A Family of Solitary Waves in Frenkel-Kontorova Lattice

Basant Lal Sharma†

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Abstract

A family of solitary waves is constructed in Frenkel-Kontorova model and its continuum and quasi-continuum approximations. Each solitary wave is characterised by the number of local maxima in its profile and a relation between external force and the velocity of wave. Such waves may be interpreted as a coherent motion, with constant velocity, of two dislocations of opposite sign or of kink-antikink pair.

Keywords: Frenkel-Kontorova Model, Lattice Model, Solitary Wave, Dislocation, Kinetic Relation

0 Introduction

Plasticity and dislocations have been the focus of active research for more than a century. After a scheme was presented by Prandtl [32] and Dehlinger [11], a one-dimensional model of lattice was suggested by Frenkel and Kontorova [18] to understand plasticity in crystals. In these pioneering investigations and others, mainly dynamics of a dislocation is considered and results are obtained in the long wavelength limit [36, 17, 38, 37]. The Frenkel-Kontorova lattice model, as a Hamiltonian system, involves an onsite potential with more than one energy wells [18] or, as called in the paper, different phases. Thus, at least two types of travelling waves can be studied:

Type 1: This is the case when particles at ±∞ are in different phases. This travelling wave may be interpreted as dislocation or kink and has been extensively studied before in the context of plasticity and phase transformation (e.g. Atkinson and Cabrera [5], Earmme and Weiner [15], Abeyaratne and Vedantam [2], Kresse and Truskinovsky [25], Carpio and Bonilla [8]), where it is commonly known as Frenkel-Kontorova dislocation. Due to the presence of external driving force, there is radiation of elastic waves.

Type 2: In this case, except some particles that are in different phases those at ±∞ are in the same phase. This configuration can be associated with a uniformly moving dislocation dipole or kink-antikink pair [38].

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†(bs72@cornell.edu) Department of Theoretical and Applied Mechanics, Cornell University, Ithaca, NY 14853. Present address: (bls@iitk.ac.in) Department of Mechanical Engineering, Indian Institute of Technology Kanpur, Kanpur, U. P. 208016, India
In long wavelength limit of Frenkel-Kontorova model, traditionally known as sine-Gordon equation, the type 1 configuration appears as Heteroclinic orbit, and such configuration is sometimes called sine-Gordon kink or soliton. In the same limit, the type 2 configuration appears as Homoclinic orbit where it is also called sine-Gordon kink-antikink pair. The creation of kink-antikink pair in a dislocation in the presence of an applied stress and thermal fluctuations was treated by Seeger and Schiller [38]. Recent numerical experiments by Dmitriev et al. [12, 13] have demonstrated the possibility of the creation of a kink-antikink pair in the Frenkel-Kontorova model due to the interaction of two breathers [23] in the absence of a driving force. For a two dimensional Frenkel-Kontorova model at non-zero temperature, nucleation and propagation of kink-antikink pair on a dislocation has been demonstrated through computer simulations by Gornostyrev et al. [20]. However, to our knowledge a plethora of such type 2 waves and the corresponding family of force-velocity relations [43, 1] have not been discussed in the literature on Frenkel-Kontorova lattice model [6]; a connection with Yoffe’s problem is anticipated Yoffe [47] and Georgiadis and Theocaris [19].

In this paper we discuss type 2 waves only. We assume that all particles in the lattice, except a few localised within a finite neighbourhood of second phase, are in one phase. The conventional Frenkel-Kontorova model with a periodic onsite potential can be thus replaced by a model with double well potential. Weiner and Sanders [46] and Atkinson and Cabrera [5] presented the Frenkel-Kontorova lattice model for a special choice of onsite potential that allowed representation of type 1 waves in closed form. The choice of onsite potential in this paper is same as that of Atkinson and Cabrera [5]. As the situation discussed here is similar to the juxtaposition of two dislocations with opposite sign, we may refer to the dislocation on right side as first dislocation and the other dislocation as second dislocation. These solitary waves exhibit a coherence that is reflected in wave profile as well as relation between force and velocity and persist in continuum and quasicontinuum [26] approximations of the lattice model.

This paper is organized as follows. In the next section we formulate the one-dimensional lattice model and present the Euler-Lagrange equations. In second section we present a general expression for family of the solitary waves in the lattice model and corresponding force-velocity relation. Then we present the same for continuum and quasicontinuum approximations that capture type 2 waves and finally we conclude with some remarks.

1 Lattice Model

Consider a one-dimensional lattice of particles. Let the set of integers, denoted by $\mathbb{Z}$, be identified with the particles constituting the lattice. Let $\tilde{a}_n(t)$ denote the displacement of $n$th particle, which is located at position $n\varepsilon$ in the lattice, for each $n \in \mathbb{Z}$ and $t \in \mathbb{R}$. By $\varepsilon$ we denote the lattice parameter. Suppose the lattice is attached to a rigid foundation by bistable springs with energy density $w$ such that $w(0) = w(a) = 0, w'(0) = w'(a) = 0$, and $w''(0) = w''(a) = c > 0$, for some $a > 0$. Further assume that each particle interacts with only its nearest neighbour particle through harmonic forces captured by elastic modulus $E$. This means that $n$th particle experiences the force due to potential energy $\varepsilon \tilde{u}(\tilde{a}_n)$, in addition to the force due to harmonic potential involving the discrepancy with the displacements of its
nearest neighbours, $\tilde{u}_{n-1}$ and $\tilde{u}_{n+1}$. Finally, we introduce an external force, per unit length and independent of $n$, on each particle and call it $\tilde{\sigma}$. We use the Lagrangian

$$\mathcal{L}(\{\tilde{u}_i\}_{i \in \mathbb{Z}}) = \sum_{n \in \mathbb{Z}} \frac{1}{2} \rho \varepsilon \dot{\tilde{u}}^2_n - \sum_{n \in \mathbb{Z}} \left\{ \frac{1}{2} E \varepsilon ((\tilde{u}_{n+1} - \tilde{u}_n)/\varepsilon)^2 + \varepsilon \tilde{w}(\tilde{u}_n) - \varepsilon \tilde{\sigma} \tilde{u}_n \right\}$$

where $\rho$ is the mass density per unit length along the lattice, $\dot{\tilde{u}} = d\tilde{u}_n(t)/dt$ and we suppress the dependence on $t$ in these expressions. The Euler-Lagrange equation describing the motion for $n$th particle is

$$\rho \varepsilon \ddot{\tilde{u}}_n - \frac{E}{\varepsilon} (\tilde{u}_{n+1} - 2\tilde{u}_n + \tilde{u}_{n-1}) + \varepsilon [\tilde{w}'(\tilde{u}_n) - \tilde{\sigma}] = 0, \forall n \in \mathbb{Z}.$$  

