A Solution to the Frenkel-Kontorova Dislocation Model

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A Solution to the Frenkel-Kontorova Dislocation Model*

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An exact solution to the nonlinear difference equation which describes a static configuration in the Frenkel-Kontorova dislocation model is given. The solution is in terms of a power series which is proved convergent. Previously, only approximate solutions had been obtained by replacing the difference equation by a differential equation. A numerical comparison is made between the exact and the approximate solutions and the Peierls energies they give.

I. INTRODUCTION

THE concept first introduced by Peierls of a barrier to the motion of a dislocation due to the discreteness of the crystal lattice has been widely used to explain the critical shear stress and the temperature dependence of creep. Theoretical estimates of the magnitude of this barrier can only be obtained with drastic simplifying assumptions or for unrealistic models, and have at most an order of magnitude significance. In most calculations, as for instance in the Peierls-Nabarro model, an essential approximation is made when the dislocation configuration is obtained from a continuum approximation, but the energy of the configuration is calculated by summing over the points of a discrete lattice.[1]

In the case of the simple one-dimensional model of Frenkel and Kontorova[2] it is not necessary to make this approximation since we have been able to obtain a series solution to the difference equation describing a static configuration. This solution may be of considerable interest in itself since the model has been studied by several authors[3–5] with a variety of applications and always the approximation of replacing differences with differentials was used.[6]

No extensive program of calculations with the solution obtained has been carried out since we believe that the results would have only a qualitative character when applications to actual cases are attempted. A numerical example is presented to give an idea of the error involved in the continuum approximation.

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II. SOLUTION TO THE DIFFERENCE EQUATION

The Frenkel-Kontorova dislocation model consists of a linear chain of equal mass points, referred to as atoms, connected by identical springs with each atom subjected to a sinusoidal substrate force. If y_n designates the displacement of the nth atom relative to the nth potential minimum, the static energy of the linear chain is

$$E=\tfrac{1}{2}\kappa\sum_n(y_{n+1}-y_n)^2+\frac{\alpha a^2}{4\pi^2}\sum_n\left(1-\cos\frac{2\pi y_n}{a}\right), \quad (1)$$

where κ is the spring constant, a is the lattice parameter, and α is the substrate force constant. The equations of equilibrium are then

$$k(\psi_{n+1}-2\psi_n+\psi_{n-1})=\sin\psi_n, \quad (2)$$

where $\psi_n\equiv 2\pi y_n/a$ and $k=\kappa/\alpha$.

We are looking for the particular solution to (2) describing a chain in which there is one atom in excess (or defect) over the number of potential minima. Using appropriate labeling, it is then seen that an asympototic solution of (2) for $n\to+\infty$ is of the form $A\exp(-\lambda n)$ with $\lambda>0$.

This suggests looking for a solution to (2) in the form of a series of odd powers of $A\exp(-\lambda n)$. Actually in this way we obtain a family of solutions depending on the positive valued parameter A. We can then introduce a continuous variable $\xi=A\exp(-\lambda n)$ and consider the power series

$$C_1\xi-C_3\xi^3+C_5\xi^5-C_7\xi^7+\cdots, \quad (3)$$

with $C_1\equiv 1$. Substituting in (2), expanding $\sin\psi_n$ in powers of ψ_n, and matching coefficients of ξ^N on both sides, we obtain for $N=1$

$$k(e^{-\lambda}-2+e^{\lambda})=1, \quad (4)$$

and for odd integer values of $N\geqslant 3$

$$C_N=\mathbf{S}(C_1,C_3,\cdots,C_{N-2})\left(\frac{\cosh N\lambda-1}{\cosh\lambda-1}-1\right)^{-1}. \quad (5)$$

The symbol $\mathbf{S}$ is defined by

$$\mathbf{S}(a_1,a_3,\cdots,a_{N-2})=\sum_{\substack{M=3\\(\text{odd})}}^{N}\frac{1}{M!}\sum_{\Omega(N,M)}a_{\alpha_1}a_{\alpha_2}\cdots a_{\alpha_M}, \quad (6)$$

TABLE I. Comparison of exact and approximate solutions.

n	ψ_n^{I}	ψ_n^{II}	V_n	$V_{n+\frac{1}{2}}$	$\bar{\psi}_n^{\mathrm{I}}$	$\bar{\psi}_n^{\mathrm{II}}$	$\bar{V}_n$	$\bar{V}_{n+\frac{1}{2}}$
0	3.1417	2.0286	−0.2802	+0.1364	3.1416	2.1436	+0.1662	−0.0744
1	1.2900	0.7772	+0.0021	+0.0135	1.3560	0.8256	−0.0127	+0.0192
2	0.4819	0.2875	+0.0035	+0.0016	0.4952	0.2952	−0.0094	+0.0037
3	0.1777	0.1095	+0.0006	+0.0002	0.1756	0.1044	−0.0013	+0.0004
4	0.0654	0.0389			0.0620	0.0368	−0.0002	
5	0.0241	0.0143			0.0220	0.0132	−0.0001	

where $\Omega(N,M)$, for $N\geqslant M\geqslant 3$, is the set of all M-tuples $(\alpha_1,\alpha_2,\cdots\alpha_M)$ of odd integers $\alpha_k=1,\ 3,\cdots,\ N\text{-}2$ whose sum is N.

