1980


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THE SOLUTION TO SINGLE KINK SOLITARY WAVE TRANSPORT FOR SYSTEMS DESCRIBED BY A GENERALIZED FRENKEL-KONTOROVA EQUATION

The Louisiana State University and Agricultural and Mechanical Col.

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THE SOLUTION TO SINGLE KINK SOLITARY WAVE TRANSPORT FOR SYSTEMS DESCRIBED BY A GENERALIZED FRENKEL-KONTOROVA EQUATION

A Dissertation

Submitted to the Graduate Faculty of the Louisiana State University and Agricultural and Mechanical College in partial fulfillment of the requirements for the degree of Doctor of Philosophy

in

The Department of Physics and Astronomy

by

Louis William Adams, Jr.
B.S., Youngstown State University, 1973
M.S., New Mexico State University, 1975
August 1980
ACKNOWLEDGEMENTS

I like this dissertation and that is a happy coincidence. My advisor, J.C. Kimball, allowed me the freedom to pursue this work in my own style while being The Source when I could not resolve some difficulty. So, I thank him for suggesting this problem, maintaining a comfortable distance, but helping selflessly when appropriate. I also thank him for permission to use Fig. 7 from his own work.

Correspondence with K. Nakajima, P.M. Marcus and especially M. Büttiker has been important and I thank them for responding to my letters. A.R.P. Rau brought the content of Chapter III, Section F, to my attention and I appreciate such a satisfying observation about the mathematical analysis I adopted for this work.

Past enthusiasm of J.D. Zund and E.P. Wigner in matters mathematical and physical, respectively, have influenced my approach and thinking about this work, and their influence on me has worked its way into my writing. This can only help.

Ultimately, any errors in this work are strictly my own.
"... Enter now the marching cordon,

flying banners of sine Gordon! ... "

J.A. Krumhansl
from "Solitons in Oxford"
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ABSTRACT

A numerical procedure to solve the differential equation for solitary waves via iteration for a generalized Frenkel-Kontorova model is presented. The generalization consists of adding a constant force proportional to particle velocity. The equation of motion is cast into integral form using a Green's function.

The introductory chapter briefly reviews recent progress in nonlinear dynamics using the sine-Gordon equation as an example. Emphasis is placed on the concept of "nonlinear modes" and its relevance in theoretical descriptions of transport processes.

After a second chapter defining the generalized Frenkel-Kontorova equation, its dimensionless reparametrization and an outline of the iteration scheme, the third chapter defines and solves the continuum approximation of a single kink transport problem. An exact functional relationship connecting applied force, friction and the resulting solitary wave velocity is given. Use is made of the sine-Gordon equation and a power balance formula in choosing a good trial solution. The numerical solution of the transport problem is given and compared with the work of others as well as the exact solutions of two similar
problems. I also demonstrate how the calculation is related to a variational principle.

In the fourth chapter the full discrete case is examined. How this differs from the continuum approximation is discussed as well as why the continuum approximation fails to adequately model aspects of transport processes in such applications as crystal defect propagation and superionic conductors. After presenting the solution to a related solvable model, I present results of my calculations.

Throughout this work the Green's function used in the numerical analysis is shown to have physical meaning and is used in particular to clarify the role of discreteness in transport processes. No simplifying assumptions are made.
A. The Recent Revival of Interest in Nonlinear Dynamics

There is no general prescription for solving nonlinear differential equations. The tricks and guesses used to obtain solutions in specific cases rarely apply to other situations. Sometimes even an adequate numerical solution may be very difficult to obtain. This is unfortunate because many interesting physical problems are nonlinear. Turbulence as described by the nonlinear equations of hydrodynamics is one example of a physical process lacking quantitative mathematical and numerical treatment.

The recent development of new mathematical means to systematically construct analytical solutions as well as the increasing computational power of computers has dramatically increased the amount of research being done in the nonlinear problems of physics. Indeed, this progress has been significant enough to serve as a unifying interest among different disciplines. This will be evident later in my presentation.

Systems having nonlinear dynamics can have solutions such as travelling or standing waves which persist rather than disperse. Nonlinear processes are frequently
described as self organizing for this reason. In linear systems dispersion relations summarize an opposite tendency: The tendency to disperse.

Systematic means to find solutions to physically interesting nonlinear differential equations is important because such solutions are frequently not accessible to finite order linear perturbation theory.\(^1\) The particular mathematical breakthrough for finding analytical solutions to some differential equations which is responsible for much of the recent progress is the "inverse scattering transform". A succinct description of the inverse scattering transform which highlights its relevance to physics is given by A.R. Bishop who writes that it is\(^2\)

\[\text{... a canonical transformation to functions of generalized action-angle variables, which serve to label allowed types of excitation ('non-linear normal modes') in the system ...} \]

Thus the solution of an arbitrary initial value problem can be 'labelled' by its nonlinear mode components, and can indeed be expressed in the form of a generalized Fourier transform with respect to these.

It would not serve the purposes of this presentation to provide a detailed discussion of this method, but the next two sections will provide relevant concrete examples clarifying what is meant by "non-linear modes".
B. Sine-Gordon Equation

Of particular interest to the new interdisciplinary study of nonlinear dynamics are solutions which are pulse-like or localized in some way. As a specific example I will discuss the sine-Gordon equation

\[ U_{TT}(X,T) = U_{XX} - \sin U \]  \hspace{1cm} (1)

Assume \( X \) and \( T \) are spatial and temporal coordinates of a wave having amplitude \( U(X,T) \). Let me list five solutions to this equation along with what they have been named. \(^3\)

**Soliton**

\[ U = 4 \arctan\left(\exp\left(\frac{X-vT}{\sqrt{1-v^2}}\right)\right) \]  \hspace{1cm} (2a)

**Antisoliton**

\[ U = 4 \arctan\left(\exp\left(-\frac{X-vT}{\sqrt{1-v^2}}\right)\right) \]  \hspace{1cm} (2b)

**Soliton-Soliton Collision**

\[ U = 4 \arctan\left(\frac{\sinh\left(X/\sqrt{1-v^2}\right)}{\cosh\left(vT/\sqrt{1-v^2}\right)}\right) \]  \hspace{1cm} (2c)

**Soliton-Antisoliton Collision**

\[ U = 4 \arctan\left(\frac{\sinh\left(vT/\sqrt{1-v^2}\right)}{v \cosh\left(X/\sqrt{1-v^2}\right)}\right) \]  \hspace{1cm} (2d)
Soliton-Antisoliton Bound State (Breather)

\[ U = 4 \arctan\left( \frac{\sin \epsilon \sin((\cos \epsilon)T)}{\cos \epsilon \cosh((\sin \epsilon)X)} \right) \]

\[ 0 < \epsilon < \frac{\pi}{2} \]  \hspace{1cm} (2e)

Because the sine-Gordon equation is Lorentz invariant under the Lorentz transformations

\[ X' = \frac{X - v'T}{\sqrt{1 - (v')^2}} \]  \hspace{1cm} (3a)

\[ T' = \frac{T - v'X}{\sqrt{1 - (v')^2}} \]  \hspace{1cm} (3b)

so are each of the solutions given by Eqs. (2).

The first two solutions, Eqs. (2a) and (2b), are travelling waves. The wave amplitude \( U \) is a function of \( X - vT \) so they are waves of permanent profile travelling at a constant velocity \( v \). These travelling waves are also solitary waves. A solitary wave is a travelling wave which, as a disturbance, is localized. Because the soliton and antisoliton solutions are solitary waves, dispersion is absent. It is a consequence of the nonlinearity of \( \sin(U) \) that these step like solutions hold themselves together. Dispersion occurs when the different Fourier contributions to a wave travel at different velocities and nonlinearity causes the contribution of higher frequency components of the Fourier terms to increase.\(^5\) (One example of this latter mechanism is obvious in the peaking and curling of ocean waves.) These two tendencies balance precisely in
Eqs. (2a) and (2b). When dissipation processes like friction are present, they can also balance a nonlinearity of this kind.