Let $t = \tilde{t}/(\varepsilon/\sqrt{E/\rho}), u_n = (2\tilde{u}_n/a - 1), \sigma = \tilde{\sigma}/(ac)$ and $w(u_n) = 2/(ca^2)\tilde{w}(\tilde{u}_n)$. Let $x = \tilde{x}/\varepsilon$ describe the one-dimensional lattice in physical space. The Euler-Lagrange equations, in the dimensionless formulation of the lattice model, can be rewritten as

$$\ddot{u}_n - (u_{n+1} - 2u_n + u_{n-1}) + \chi^2 [w'(u_n) - \sigma] = 0, \forall n \in \mathbb{Z},$$  

(1)

where $\chi = \varepsilon \sqrt{2c/E}$ is a structural parameter. The function $w$ has global minima at $\pm 1$ and also a local maxima at 0. By the phrase ‘$n$th particle in the lattice is in the first (second)
phase’, it is meant that \( u_n < 0(> 0) \). We consider a special potential function for \( w \), so that we can present solutions in closed form,

\[
w(u) = \frac{1}{2}(u + 1)^2H(-u) + \frac{1}{2}(u - 1)^2H(u),
\]

where \( H(x) = 1 \) for \( x \geq 0 \) and 0 otherwise is the Heaviside step function. This square well potential function is also shown in Fig. 1 along with a quartic well potential function \( w(u) = \frac{1}{8}(u - 1)^2(u + 1)^2 \) and sinusoidal potential function \( w(u) = \frac{1}{\pi^2}(1 + \cos \pi x) \) with the same curvature at \( \pm 1 \). In the context of dislocation, an approximation of a nonlinear function by piecewise linear function has been used by Maradudin [28], Sanders [35], Celli and Flytzanis [10] and Ishioka [22] for a screw dislocation, and by Kratochvíl and Indenbom [24], Weiner and Sanders [46], and Atkinson and Cabrera [5] for Frenkel-Kontorova model.

In general, one would like to investigate the behaviour of \( \{u_n(t)\}_{n \in \mathbb{Z}} \) with given initial and boundary conditions as well as given force \( \sigma \) and parameter \( \chi \). However, in this paper we discuss only solitary waves.

## 2 Solitary Wave in Lattice Model

Let \( z = n - vt \), \( u(z) = u_n(t) \) in (1) where \( v \) is the velocity of solitary wave. The piecewise linear differential-difference equation that determines \( u(z) \) is

\[
v^2\frac{d^2u}{dz^2} - (u(z + 1) - 2u(z) + u(z - 1)) + \chi^2[u(z) - \sigma + 1 - 2H(u)] = 0.
\]

Assume that

\[
|u(z)| > z_0; \quad u(z) > 0, |z| < z_0.
\]

Also we assume that \( u(z) \to \text{const. as } |z| \to \infty \). The assumption \( (4) \), similar to that used by Atkinson and Cabrera [5], Earmme and Weiner [15] and Kresse and Truskinovsky [25] owing to the special choice of onsite potential function, leads to the following linear differential-difference equation

\[
v^2\frac{d^2u}{dz^2} - (u(z + 1) - 2u(z) + u(z - 1)) + \chi^2[u(z) - \sigma + 1 - 2H(z_0 - |z|)] = 0.
\]

By using Fourier Transforms, we can construct the solitary wave\(^1\) from equation (5)

\[
u(z) = \sigma - 1 + 2\chi^2 \left\{ \begin{array}{l}
2i \sum_{\xi \in S^+} e^{-i\xi z} \sin(\xi z_0)/(L'(\xi)\xi) \\
1/\chi^2 + \sum_{\xi \in S^+} e^{-i\xi z} e^{i\xi z_0}/(L'(\xi)\xi) \\
+ \sum_{\xi \in S_u} e^{-i\xi z} e^{i\xi z_0}/(L'(\xi)\xi) \\
-2i \sum_{\xi \in S^d} e^{-i\xi z} \sin(\xi z_0)/(L'(\xi)\xi)
\end{array} \right. \quad z \leq -z_0,
\]

\[
\frac{1}{\chi^2} + \sum_{\xi \in S_u} e^{-i\xi z} e^{i\xi z_0}/(L'(\xi)\xi) \quad |z| < z_0,
\]

\[
-2i \sum_{\xi \in S^d} e^{-i\xi z} \sin(\xi z_0)/(L'(\xi)\xi) \quad z \geq z_0,
\]

with \( L(\xi) = \chi^2 + 4\sin^2 \xi/2 - v^2\xi^2, S^\pm = \{\xi \mid L(\xi) = 0; \text{Im } \xi \geq 0\}, S_u = \{\xi \mid L(\xi) = 0; \text{Im } \xi = 0, \xi \neq 0\} \). By assumption \( (4) \), using \( u(z_0) = 0 \), the constant force \( \sigma \) is given by

\[
\sigma = 1 + 4\chi^2 i \sum_{\xi \in S^d} e^{-i\xi z_0} \sin(\xi z_0)/(L'(\xi)\xi)
\]

\(^1\)For details please see appendix A.
and by using \( u(-z_0) = 0 \), \( z_0 \) is determined by

\[
\sum_{k \in S_u \cap \mathbb{R}^+} \sin^2 k z_0 / (L'(k)) = 0. \tag{8}
\]

Let us define \( u(z_0^+) = \lim_{z \searrow z_0} u(z), u(z_0^-) = \lim_{z \nearrow z_0} u(z) \). We can show that \( u'(z_0^+) = u'(z_0^-), u'(-z_0^+) = 4 \chi^2 \sum_{\xi \in S_u \cap \mathbb{R}^+} \sin(2kz_0') / L'(k) - u'(z_0^+), u'(-z_0^-) = -u'(z_0^+) \), therefore

\[
u'(z_0^+) = -u'(-z_0^-) \Leftrightarrow \sum_{\xi \in S_u \cap \mathbb{R}^+} \sin(2kz_0') / L'(k) = 0. \tag{9}\]

The function (6) is a solution of (3) only if the particles in the interval \((-z_0, z_0)\) lie in second phase according to the assumption (4). We present below an interval of \( v \) where the solution (6) may hold.