III. CONVERGENCE OF THE SERIES SOLUTION

In order to prove that the series (3) is convergent, consider the equation

$$d^2\psi/dx^2=\sin\psi, \tag{7}$$

which, taking $\lambda n=x$, is the limiting form of (2) as $k\to+\infty$. By (4) this is the continuum limit in which $\lambda\to 0$. We look for a solution to (7) in the form of a power series in $\xi=Ae^{-x}$.

$$\psi(x)=C_1'\xi-C_3'\xi^3+C_5'\xi^5-C_7'\xi^7+\cdots, \tag{8}$$

with $C_1'\equiv 1$, and go through the same steps as before, obtaining

$$C_N'=(N^2-1)^{-1}\mathbf{S}(C_1',C_3',\cdots,C_{N-2}') \tag{9}$$

for $N\geqslant 3$. On the other hand, we know a solution to (7) of the form (8),

$$\psi(x)=4\tan^{-1}\left(\frac{Ae^{-x}}{4}\right)=\xi-\frac{\xi^3}{4^23}+\frac{\xi^5}{4^45}-\frac{\xi^7}{4^67}+\cdots, \tag{10}$$

which is absolutely convergent for $|\xi|<4$ and is twice differentiable term by term. Hence we can identify (10) with (8) term by term.

We can now prove that the series (3) is also absolutely convergent for $|\xi|<4$. From (5) and (9) with (6) it is clear that $C_N>0$ and $C_N'>0$. Thus, for the comparison test of convergence, we need only to show that $C_N'\leqslant C_N$. We first note that for $N>1$

$$\frac{\cosh N\lambda-1}{\cosh\lambda-1}=\frac{\dfrac{(N\lambda)^2}{2!}+\dfrac{(N\lambda)^4}{4!}+\dfrac{(N\lambda)^6}{6!}+\cdots}{\dfrac{\lambda^2}{2!}+\dfrac{\lambda^4}{4!}+\dfrac{\lambda^6}{6!}+\cdots}>N^2. \tag{11}$$

From (5), (9), and (11)

$$\frac{C_N'}{C_N}<\frac{\mathbf{S}(C_1',C_3',\cdots,C_{N-2}')}{\mathbf{S}(C_1,C_3,\cdots,C_{N-2})}. \tag{12}$$

The proof that $C_N'\leqslant C_N$ follows at once from (12) by induction starting with $C_1=C_1'=1$ and using the definition (6). So by the comparison test, the series (3) is absolutely convergent for $|\xi|<4$. For $|\xi|<4\exp(-\lambda)$, this justifies the previous formal steps (4) to (6) which assure that (3) is a solution to (2).

IV. THE PEIERLS ENERGY

The solution obtained can be continued outside of the range $|\xi|<4$ by direct use of the difference equation, for an arbitrary positive value of the parameter A. For $n\to-\infty$ with most values of A the amplitude of ψ_n increases indefinitely. We are, however, only interested in the case of one excess atom. In this case the limiting value of ψ_n as $n\to-\infty$ must be 2π. For two symmetric configurations we are assured of this behavior. The first (I) is a solution symmetric about some maximum of the substrate potential. Labeling the central atom zero, this means that A^{I} must be chosen so that $\psi_0^{\mathrm{I}}=\pi$. The second (II) is a solution symmetric about some minimum of the substrate potential. Labeling zero the atom just to the right of the center, this means that A^{II} must be chosen so that $\psi_{-1}^{\mathrm{II}}+\psi_0^{\mathrm{II}}=2\pi$ and $\psi_0^{\mathrm{II}}<\pi<\psi_{-1}^{\mathrm{II}}$. The difference $E^{\mathrm{I}}-E^{\mathrm{II}}$ in the energy of these two configurations is defined to be the Peierls energy and can be obtained by use of (1).