It is customary to designate a solution which changes by a fixed value over a limited region a kink. This fixed value is $2\pi$ in Eqs. (2a) and (2b) and they are for this reason single kink and single antikink solutions. The kink and antikink solutions behave like classical particles in that their shapes are constant, but their widths undergo a contraction as a function of $v$ following the usual formula of the relativistic Lorentz contraction. Note multiples of $2\pi$ may be added to Eqs. (2) and the results still satisfy Eq. (1), the sine-Gordon equation.

When Eq. (2c) is carefully examined, it looks like a collision between two kinks like that of Eq. (2a). In fact when the two kinks comprising this solution are far apart, this third solution analytically reduces to two formulas like the first solution. So Eq. (2c) is a two kink solution. Note, however, Eq. (2c) does not arise from the simple addition of two single kink solutions. Linear superposition fails here. Similarly Eq. (2d) is, as its name implies, interpretable as the collision of a kink and antikink as given by Eqs. (2a) and (2b). But it is not a linear combination of them.

The "breather" solution can be considered to be the bound state of a kink-antikink pair. It is localized in space and undergoes periodic oscillations in time.
Numerical simulations have demonstrated that when dissipative effects are included in the sine-Gordon equation, a kink and antikink can indeed collide to form such a solution. I might add too that in such a collision little ripples leak off which is termed "radiation".

All of the solutions are termed **solitons** because of the shape preserving nature of the collisions. These pulse-like solutions have the same shapes and speeds after a collision as before and this is a general property: There are an indefinitely large number of solutions of the sine-Gordon equation (and other equations) which behave this way as a class. I will say more about this in the next section. Note that a soliton is a solitary wave, but a solitary wave need not be a soliton.

The select solutions that I have presented for the sine-Gordon equation are for infinite systems: The domain of $X$ is infinite. Analytical solutions to the sine-Gordon equation for finite systems have been recently derived in terms of Jacobian elliptic functions which are completely analogous to these solutions for the infinite systems. Consequently there is a wealth of analytical information for this particular equation. For this reason it has been extensively applied in physics. So far my discussion of the sine-Gordon equation may give the impression that all one can look forward to are cookbook like listings of known solutions. This is where the inverse scattering transform and the idea of "nonlinear modes" enters.
C. Nonlinear Modes

Clearly Eqs. (2), as solutions to a nonlinear differential equation, cannot be linearly superposed to obtain more general solutions. No linear superposition principle holds. Indeed, the mathematical structure of the two kink solution Eq. (2c) looks very different from the single kink solution Eq. (2a) even though Eq. (2a) is a special case of Eq. (2c). Actually there is a mathematical rule called the Bäcklund transformation which can take any solution of the sine-Gordon equation and be used to produce a new solution of the sine-Gordon equation. The single kink solution can, for example, even be generated from the no kink solution ("vacuum") \( U = 0 \). Another related rule can take any two solutions and create a third. The two kink solution, Eq. (2c), can be generated from two one kink solutions having the form of Eq. (2a). And so on. Therefore we effectively have an instance of a nonlinear superposition principle.

For this reason, all of these solutions can be designated "nonlinear modes". They are modes in that they can be treated as elementary solutions upon which more complex solutions can be constructed. The earlier quote by A.R. Bishop will make more sense when read with this definition in mind.

Now the question is, do these identifiable modes have any relevance in "real" problems? After all, if the nonlinear modes will only appear if initial conditions are
just so, how can this be used as a basis for a more complete analysis? The answer is that arbitrary initial waveforms break up (evolve in time) into these persistent nonlinear modes and nonpersistent waves called continuum modes or simply "radiation" or "phonons". I point out that this property is not confined only to the sine-Gordon equation. And in some cases nonlinear superposition relationships are known for both the nonlinear modes and the continuum modes combined. These observations culminate in the conclusion that is is not unreasonable to study nonlinear modes as things-in-themselves.

If nonlinear modes of physical systems were truly solitons, then this would imply a violation of the assumption of ergodicity in statistical mechanics. They would radically alter how such a system would thermalize or prevent it from thermalizing at all. This would occur because the solitons would not share their energy with the rest of the system or each other. Of course, this presumes solitons can survive thermal perturbations. Simulations suggest this may be the case and in addition thermal effects can generate kink-antikink pairs. However, simulations by necessity have dispersive and discrete characteristics built in that will not precisely emulate the ideal properties of equations like sine-Gordon.
D. Transport

Information about physical systems like solids is typically obtained by applying a force either as a stress or electromagnetic field. A steady state can be established where the power delivered by the external force is balanced by dissipative effects. Therefore it is natural to seek travelling wave solutions of linear or nonlinear systems in problems involving the transport of mass or charge or whatever.

With the addition of such realistic details as dissipation and/or applied field to models supporting soliton solutions, the nice properties described in the previous section tend to dissappear. The travelling waves described by the modified equation may be solitary waves, but not solitons. Even if solitary waves do not survive collisions they may significantly affect transport processes if their lifetimes are long enough. So again it is appropriate to concentrate on particular solitary waves as a first step in modeling a generally complex transport process.

One need not totally abandon hope of making use of known soliton solutions in the modified equations. "Real" travelling waves may be small perturbations on solitons. Solitons can be dressed with perturbations for more realistic circumstances. After discovering solitary wave solutions in ideal circumstances, one may perform perturbations "about" these nonlinear modes. A multisoliton perturbation
theory for equations like the sine-Gordon equation has been developed\textsuperscript{15} which is capable of determining, for example, the radiation produced by solitons accelerated by applied forces.

A word of caution is advisable when such realistic additions are made. Sometimes unexpected features may arise. As an example, the sine-Gordon equation has solutions representing two solitons travelling in the same direction with different speeds. However, no solution exists for two solitons travelling in the same direction when the speeds are the same. Yet when friction and an applied force are added, such solutions do exist and are stable.\textsuperscript{16}

E. Summary and Objective

Good molecular dynamics calculations which attempt to completely compute the evolution of many particle systems amenable to classical theory are probably the best way of trying to predict transport behaviour of systems. However, even at the present time these calculations are difficult and it is hard to study the role of particular modes. There are indications that with the addition of friction and even discreteness (i.e., the fact that the particles of the system are separate and do not constitute a continuous material) solitary wave solutions exist.\textsuperscript{17} Consequently I reiterate it is reasonable to pick an elementary nonlinear mode for study of a suitable generalization of the sine-
Gordon equation. This is what I will consider in the remainder of this work and I will choose the single kink mode analogous to Eq. (2a). In order to avoid perturbation theories, complete function expansions and finite difference approximations of derivatives, I have developed a practical iterative technique for a commonly used generalization of the sine-Gordon equation. This equation supports solitary wave motion in a one dimensional system of harmonically coupled discrete particles moving in a spatially periodic external potential. The system has dissipative effects (phenomenological friction) and a compensating constant external force.
A. Definition of the Equation and Specification of the Transport Problem

In what follows the reader may wish to refer to Fig. 1 which provides an analog for the equations to be discussed.

One physical interpretation of the sine-Gordon equation

$$\mu_{tt}(x,t) = k a^2 u_{xx} - V_0 \sin(\frac{2\pi u}{a})$$  \hspace{1cm} (4)

is that particle n, where n is an integer, is displaced u(na,t) from position na. The particles all have mass m and interact with each other through nearest neighbor harmonic forces approximated by $ka^2 u_{xx}(na,t)$. The periodic force of amplitude $V_0$ and spatial period "a" can represent the net force produced by an immobile lattice of other particles.

The Frenkel-Kontorova equation differs from the sine-Gordon equation by having the particles interact in truly harmonic fashion with harmonic force constant k.

$$\mu_{tt}(na,t) = k[u((n+1)a,t)-2u(na,t)+u((n-1)a,t)] - V_0 \sin(\frac{2\pi u}{a})$$  \hspace{1cm} (5)
Figure 1a The above diagram indicates a physical model for the generalized Frenkel-Kontorova equation, Eq. (7). Masses connected by (invisible) springs move on a sinusoidal surface. The series of sketches schematizes the transport of one vacancy via a one kink solitary wave. The various parameters are explained in the text.
Figure 1b Complementary to Fig. 1a, the above diagram represents the transport of one interstitial via a one anti-kink solitary wave.
In the "continuum approximation"

\[ u((n+1)a,t) - 2u(na,t) + u((n-1)a,t) = \varepsilon \partial^2 u_{xx}(na,t) \]  

(6)

the Frenkel-Kontorova equation, Eq. (5), reduces to the sine-Gordon equation, Eq. (4).