When \( v > v_c^1 \), where \( v_c^1 \) is the maximum phase velocity that equals the group velocity for the same non-zero wave number [5, 33], as shown in Fig. 2, we get \( S_u = \{k_0, -k_0\} \). From (8) we obtain \( z_0 = n\pi / k_0, n \in \mathbb{Z}, n > 0 \) and the condition (9) is automatically satisfied. Thus a countable number of solitary waves may exist for given velocity \( v > v_c^1 \). For \( v < v_c^1 \), the expression (6) may not be a solution of (3) as we could not find \( v \) and \( z_0 \), numerically, satisfying condition (9) and assumption (4), similar to the case of one dislocation [5, 10]. We also discuss this issue at the end of the paper.

![Figure 2: \( v_c^1 \) for \( \chi = 0.5 \).](image)

For solitary waves presented here the velocity of propagation should be read as speed of propagation since the wave (6) with prescribed velocity do not depend on the sign of \( v \). As shown in Fig. 3, symbol \( n \) corresponds to the number of local maxima in wave profile (6), or bumps in the second phase. The solitary wave profile is shown in Fig. 3 for one and more bumps in the region with second phase and these waves have been grouped together with respect to same velocities of propagation. At small velocities there is a notable difference in

\[\text{For details please see Claim 3 in appendix A.}\]
the profiles for different values of \( n \) but at large velocities the wave profiles resemble each other very closely. Also at large velocities, starting around \( v = 1 \), the displacements become so large that dislocation dissociation may be favored similar to the case of one dislocation [14].

Figure 3: Solitary waves in Frenkel-Kontorova Lattice for \( \chi = 0.5 \). The wave profiles have been shifted a little in order distinguish them visually. The solid curves stands for \( n = 1 \), small dashed curve for \( n = 2 \), dash-dot-dash curve for \( n = 3 \), and long dashed curve for \( n = 4 \).

Note that the size of second phase zone, twice of \( z_0 \) (8), depends only on the non-zero and real wave numbers, \( k \in S_\nu \), satisfying the condition \( L(k) = 0 \), or equivalently \( \omega(k) = vk, k \in \mathbb{R} \), where \( \omega(k) = \chi^2 + 4 \sin^2 k/2 \) is the dispersion relation for the lattice. This is reminiscent of the possibility of macroscopic dissipation in the form of microscopic waves in the analysis of Frenkel Kontorova dislocation [5, 25, 8] and also in the analysis of a screw dislocation [10, 41, 40], where a dislocation moves due to the action of a configurational force and work done in this way at macroscale is converted into energy radiated in microscopic waves. It can be observed that, in case of one dislocation, use of inverse radiation condition leads to motion of dislocation against the configurational force. In other words, the energy contained in waves is converted into potential energy of configurational type and this can be interpreted as non-dissipative motion.

In fact, in each solitary wave, energy (in waves) is radiated by the first dislocation and it is macroscopically dissipative and the second dislocation with opposite sign is activated.
by these radiated waves to move against the action of configurational force and is non-
dissipative. Taking sum of both there is no dissipation and also there is no work done by
configuration forces when the dislocation dipole moves. Indeed, one interpretation of these
solitary waves is that they represent two dislocations of opposite sign moving together in such coherence that one dislocation emits lattice waves in a manner that supplies the right condition for the propagation of the other dislocation\(^3\). This is a much stronger interaction between waves and dislocation than that studied by Leibfried [27], Nabarro [31] and Eshelby [16] where a wave is considered as a small perturbation leading to oscillatory motion of a dislocation.

If the two dislocations are separated by a large distance, i.e. \(n \to \infty\), then the force
needed to move second dislocation is independent of the other and in this limiting case \(\sigma v\)-
relation (7) is same as the kinetic relation [43, 1] for one dislocation obtained by Atkinson and Cabrera [5]. Therefore, we can interpret the relation (7) between external force and velocity as the kinetic relation for first dislocation modified by the presence of the second dislocation of opposite sign moving with the same velocity. For simplicity, we call the relation between force, \(\sigma\), and velocity, \(v\), of a solitary wave as \(\sigma v\)-relation. For the case \(v > v_c\), \(S_u = \{k_0, -k_0\}\) and \(\sigma v\)-relation (7) reduces to

\[
\sigma = 2\chi^2 \sum_{\xi \in S_u} (1 - e^{-2i\xi n\pi/k_0})/(L'(\xi)\xi).
\]

Thus there is a unique stress level \(\sigma\) associated with the propagation of a solitary wave with a given number of bumps \(n\) and a given velocity \(v\). We present \(\sigma v\)-relations in Fig. 4 along with the Peierls stress reported by Sharma [39]. As mentioned above, \(\sigma v\)-relation of type 2 waves approaches that for type 1 waves as \(n\) increases to infinity. Note also that \(\sigma\) is almost independent of \(n\) for \(v \geq 1\). This is resonant with resemblance in the wave profiles at large velocities in Fig. 3. This is because ‘core’ of both dislocations shrinks at large velocity and therefore, the effective distance between them also becomes large and the resulting \(\sigma v\)-relations coincide with the kinetic relation for one dislocation.

In the following section, we construct the solitary wave in continuum and quasicontinuum approximations of Frenkel-Kontorvva lattice model [25].

