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# Multi-kinks in modulated crystals: the soliton lattice of the frustrated $\phi^4$ model

J J M Slot† and T Janssen

Institute for Theoretical Physics, University of Nijmegen, Toernooiveld, 6525 ED Nijmegen, The Netherlands

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**Abstract.** The dynamics of multi-kinks (soliton lattices) in a linear chain system with frustration, in which incommensurate phases occur, is studied using a combination of analytical and numerical techniques. The multi-kinks are found to have a complex structure when frustration is present in the system, in contrast to multi-kinks in non-frustrated systems.

## 1. Introduction

In a recent paper [1] (hereafter referred to as I) we studied the dynamics of single kinks in a model for crystals with a quasiperiodic distortion, the so-called incommensurate displacively modulated crystal structures. This model, the DIFFF (discrete frustrated $\phi^4$) model, consists of a chain of classical particles. Each particle has one degree of freedom denoted by $x_n$, and is harmonically coupled to its nearest and next-nearest neighbours. In addition, each particle moves in a anharmonic (quartic) site potential. The Hamiltonian of the system is therefore given by

$$H=\sum_n\left(\tfrac{1}{2}p_n^2+\tfrac{1}{2}Ax_n^2+\tfrac{1}{4}x_n^4+Bx_nx_{n-1}+Dx_nx_{n-2}\right). \tag{1.1}$$

The ground state of the model was studied in detail as a function of the parameters [2]. This ground state depends on the two ratios $A/D$ and $B/D$. Figure 1 shows the various ground-state configurations as a function of these ratios. When $|B/D|<4$ an incommensurate ground state is possible (hatched regions). Essential for this is the competition between first-and second-neighbour interaction, in particular a non-zero value of $D$.

The strategy we followed in I to study the dynamics corresponding to the above Hamiltonian was twofold. On the one hand we numerically integrated the corresponding equations of motion for finite chains but in doing so we were guided by the results we obtained from an analysis of a continuum approximation to (1.1). Within this one-mode continuum approximation which is valid for a system with a ground state in one of the so-called 'sinusoidal' regions of the phase diagram (figure 1), we found the explicit form of the single kink. This solution of the equations of motion of the continuum model consists of a non-trivial variation of the amplitude and the phase of the ground-state configuration. This kink is different from the well known kink of the ordinary (non-frustrated) $\phi^4$ model. For instance its so-called topological charge, i.e. the asymptotic phase difference in units of $2\pi$ which the kink spans, is not fixed

† Present address: Developmental Technologies BV, Sourethweg 9, 6422 PC Heerlen, The Netherlands.

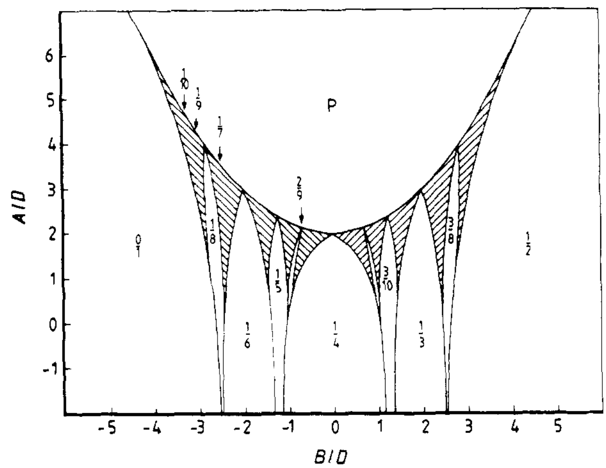


**Figure 1.** Phase diagram of the discrete frustrated $\phi^4$ model. Each point in this diagram corresponds to a ground state of the model. Indicated are the small-period commensurate phases by their wavevector. The shaded regions correspond to incommensurate phases and to long-period commensurate phases.

to $\frac{1}{2}$ as for the ordinary $\phi^4$ kink, but can have any value between 0 and 1 depending on the parameters of the model ($A$, $B$ and $D$), the wavevector of the ground-state configuration and the velocity of propagation. The reason for this difference can be found in the appearance, in general, of the so-called Lifshitz term in the Landau-Ginzburg-like continuum Hamiltonian which can be derived starting from (1.1). The equations of motion of the continuum approximation are formally identical to those for a particle with two degrees of freedom in a potential. The coefficient of this Lifshitz term can be interpreted as a magnetic field strength, as was shown in I. Now when this strength goes to zero the 'frustrated' kink reduces to the 'non-frustrated' continuum kink. We also showed in I that, when we use this 'frustrated' continuum kink as the initial configuration in the integration of the discrete equations of motion for a finite system, it very rapidly relaxes to a 'frustrated' discrete kink.

For the ordinary $\phi^4$ model, but also for other models like the sine-Gordon model and the Takayama-Lin Liu-Maki (TLM) model for trans-polyacetylene, one can also find, besides the single-kink solution, the so-called soliton lattice solution or multi-kink solution. This was for instance done by Horovitz [3] in the case of the TLM model. The soliton lattice in these models consists of regularly spaced alternating kinks and anti-kinks. Such a solution can also be found in the one-mode continuum limit of the DIFFF model, although as we will see this will not be a periodic solution in general. This solution and some of its properties will be the main subject of the present paper. Furthermore, we will give some numerical evidence of the existence of a corresponding solution in the discrete system.

In the next section we will briefly recall the continuum model in the one-mode approximation starting from Hamiltonian (1.1). More details of this derivation can be found in I. Furthermore in this section we will discuss briefly the single-kink solution of the corresponding equations of motion. The third section is devoted to the actual soliton lattice solution in both the continuum and discrete model. The soliton lattice solution in the continuum model is a more general solution of the corresponding equations of motion than the single-kink solution. Therefore, this single-kink solution can be recovered from the soliton lattice solution by taking an appropriate limit. This limit will be discussed in appendix 2. Finally, some conclusions will be given in § 4.