I generalize the Frenkel-Kontorova equation like so.

\[ \mu u_{tt}(na,t) = ku((n+1)a,t) - 2u(na,t) + u((n-1)a,t)) 
- Du_t - V_0 \sin(\frac{2\pi u}{a}) - F \]  

(7)

A velocity dependent force with friction constant \( D \) provides an energy sink, and a constant external force \( F \) provides an energy source. If \( D \) and \( F \) are zero, Eq. (7) reduces to the Frenkel-Kontorova equation, Eq. (5). I will always refer to this as the generalized Frenkel-Kontorova equation. It has frequently been used in lattice defect propagation, but is applicable whenever discreteness cannot be ignored and transport is induced.

There are unrealistic aspects of this equation as a basis for modeling physical processes. The phenomenological friction term provides an energy sink for the moving particles and, as such, could represent the effects of collisions with a lattice, thermalization, production of induced electrical currents, et cetera. But this energy simply vanishes from the mathematical model, and this is unphysical.

In real systems where this equation is applied, there is a hard core repulsion force between the particles.
However, the particles are described in the equation as transparent to one another because of the harmonic interaction. In addition this interaction is strongly attractive as the displacement between particles increases between nearest neighbors. A net repulsive interaction is simulated in one aspect: The mass chain finds it energetically favorable for the particles to be evenly spaced, ignoring the effect of the lattice potential.

Seeking only travelling wave solutions of Eq. (7) allows us to introduce a dynamical constraint simplifying the analysis.

\[ u(a_n, t) = u(a_n - vt) \]  

(8)

The function \( u \) only depends on one variable, \( a_n - vt \). Here the parameter \( v \) is the travelling wave velocity. It will always be a positive number in this presentation. When friction is nonzero the external force \( F \) is necessary to maintain the shape and velocity of a solitary wave. The primary goal of this work is to determine the relationship between the velocity of a single kink solution comparable to Eq. (2a), and the external force required to maintain it. I will write "transport" when I refer to the velocity versus applied force relationship. The boundary conditions of this single kink solution are
\begin{align*}
    u(+ \infty) &= a(1 - \frac{\arcsin(F/V_0)}{2\pi}) \quad (9a) \\
    u(- \infty) &= -a \frac{\arcsin(F/V_0)}{2\pi} \quad (9b)
\end{align*}

These follow from Eq. (7) because the derivatives must vanish at \( x = \pm \infty \). There are seven physical parameters in this problem: \( m, k, D, V_0, F, a \) and \( v \).

So far I have not been very specific about what it is that is being transported. Fig. 1a indicates what I have in mind. The particles help one another over the sinusoidal barriers via harmonic interaction in response to one vacancy in the mass chain. The vacancy moves in the opposite direction of the applied force \( F \) while all of the particles move in the same direction by one lattice constant. In this way it mimics Eq. (2a). So the solitary wave moves in the same direction as the vacancy, towards the right in Fig. 1a.

Fig. 1b illustrates the situation when, instead of a vacancy, an extra particle is in the mass chain. Because of the nature of the equation of motion, the one vacancy problem is equivalent to the one interstitial particle problem, as far as the resulting force versus velocity relationship is concerned. So if Eq. (2a) corresponds to a one vacancy solution, Eq. (2b) corresponds to a one interstitial solution in the absence of \( F \) and \( D \). Since vacancy motion and interstitial motion are both supported by the equation of motion (this can be formally proven) it is not
impossible that "kink-antikink creation" could occur in the springs and masses model: Perhaps a thermal perturbation could produce a vacancy moving in the opposite direction of F (a kink) and an interstitial moving in the same direction as F (an antikink). A current of unit mass would be established and the net result is one unit of mass carried to minus infinity.

B. Dimensionless Parametrization

My dimensionless parametrization of Eqs. (7), (8) and (9) is somewhat involved and begins with these definitions:

\[ u(na,t) = aU(na,t) \quad (10a) \]
\[ f = \frac{F}{V_0} \quad (10b) \]
\[ K = \frac{ka}{2\pi V_0} \quad (10c) \]
\[ \bar{X} = \sqrt{\frac{2\pi V_0}{ka}} n = \frac{n}{\sqrt{K}} \quad (10d) \]
\[ c = \sqrt{\frac{ka^2}{m}} \quad (10e) \]
\[ T = \sqrt{\frac{2\pi V}{ma}} t = \frac{ct}{a/\sqrt{K}} \quad (10f) \]
\[ \bar{g} = \sqrt{\frac{a}{2\pi maV_0}} \quad (10g) \]

With these definitions the equation of motion reduces to
\[ U_{TT}(n_a,t) = K(U((n+1)a,t)-2U(na,t)+U((n-1)a,t)) \]

\[ - \frac{\partial}{\partial t} U_T - \left( \frac{\sin 2\pi U + f}{2\pi} \right) \]  

(11)

To complete the reparametrization let

\[ g = \frac{g}{\sqrt{1-V^2}} \]  

(12a)

\[ U(an,t) = U(\sqrt{\frac{1+g^2}{1-V^2}}(X-VT)) = U(X) \]  

(12b)

\[ h = \sqrt{\frac{4+g^2}{K(1-V^2)}} \]  

(12c)

The final equation is

\[ (h,\nabla)^2 U(X) + \frac{g}{\sqrt{4+g^2}} U' - \left( \frac{\sin 2\pi U + f}{2\pi(4+g^2)} \right) = 0 \]  

(13a)

where I have defined an operator

\[ (h,\nabla)^2 U(X) = \frac{1}{1-V^2} \left( \frac{U(X+h)-2U(X)+U(X-h)}{h^2} - \nabla^2 U''(X) \right) \]  

(13b)

The boundary conditions are now

\[ U(+\infty) = 1 - \frac{\arcsin f}{2\pi} \]  

(14a)

\[ U(-\infty) = -\frac{\arcsin f}{2\pi} \]  

(14b)

I presented the above equations in that order which leads to Eqs. (13) and (14) most easily. A more convenient list of the parameters is given below.
The dimensionless parametrization of the generalized Frenkel-Kontorova equation involves ultimately only four parameters: \( f, g, \overline{v} \) and \( h \). This is about half the number of the original equation, Eq. (7). Each of these dimensionless parameters has a clear physical interpretation.

The constant \( c \) of Eq. (15e) is the velocity at which small amplitude periodic waves propagate at long wavelengths; i.e., the "sound velocity". This can be verified by linearizing Eq. (7), ignoring friction and the external force, and making the continuum approximation, Eq. (6). Therefore Eq. (15d) implies \( \overline{v} \) is the velocity of the solitary wave in units of the velocity of sound. The presence of \( \sqrt{1-\overline{v}^2} \) in the parametrization implies \( \overline{v} \leq 1 \).
The external force and friction parameters F and D are proportional to f and g, respectively. For the propagation of solitary waves, f can be no larger than 1. If it were greater than 1, all particles would be pushed over the sinusoidal potential. In addition, Eqs. (14) for the boundary conditions would make no sense. By absorbing an additional factor of $\sqrt{4 + g^2}$ into the argument of U (see Eq. (12b)) an advantage in the numerical calculations is gained even though some formulas will be more complicated than necessary. The advantages will be indicated later.