### 3 Solitary Wave in Continuum and Quasicontinuum Approximations of Lattice Model

The phonon dispersion relation for the lattice model is given by

\[
\omega(k)^2 = 4 \sin^2 \frac{k}{2} + \chi^2, \forall k \in \mathbb{C}.
\] (10)

As the first approximation of lattice model, we get a dispersion relation for the classical continuum model

\[
\omega^2 = k^2 + \chi^2 + o(k^2),
\] (11)

\(^3\)This comment is due to Lev Truskinovsky.
Figure 4: \( \sigma v \)-relations for solitary waves in Frenkel-Kontorova lattice for \( \chi = 0.5 \). Peierls stresses are obtained in [39] as \( k \to 0 \). This corresponds to equation of motion,

\[
 u_{tt} = u_{xx} - \chi^2[w'(u) - \sigma],
\]

and reduces to the ubiquitous sine-Gordon equation [36, 23] or Enneper equation [37] in a special case of \( \sigma = 0 \) and sinusoidal potential function \( w(u) = \frac{1}{\pi^2}(1 + \cos \pi x) \). Using \( u(x, t) = u(x - vt) = u(z) \) and the boundary conditions, \( \lim_{z \to \infty} u(z) = \lim_{z \to -\infty} u(z) \), it can be found that there are no type 2 solitary waves for \( \sigma = 0 \), but for \( \sigma > 0 \),

\[
 \pm \int_{u(0)}^{u(z)} du / \{w(u) - \{w(\sigma - 1) + w'(\sigma - 1)(u - \sigma - 1)\}\}^{1/2} = \chi \sqrt{2z/\sqrt{1-v^2}}.
\]

The solitary wave for \( w \) given by (2) is shown in Fig. 5 where \( z \)-axis has been scaled by a factor of \( \chi \sqrt{2/\sqrt{1-v^2}} \). The \( \sigma v \)-relation is trivial in this case, namely, any \( \sigma \in (0, 1) \) is associated with any \( |v| < 1 \).

A higher gradient continuum with negative capillarity, and not conventional positive capillarity [44, 7, 9], by an approximation of the lattice model is possible if we include the next term in the Taylor series expansion of the relation (10). So we get a dispersion relation

\[
 \omega^2 = k^2(1 - \lambda k^2) + \chi^2 + o(k^4),
\]

as \( k \to 0 \), with\(^4 \) \( \lambda = 1/12 \). This is a second gradient elastic model, also called Boussinesq

\(^4\)For \( \lambda < 0 \), there are no type 2 waves. Besides this value, \( \lambda \) can be also considered as a parameter [41]
approximation sometimes [25, 3], with the equation of motion

$$u_{tt} = u_{xx} + \lambda u_{xxxx} - \chi^2 [u'(u) - \sigma].$$  \hspace{1cm} (14)

We call this model as Model 1. Using \(u(x, t) = u(x - vt) = u(z)\), the equation for travelling waves is

$$\lambda u_{zzzz} + (1 - v^2)u_{zz} - \chi^2 [u(z) - \sigma + 1 - 2H(u)] = 0.$$  \hspace{1cm} (15)

Assume \(u > 0\) for \(z \in (-z_0, z_0)\) and \(u < 0\) for \(z \in \mathbb{R} \setminus (-z_0, z_0)\). With \(\lim_{z \to \infty} u(z) = \lim_{z \to -\infty} u(z) = \text{const.}\) and the condition that all derivatives of \(u\) approach 0 as \(z \to \pm\infty\), and the jump conditions, easily derivable from the weak form of (15), \([u] = [u_z] = [u_{zz}] = [u_{zzz}] = 0\) at \(z = \pm z_0\), the solution\(^5\) can be expressed as

$$u(z) = \sigma - 1 + 2 \begin{cases} \sinh(n\pi r)e^{-r_1|z|/(r^2 + 1)}, & z < -n\pi/r_3, z > n\pi/r_3, \\ 1 - (e^{-n\pi r} \cosh r_1 z + r^2(-1)^n \cos r_3 z)/(r^2 + 1), & z \in [-n\pi/r_3, n\pi/r_3]. \end{cases}$$  \hspace{1cm} (16)

where \(n\) is a positive integer and \(r_1 = \sqrt{-(1-v^2) + R_1/2\lambda}, r_3 = \sqrt{(1-v^2) + R_1/2\lambda}\), with \(R_1 = \sqrt{(1-v^2)^2 + 4\chi^2\lambda}\) and \(r = r_1/r_3 = 4\chi^2\lambda/\{(1-v^2) + R_1\}\). and

$$\sigma = \frac{r^2 + e^{-2n\pi r}}{r^2 + 1}.\)
Using $\lambda = 1/12$, the external driving force $\sigma$ has been plotted against velocity $v$ in Fig. 6.

A Padé approximation of the relation (10) gives a dispersion relation representing a class of continuum models with velocity gradients [30, 34, 25, 40]

$$\omega^2 = \frac{k^2}{1 + \kappa k^2} + \chi^2,$$

(17)

with $^{6}\kappa = 1/12$. The equation of motion for this continuum model with first order ‘micro-kinetic’ energy [42, 25] is

$$\kappa v^2 u_{zzzz} + (1 - v^2 + \kappa \chi^2) u_{zz} - \chi^2 [u(z) - \sigma + 1 - 2H(u)] = 0.$$

(19)

With $\lim_{z \to \infty} u(z) = \lim_{z \to -\infty} u(z)$ and the condition that all derivatives of $u$ approach 0 as $z \to \pm \infty = \text{const.}$ and the jump conditions $[u] = [u_z] = [u_{zzz}] = 0$, $v^2 [u_{zz}] = 2\chi^2$ at $z = \pm z_0$, the solution can be written as $^7$

$$u(z) = \sigma - 1 + \begin{cases} A_1 e^{-r_1|z|}, & |z| > z_0, \\ 2 + 2B_1 \cosh r_1 z + 2B_3 \cosh r_3 z, & z \in [-z_0, z_0] \end{cases}$$

(20)

where $A_1 = 2 \sinh r_1 z_0 \frac{\chi^2 / v^2 + r_3^2}{r_1^2 - r_3^2}$, $B_1 = e^{-r_1 z_0} \frac{\chi^2 / v^2 + r_3^2}{r_1^2 - r_3^2}$, $B_3 = \frac{\chi^2 / v^2 + r_3^2}{(r_1^2 - r_3^2) \cosh r_3 z_0}$, $z_0 = \frac{i n \pi}{r_3}$, with $n$ being a positive integer and $r_1 = \sqrt{-\frac{(1 - v^2 + \kappa \chi^2) + r_3^2}{2\kappa v^2}}$, $r_3 = i \sqrt{\frac{(1 - v^2 + \kappa \chi^2) + r_3^2}{2\kappa v^2}}$.