Usually ψ_n^{I} is approximated by $\bar{\psi}_n^{\mathrm{I}}=\psi(k^{-\frac{1}{2}}n)$, that is, by the solution (8) to (7), with $A=4$ so that $\psi(0)=\pi$. Similarly, ψ_n^{II} is approximated by $\bar{\psi}_n^{\mathrm{II}}=\psi[k^{-\frac{1}{2}}(n+\frac{1}{2})]$. In order to give an idea of the error involved in this approximation, a numerical calculation has been performed for the case $\lambda=1$, corresponding to $k=0.921$ by (4). For several central atoms Table I gives the displacements and the Peierls energy densities in units of $\alpha a^2/4\pi^2$ according to both the exact series solution (3) and the continuum approximation (8). The Peierls energy density is defined by

$$V_s=1-\cos\psi_s^{\mathrm{I}}-\tfrac{1}{2}k(\psi_{s-1}^{\mathrm{II}}-\psi_s^{\mathrm{II}})^2 \tag{13a}$$

for integer values of s, and by

$$V_s=\tfrac{1}{2}k(\psi_{s-\frac{1}{2}}^{\mathrm{I}}-\psi_{s+\frac{1}{2}}^{\mathrm{I}})^2-(1-\cos\psi_{s-\frac{1}{2}}^{\mathrm{II}}) \tag{13b}$$

for half-integer values of s. The approximate Peierls energy density $\bar{V}_s$ is similarly defined in terms of $\bar{\psi}_s^{\mathrm{I}}$ and $\bar{\psi}_s^{\mathrm{II}}$.

V. CONCLUDING REMARKS

A point to notice about this table is that, even though the displacements calculated from the series (ψ_n^{I} and ψ_n^{II}) and from the approximation ($\bar{\psi}_n^{\mathrm{I}}$ and

$\bar{\psi}_n^{II}$) agree fairly well, the Peierls energy density contributions show hardly any agreement even as to sign. Summing V_s over integers and half-integers, the resulting Peierls energy is 0.036 ($\alpha a^2/4\pi^2$) according to the series and is 0.017 ($\alpha a^2/4\pi^2$) according to the approximation.

To get an idea of the order of magnitude of this Peierls energy, we can correlate the model with an actual edge dislocation in silicon or germanium. We choose these materials because the dislocation of our numerical example has a very narrow core. The substrate constant α can be related to a properly defined shear modulus G of the material by $\alpha=Ga$, where a is of the order of the lattice constant. Taking $G=0.5\times10^{12}$ d/cm^2 and $a=5$ A for silicon or germanium, it turns out that $\alpha a^2/4\pi^2\simeq1$ ev. Thus, the Peierls energy is a few hundreths of an ev per atom plane along the dislocation line, a very reasonable result for such a simplified model.

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Kinking and the Fracture of Ionic Solids

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A single crystal undergoing plastic bending develops constraints due to the gradient in lateral contraction across the beam. These constraints result in lateral stresses which may be relieved by the process of anticlastic kinking. Anticlastic kink boundaries in rocksalt structure solids consist of arrays of {121}⟨110⟩ edge dislocations formed by the interaction of two systems of {110}⟨110⟩ glide dislocations, one system being responsible for slip in the main part of the crystal beam, the other confined to its corner.

Temperature affects the structure of kink boundaries and their subsequent role in initiating fracture.

I. At high temperatures (~0.3 Tm). The resultant edge dislocations in the boundary can move over their {121} slip planes and the kinks become sharp. The resultant dislocations are ineffective barriers to slip and the crystals are ductile.

II. At low temperatures (~0.1–0.2 Tm). The resultant edge dislocations are immobile and the kinks consist of a diffuse array. The resultant dislocations provide strong barriers to slip and cracks nucleate at the kink boundary.

III. At very low temperatures (~0.1 Tm). Fracture occurs before the second set of {110}⟨110⟩ glide dislocations have been activated to generate anticlastic kinks. Relaxation of the lateral stress results in a complex fracture.

INTRODUCTION

It is important at the outset to distinguish between two kinds of kinking. The first arises from the elastic interaction between edge dislocations of the same Burgers vector moving on a set of parallel planes while the second arises from the interaction between families of dislocations with different Burgers vectors moving on intersecting slip planes. The first is more familiar in metals and is particularly associated with the compression of hexagonal close-packed single crystals. The crystals become locally plastically unstable and the lattice buckles and kinks by the organized movement of edge dislocations on parallel planes in the manner described by Orowan.[1] Catastrophic buckling of this kind accompanied by large stress drops has been observed and recorded in detail for cesium iodide and other ionic solids by Klassen-Neklyudova *et al.*[2] A similar, though less catastrophic, process is involved in the formation of primary deformation bands which accommodate the crystal lattice rotation relative to the loading axis during tensile deformation. These may also be seen in certain ionic solids (sodium chloride single crystals, for example) elongated in tension at room temperature.

The second type of kink band which is the chief concern of the present paper is associated with the deformation of ionic solids under loading conditions where there is an imposed constraint. Their occurrence has been stressed by numerous Russian workers[2–4] and by Pratt and co-workers.[5,6] Originally these kink bands were discovered by Brilliantov and Obreimov,[7] who compressed squat, and therefore constrained, slabs of sodium chloride. Their appearance led these authors to refer to the kinks as "irrational twins," although it is now appreciated that this is a misnomer since they originate by glide. Klassen-Neklyudova *et al.*[2] have suggested that they now be referred to as "Brilliantov-Obreimov" bands. Similar kinking has been observed

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