I call h the "discreteness" parameter because its size determines how important the discrete mass character of the system affects the dynamics. The distance between the mass particles in dimensionless units is h. When h tends to zero, the finite difference of Eq. (13b) tends to $U''(X)$. In fact

$$\lim_{h \to 0} (h, \bar{v}^2)_{X} = (0, \bar{v}^2)_{X} = \frac{d^2}{dX^2}$$

(16a)

The harmonic interaction dominates the inertial contribution in this case. Further

$$\lim_{h \to \infty} (h, \bar{v}^2)_{X} = (\infty, \bar{v}^2)_{X} = -\frac{\bar{v}^2}{1 - \bar{v}^2} \frac{d^2}{dX^2}$$

(16b)

Here the inertial contribution dominates the harmonic interaction. In Chapter II, Section E, a solution is presented where these two contributions always cancel.
C. Two Invariants

There seems to be little that can be done with Eqs. (13) analytically. But nonlinear equations sometimes have invariants, conserved quantities, which are constants of motion. I will present two such invariants for Eqs. (13). (The sine-Gordon equation has an infinite number of constants of motion.)

The first is derived by integrating Eqs. (13) over X from minus infinity to plus infinity and utilizing the boundary conditions, Eqs. (14). The result is

\[ 2\pi g\sqrt{4+g^2} = \int_{-\infty}^{+\infty} (\sin 2\pi U(X) + f) dX \]  

This "moment" of the differential equation indicates the balance which must be maintained between the momentum supplied by the external force (with due consideration to the lattice potential) and the momentum lost because of the dissipative force. Without this balance solutions would "run away" as momentum accumulates: Solitary wave solutions would not be possible.

The second identity is derived by multiplying Eq. (13a) by \(U'(X)\) and again integrating as before. The result this time is

\[ f = 2\pi g\sqrt{4+g^2} \int_{-\infty}^{+\infty} (U'(X))^2 dX \]  

This "first velocity moment" of the differential equation quantifies the requirement that there be a balance between
the power supplied by the applied field and the power dissipated by friction. Again, without this balance, solitary waves will not be possible. This interpretation comes from noting the derivation is accomplished by integrating force times velocity: total power. I will use this invariant numerically as described later.

The finite difference term in Eq. (13b) represents the harmonic interaction between nearest neighbor particles and constitutes internal forces of the system. As such, these forces do not contribute to either of the invariants. It can be rigorously be shown they cancel upon integration.

D. Fundamental Identity

Let me rewrite the dimensionless equation of motion, Eq. (13a), as follows.

\[
(h,\sqrt{\alpha}) \frac{d^2 U(x)}{dx^2} + \frac{E}{\sqrt{4 + g^2}} U' - \frac{1}{4 + g^2} U = \frac{\sin 2\pi U - 2\pi U + f}{2\pi(4 + g^2)}
\]  

(18a)

If the right side of the equation were zero, the remaining left side would be a tractable linear differential equation. In fact it would resemble the equation of motion of harmonically coupled oscillators. We can formally treat the right side of the equation

\[
S[U(x)] = \frac{\sin 2\pi U - 2\pi U + f}{2\pi(4 + g^2)}
\]  

(18b)

containing the nonlinearity \( \sin 2\pi U \) as a source term driving a system which has an equation of motion given by the
left side. This is a common technique in mathematical physics. It allows me to cast the equation of motion into integral form via a Green's function.

Using Green's functions with a nonlinear differential equation may seem strange, and in order to avoid any misunderstandings I present a derivation.¹⁹ Let me denote

\[ L_X = (h, \nabla^2)_X + \frac{\xi}{\sqrt{4 + \xi^2}} \frac{d}{dx} - \frac{1}{4 + \xi^2} \]  

so Eqs. (18) can be written as

\[ L_X U(X) = S[U(X)] \]  

I introduce \( G(X-X') \), the Green's function for the operator \( L_X \), and note the following identity is a simple consequence of integration by parts. Note carefully when \( X \) is and is not primed.

\[
\int_{-\infty}^{+\infty} G(X-X')(L_X U(X'))dX' = \int_{-\infty}^{+\infty} (L_X G(X-X')) U(X')dX' \\
+ \left[ \frac{\xi}{\sqrt{4 + \xi^2}} G(X-X') U(X') \right]_{-\infty}^{+\infty} \\
- (\frac{\nabla}{1-\nabla^2})(G(X-X') \frac{dU(X')}{dX'}) \\
- \frac{dG(X-X')}{dX'} U(X')) \right]_{-\infty}^{+\infty} 
\]

So far I have not specified any properties of \( G(X-X') \) beyond those implicitly assumed by allowing integration by parts. Now I make the choices
\[ G(\pm\infty) = 0 \]  \hspace{1cm} (21a)

\[ G'(\pm\infty) = 0 \]  \hspace{1cm} (21b)

\[ L'G(X-X') = d(X-X') \]  \hspace{1cm} (21c)

where \(d(X-X')\) is my notation for the Dirac delta function.

With these choices Eq. (20) reduces to what I will now on refer to as "the identity".

\[ U(X) = \int_{-\infty}^{+\infty} G(X-X')S[U(X')]dX' \]  \hspace{1cm} (21d)

Because this identity is valid irrespective of the boundary conditions on \(U\), its solution is not unique. Boundary conditions must supplement Eq. (21d). Note the Green's function does not involve \(U\) in any way.

Given \(G\), I can use some well-known techniques for analyzing linear systems in this nonlinear problem. What I will do is use Eq. (21d) as an iteration equation for \(U\) to determine single kink solutions. There are no approximations in this approach, nor is it a perturbation theory in the usual sense of an expansion in some small parameter.

E. Green's Function

In a more expanded form Eq. (20c) is

\[ (h\nabla^2)G(X) + \frac{g}{\sqrt{4+g^2}}G' - \frac{1}{4+g^2}G = d(X) \]  \hspace{1cm} (22)
This equation indicates the Green's function contains no information about the applied field nor about the mechanics of motion over the potential barriers between two successive minima of the sinusoidal potential. It is essentially the equation of motion of harmonically coupled particles, each of which sit in a parabolic potential. The delta function is a travelling impulse (since \( X = \overline{X} - \overline{V} T \) which strikes each mass once in succession in time intervals of \( a/V_0 \). The solution to Eq. (22), the Green's function, will indicate the response of the system to these impulses. Its normalization is

\[
\int_{-\infty}^{+\infty} G(X) dX = -(4+g^2) \tag{23}
\]

as can be determined by integrating Eq. (22).

The Green's function can be found in integral form using the fourier transform. Let

\[
G(X) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \mathcal{G}(k) e^{ikX} dk \tag{24a}
\]

\[
d(X) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \frac{1}{\sqrt{2\pi}} e^{ikX} dk \tag{24b}
\]

Applying the fourier transform to Eq. (22) we find

\[
\mathcal{G}(k) = -\frac{1}{\sqrt{2\pi}} \left[ \frac{1}{1-V^2} \left( \frac{\sin \left( k \frac{h}{\sqrt{2}} \right)}{h/2} \right)^2 - V^2 k^2 \right]^{-1} \left( \frac{k}{\sqrt{4+g^2}} \right) \frac{1}{\sqrt{4+g^2}} \tag{25}
\]

If we care to identify \( e^{ikX}/\sqrt{2\pi} \) in Eq. (24a) as a phonon of the lattice of particles with (dimensionless) wavevector \( k \), then \( \mathcal{G}(k) \) is essentially a phonon density of states. That
is, the relative number of phonons of wavevector $k$ comprising the Green's function and generated in response to the series of unit impulses is

$$dn(k) = \frac{1}{\sqrt{2\pi}} \left( \frac{G(k)}{G(0)} \right) dk$$  \hspace{1cm} (26a)$$

where

$$n = \int_{-\infty}^{+\infty} \left( \frac{dn(k)}{dk} \right) dk = 1$$  \hspace{1cm} (26b)$$

which follows from Eq. (24a).