## 2. Continuum model

In this section we will briefly discuss the continuum limit of the discrete Hamiltonian (1.1) in the so-called one-mode approximation. This procedure was treated at length in I. Therefore we will present here only the result and the main line of reasoning. The idea of the one-mode approximation stems from the observation that when the model parameters $A$, $B$ and $D$ are chosen such that we are in a region of the phase diagram (figure 1) just below the transition line from the P (para) phase to one of the modulated phases, the ground-state configuration is approximately described by

$$x_n^{(0)} = \Delta \sin(qn + \phi). \tag{2.1}$$

This ground-state configuration can be periodic (a superstructure) or incommensurate. The latter we also approximate by a superstructure. Therefore we can write

$$q = 2\pi L/N \tag{2.2}$$

with $L$ and $N$ coprime and possibly very large. Various values of $L/N$ are shown in figure 1. In the remainder of this paper we will restrict ourselves to the case $N \neq 1, 2$ or 4. The reason is that both cases $N = 1$ and $N = 2$ lead to the ordinary $\phi^4$ model and thus to the ordinary $\phi^4$ soliton lattice solution. The case $N = 4$ is more complicated as we showed in I. However, in the so-called constant amplitude approximation (CAA) [4] the continuum model reduces to the well known sine-Gordon model [1], and leads therefore to the soliton lattice solution corresponding to this model [5]. The ground-state configuration (2.1) with fundamental 'wavevector' $q$ (2.2) is an $N$-fold superstructure. This superstructure will be $M$-fold degenerate, where $M = N$ if $N$ is even and $M = 2N$ if $N$ is odd. These $M$ degenerate phases all have the same amplitude $\Delta$, but a different phase angle $\phi$, i.e.

$$\phi = \phi^{(j)} \equiv 2\pi \frac{j}{M} + \text{constant} \qquad (j = 0, \dots, M-1). \tag{2.3}$$

It is clear that, due to this degeneracy of the ground state, kinks or domain walls naturally appear as low-lying static excitations of the system, because they locally connect different degenerate ground-state phases.

To derive the appropriate continuum Hamiltonian in this 'sinusoidal' region of the phase diagram, we make the following ansatz:

$$x_n(t) = e^{iqn} Q(n, t) + e^{-iqn} Q^*(n, t) \tag{2.4}$$

where the complex 'order-parameter' field $Q(\xi, t)$ is a slowly varying function of $\xi$. By slowly varying we mean here that if

$$Q = O(1) \qquad \text{then } Q' \equiv \frac{\partial Q}{\partial \xi} = O(\varepsilon) \qquad \text{and } Q'', Q'^2 = O(\varepsilon^2) \text{ etc} \tag{2.5}$$

where $\varepsilon \ll 1$. This assumption is justified when the typical width of a kink in the system is large enough ($\geqslant 3$ unit cells). The procedure to follow consists of substituting (2.4) in the Hamiltonian (1.1), sum out all the fast varying terms (i.e. those terms which have as a factor some power of $\exp(iqn)$), replace the sum over $n$ by an integral over $\xi$ and eliminate all appearing 'surface' terms.

As was shown in I the equations of motion for $Q$ and $Q^*$, or more conveniently for the real fields $u$ and $v$ defined by $Q=(u-iv)/2$, are in their stationary form given by

$$\begin{aligned} u'' &= ru + Hv' + su(u^2+v^2) \\ v'' &= rv - Hu' + sv(u^2+v^2). \end{aligned} \tag{2.6}$$

The parameters $r$, $s$ and $H$ in (2.6) are defined by

$$r \equiv \frac{a}{c^2} < 0 \qquad s \equiv \frac{3}{4c^2} \qquad \text{and} \qquad H \equiv \frac{2b}{c^2} \tag{2.7}$$

where

$$\begin{aligned} a &\equiv A + 2B\cos(q) + 2D\cos(2q) \\ b &\equiv B\sin(q) + 2D\sin(2q) \\ c^2 &\equiv -(B\cos(q) + 4D\cos(2q)). \end{aligned} \tag{2.8}$$

It is sufficient to study (2.6) because any travelling solution to the full time-dependent equations of motion can be obtained from a solution of (2.6) by a mere 'boost' [1]. By viewing $\xi$ as a 'time' variable, (2.6) can be interpreted as the equations of motion of an integrable classical system with two degrees of freedom, i.e. a particle moving in a plane perpendicular to a homogeneous magnetic field with strength $H$, in a non-linear central potential (inverted 'mexican hat')

$$\begin{aligned} U(\rho) &= -\tfrac{1}{2}r\rho^2 - \tfrac{1}{4}s\rho^4 - \frac{r^2}{4s} = -\tfrac{1}{4}s(\rho^2-\rho_0^2)^2 \\ \rho^2 &\equiv u^2+v^2 \qquad \rho_0^2 \equiv -\frac{r}{s}. \end{aligned} \tag{2.9}$$

It is integrable because there are two integrals of the motion, namely the 'energy' $\varepsilon$ and the 'angular momentum' $L_\perp$

$$\varepsilon = \tfrac{1}{2}(u'^2+v'^2) + U(\rho) \tag{2.10}$$

$$L_\perp = uv' - u'v + \tfrac{1}{2}H(u^2+v^2). \tag{2.11}$$

The solution of the stationary problem is completely determined once these two integrals are specified. For instance in I we showed that the single-kink solution, which we referred to as the $H \neq 0$ solitary wave, corresponds to

$$\varepsilon = 0 \qquad \text{and} \qquad L_\perp = -\frac{rH}{2s} = \tfrac{1}{2}H\rho_0^2. \tag{2.12}$$

This solution, which only exists for $H^2 < -2r$, is given by

$$\begin{aligned} u(\xi) &= \sqrt{\Omega(\xi)}\sin\phi(\xi) \\ v(\xi) &= \sqrt{\Omega(\xi)}\cos\phi(\xi) \end{aligned} \tag{2.13}$$

with

$$\Omega(\xi) = -\frac{r}{s} - \frac{\nu^2}{2s}\operatorname{sech}^2(\tfrac{1}{2}\nu\xi) \qquad \nu^2 \equiv -(H^2+2r) > 0 \tag{2.14}$$

and

$$\phi(\xi) = \phi(-\infty) - \tan^{-1}\left(\frac{\nu}{H}\right) - \tan^{-1}\left(\frac{\nu}{H}\tanh(\tfrac{1}{2}\nu\xi)\right). \tag{2.15}$$

So the topological charge or winding number of $\eta$ of this solution is equal to

$$\eta \equiv \frac{\phi(+\infty) - \phi(-\infty)}{2\pi} = -\frac{1}{\pi}\tan^{-1}\left(\frac{\nu}{H}\right). \tag{2.16}$$

In the next section we will construct the soliton lattice solution of (2.6).