$^6$\kappa can also be considered as a parameter [40].

$^7$Please see appendix B.
\[ R_2 = \sqrt{(1 - v^2 + \kappa \chi^2)^2 + 4\chi^2\kappa v^2}. \]

The Kinetic relation is

\[ \sigma = \frac{\chi^2/v^2 + r_1^2 + (\chi^2/v^2 + r_3^2)e^{-2i\pi r_1/r_3}}{r_1^2 - r_3^2}. \]

Using \( \kappa = 1/12 \), the external driving force \( \sigma \) necessary to sustain the motion of the solitary waves has been plotted against velocity \( v \) in Fig. 7. For model 2, as \( v \to 0, \sigma \to 1, \forall n < \infty \) in contrast with the case of model 1.

4 Some Remarks

(1) From the solitary wave profiles and \( \sigma v \)-relations, as shown in Fig. 8 and Fig. 9 respectively, for comparison between lattice model, model 1 and model 2, we can see that these models behave differently in the small velocity regime. For sufficiently large velocities the continuum approximations capture the effects due to discreteness, similar to the case of type 1 waves [25, 3]. From a point of view of modelling discrete systems using continuum formulation, these results present an example of travelling waves in a lattice model which are very well approximated by quasicontinuum approximations although may not be captured by all continuum schemes.

(2) Similar to the waves of type 1 [25, 29], without proof we conjecture that there exists a lower bound in the velocity, denoted by \( v^*_n \), of such solitary waves. So only those solitary waves with \( n \) number of bumps and which satisfy the property \( v \geq v^*_n \) propagate in lattice with formal representation (6). An estimate of \( v^*_n \), which we call \( \hat{v}_n \), is possible by using a local condition that needs to be satisfied for all such acceptable velocities. This estimate is
Figure 8: Solitary waves for \( n = 1, 2, 3, 4 \).

given by

\[
\hat{v}_n := \inf \{ v : u'(n\pi/k_0(v)) < 0, L(k_0(v)) = 0 \}.
\]

which gives

\[
\hat{v}_n = \inf \{ v : i \sum_{\xi \in S^a} (1 - e^{-2i\xi(n\pi/k_0(v))} - L'(\xi) < 0, L(k_0(v)) = 0 \}. \tag{21}
\]

This also yields a lower bound \( \hat{v}_{\infty} \) on the velocity of propagation of travelling waves of type 1 \([29, 25, 4]\) and we state the results as a conjecture without proof of monotonicity of \( \hat{v}_n \) \( \tag{21} \) as \( n \) increases,

\[
\hat{v}_{\infty} := \inf_{\hat{v}_n} \{ v : \sum_{\xi \in S^a} \text{Im} L'(\xi)/|L'(\xi)|^2 < 0 \}. \tag{22}
\]

As shown in Fig. 4, \( n \) increases, \( \sigma(\hat{v}_n) \) appears to decrease almost as fast as \( \sigma_p^a \). Note that the velocity of solitary waves is unique if \( \sigma \) is such that it is greater than \( \sigma \) corresponding to \( v = \hat{v}_n \) \( \tag{21} \).

At this point we do not know how to complete the picture between \( v = 0 \) and \( v = \hat{v}_n \) \( \tag{21} \) for each \( n \). This is similar to the question that concerns situation for the Frenkel-Kontorova dislocation at small velocities \([5]\) and the enigma of kinematic resonances \([33]\) in this regime.
Figure 9: Kinetic relations for solitary waves for $\chi = 0.5$.

(3) The solitary wave profiles shown in Fig. 3 have been also shown in Fig. 10, but they have been grouped with respect to number of bumps in the second phase. In Fig. 11, we present the solitary wave profiles possible under the same external stress $\sigma$ and also the same number of bumps. As the number of bumps increases the difference in the two velocities for the same external stress also decreases. For any given $n$ number of bumps, this difference vanishes when $\sigma = \sigma_c^n$, which is the critical point such that for $\sigma < \sigma_c^n$ the solitary wave with $n$ bumps ceases to exist. Thus $\sigma_c^n$ behaves like the dynamic Peierls stress \cite{45, 5} and reduces to the value for one dislocation in the limiting case of an infinite number of bumps, when effectively the solitary wave reduces to one dislocation or kink. The solitary wave profiles at $\sigma_c^n$ have been shown in Fig. 12, where $v_c^n$ denotes the unique velocity when $\sigma = \sigma_c^n$ for given $n$.

(4) At this point, an observation can been made regarding the relationship between solitary waves and equilibrium states \cite{39}. We find that $\hat{v}_n$ is close to 0.3 for $\chi = 0.5$, so using this rough estimate, we have shown the wave profile at $v = 0.3$ and compared it with the equilibrium states obtained in the presence of $\sigma = \sigma_p^n$ where $n$ denotes the number of particles in the second phase and $\sigma_p^n$ is the Peierls stress for the corresponding static equilibrium configuration. As shown in Fig. 13, there is one to one correspondence between the number of bumps in second phase of the solitary waves and the number of particles in second phase of the equilibrium states.

(5) This paper is a result of an accidental observation of solitary waves of type 2 in continuum approximations of Frenkel-Kontorova lattice. Soon we found that these waves persist in the lattice model and exhibit a rich behaviour in wave profiles as well as $\sigma v$-
relations. Recently we were able to gain more insight into the kink-antikink equilibrium states corresponding to the solitary waves of type 2 [39]. The study of change in free energy [39] associated with transitions between such equilibrium states indicates towards the instability of solitary waves in Frenkel-Kontorova lattice [21]. The instability has been observed when we solved the Euler-Lagrange equations (1), numerically, using MATLAB but we just mention these facts here and leave the question for future.