The Green's function is not a trivial function as can be made most evident by simply writing it out completely.

$$G(X) = -\frac{1}{2\pi} \int_{-\infty}^{+\infty} \frac{e^{ikX} dk}{1 - \frac{1}{2} \left[ \left( \frac{\sin k\hbar}{\hbar} \right)^2 - \frac{\varepsilon}{\sqrt{4 + \varepsilon^2}} \right] - \frac{\varepsilon}{\sqrt{4 + \varepsilon^2}} \frac{1}{4 + \varepsilon^2}}$$  \hspace{1cm} (27)$$

There are two limiting cases for which elementary formulas for the Green's function can be easily derived using contour integration and Eqs. (16). They are

$$G_0(X) = \lim_{h \to 0} G(X) = -\exp\left(-\frac{\varepsilon}{\sqrt{4 + \varepsilon^2}} + \text{sgn}(X)X\right)$$  \hspace{1cm} (28)$$

and

$$G_\infty(X) = \lim_{h \to \infty} G(X) = \frac{1}{w} \left( \frac{1 - \sqrt{w^2}}{\sqrt{w^2}} \right) \exp(eX) \sin(wX) H(-X)$$  \hspace{1cm} (29a)$$

where

$$e = \frac{1}{2} \left( \frac{1 - \sqrt{w^2}}{\sqrt{w^2}} \right) \frac{\varepsilon}{\sqrt{4 + \varepsilon^2}}$$  \hspace{1cm} (29b)$$
Here the signum and Heaviside functions are

\[ \text{sgn}(X) = \begin{cases} +1 & X > 0 \\ -1 & X < 0 \end{cases} \]  

(30a)

and

\[ H(X) = \begin{cases} +1 & X > 0 \\ 0 & X < 0 \end{cases} \]  

(30b)

respectively.

Both of these special cases for G satisfy Eqs. (21) whenever a finite velocity and friction is present.

F. General Remarks on Numerical Calculations

Combining Eqs. (21d) and (23), the identity can be written as

\[ U(X) = -\frac{f}{2\pi} + \frac{1}{4\pi g^2} \int_{-\infty}^{\infty} G(X-X') \left( \frac{\sin 2\pi U(X')}{2\pi} - U(X') \right) dX' \]  

(31a)

This integral identity is more attractive from a numerical standpoint than the original differential equation. Integration is a safe numerical calculation while differentiation is not, in the context of solving nonlinear differential equations. Recall Eq. (17b) which I here renumber.

\[ f = 2\pi g \sqrt{4\pi g^2} \int_{-\infty}^{\infty} (U'(X))^2 dX \]  

(31b)

Eqs. (31) are the basis for my numerical approach.

After choosing a trial solution for f and U, I use Eq. (31a)
to give a new trial solution more closely satisfying the equation of motion. This in turn is substituted into Eq. (31b) to determine the new trial value of $f$. Remember Eq. (31b) constrains $f$ to be a value consistent with power balance, solutions which do not accelerate. I can repeat this process until sufficient convergence is achieved. If superscripts indicate iteration number, we can denote this algorithm by

$$U^{(n+1)}(X) = -\frac{f^{(n)}}{2\pi} + \frac{1}{4\pi g} \int_{-\infty}^{\infty} G(X-X') \left( \frac{\sin 2\pi U^{(n)}(X')}{2\pi} - U^{(n)}(X') \right) dX'$$

(32a)

$$f^{(n+1)} = 2\pi g \sqrt{4 + g^2} \int_{-\infty}^{\infty} ((U^{(n+1)}(X))^2) dX$$

(32b)

In actual practice $U(X)$ is represented by a finite number of values over a limited domain of $X$. Because of this, the convergence of the iteration is significantly accelerated by introducing newly iterated point values of $U$ at those values of $X$ in the mesh into the iteration as soon as they are computed rather than waiting until an entirely new $U$ over all values of $X$ is determined. The notation needed to communicate this more clearly is so cumbersome and obscuring that I refer the reader to an appendix where a sample computer program is provided.

In any event, generally speaking $G$ is exponentially damped for large magnitude $X$ and this aids in the convergence of the iteration. In addition, for small values of $U$, the sinusoidal term and the linear term nearly cancel in
Eq. (32a). I intentionally built this into the identity to aid convergence of the iteration. More generally, far from the origin where the kink will be centered in my trial solutions for \( U \), the iteration convergence tends to be quadratic in the difference between successive iterations. To see this, Eq. (32a) can be used. Defining

\[
e_n(X) = U^{(n)}(X) - U^{(n-1)}(X) \tag{33a}
\]

and

\[
\bar{U}_n(X) = \frac{1}{2}(U^{(n)}(X) + U^{(n-1)}(X)) \tag{33b}
\]

then the subtraction of two successive iterations gives

\[
e_n(X) = \frac{1}{4\pi g^2} \int_{-\infty}^{+\infty} G(X-X')(\frac{1}{\pi}\cos(2\pi \bar{U}_{n-1}(X'))\sin(\pi e_{n-1}(X')) - e_{n-1}(X'))dX' \tag{33c}
\]

When \( X \) is large in magnitude let me assume for the sake of this argument that iterations always obey the boundary conditions and

\[
\cos(2\pi \bar{U}_{n-1}) = \cos(2\pi \bar{U}_{n-1}(\pm \infty)) = \sqrt{1-r^2} \tag{34a}
\]

(See Eqs. (14).)

\[
\sin(\pi e_{n-1}(X)) \approx \pi e_{n-1}(X) - \frac{\pi^2}{2} e_{n-1}(X) \tag{34b}
\]

Because \( G \) is significant only when \( X \) is comparable to \( X' \) in the integrand, when \( X \) is large Eqs. (34) permit the approximations
If the maximum difference between iterations \( n-2 \) and \( n-1 \) is \( \text{Max}(e_{n-1}(X))=0.1 \), then \( e_n(X) \leq 0.02 \), etcetera. This derivation is not meant to be rigorous, but it suggests that if convergence occurs, it ought to quadratically converge from the ends towards the center.

Determining the Green's function in the general case means numerically computing a fourier transform indicated by Eq. (27), or, at least, its real part since the imaginary part vanishes. Because this computation must be performed on a finite mesh, small spurious oscillations may appear. But the iteration requires integration and these oscillations will be smoothed out in the convolution. This is another bonus using such an identity. Oscillations grow when differentiation is numerically computed unless great care is taken. No special numerical techniques are required to perform any part of the calculations.

Later I will demonstrate the relationship between my approach and a variational calculation. And I will indicate how the Green's function contains important physical information about \( U \) and the transport solution that would be hard to discover short of knowing the exact answer.
CHAPTER III
CONTINUUM APPROXIMATION SOLUTION

A. What the Approximation Means

In the limit as h tends to zero, equations simplify as indicated earlier and I list the relevant equations below.

\[ U''(X) + \frac{g}{\sqrt{4+g^2}} U' - \left( \frac{\sin 2\pi U + f}{2\pi(4+g^2)} \right) = 0 \]  \hfill (36a)

\[ G_0''(X) + \frac{g}{\sqrt{4+g^2}} G_0' - \frac{1}{4+g^2} G_0 = d(X) \]  \hfill (36b)

\[ G_0(X) = -\exp\left(-\frac{X}{\sqrt{4+g^2}} \right) \]  \hfill (36c)

\[ U(X) = -\frac{f}{2\pi} + \frac{1}{4+g^2} \int_{-\infty}^{+\infty} G_0(X-X') \left( \frac{\sin 2\pi U(X')}{2\pi} \right) - U(X')) dX' \]  \hfill (36d)

\[ f = 2\pi g \sqrt{4+g^2} \int_{-\infty}^{+\infty} (U'(X))^2 dX \]  \hfill (36e)

What has been assumed is called the continuum approximation. Recall Eq. (6). In terms of dimensionless quantities this can be restated as

\[ \frac{U(X+h)-2U(X)+U(X-h)}{h^2} \approx U''(X) \]  \hfill (37a)

When h is sufficiently small, the approximation appears reasonable. Discreteness is defined as small when

\[ h = \frac{\sqrt{4+g^2}}{K(1-v^2)} \ll 1 \]  \hfill (37b)
Because

\[ K = \frac{ka}{2\pi V_0} \]  

(37c)

h will be small when the interaction between particles is much stronger than the sinusoidal lattice force quantified by ka and \( V_0 \), respectively. This not a sufficient condition that the continuum approximation be valid. The parameter h may be numerically small, but \( U \) may still be so wildly oscillatory that h is not small enough for Eq. (37a) to be appropriate. If higher even order derivatives of \( U(X) \) than the second are small compared to the second derivative this condition will be satisfied if in addition h is small. At least, this is a reasonable argument if a Taylor series expansion of \( U(X \pm h) \) is performed in Eq. (37a).

