant b$. Let the fixed point A ($x = 0$, $y = 0$) correspond

to the C phase. Different solutions of equations (4) lie on the invariant curves of the transformation T. In particular, a single-soliton solution lies precisely on separatrices. In the continuous approximation the separatrix starts from the fixed point A and goes back to the same point. The discreteness results in a splitting of the separatrix into two curves Γ_1 and Γ_2, one of which, Γ_1, goes out from the point A while the second one Γ_2 enters it. The separatrices Γ_1 and Γ_2 intersect each other in an infinite set of so-called homoclinic points. A single-soliton configuration is formed by a subset of homoclinic points shown in figure 1 by open circles. It is just the intersection of separatrices which is the cause of a soliton pinning by a lattice. The translation of a soliton over the period $b(x_n \to x_{n+1})$ does not change the energy (1). The continuous transition between the configurations differing by a translation over the period can be realised by a saddle-point trajectory $x_n(s)$. The difference between the maximal and minimal energy along this trajectory is precisely the pinning energy. It has been estimated by Pokrovsky (1981) as $E_{\text{pin}} \sim \exp(-\pi^2 V^{-1/2})$. The saddle-point configuration corresponds to an extremal value of the energy (1) and satisfies the same boundary conditions as the single-soliton configuration. Since the transformation T conserves the orientation of intersecting curves, the homoclinic points corresponding to the single-soliton and saddle-point configurations alternate. The simplest situation is depicted in figure 1, where the saddle-point configuration is shown by the full circles.

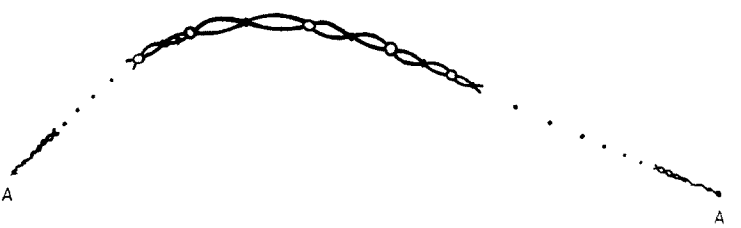

Figure 1. The splitting of a separatrix. The open circles correspond to a single-soliton solution. The other homoclinic points correspond to a saddle-point configuration.

We consider now a multi-soliton structure ($\delta > \delta_{c1}$). In the misfit interval (3) the intersoliton distance z is much larger than the soliton width l_0. So solitons can be considered as particles with the interparticle interaction $U(z) \sim \exp(-z/l_0)$, whilst their interaction with a lattice is described by the periodic pinning potential

$$V_p(x) = E_{\text{pin}} \cos(2\pi x/b).$$

The energy of such a system has the form

$$E_s = \tfrac{1}{2} \sum_{n \neq m} U(z_n - z_m) + \sum_n V_p(z_n) - \mu N \tag{5}$$

where z_n are coordinates, $\mu \sim (\delta - \delta_{c1})$ is a chemical potential of solitons, and N is their total number.

In a small vicinity of δ_{c1} ($\delta - \delta_{c1} \ll \delta_{c2} - \delta_{c1}$) the interaction between solitons is much weaker than the magnitude of the pinning energy E_{pin}. So it is possible to regard solitons as being located at the minima of the potential $V_p(z)$. Now the problem is reduced to the choice of the integers z_n minimising the total energy:

$$\tilde{E}_s = \tfrac{1}{2} \sum_{n \neq m} U(z_n - z_m) - \mu N \tag{6}$$

(we put here $b = 1$). This problem can be solved by a well known linear-programming method as has been done by Hubbard (1978) and Pokrovsky and Uimin (1978). Within the misfit range (3) the lowest energy corresponds to periodic soliton structures. In the first approximation such a structure represents the simple soliton lattice with the period m. The number m is an integer closest to the minimum point of the function

$$F(z) = z^{-1}[U(z) - \mu].$$

We denote by μ_m a special value of μ which satisfies the condition $F(m) = F(m+1)$. A more complex periodic structure appears in a small vicinity of each μ_m. The elementary cell of such a structure contains an ordered sequence of intervals of lengths m and $m+1$. The scaling transformation reduces the new structures to the preceding soliton structures by considering the interval 'm' as a particle and the interval '$m+1$' as an empty site. The new cascade of periodic structures is subjected to a tiny splitting which is connected with the next scaling transformation. The values of μ_m can easily be evaluated as $\mu_m \sim \exp(-m/l_0)$. The range of μ near μ_m, in which the degeneration results in the next cascade of periodic structures, is $\Delta\mu \sim \mu_m^2$. The hierarchy of structures of a different complexity degree is represented in figure 2.

The same result can be explained in the language of the T transformation. Simple structures with the period m are represented by the periodic trajectories of T consisting of m points on the torus. The structures of the next type

$$\underbrace{m, m, \ldots, m}_{s \text{ times}}, m+1$$

can be presented by a periodic trajectory containing $(ms + m + 1)$ points and encircling the torus $(s+1)$ times. On these periodic trajectories the energy (1) takes the minima in a finite range of $\delta: \delta_{c1} \leqslant \delta \leqslant \delta_r$. We conjecture that the RHS of this inequality coincides with the misfit value δ_{c2}, which is the threshold for a transition to the

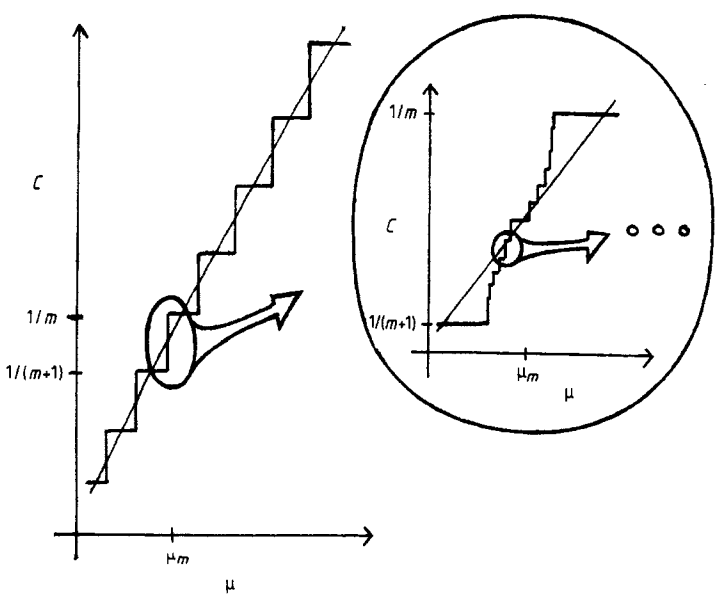

Figure 2. A schematic representation of the scaling hierarchy of periodic soliton structures. The graph shows the resulting concentration C of particles via the chemical potential μ.

Kolmogorov–Arnold–Moser trajectories. On these trajectories the pinning energy vanishes.

A similar consideration can straightforwardly be applied for the determination of a ground-state structure of the Frenkel–Kontorova model with a strong potential $V \gg 1$.

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