A Construction of Solitary waves for the Lattice model using Fourier Transforms

Similar to the method adopted in [5, 25], using (4) we introduce a part of the Fourier Transform, and from (3) we get

\[
v^2 \int_{z_0}^{\infty} e^{i\xi z} \frac{d^2 u}{dz^2} dz - (\int_{z_0}^{\infty} e^{i\xi z} u(z + 1) dz - 2 \int_{z_0}^{\infty} e^{i\xi z} u(z) dz + \int_{z_0}^{\infty} e^{i\xi z} u(z - 1) dz) + \chi^2 [\int_{z_0}^{\infty} e^{i\xi z} u(z) dz - (\sigma - 1) \int_{z_0}^{\infty} e^{i\xi z} dz] = 0.\]

Figure 10: Solitary waves in Frenkel-Kontorova Lattice for \( \chi = 0.5 \), same as shown in the pervious figure but arranged with respect to the number of peaks \( n \). The solid curves stands for \( v = 0.3 \), small dashed curve for \( v = 0.6 \), dash-dot-dash curve for \( v = 0.9 \), and long dashed curve for \( v = 1.01 \).
Using integration by parts and the definitions

\[ L(\xi) = \chi^2 + 4 \sin^2 \frac{\xi}{2} - v^2 \xi^2, \]

\[ \hat{u}_r(\xi) = \int_{z_0}^{\infty} e^{i\xi z} u(z) dz, \]

we get a part of \( \hat{u}, \)

\[
\hat{u}_r(\xi) = \frac{1}{\sqrt{2\pi L(\xi)}} \left[ v^2 e^{i\xi z_0} u'_+(z_0) - i\xi v^2 e^{i\xi z_0} u_+(z_0) - \int_{z_0}^{2z_0+1} e^{i\xi(y-1)} u(y) dy 
+ \int_{z_0-1}^{z_0} e^{i\xi(y+1)} u(y) dy + \chi^2(\sigma - 1) \int_{z_0}^{\infty} e^{i\xi z} dz \right].
\] (23)

Similarly other parts of Fourier Transform of \( u \) with definition, \( \hat{u}_l(\xi) = \int_{-\infty}^{-z_0} e^{i\xi z} u(z) dz, \)

\( \hat{u}_c(\xi) = \int_{-z_0}^{z_0} e^{i\xi z} u(z) dz, \)

are given by

\[
\hat{u}_l(\xi) = \frac{1}{\sqrt{2\pi L(\xi)}} \left[ -v^2 e^{-i\xi z_0} u'_+(-z_0) + i\xi v^2 e^{-i\xi z_0} u_+(-z_0) + \int_{-z_0}^{-z_0+1} e^{i\xi(y+1)} u(y) dy 
- \int_{-z_0-1}^{-z_0} e^{i\xi(y+1)} u(y) dy + \chi^2(\sigma - 1) \int_{-\infty}^{-z_0} e^{i\xi z} dz \right].
\] (24)
and

\[ \hat{u}_c(\xi) = \frac{1}{\sqrt{2\pi L(\xi)}} \left[ -v^2 e^{i\xi z_0} u'(z_0) + v^2 e^{-i\xi z_0} u'(-z_0) \right. \\
\left. + i\xi e^{i\xi z_0} v^2 u_-(-z_0) - i\xi e^{-i\xi z_0} v^2 u_-(-z_0) - \int_{-z_0}^{-z_0+1} + \int_{-z_0+1}^{z_0} e^{i\xi(y-1)} u(y)(\xi) \\
+ \int_{-z_0}^{-z_0} - \int_{z_0-1}^{z_0} e^{i\xi(y+1)} u(y)dy + \chi^2(2 + \sigma - 1) \int_{-z_0}^{z_0} e^{i\xi z} dz \right]. \]  

(25)

Combining all three parts (23), (24) and (25), and assuming continuity and differentiability of \( u \) at \( z = \pm z_0 \), we get the full function \( \hat{u} \), the Fourier Transform of \( u \). From the inverse Fourier Transform of \( \hat{u} \), we obtain

\[ u(z) = \frac{1}{2\pi} \chi^2 \int_{-\infty}^{\infty} e^{-i\xi z} \frac{e^{-i\xi z}}{L(\xi)} [(\sigma - 1) \int_{-\infty}^{\infty} e^{i\xi z} dz + 2 \int_{-z_0}^{z_0} e^{i\xi z} dz] d\xi \]

\[ = \sigma - 1 + \frac{2\chi^2}{\pi} \int_{-\infty}^{\infty} \frac{e^{i\xi(z_0-z)} + e^{-i\xi(z_0+z)}}{2iL(\xi)} d\xi. \]  

(26)

Assume \( z_0 \neq 0 \), so there is no pole at \( \xi = 0 \). Also due to lack of radiative damping as \( |z| \to \infty \), we don’t expect any elastic waves in the solution for \( |z| > z_0 \). Therefore, in order to invoke the residue theorem, we complete the integration along a contour so that all the real valued poles of the integrand are excluded.

For \( z > z_0 \), we consider a contour that lies in the lower half of the complex plane, \( C_2 \) as

![Figure 12: Solitary waves at the minimum value of \( \sigma \) for \( \chi = 0.5 \) and the case of \( n = 1, 2, 3 \) and 4 number of bumps.](image)
Figure 13: Solitary waves for \( n = 1, 2, 3, 4 \) for \( v = 0.3 \) and static equilibria [39] for \( \chi = 0.5 \). Solitary wave with \( n \) bumps can be identified with an equilibrium state involving \( n \) particles in second phase.

shown in Fig. 14, and by using residue theorem, we get from (26)

\[
u(z) = \sigma - 1 - 4\chi^2 i \sum_{\xi \in S_d^-} \frac{e^{-i\xi z} \sin(\xi z_0)}{L'(\xi)\xi}, S_d^- = \{\xi \mid L(\xi) = 0; \text{Im } \xi < 0\}.\]

For \( z < -z_0 \), we consider a contour that lies in the upper half of the complex plane, \( C_1 \) as shown in Fig. 14, and using the Residue theorem, we get from (26)

\[
u(z) = \sigma - 1 + 4\chi^2 i \sum_{\xi \in S_d^+} \frac{e^{-i\xi z} \sin(\xi z_0)}{L'(\xi)\xi}, S_d^+ = \{\xi \mid L(\xi) = 0; \text{Im } \xi > 0\}.\]

We require that \( u(-z_0) = 0 \), according to the assumption (4), and it is equivalent to the following claim.