Merely assuming the continuum approximation to be valid means throwing away certain dynamical degrees of freedom available to the particles. This is suggested by the Green's function, Eq. (36c): In the continuum approximation the chain of masses responds rather simply with no oscillatory motion evident that we might expect to occur because the particles move in the bottom of parabolic potentials. In the continuum approximation the system of masses behaves like an elastic band, a continuous mass distribution.20

The continuum approximation need not be considered a degraded version of the full discrete model. It can be treated as a new model in its own right like the sine-Gordon equation.
B. Consequences of Reduced Parametrization

In the continuum approximation the differential equation for the solitary wave, Eq. (36a), depends only on the two parameters \( f \) and \( g \). This is a reduction by almost a factor of four from the original number of parameters. All possible friction and velocity combinations are implicit in \( g \). See Eq. (15b). This means given \( g \) only one value of \( f \), the external force, will yield solitary wave solutions. The relation representing the general solution to the transport problem for the single kink solution will be symbolized by

\[
f = f(g)
\]  

(38a)

or conversely

\[
g = g(f) = \frac{g_V}{\sqrt{1 - V^2}}
\]  

(38b)

For a particular transport problem \( V_0 \) and "a" are constant. Let me define a function \( A \) depending only on \( f \) in the following way.

\[
g = \sqrt{\frac{a}{2\pi m V_0}} A(f)
\]  

(39a)

Noting from Eq. (15c)

\[
\bar{g} = \sqrt{\frac{a}{2\pi m V_0}} D
\]  

(39b)

and using Eq. (38b) I conclude
\[ \bar{v}(D,f) = \frac{A(f)}{\sqrt{D^2 + A^2(f)}} \]  

This solution to the transport problem in the continuum approximation is perfectly general regardless of the type of wave of unchanging shape and constant velocity supported by the equation of motion, Eq. (36a). No specific boundary conditions are assumed so multikink solutions, if they exist, satisfy this functional relationship. In fact, the result is insensitive to the precise form of the lattice potential.

My choice of parametrization is very similar to that adopted by Marcus and Imry except for my factors of \((4+g^2)\) appearing in the differential equation. As \(\bar{v}\) tends to 1, \(g\) tends to infinity. My form of the differential equation gives a Green's function, Eq. (36c), with finite exponential damping in this instance. This is an advantage in numerical calculations because it expands the region over which the integration is computed since the Green's function damps out in a more reasonable way.

C. Green's Function and Trial Solution to the Transport Problem

The Green's function, Eq. (36c), is graphed in Fig. 8a. When \(g\) is zero, \(G\) is symmetric and is represented by the dashed curve. Increasing \(g\) causes the "front" \((X=\bar{x}-\bar{v}T>0)\) to become steeper and the relaxing tail \((X=\bar{x}-\bar{v}T<0)\) becomes longer. This is reminiscent of the profile in a foam
cushion caused by a finger pressed into it which moves along its surface at a uniform velocity. The faster the finger moves across the surface, the more abrupt the front and the longer the tail as seen from the perspective of the finger. The simple exponential decay of the Green's function is welcome for numerical calculations.

When friction is zero, $g=0$ and no force is required to transport the solitary wave: $f=0$. Eq. (36a) reduces to the sine-Gordon equation. The appropriate single kink solution is

$$U(X) = \frac{2}{\pi} \arctan(\exp(\frac{1}{2}X)) \quad (40)$$

obeying the boundary conditions

$$U(\pm\infty) = H(\pm\infty) \quad (41)$$

where $H$ is the Heaviside function of Eq. (30b). Besides this one solution, I know of one other and will present it in Chapter III, Section E.

I need a trial solution to begin the iteration. I choose it to be

$$U_t(X) = -\frac{\arcsin f}{2\pi}$$

$$+ \frac{2}{\pi} \arctan(\exp(\frac{1}{2} \sqrt{\frac{1-t^2+g^2}{4+g^2}} + \frac{g}{\sqrt{4+g^2}} \text{sgn}(X))X) \quad (42)$$

It is easy to demonstrate several properties of $U_t$: The boundary conditions Eqs. (14) are satisfied, the exact
solution Eq. (40) is obtained when \( g = f = 0 \), and for large magnitude \( X \) it has the correct asymptotic exponential damping exponents. These exponents were determined by linearizing Eq. (36a) and finding the exponential solutions. The slope discontinuities at \( X = 0 \) is unphysical but it does not lead to any difficulties. Experience has shown me that Eq. (42) is a good global trial solution: It has the proper qualitative behaviour for all reasonable values of \( f \) and \( g \).

A trial solution for \( f(g) \) is also desirable and Eq. (36e) will provide it.

\[
2 \pi g \sqrt{4 + g} \int_{-\infty}^{+\infty} f(U_t(X)) \, dX = \frac{2}{\pi} g \sqrt{4 + g} + g^2
\]  

(43)

Therefore

\[
f_t = \frac{2}{\pi} g \sqrt{4 + g} + g^2
\]

(44a)

implying

\[
f_t(g) = \left( \frac{4g}{\pi} \right) \sqrt{1 + \left( \frac{1}{4} - \left( \frac{\pi}{8} \right)^2 \right) \left( \frac{4g}{\pi} \right)^4 - \left( \frac{1}{2} - \left( \frac{\pi}{8} \right)^2 \right) \left( \frac{4g}{\pi} \right)^2}
\]

(44b)

or

\[
g_t(f) = \sqrt{1 - \left( \frac{\pi}{8} \right)^2 f^2} - \sqrt{1 - f^2}
\]

(44c)

The last equation can be used in Eqs. (39). Eq. (44b) will be shown to be an excellent trial solution. It is evident from Eq. (44c) that when \( f = 1 \)
\[ g_{t, \text{max}} = g_t(1) = \frac{\sqrt{\pi}}{2} \]  

Equation (44d)

\( f_t \) increases monotonically as a function of \( g \) until \( g = \sqrt{\frac{\pi}{2}} \) where it levels out to zero slope. Expanding Eq. (44b) in \( g \) gives

\[ f_t = \frac{4}{\pi} g + O(g^3) \]

\[ = \frac{4}{\pi} \frac{\overline{E} \overline{V}}{\sqrt{1-\overline{V}^2}} + O(g^3) \]  

Equation (44e)

This is exactly what perturbation theories and phenomenological calculations predict.\(^{22}\)

Summarizing, Eqs. (42) and (44b) are starting solutions for the iteration of \( U(X) \) and \( f \) thru Eqs. (36c), (36d) and (36e).

D. Exact Solution for a Similar Problem

Many analytical solutions are known for the sine-Gordon equation, but the exact analytical solution to the transport problem I have indicated has not been solved to my knowledge. Surprisingly if a term quadratic in velocity rather than linear in velocity is used to represent the phenomenological friction, the transport problem can be completely solved in an elementary way.\(^{23}\)

We begin with an equation of motion
Here $x=na$ if the system is discrete. The single kink solitary wave solutions I have presented so far satisfy

$$u_t(x,t) < 0$$

and I will assume this to be the case here. Our result will not contradict this. The particles all move in the direction of the applied force $F$, in the minus $x$ direction. Therefore

$$mu_{tt}(x,t) = ka^2 u_{xx} - D'|u_t|^2 - V_0 \sin \left( \frac{2\pi u}{a} \right) - F$$

Dimensionless parameters now follow.

$$T = \sqrt{\frac{2\pi V_0}{ma}} t$$

$$X = \sqrt{\frac{2\pi V_0}{ka}} \frac{x}{a}$$

$$U = u/a = U \left( \frac{X-VT}{\sqrt{1-V^2}} \right) = U(X)$$

$$g = \frac{D'a}{\pi m}$$

And now

$$U''(X) + \pi g^2 (U'(X))^2 = \frac{\sin 2\pi U + f}{2\pi}$$
Here comes the trick. Clearly
\[ \frac{dU}{dX} \frac{d^2 U}{dX^2} = \frac{d}{dX}\left( \frac{1}{2} \left( \frac{dU}{dX} \right)^2 \right) \] (48a)

but being cavalier with differentials allows this to be re-arranged to read
\[ \frac{d^2 U}{dX^2} = \frac{d}{dU} \left( \frac{1}{2} \left( \frac{dU}{dX} \right)^2 \right) \] (48b)

Eq. (47) in turn can be written
\[ \frac{d}{dU} \left( \frac{1}{2} (U')^2 \right) + 2\pi g^2 \left( \frac{1}{2} (U')^2 \right) = \frac{\sin 2\pi U + f}{2\pi} \] (49)

The original second order nonlinear differential equation in \( U(X) \) has now been turned into a first order linear differential equation for \( \frac{1}{2} (U')^2 \) which is a function of \( U \).