## 3. Soliton lattice solution

The origin of the specific values (2.12) for the two integrals of the motion in the case of the single kink is to be found in the boundary conditions for the single kink, namely

$$\lim_{\xi\to\pm\infty}\begin{bmatrix} u'(\xi) \\ v'(\xi) \end{bmatrix} = 0 \qquad \text{and} \qquad \lim_{\xi\to\pm\infty} \rho^2(\xi) = \rho_0^2 \tag{3.1}$$

because, by definition, a single kink connects in an asymptotic sense two degenerate ground-state phases $\{\rho = \rho_0;\ \phi \in [0, 2\pi)\}$ and has a finite creation energy with respect to the ground-state energy. The interpretation of these boundary conditions is clear within the mechanical model. The mechanical particle has to start in the infinite past on the brim of the inverted mexican hat with an infinitesimal velocity directed inwards, in order to end in the infinite future on that same brim with a zero velocity. When its angular momentum $L_\perp$ is non-zero it will experience a centrifugal repulsion near the origin and will therefore avoid the origin during its course through the inside of the inverted mexican hat. The condition for the existence of the single kink which we mentioned in the previous section, i.e. $H^2 < -2r$, is in fact a condition for the existence of a local minimum between 0 and $\rho_0$ of the effective radial potential, as was shown in appendix B of I. It is easy to verify that the effective radial potential (see appendix 1) maximally has one local minimum in combination with one local maximum, the condition for this being in general

$$0 \leqslant L_\perp^2 < \tfrac{4}{27}s(\rho_0^2 + H^2/4s)^3. \tag{3.2}$$

It is clear because of the unboundedness of the inverted mexican hat, and therefore of the effective radial potential, that one needs such a local minimum in order to have a bounded motion of the mechanical particle. For an angular momentum $L_\perp$ which satisfies (3.2) these local extrema are located at

$$\begin{aligned} \rho_{\min} &\equiv \left\{\tfrac{1}{3}\left(\rho_0^2 + \frac{H^2}{4s}\right)\left[1 - 2\cos\left(\frac{\pi}{3} + \frac{\alpha}{3}\right)\right]\right\}^{1/2} \\ \rho_{\max} &\equiv \left[\tfrac{1}{3}\left(\rho_0^2 + \frac{H^2}{4s}\right)\left(1 + 2\cos\frac{\alpha}{3}\right)\right]^{1/2} \end{aligned} \tag{3.3}$$

where $\alpha$ is defined through

$$\cos\alpha = 1 - \frac{L_\perp^2}{2s}\left[\tfrac{1}{3}\left(\rho_0^2 + \frac{H^2}{4s}\right)\right]^{-2}. \tag{3.4}$$

For instance in the case of the single kink one has $\rho_{max} = \rho_0$. In general, however, $\rho_{max}$ can be everywhere with respect to $\rho_0$. The same is true for $\rho_{min}$, although one always has $\rho_{min} < \rho_{max}$.

It is clear that the motion of the mechanical particle is completely determined once we specify its initial position and its initial velocity (four initial conditions). Alternatively we can also specify $L_\perp$, $\rho_1 \equiv \rho(0)$ and $\rho_1' \equiv \rho'(0)$. Of course in this case the motion is not completely determined, because the initial phase $\phi_1 \equiv \phi(0)$ is still free. Without losing generality one can always assume that the initial point is a so-called turning point of the motion, i.e. $\rho_1' = 0$. The initial angular velocity $\phi_1' \equiv \phi'(0)$ and the energy $\varepsilon$ now follow from

$$\phi_1' = \tfrac{1}{2}H - \frac{L_\perp}{\rho_1^2} \tag{3.5}$$

$$\varepsilon = \tfrac{1}{2}\rho_1^2\phi_1'^2 - \tfrac{1}{4}s(\rho_1^2 - \rho_0^2)^2. \tag{3.6}$$

Furthermore, one can always assume that $\rho_{min} \leqslant \rho_1 \leqslant \rho_{max}$. It is now easy to see that when $\phi_1' = 0$ one can only have $\rho_1 \leqslant \rho_0 \leqslant \rho_{max}$. For a non-zero $\phi_1'$ one can also have $\rho_0 \leqslant \rho_1$.

Generally speaking, a soliton lattice is a configuration which consists of a regular array of degenerate (near-)ground-state phases separated by domain walls. This is why one also uses the name multi-kink or kink lattice for such a configuration. Furthermore one usually assumes that the typical width of the kinks is small compared to their mutual distance, so large portions of ground-state phase are separated by narrow walls. This means that the order-parameter field $Q$ will show a slow variation between two kinks, and a relatively fast variation when passing through a kink. Now let us translate all of this in terms of our mechanical model. First of all we have to bear in mind that every orbit of the mechanical particle corresponds to an order parameter varying in the system, i.e. an order-parameter field $Q(\xi)$, and that the velocity field of the particle therefore corresponds to $Q'(\xi)$. We know that near a classical turning point (here we have actually a turning circle) the particle will have a small radial velocity which eventually becomes zero at the turning point. The angular velocity, however, does not have to be small near or at a turning point. The motion near one of the turning circles has to correspond to a (near)-ground-state phase. Thus one of the turning circles $\rho = \rho_1$ or the other one has to be close to $\rho = \rho_0$. Now when the angular velocity is non-zero at the turning circle closest to the ground state $\rho = \rho_0$, one will have no single (near-)ground-state phase between two kinks, but one will pass gradually through a whole bunch of (near-)ground-state phases in going from one kink to the next one. So we have to conclude that our soliton lattice solution has to correspond to a motion for which $\phi_1'$ is small. We take here the extreme case $\phi_1' = 0$ and thus $\rho_1 \leqslant \rho_0$. We can therefore write

$$\rho_1^2 = \rho_0^2 - \Delta \qquad \Delta \geqslant 0 \text{ and small.} \tag{3.7}$$

Furthermore from (3.5) and (3.6) it follows that for a soliton lattice solution we have

$$L_\perp = \tfrac{1}{2}H\rho_1^2 = \tfrac{1}{2}H\rho_0^2 - \tfrac{1}{2}H\Delta \tag{3.8}$$

and

$$\varepsilon = U(\rho_1) = -\tfrac{1}{4}s(\rho_1^2 - \rho_0^2)^2 = -\tfrac{1}{4}s\Delta^2 < 0. \tag{3.9}$$