**Claim 1:**

\[
\sum_{\xi \in S_d^-} \frac{e^{-i\xi z_0} \sin(\xi z_0)}{L'(\xi)\xi} + \sum_{\xi \in S_d^+} \frac{e^{i\xi z_0} \sin(\xi z_0)}{L'(\xi)\xi} = 0.
\]

**Proof:** Since \( \xi \in S_d^- \Leftrightarrow \xi^* \in S_d^+ \), and \( L'(\xi) = 2(\sin \xi - v^2 \xi) \), so \( L'(\xi^*) = L'(\xi)^* \); we get

\[
\sum_{\xi \in S_d^-} \left\{ \frac{e^{-i\xi z_0} \sin(\xi z_0)}{L'(\xi)\xi} + \frac{e^{i\xi z_0} \sin(\xi z_0)}{L'(\xi)\xi^*} \right\} = \sum_{\xi \in S_d^+} \left\{ \frac{e^{-i\xi z_0} \sin(\xi z_0)}{L'(\xi)\xi} + \frac{e^{-i\xi z_0} \sin(\xi z_0)}{L'(\xi)\xi^*} \right\}.
\]

Since \( \xi \in S_d^- \Leftrightarrow -\xi^* \in S_d^-, \) and \( L'(-\xi^*) = -L'(\xi) \), the claim follows. QED
Figure 14: Contours $C_1, C_2, C_+$ for Integration. The radius is considered to go to infinity in the evaluation of the integrals and the contribution from the peripheral part goes to zero very fast due to the presence of exponentially decaying term in the integrand.

For $|z| < z_0$, we cannot exclude real valued poles in the integral term of (26). However, we dissect the expression of integral into two integrals

$$
\int_{-\infty}^{\infty} \frac{e^{i\xi(z_0-z)} - e^{-i\xi(z_0+z)}}{2iL(\xi)\xi} d\xi = \int_{-\infty}^{\infty} \frac{e^{i\xi(z_0-z)}}{2iL(\xi)\xi} d\xi - \int_{-\infty}^{\infty} \frac{e^{-i\xi(z_0+z)}}{2iL(\xi)\xi} d\xi.
$$

For the first integral, consider the contour $C_+$, as shown in the second of Fig. 14, that lies in the upper half of the complex plane but also includes the real axis and for the second integral consider a contour $C_-$, as shown in Fig. 14, that lies, strictly, in the lower half of the complex plane. After the breakup of the contour integrals, we do get a contribution from the pole at $\xi = 0$ for the first integral. Thus for $|z| < z_0$,

$$u(z) = \sigma - 1 + 2 + 2\chi^2 \left[ \sum_{\xi \in S_u^+ \cup S_u} \frac{e^{-i\xi z} e^{i\xi z_0}}{L'(\xi)\xi} + \sum_{\xi \in S_u^+} \frac{e^{-i\xi z} e^{-i\xi z_0}}{L'(\xi)\xi} \right],$$

with $S_u = \{ \xi \mid L(\xi) = 0; \text{Im} \ \xi = 0, \xi \neq 0 \}$.

We also need that $u(z) \rightarrow 0$ as $z \rightarrow \pm z_0$ with $|z| \leq z_0$. These two conditions can be simplified to an identity proved in the claim below and the condition

$$
\sum_{k \in S_u} e^{2ikz_0}/(L'(k)k) = \sum_{k \in S_u} 1/(L'(k)k).
$$

Claim 2:

$$1 + \chi^2 \sum_{L(\xi) = 0, \xi \neq 0} \frac{1}{L'(\xi)\xi} = 0,$$

(28)
**Proof:** Consider the contour $C_-$ that lies in the lower half of the complex and the contour $C_+$ that lies in the upper half complex plane including the real axis. Then \( \int_{C_-} \frac{1}{L(\xi)} \, d\xi = \int_{C_+} \frac{1}{L(\xi)} \, d\xi = -2\pi i \sum_{\xi \in S_u} \frac{1}{L(\xi)} \), but also \( \int_{-\infty}^{\infty} \frac{1}{L(\xi)} \, d\xi = \int_{C_+} \frac{1}{L(\xi)} \, d\xi + \sum_{\xi \in S_u^+} \frac{1}{L(\xi)} \). Therefore

\[
\frac{1}{L(0)} + \sum_{k \in S_u} \frac{1}{L'(k)} + \sum_{\xi \in S_u^+} \frac{1}{L'(\xi)} + \sum_{\xi \in S_u^-} \frac{1}{L'(\xi)} = 0.
\]

Since \( L(0) = \chi^2 \), the identity (29) follows. QED

In the construction of the solitary waves, using the Fourier Transform of \( u \), we assume the continuity of the derivative of \( u \). For the derivative, as \( z \searrow z_0 \),

\[
u' (z_0^-) = -4\chi^2 \sum_{\xi \in S_d^-} e^{-i\xi z_0} \sin(\xi z_0) = 2i\chi^2 \sum_{\xi \in S_d^-} \frac{1 - e^{-2i\xi z_0}}{L'(\xi)},
\]

and as \( z \nearrow z_0 \),

\[
u' (z_0^+) = -i2\chi^2 \sum_{\xi \in S_d \cup S_d^- \cup S_d^+} \frac{1}{L'(\xi)} + i2\chi^2 \sum_{\xi \in S_d^-} \frac{1 - e^{-2i\xi z_0}}{L'(\xi)}
\]

\[= -i2\chi^2 \sum_{\xi \in S_u \cup S_d^- \cup S_d^+} \left[ \frac{1}{L'(\xi)} + \frac{1}{L'(-\xi)} \right] + i2\chi^2 \sum_{\xi \in S_d^-} \frac{1 - e^{-2i\xi z_0}}{L'(\xi)}
\]

\[= i2\chi^2 \sum_{\xi \in S_d^-} \frac{1 - e^{-2i\xi z_0}}{L'(\xi)} = u' (z_0^+).
\]

Thus, the solitary waves are continuously differentiable at \( +z_0 \). However we find that the continuity of derivative at \( z = -z_0 \) imposes a restriction on \( z_0 \) itself as condition (9). In the following claim we prove this condition as necessary.