This means
\[ \frac{1}{2} (U')^2 = A \cos 2\pi U + B \sin 2\pi U + C \] (50a)

where \( A, B \) and \( C \) are constants to be determined by substitution into Eq. (49). When this is done we find
\[ \frac{1}{2} (2\pi U')^2 = -\frac{1}{1+g^4} \cos 2\pi U + \frac{g^2}{1+g^4} \sin 2\pi U + \frac{f}{g^2} \] (50b)

Imposing the boundary conditions on this first integral, Eqs. (14), immediately gives the transport solution
\[ f(g) = \frac{g^2}{\sqrt{1+g^4}} \] (51a)
or

\[ \bar{v} = \sqrt{\frac{f}{g}} \sqrt{1-f^2} \]  

(51b)

These are graphed in Figs. 2. The solitary wave can have velocities ranging from zero to the speed of sound. For a given velocity, the larger the amount of friction \( g \), the larger the force \( f \) required to move the solitary wave. There are no surprises here.

Using Eq. (51a), Eq. (50b) can be written as

\[ (2\pi U')^2 = \frac{4}{\sqrt{1+g^4}} \sin^2(\frac{1}{2}(2\pi U+\arcsin f)) \]  

(52)

Performing the one remaining elementary integral gives

\[ U(X) = -\frac{\arcsin f}{2\pi} + \frac{2}{\pi} \arctan(\exp(-\frac{X}{(1+g^4)^{1/2}})) \] 

(53)

This resembles my trial solution Eq. (42). The problem can actually be solved for more flexible boundary conditions than I have used here. See the previous reference, Ref. 23, for details.

E. Results and Comparison With the Work of Others

In Appendix I is a listing of the computer program I developed for computations in the continuum approximation. A sample output is also provided. The iteration equations are Eqs. (36d) and (36e); trial solutions are Eqs. (42) and (44b). The simple trapezoidal rule is used in the integration for iterating \( U \). An IBM 3033 computer requires less than \( \frac{1}{2} \) second for one iteration of \( U \) and \( f \) when 100 points
specify U. For 300 points about 4 seconds is required for one such iteration. The larger \( g \) is, the larger the number of points required for the same level of precision in \( f \). This is because of the longer tail which develops in \( U \) and \( G \): More points are needed to represent longer functions. For \( g \) less than 0.8 adequate convergence (i.e., a precision deemed better than 1%) is achieved after about 5 iterations using 200 points. I never needed more than 10 iterations or 400 points in the results I now present.

Figs. 5 show two iterated solutions for \( U \) where \( g \) is equal to \( \frac{1}{2} \) and 1. Dashed curves are trial functions. Note the wavefront is well guesses by the trial solution, but the tail relaxes quicker than trial solutions predict. The discontinuity in the trial solution is evident for the larger value of \( g \). Keep in mind Eq. (15i) when comparing solutions (or Green's functions): Changing the values of parameters changes the numerical relationship between the dimensionless coordinate \( X \) and the dimensioned coordinates \( x \) and \( t \).

Figs. 4 give the transport curves. In Fig. 4a is the general solution and note how well the analytical approximation, Eq. (44b), agrees with it. This reflects a good choice in the original shape of the trial function for \( U \). The dashed line in Fig. 4a is the perturbation result, Eq. (44e). My computed solution is appropriately asymptotic to it for \( g \) tending to zero. Fig. 4b shows specific
velocity versus force curves for specific amounts of friction $\bar{g}$.

There is a surprise, a feature not arising in the exact solution of the problem considered in the previous section. I find a maximum value which $g$ can have before the solution runs away because $f=1$.

$$g_{\text{max}} \approx 1.13 \quad (54a)$$

My trial solution also indicated this would occur. Referring to Eq. (44d) the prediction was

$$g_{t,\text{max}} = \sqrt{\frac{\pi}{2}} \approx 1.25 \quad (54b)$$

Through Eq. (15b), the definition of $g$ in terms of $\bar{g}$ and $\bar{v}$, this maximum $g$ means a maximum velocity exists for the one kink solution in the presence of friction.

$$\bar{v}_{\text{max}}(\bar{g}) = (1 + \left(\frac{\bar{g}}{1.13}\right)^2)^{-\frac{1}{2}} \quad (54c)$$

If there is no friction, $\bar{g}=0$ and so $\bar{v}_{\text{max}}=1$. If $\bar{g}=1$ then $\bar{v}_{\text{max}} \approx 3/4$.

In Chapter IV, Section C, I will derive the solution to the same transport problem where the sinusoidal lattice potential is replaced by parabolic sections. To determine whether my program somehow overestimated $f$ when $g$ was large, I used this result for the parabolic lattice potential as a test case. Figs. 3 is a graph of the transport solution. It much more closely resembles my result for the sinusoidal
Figure 2a General transport curve when the friction force is quadratic in velocity. See Eqs. (46) and Section D of this chapter. For specific velocity versus force curves see Fig. 2b.
Figure 2b Transport curves based on the general solution shown in Fig. 2a. Compare this with Figs. 3b and 4c.
Figure 3a General transport curve when the lattice potential is made of parabolic sections as described in Chapter IV, Section C. For specific velocity versus force curves, see Fig. 3b.
Figure 3b  Transport curves based on the general solution shown in Fig. 3a.
Figure 4a. The long curve is the general solution to single kink transport for the continuum approximation of the generalized Frenkel-Kontorova equation. It terminates at $g=1.13$. The short solid curve is part of the trial solution, Eq. (44b). Below $g=\frac{1}{2}$, it is very close to the exact solution. It peaks for $g=\sqrt{\pi}/2$ with $f=1$ before declining in value.
Figure 4b The dashed curve is the solution of the transport problem reproduced from Fig. 4a. Solutions obtained by Nakajima et. al. are indicated by the values of $g$ used in their calculations. If all the curves were the correct solutions, they would all lie on top of the dashed curve. See text for discussion. See also Fig. 4c.
Figure 4c Solid lines are based on the general result shown in Fig. 4a. Three solutions of Nakajima et al. are dashed lines. See Fig. 4b.
Figure 5a The dashed line is the trial solitary wave of Eq. (42) with $f=0.593$. The solid curve is the final result which required about 2 iterations, where $f=0.599$. For this calculation 200 points represented $U(X)$. See Fig. 5b.
Figure 5b  This is a continuation of Fig. 5a. Here the trial solution has $f=0.951$ and about 7 iterations were required yielding $f=0.97$. Note the obvious slope discontinuity of the trial solution, Eq. (42), for this large amount of friction.
lattice potential than the quadratic velocity dissipation case of Fig. 2. In the case of a parabolic lattice potential $g$ does tend to infinity because $v_{\text{max}} = 1$ irrespective of friction. At $g=7$ the exact $f$ is within $4\%$ of its maximum value of $\pi$. Using 400 points in a calculation, the value of $f$ obtained is too small by about $2\%$. For values of $g$ much larger, the program suffers from underflow problems because of the long tails on $G$ and $U$. Generally in such an instance $f$ is too small because part of $U$ is outside the range of of program causing $f$ to be too small because of Eq. (36e). Therefore I am confident the program has not improperly given too large a value of $f$ at $g=1.13$ when the sinusoidal lattice potential is treated.