By using the equations of motion for $u$ and $v$ (2.6) and the two integrals $\varepsilon$ and $L_\perp$ (2.10) and (2.11) and doing a little algebra, it is not hard to derive the following equation for $u^2+v^2$, which we will denote by $\Omega$ from now on:

$$\Omega'' = 4\varepsilon + 2HL_\perp + r^2/s + (4r - H^2)\Omega + 3s\Omega^2. \tag{3.10}$$

The constant term in this equation is positive. This can be deduced using (3.8) and (3.9)

$$4\varepsilon + 2HL_\perp + \frac{r^2}{s} = (H^2 + 2s\Delta)\Omega_1 + s\Omega_1^2 > 0 \tag{3.11}$$

with $\Omega_1 \equiv \rho_1^2$. By integrating (3.10) once we get

$$\tfrac{1}{2}\Omega'^2 - [(H^2+2s\Delta)\Omega_1 + s\Omega_1^2]\Omega + \tfrac{1}{2}(H^2-4r)\Omega^2 - s\Omega^3 = \text{constant}. \tag{3.12}$$

The value of this constant follows from the boundary condition

$$\Omega' = 0 \qquad \text{when} \qquad \Omega = \Omega_1. \tag{3.13}$$

Therefore it is easy to see that this constant is equal to $-\frac{1}{2}H^2\Omega_1^2$. Thus (3.12) can be written as

$$\Omega'^2 = 2s\left\{\Omega^3 - \left(2\Omega_0 + \frac{H^2}{2s}\right)\Omega^2 + \left[\Omega_1^2 + 2\left(\Delta + \frac{H^2}{2s}\right)\Omega_1\right]\Omega - \frac{H^2}{2s}\Omega_1^2\right\}. \tag{3.14}$$

The solution of this last equation is implicitly given by the quadrature

$$\xi = \xi^{(0)} + \frac{1}{\sqrt{2s}}\int_{\Omega^{(0)}}^{\Omega} \mathrm{d}t \frac{1}{\sqrt{R(t)}} \tag{3.15}$$

with $R(t)$ the following third-order polynomial in $t$:

$$R(t) = t^3 - \left(2\Omega_0 + \frac{H^2}{2s}\right)t^2 + \left[\Omega_1^2 + 2\left(\Delta + \frac{H^2}{2s}\right)\Omega_1\right]t - \frac{H^2}{2s}\Omega_1^2. \tag{3.16}$$

The zeros of this polynomial can easily be found and are given by

$$\Omega_1 = \Omega_0 - \Delta \tag{3.17}$$

$$\Omega_\pm = \tfrac{1}{2}(\Omega_0 + \Delta + H^2/2s) \pm \tfrac{1}{2}[(\Omega_0 + \Delta - H^2/2s)^2 + (4H^2/s)\Delta]^{1/2}. \tag{3.18}$$

These zeros are arranged in a definite order

$$0 < \Omega_- < \Omega_1 < \Omega_0 + \Delta < \Omega_+. \tag{3.19}$$

The proof of this ordering is given in appendix 1. In this same appendix we show, by an analysis of the effective radial potential, that the condition for the existence of a non-trivial motion is given by (equivalent to (3.2))

$$0 < \Omega_- < \Omega_1. \tag{3.20}$$

For a non-zero value of $\Delta$ this is always true, irrespective of the value of the magnetic field $H$. This is in contrast to the case of the single kink ($\Delta = 0$), because there a similar condition to (3.2) is only fulfilled when

$$H^2 < -2r \tag{3.21}$$

as was shown in I. Now the radial motion of the mechanical particle takes place between the following bounds:

$$\Omega_- \leqslant \Omega \leqslant \Omega_1. \tag{3.22}$$

As initial position we take for reasons of convenience $\Omega(0)=\Omega_-$ instead of $\Omega(0)=\Omega_1$. Thus (3.15) becomes

$$\xi=\frac{1}{\sqrt{2s}}\int_{\Omega_-}^{\Omega}\mathrm{d}t\frac{1}{[(t-\Omega_-)(\Omega_1-t)(\Omega_+-t)]^{1/2}}. \tag{3.23}$$

This last integral can be expressed as an incomplete elliptic integral of the first kind $F(\phi, k)$ (see for instance [6]), namely

$$\xi=\frac{1}{\lambda}F\left[\sin^{-1}\left(\frac{\Omega-\Omega_-}{\Omega_1-\Omega_-}\right)^{1/2}, k\right] \tag{3.24}$$

with

$$\lambda\equiv\left(\frac{s(\Omega_+-\Omega_-)}{2}\right)^{1/2}$$

and elliptic modulus

$$k=\left(\frac{\Omega_1-\Omega_-}{\Omega_+-\Omega_-}\right)^{1/2}$$

where $0<k<1$ on account of (3.19). Therefore $\Omega(\xi)$ can be expressed in terms of the Jacobi elliptic function $\mathrm{sn}(u, k)$, the so-called sine amplitude, by inverting (3.24)

$$\Omega(\xi)=\Omega_-+[\Omega_1-\Omega_-]\,\mathrm{sn}^2(\lambda\xi, k). \tag{3.25}$$

This sine amplitude $\mathrm{sn}(u, k)$ is a periodic function of $u$ with period

$$4K(k)\equiv 4F(\tfrac{1}{2}\pi, k)\equiv 4\int_0^{\pi/2}\frac{\mathrm{d}\theta}{(1-k^2\sin^2\theta)^{1/2}}. \tag{3.26}$$

$K(k)$ is known as the complete elliptic integral of the first kind. Because $\mathrm{sn}(-u, k)=-\mathrm{sn}(u, k)$, we have that $\Omega$ is periodic with period

$$T\equiv\frac{2K(k)}{\lambda}. \tag{3.27}$$

This period lies somewhere between

$$\frac{\pi}{\lambda}\left(=\frac{2K(0)}{L}\right) \qquad \text{and} \qquad \infty\left(=\frac{2K(1)}{\lambda}\right).$$