**Claim 3:** Condition (9) is necessary for the continuity of derivative of solitary wave.

**Proof:** As \( z \searrow -z_0 \),

\[
u' (-z_0^+) = -i2\chi^2 \sum_{\xi \in S_u} \frac{e^{2i\xi z_0}}{L'(\xi)} - i2\chi^2 \sum_{\xi \in S_d^+} \frac{e^{2i\xi z_0}}{L'(\xi)} - i2\chi^2 \sum_{\xi \in S_d^-} \frac{1}{L'(\xi)}
\]

\[= -i2\chi^2 \left\{ \sum_{\xi \in S_u} \frac{e^{2i\xi z_0}}{L'(\xi)} + \sum_{\xi \in S_d^+} \frac{e^{2i\xi z_0}}{L'(\xi)} + \sum_{\xi \in S_d^-} \frac{e^{-2i\xi z_0}}{L'(\xi)} \right\} = u' (z_0^-).
\]
But
\[
\sum_{\xi \in S_u} \frac{e^{2i\xi_0}}{L'(\xi)} + \sum_{\xi \in S_u^+} \frac{e^{2i\xi_0}}{L'(\xi)} + \sum_{\xi \in S_u^-} \frac{e^{-2i\xi_0}}{L'(\xi)} = \sum_{\xi \in S_u} \frac{e^{2i\xi_0}}{L'(\xi)} + \sum_{\xi \in S_u^+} \left( \frac{e^{2i\xi_0}}{L'(\xi)} + \frac{e^{-2i\xi_0}}{L'(-\xi)} \right) (\xi \in S_u^- \Leftrightarrow \xi^* \in S_u^-)
\]
\[
= \sum_{\xi \in S_u} \frac{e^{2i\xi_0}}{L'(\xi)} + \sum_{\xi \in S_u^+} \left( \frac{e^{2i\xi_0}}{L'(\xi)} + \frac{e^{2i\xi_0}}{L'(-\xi)} \right) (\xi \in S_u^- \Leftrightarrow -\xi^* \in S_u^+)
\]
\[
= 2i \sum_{\xi \in S_u \cap \mathbb{R}^+} \frac{\sin(2k\xi_0)}{L'(k)}.
\]

So \(z \searrow -z_0, u'(-z_0^+) = 4\chi^2 \sum_{\xi \in S_u \cap \mathbb{R}^+} \frac{\sin(2k\xi_0)}{L'(k)} - u'(z_0^+)\). And as \(z \nearrow -z_0\),
\[
u'(-z_0^-) = 4\chi^2 \sum_{\xi \in S_u^-} \frac{e^{-2i\xi_0}}{L'(\xi)} = -u'(z_0^+).
\]

Thus the continuity of derivative of \(u\) at \(-z_0\) implies the restriction (9). QED

**B  Solitary waves in Continuum Models**

To obtain solitary waves in the continuum model with second order strain energy (15), the method is similar to the one shown here. We now describe the method used to obtain solitary waves for the continuum approximation (18). Let \(u\) be given by the ansatz
\[
u(z) = \sigma - 1 + \begin{cases} \sum_{i=1}^4 A_i e^{-r_i|z|}, & z < -z_0, \\ 2 + \sum_{i=1}^4 B_i e^{-r_i z}, & z \in [-z_0, z_0] \\ \sum_{i=1}^4 A_i e^{-r_i|z|}, & z > z_0 \end{cases}
\]

with \(r_{1,2} = \pm \sqrt{-\left(1-v^2+\kappa \chi^2\right) + R_{2en^2}}, r_{3,4} = \pm i \sqrt{\left(1-v^2+\kappa \chi^2\right) + R_{2en^2}}\), and
\[
R = \sqrt{\left(1-v^2+\kappa \chi^2\right)^2 + 4\chi^2 \kappa v^2}.
\]

With \(\lim_{z \to -\infty} u(z) = \lim_{z \to -\infty} u(z)\) and all derivatives of \(u\) approach 0 as \(z \to \pm \infty\), and
the jump conditions $[u] = [u_z] = [u_{zzz}]= 0$, $v^2 [u_{zz}]= 2 \chi^2$ at $z = \pm z_0$,

\[
\begin{align*}
A_i' e^{-r_1 z_0} &= 2 + \sum_{i=1}^4 B_i e^{-r_i z_0}; & A_i' e^{-r_1 z_0} &= 2 + \sum_{i=1}^4 B_i e^{r_i z_0}, \\
-r_1 A_i' e^{-r_1 z_0} &= -\sum_{i=1}^4 r_i B_i e^{-r_i z_0}; & r_1 A_i' e^{-r_1 z_0} &= -\sum_{i=1}^4 r_i B_i e^{r_i z_0}, \\
\frac{1}{r_1^3} A_i' e^{-r_1 z_0} &= \sum_{i=1}^4 \frac{1}{r_i^3} B_i e^{-r_i z_0} - 2 \chi^2 / v^2; & \frac{1}{r_1^3} A_i' e^{-r_1 z_0} &= \sum_{i=1}^4 \frac{1}{r_i^3} B_i e^{r_i z_0} + 2 \chi^2 / v^2, \\
-\frac{1}{r_1^3} A_i' e^{-r_1 z_0} &= -\sum_{i=1}^4 \frac{1}{r_i^3} B_i e^{-r_i z_0}; & -\frac{1}{r_1^3} A_i' e^{-r_1 z_0} &= -\sum_{i=1}^4 \frac{1}{r_i^3} B_i e^{r_i z_0}.
\end{align*}
\]

After simplification we get $A_2 = A_1' = A_1, B_1 = B_2, B_3 = B_4$ and

\[
A_1 = -2 \sinh r_1 z_0 \frac{-\chi^2 / v^2 - r_3^2 / r_1^2}{r_3^2 - r_1^2}, B_1 = e^{-r_1 z_0} \frac{-\chi^2 / v^2 - r_3^2 / r_1^2}{r_3^2 - r_1^2}, B_3 = \frac{-\chi^2 / v^2 - r_1^2 / r_3^2}{(r_1^2 - r_3^2) \cosh r_3 z_0},
\]

and $z_0 = \frac{\pi n}{r_3}$, where $n$ is a positive integer.

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