The equation for the phase $\phi(\xi)$ is easily obtained by transforming $L_\perp$ (2.11) using (2.13)

$$L_\perp=\tfrac{1}{2}H\Omega_1=-\Omega\phi'+\tfrac{1}{2}H\Omega \tag{3.28}$$

or

$$\phi'=\tfrac{1}{2}H\left(1-\frac{\Omega_1}{\Omega}\right). \tag{3.29}$$

If we now substitute (3.25) in this expression, we end up after some algebra with

$$\phi'(\xi)=\tfrac{1}{2}H\beta^2\frac{1-\mathrm{sn}^2(\lambda\xi, k)}{1-\beta^2\,\mathrm{sn}^2(\lambda\xi, k)} \qquad \beta^2\equiv 1-\frac{\Omega_1}{\Omega_-} \tag{3.30}$$

or

$$\phi(\xi)=\phi(0)+\frac{H}{2\lambda}\beta^2\int_0^{\lambda\xi}du\frac{1-\text{sn}^2(u,k)}{1-\beta^2\,\text{sn}^2(u,k)} \tag{3.31}$$

where on account of (3.19) we have $0<-\beta^2<\infty$. Again we can express this last integral in terms of an incomplete elliptic integral, but now one of the third kind $\Pi(\phi,\beta^2,k)$ [6], namely

$$\phi(\xi)=\phi(0)+\frac{H}{2\lambda}\{\lambda\xi+(\beta^2-1)\Pi(\text{am}(\lambda\xi,k),\beta^2,k)\} \tag{3.32}$$

where the amplitude $\text{am}(u,k)$ is defined by

$$\sin(\text{am}(u,k))\equiv\text{sn}(u,k) \tag{3.33}$$

and $\Pi(\phi,\beta^2,k)$ by

$$\Pi(\phi,\beta^2,k)=\int_0^{\phi}\frac{d\theta}{(1-\beta^2\sin^2\theta)(1-k^2\sin^2\theta)^{1/2}}. \tag{3.34}$$

The phase $\phi(\xi)$ (3.32) has the following property. If we write $\xi$ as

$$\xi=nT+\hat{\xi}\qquad\text{for some } n\in Z \tag{3.35}$$

with $T$ given by (3.27) and $-\frac{1}{2}T<\hat{\xi}\leq\frac{1}{2}T$ (this is unique), then

$$\phi(\xi)=\phi(\hat{\xi})+n\Delta\phi \tag{3.36}$$

where

$$\Delta\phi\equiv\frac{H}{\lambda}\{K(k)+(\beta^2-1)\Pi(\tfrac{1}{2}\pi,\beta^2,k)\} \tag{3.37}$$

which we define as the phase difference of the soliton lattice. It now follows that, when this phase difference is some rational multiple of $2\pi$, we have a periodic soliton lattice, i.e. when

$$\Delta\phi=2\pi n/m\qquad\text{for some } n,m\in Z. \tag{3.38}$$

When this is not the case we have an incommensurate soliton lattice. Figure 2 shows an example of the phase and amplitude of an incommensurate soliton lattice. Needless to say, a moving solition lattice can be obtained by boosting [1]. This will again imply, just as in the case of the single kink, that the phase difference will depend on the velocity of propagation $v$. The total energy of a static soliton lattice configuration is, of course, infinite. However, because the energy density (Hamiltonian density) can be expressed entirely in terms of $\Omega(\xi)$, we can calculate the energy per period $T$ (3.27), i.e.

$$E_0=\tfrac{1}{2}c^2\int_{-T/2}^{T/2}d\xi\{\tfrac{1}{2}(u'^2+v'^2)+\tfrac{1}{2}H(uv'-u'v)+\tfrac{1}{2}r(u^2+v^2)+\tfrac{1}{4}s(u^2+v^2)^2+r^2/4s\}. \tag{3.39}$$

This can be written, using the integrals of the motion, as

$$E_0=\frac{sc^2}{2\lambda}\int_{-K(k)}^{K(k)}dw\{\tfrac{1}{4}\Delta^2+(\Delta+H^2/4s)(\Omega_1-\Omega_-)\,\text{cn}^2(w,k)+\tfrac{1}{2}(\Omega_1-\Omega_-)^2\,\text{cn}^4(w,k)\} \tag{3.40}$$

with $\text{cn}(w,k)$ the so-called cosine amplitude, which is related to the sine amplitude

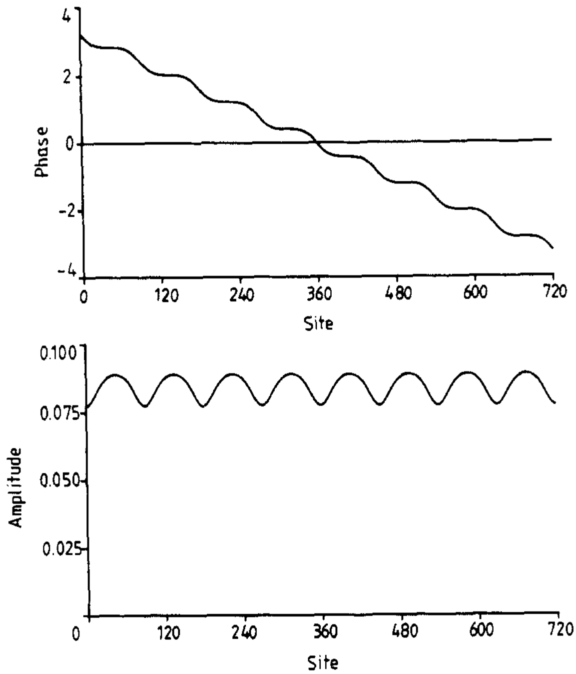


**Figure 2.** Sketch of the phase $\phi$ and the amplitude $\rho \equiv \sqrt{\Omega}$ as a function of $\xi$.

via $\mathrm{cn}^2(w, k) = 1 - \mathrm{sn}^2(w, k)$. All the integrals in (3.40) can be done, leading to

$$E_0 = \frac{sc^2}{2\lambda}\{K(k)\Delta^2 + 2[\Delta + H^2/4)s](\Omega_+ - \Omega_-)[E(k) - (1-k^2)K(k)]$$
$$+\tfrac{2}{3}(\Omega_+ - \Omega_-)^2[(2k^2-1)E(k) + \tfrac{1}{2}(1-k^2)(2-3k^2)K(k)]\}. \quad (3.41)$$

In this last expression $E(k)$ is the so-called complete elliptic integral of the second kink, which is defined by

$$E(k) = E\left(\frac{\pi}{2}, k\right) = \int_0^{\pi/2} (1 - k^2 \sin^2\theta)^{1/2}\,\mathrm{d}\theta. \quad (3.42)$$

In the case of the single kink we argued in I that it is linearly unstable. The main reason for this instability is the fact that the initial phase is a free parameter combined with the fact that the potential in the one-mode continuum limit is rotationally invariant in the $u$-$v$ plane. The same is true for the soliton lattice solution. Therefore we may expect that this solution is also linearly unstable in this continuum limit. The proof of this conjecture is, however, far more difficult than in the case of the single kink and is at the present time not known to us.

Mechanisms, like we discussed in I, which pin the phase of the single kink are of course also valid for the soliton lattice solution, i.e. phase pinning via coupling to higher harmonics of the fundamental mode.

We will end this section with a short discussion concerning the existence of the soliton lattice configuration in the discrete system. One way to reveal such a solution in a discrete system is to integrate the discrete equations of motion, thereby using the continuum solution as an initial condition. The hope is then that this continuum solution is near the discrete one, so that it quickly relaxes to this discrete solution.

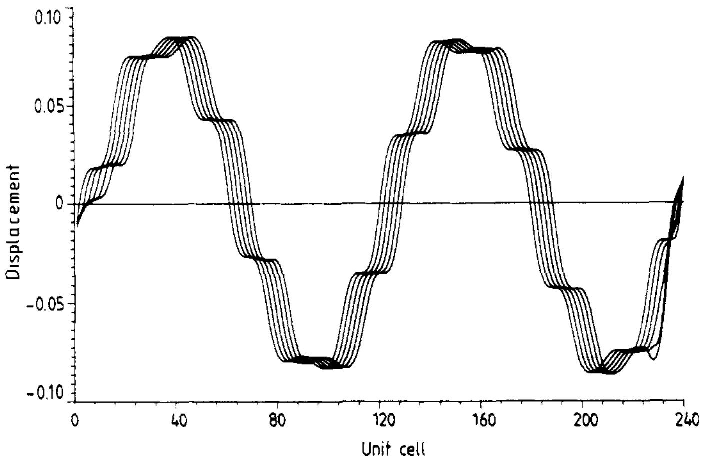


**Figure 3.** Propagating soliton lattice within a $N = 6$ superstructure. The displacement of the third particle in each unit cell is given for six successive times separated by 20 time steps.

The details of the method we use for integrating the discrete equations of motion can be found in I.

The result of one such calculation is shown in figure 3. In this picture we have plotted the displacement of every third site in each of the 240 unit cells, containing six particles each, of this finite system, at successive intervals of 20 time steps. The parameters $A$, $B$ and $D$ are in this case 0.734, −0.480 and 0.260, which implies that $A/D = 2.833$ and $B/D = -1.846$. In the phase diagram (figure 1) this corresponds to a point in the 'sinusoidal' region of the $N = 6$ superstructure phase. The reason for looking at each third site is, of course, to eliminate the fast varying $n$ dependence ($e^{ilqn}$) in $x_n$ (cf (2.4)). The value of $\Delta$ we took was $10^{-4}$, which is small with respect to the current value of $\Omega_0$, namely $8 \times 10^{-3}$. The initial velocity we took was $v = 0.525$. With these values of the parameters the period $T$ of $\Omega$ in the initial configuration is about 90 lattice constants and the phase difference $\Delta\phi$ is near $\pi/4$, actually $\Delta\phi = -0.2578\pi$ (which makes it a so-called incommensurate soliton lattice). The whole system ($16 \times 90 = 1440$ sites) makes up nearly two whole periods of the soliton lattice. Concluding we can say that this figure clearly demonstrates the existence of a propagating soliton lattice in the discrete system with no shape change during its propagation through the system. At both ends one notices some disturbance, but this is entirely due to the fixed BC we use in the calculation. Notice that such a kink lattice with $\Delta\phi \approx \frac{1}{4}\pi$ does not connect degenerate ground states ($\Delta\phi = \pi/3$) and can, therefore, only occur in this sinusoidal region. Actually it is surprising that it is so stable in the numerical example.

This example just shows that there exists a solution with a rather long lifetime consisting of a moving lattice of kinks. A more systematic treatment of these solutions and their stability is in progress.

## 4. Concluding remarks

We have investigated the presence and some of the properties of a multi-kink or soliton lattice in a linear chain system with frustration in which incommensurate modulations occur. The procedure was, as in the case of the single kinks [1] a combination of analytical techniques applied to a continuum approximation of the model and numerical integration of the equations of motion. The main results are the following.

In contrast to soliton lattices in systems without frustration, the soliton lattices in a system with frustration have a rather complex structure.

A soliton lattice in a frustrated system does not have to be periodic at the level of the continuum approximation. This is due to the fact that the amplitude of the soliton lattices, which is a periodic function, and the increase in the phase in such a period are in general incommensurate with respect to one another.

Even if the soliton lattice is commensurate in the above sense, it will in general be incommensurate with respect to the underlying discrete lattice.

Just as in the case of the single kinks we have again that the phason velocity is the upper limit for the velocity of propagating soliton lattices.

Moving soliton lattices keep their form over long distances, which establishes the presence of well defined soliton lattices in a discrete system.

## Appendix 1

In this appendix we will analyse the effective radial potential which the mechanical particle feels in the case of the soliton lattice solution. In particular we will give a proof of the definite ordering (3.19), i.e.

$$0<\Omega_-<\Omega_1<\Omega_0+\Delta<\Omega_+. \tag{A1.1}$$

This effective radial potential can be derived by first transforming the energy $\varepsilon$ of the particle ((2.10) and (3.9))

$$\varepsilon = -\tfrac{1}{4}s\Delta^2=\tfrac{1}{2}(u'^2+v'^2)-\tfrac{1}{2}r(u^2+v^2)-\tfrac{1}{4}s(u^2+v^2)^2-r^2/4s \tag{A1.2}$$

to polar variables $\rho$ and $\phi$ by using

$$\begin{aligned} u(\xi)&=\rho(\xi)\sin\phi(\xi)\\ v(\xi)&=\rho(\xi)\cos\phi(\xi). \end{aligned} \tag{A1.3}$$

This leads to

$$\varepsilon=\tfrac{1}{2}(\rho'^2+\rho^2\phi'^2)-\tfrac{1}{2}r\rho^2-\tfrac{1}{4}s\rho^4-r^2/4s. \tag{A1.4}$$

$\phi'$ can be eliminated from this last expression by using the angular momentum $L_\perp$ in polar variables

$$L_\perp=\tfrac{1}{2}H\rho_1^2=-\rho^2\phi'+\tfrac{1}{2}H\rho^2. \tag{A1.5}$$

Thus

$$\varepsilon=\tfrac{1}{2}\rho'^2+U_{\text{eff}}(\rho) \tag{A1.6}$$

with

$$U_{\text{eff}}(\rho)=-\frac{r^2}{4s}-\tfrac{1}{2}r\rho^2-\tfrac{1}{4}s\rho^4+\tfrac{1}{8}H^2\frac{1}{\rho^2}(\rho^2-\rho_1^2)^2. \tag{A1.7}$$

This potential only depends on $\rho$ through $\Omega\equiv\rho^2$. Therefore it is more convenient to analyse $\tilde{U}_{\text{eff}}(\Omega)\equiv U_{\text{eff}}(\sqrt{\Omega})$, which can be written as

$$\tilde{U}_{\text{eff}}(\Omega)=-\tfrac{1}{4}s(\Omega-\Omega_0)^2+\tfrac{1}{8}H^2\frac{1}{\Omega}(\Omega-\Omega_1)^2. \tag{A1.8}$$

The first term constitutes the inverted mexican hat $\bar{U}_{\mathrm{IMH}}(\Omega)$ and the second term the effective centrifugal potential $\bar{U}_{\mathrm{CF}}^{\mathrm{eff}}(\Omega)$. A sketch of both these potentials and their sum is shown in figure 4. It is not hard to see that the solutions of the equation

$$\bar{U}_{\mathrm{eff}}(\Omega)=\varepsilon=-\tfrac{1}{4}s\Delta^2 \tag{A1.9}$$

are given by (3.17) and (3.18), i.e.

$$\begin{aligned}\Omega_1&=\Omega_0-\Delta\\ \Omega_\pm&=\tfrac{1}{2}[\Omega_0+\Delta+H^2/2s]\pm\tfrac{1}{2}[(\Omega_0+\Delta-H^2/2s)^2+(4H^2/s)\Delta]^{1/2}.\end{aligned} \tag{A1.10}$$

For the expression for $\Omega_+$ it is immediately clear that

$$\Omega_+>\Omega_0+\Delta \tag{A1.11}$$

and because $\Delta$ is positive, we also have

$$\Omega_1=\Omega_0-\Delta<\Omega_0+\Delta. \tag{A1.12}$$

When $\Omega\to 0$ we have that $\bar{U}_{\mathrm{CF}}^{\mathrm{eff}}(\Omega)\to+\infty$, while $\bar{U}_{\mathrm{IMF}}(\Omega)$ remains finite and negative. Therefore we have that for sufficiently small values of $\Omega$

$$\bar{U}_{\mathrm{eff}}(\Omega)>\varepsilon. \tag{A1.13}$$

The same is true for $\Omega_1<\Omega<\Omega_0+\Delta$, as can be seen in figure 4. So in order to have a non-trivial motion ($\rho\neq\rho_1$, $\rho'=0$), we need that

$$0<\Omega_-<\Omega_1 \tag{A1.14}$$

or in other words

$$\bar{U}_{\mathrm{eff}}(\Omega)\leqslant\varepsilon \qquad \text{for } \Omega_-\leqslant\Omega\leqslant\Omega_1. \tag{A1.15}$$

By using (A1.10) we see that (A1.14) boils down to

$$-\Omega_0+3\Delta+\frac{H^2}{2s}<\left[\left(\Omega_0+\Delta-\frac{H^2}{2s}\right)^2+\frac{4H^2}{s}\Delta\right]^{1/2}. \tag{A1.16}$$

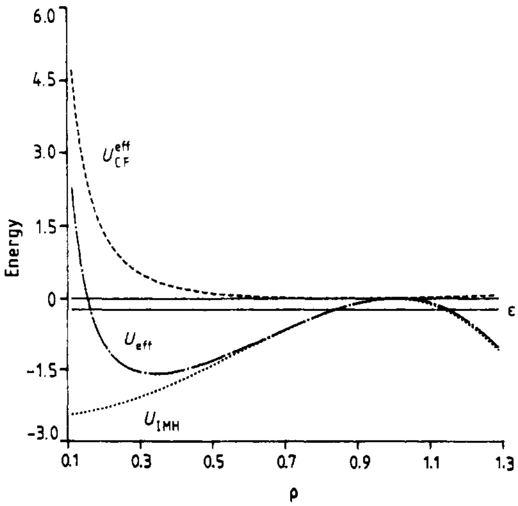


**Figure 4.** Sketch of $U_{\mathrm{IMH}}(\rho)$, $U_{\mathrm{CF}}^{\mathrm{eff}}(\rho)$ and $U_{\mathrm{eff}}(\rho)=U_{\mathrm{IMH}}(\rho)+U_{\mathrm{CF}}^{\mathrm{eff}}(\rho)$ as functions of $\rho$ (arbitrary units).

For $\Delta = 0$ this inequality is satisfied when

$$\frac{H^2}{2s} < \Omega_0 \qquad \text{or} \qquad H^2 < -2r \tag{A1.17}$$

which is the condition for the existence of the single-kink solution. Now suppose that

$$\tfrac{1}{3}\Omega_0 \leqslant \Delta < \Omega_0. \tag{A1.18}$$

Then we have $-\Omega_0 + 3\Delta \geqslant 0$ and thus $-\Omega_0 + 3\Delta + H^2/2s > 0$. In this case (A1.16) is equivalent to

$$\left(-\Omega_0 + 3\Delta + \frac{H^2}{2s}\right)^2 < \left(\Omega_0 + \Delta - \frac{H^2}{2s}\right) + \frac{4H^2}{s}\Delta. \tag{A1.19}$$

If we work this out we find $8\Delta^2 < 8\Omega_0\Delta$ or $\Delta < \Omega_0$, which is true by supposition. Thus (A1.14) is true independently of the magnetic field strength $H$ when $\Delta$ obeys (A1.18). Now suppose that

$$0 < \Delta < \tfrac{1}{3}\Omega_0. \tag{A1.20}$$

Then for $H^2/2s < \Omega_0 - 3\Delta$ we have that

$$-\Omega_0 + 3\Delta + H^2/2s < 0 \tag{A1.21}$$

and thus we must conclude that (A1.16) is trivially satisfied. On the other hand when

$$H^2/2s \geqslant \Omega_0 - 3\Delta \tag{A1.22}$$

we have again $-\Omega_0 + 3\Delta + H^2/2s \geqslant 0$ and so we can repeat the reasoning which we just gave in the complementary case (A1.18).

Therefore we can conclude that (A1.14) is always true as long as $\Delta \neq 0$. This completes the proof of the definite ordering (A1.1).

## Appendix 2

In this appendix we will discuss the single-kink limit of the soliton lattice solution. This amounts to letting $\Delta$ go to zero $(\Omega_1 \to \Omega_0)$.

First we will show that when $\Delta \to 0$ (3.25), i.e.

$$\Omega(\xi) = \Omega_- + (\Omega_1 - \Omega_-)\,\mathrm{sn}^2(\lambda\xi, k) \tag{A2.1}$$

reduces to (2.14), i.e.

$$\Omega(\xi) = -\frac{r}{s} - \frac{\nu^2}{2s}\,\mathrm{sech}^2(\tfrac{1}{2}\nu\xi). \tag{A2.2}$$

Because the single kink only exists for $\nu^2 \equiv -(H^2 + 2r) > 0$, we will impose this as an extra condition, while taking the limit $\Delta \to 0$. This condition can also be written as

$$\frac{H^2}{2s} < \Omega_0 \equiv -\frac{r}{s}. \tag{A2.3}$$

In this limit $\Omega_1$ (3.17) and $\Omega_\pm$ (3.18) go to

$$\Omega_1 \to \Omega_0$$

and

$$\Omega_- \to \frac{H^2}{2s} \qquad \Omega_+ \to \Omega_0. \tag{A2.4}$$

Therefore $\lambda$ and $k$ (3.24) go to

$$\lambda \to \tfrac{1}{2}\nu \qquad \text{and} \qquad k = \left(\frac{\Omega_1 - \Omega_-}{\Omega_+ - \Omega_-}\right)^{1/2} \to 1. \tag{A2.5}$$

In this last limit, when the elliptic modulus $k$ goes to 1, the sine amplitude will go to the hyperbolic tangent, i.e.

$$\mathrm{sn}(\lambda\xi, k) \to \tanh(\tfrac{1}{2}\nu\xi). \tag{A2.6}$$

Thus if we combine all these results, we see that $\Omega$ (A2.1) goes to

$$\Omega(\xi) \to \frac{H^2}{2s} - \left(\frac{r}{s} + \frac{H^2}{2s}\right) \tanh^2(\tfrac{1}{2}\nu\xi)$$

which is equal to (A2.2). Now let us look at the phase $\phi$ (3.32), i.e.

$$\phi(\xi) = \phi(0) + \frac{H}{2\lambda}\{\lambda\xi + (\beta^2 - 1)\Pi(\mathrm{am}(\lambda\xi, k), \beta^2, k)\} \tag{A2.7}$$

with $\beta^2 = 1 - \Omega_1/\Omega_-$. First of all when $k \to 1$, the incomplete elliptic integral of the third kind $\Pi(\phi, \beta^2, k)$ goes to (see, for instance, [6])

$$\Pi(\phi, \beta^2, k) \to \frac{-1}{\beta^2 - 1}\left[\ln(\tan\phi + \sec\phi) - \beta \ln\left(\frac{1 + \beta\sin\phi}{1 - \beta\sin\phi}\right)^{1/2}\right]. \tag{A2.8}$$

Because $\phi = \mathrm{am}(\lambda\xi, k)$ we have that $\sin\phi = \mathrm{sn}(\lambda\xi, k) \to \tanh(\tfrac{1}{2}\nu\xi)$. The coefficient $\beta$ which is imaginary (cf (3.19)) goes to

$$\beta = \mathrm{i}\left(\frac{\Omega_1 - \Omega_-}{\Omega_-}\right)^{1/2} \to \mathrm{i}\frac{\nu}{H}. \tag{A2.9}$$

Therefore $\phi$(A2.7) becomes in this limit

$$\phi(\xi) \to \phi(0) + \tfrac{1}{2}H\left[\xi - \xi + \frac{\mathrm{i}}{H}\ln\left(\frac{1 + (\mathrm{i}\nu/H)\tanh(\tfrac{1}{2}\nu\xi)}{1 - (\mathrm{i}\nu/H)\tanh(\tfrac{1}{2}\nu\xi)}\right)\right] \tag{A2.10}$$

$$= \phi(0) - \frac{1}{2\mathrm{i}}\ln\left(\frac{1 + (\mathrm{i}\nu/H)\tanh(\tfrac{1}{2}\nu\xi)}{1 - (\mathrm{i}\nu/H)\tanh(\tfrac{1}{2}\nu\xi)}\right). \tag{A2.11}$$

It is now not hard to see that this last expression is equal to

$$\phi(0) - \tan^{-1}((\nu/H)\tanh(\tfrac{1}{2}\nu\xi)) \tag{A2.12}$$

which is (2.15) apart from a constant. So both the phase and the amplitude of the single kink can be recovered from the corresponding quantities of the soliton lattice when $\Delta \to 0$. Finally, by using the following results:

$$K(k) \to \ln\frac{4}{(1 - k^2)^{1/2}} \qquad E(k) \to 1 \tag{A2.13}$$

and

$$\Delta \sim 1 - k^2 + \mathrm{O}[(1 - k^2)^2] \qquad \text{when } k \to 1 \tag{A2.14}$$

one can easily recover from (3.41), the energy of a static single kink which we calculated in I, namely

$$E_0(\text{single kink}) = \frac{\nu c^2}{2s}\left(-\tfrac{2}{3}r + \tfrac{1}{6}H^2\right). \tag{A2.15}$$

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