If it was simply a matter of poor integration yielding a value of $f$ too large, then improving the integration by using a smaller mesh could increase $g_{\text{max}}$ if in fact $g_{\text{max}}$ was infinite. Exactly the opposite occurs.

Nakajima and coworkers (from here on to be referred to simply as Nakajima) reported solutions to this same problem obtained using a finite difference scheme. They solved the equation of motion written as the general partial differential equation in $x$ and $t$ for several values of the friction constant. Their $\Gamma$ and $\Upsilon$ are my $g$ and $f$, respectively. Nakajima also found limiting velocities for the solitary waves less than the speed of sound and Table I compares their results with my predictions.

The transport curves they obtain do not agree well with
TABLE I

Comparison of Maximum Solitary Wave Velocity, $\overline{V}_{\text{max}}$, Obtained by Nakajima et. al. with Eq. (54c)

<table>
<thead>
<tr>
<th>$\bar{\varepsilon}$</th>
<th>Nakajima et. al.</th>
<th>Present Work</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.0</td>
<td>0.76</td>
<td>0.749</td>
</tr>
<tr>
<td>0.5</td>
<td>0.94</td>
<td>0.914</td>
</tr>
<tr>
<td>0.3</td>
<td>&gt;1?</td>
<td>0.967</td>
</tr>
<tr>
<td>0.1</td>
<td>0.98</td>
<td>0.996</td>
</tr>
</tbody>
</table>
my general solution as Fig. 4b indicates. Their curves ought to fall onto my general solution. For large values of $\bar{g}$ I find tolerable agreement, the differences being less than 15%. However, our results disagree substantially for small values of $\bar{g}$. Their results do not agree well with the perturbation result for small $\bar{g}$. That is, for $g$ less than about 0.4, the difference between what I have indicated as the solution and the perturbation result is less than 4%. However, the curves of Nakajima deviate substantially from the perturbation results in this regime as the friction parameter becomes smaller. This is unreasonable. I believe the reason for the discrepancy is their use of a numerical scheme involving finite differences as approximations to the derivatives appearing in the partial differential equation: They really did not solve the case of a continuum approximation. This can introduce an intrinsic dynamical friction of a kind to be described in Chapter IV. Nakajima suggested the same explanation in a private communication with me.

Marcus and Imry$^{25}$ recently published a transport curve for $\bar{g}=0.1$ and it agrees precisely with my result. They too note a discrepancy with Nakajima. Unfortunately when $\bar{g}=0.1$ then I predict $v_{\text{max}}=0.996$ and it is not possible to discern whether their graph terminates for a velocity less than that of sound. I have written to them concerning this matter but as of this writing have not received a reply.
I do not agree with the numerical calculations of Büttiker and Thomas. Their general solution $\phi(F/V) = g(f)$ does not agree with Nakajima (for large $g$), Marcus and Imry (for $g=0.1$) or myself. I recently received a letter from Büttiker acknowledging an error in the calculations. However, they correctly demonstrate a solution exists to the differential equation of motion when $f=\bar{v}=1$, potentially contradicting Nakajima and myself in regard to limiting velocities less than the speed of sound. To construct the solution I cannot use an equation with $g$ in it because $g$ diverges when $\bar{v}=1$. Instead consider the continuum approximation of Eq. (11).

$$U_{TT}(x,t) = \frac{\partial}{\partial x} \left( U_{XX} - g \frac{\partial}{\partial t} U_T - \frac{(\sin 2\pi U + f)}{2\pi} \right)$$

(55)

Assuming $\bar{v}=1$, the travelling wave constraint is

$$U(x,t) = U(\Omega-T) = U(x)$$

(56)

Upon substituting this into Eq. (55) the two second derivative terms cancel. This physically means the lattice potential and harmonic interaction between particles always cancel. (See Eqs. (16).) What remains is, after setting $f=1$,

$$U'(x) = \frac{1+\sin 2\pi U}{2\pi g} = \frac{\sin^2(\pi U + \frac{\pi}{2})}{\pi g}$$

(57)
Solving gives

\[ U(X) = \frac{1}{\pi} \arctan\left(\frac{X}{\bar{g}}\right) \]  

(58)

Therefore a solution does exist when \( \bar{v} = 1 \), namely Eq. (58). Does this mean I have incorrectly computed the transport curve?

Making no assumptions, Eq. (58) can be written as

\[ U''(\frac{X-\bar{v}T}{\sqrt{1-\bar{v}^2}}) + g \, U' - \frac{\sin 2\pi U + f}{2\pi} = 0 \]  

(59)

Here derivatives are with respect to the indicated argument of \( U \). The question is, does Eq. (59) have Eq. (58) as its solution as \( \bar{v} \) tends to 1, if that is possible. Eq. (59) can be considered the equation of motion of one particle moving along a sinusoidal surface inclined with respect to a constant gravitational field. The surface has a friction coefficient \( g \). In this analogy \( f=1 \) means the sinusoidal surface is tipped with respect to the horizontal so the potential is steplike and valleys in the total potential disappear. An argument has been proposed\(^{27}\) that \( g \) must go to infinity, and hence \( \bar{v} \) tend to 1, as \( f \) tends to 1. The trajectory of interest is one in which the particle begins at a potential minima, moves down the inclined surface over a sinusoidal bump and stops precisely at the next potential minima. The idea is that as \( f \) approaches 1 so the total potential loses its minima, the friction parameter \( g \) must diverge to keep the particle from slipping down the "steps" indefinitely. This does not convince me because I
can imagine the particle motion to be overdamped at a finite value of $g$ (i.e., $g<1.13$) so that the particle still stops at the next horizontal section of a step. My belief is that Eq. (58) represents a solution not "connected" to those for which $f$ and $\overline{v}$ are both less than 1. I argued earlier (see Eq. (16)) the harmonic interaction always dominates the inertial term in the continuum approximation. A complete cancellation of these terms is not indicated.

F. How the Identity Relates to a Variational Calculation

A.R.P. Rau has pointed out to me in a personal communication that the identity, Eq. (36d), is closely connected with a variational. By variational I mean a prescription for successively iterating the solution so a trial solution deviating from the exact solution by some small error will produce a new estimate having an error of second order in this small error.

The "constraint" of the variational is the differential equation for $U$.

$$U''(X) + \frac{g}{\sqrt{4+g^2}} U' - \frac{1}{4+g^2} U - \left(\frac{\sin 2\pi U}{2\pi(4+g^2)} \right) = 0$$

(60)

In this discussion I will assume the exact $f$ is known. Let subscripts $v$ and $t$ designate variational and trial solutions respectively. I define the variational
When $U_t = U$, the constraint Eq. (60) is satisfied and for this reason $U_v[U] = U$. The function $L_t(X,X')$ is the (trial) lagrangian multiplier. It is chosen by requiring that small variations in the trial functions lead to second order errors in $U_v$ from the exact solution of the constraint, Eq. (60). Let

$$U_t = U + dU$$

$$L_t = L + dL$$

where $dU$ and $dL$ are small valued functions representing deviations of $U_t$ and $L_t$ from $U$ and $L$. In what follows I will assume the trial solutions obey the same boundary conditions as the exact solutions. Then the boundary conditions of $dU$ and $dL$ will be zero because of Eqs. (62). Substitution of Eqs. (62) into Eq. (61) results in

$$U_v = U + dU - \int_{-\infty}^{+\infty} L_t [ (dU)' + \frac{g}{\sqrt{4+g^2}} (dU)' - \left( \frac{\cos 2\pi U}{4+g^2} - 1 \right) dU ] dx'$$

(63)

To arrive at this result I have used the constraint Eq. (60) and

$$\sin(2\pi(U + dU)) = (2\pi \cos 2\pi U) dU + O(dU')$$

(64)
Second order deviations are not of interest because I only want to insure first order terms do not contribute.

Integrating Eq. (63) by parts and absorbing the lone \( dU \) into the integrand with a delta function \( d(X-X') \) I obtain

\[
U_v = U - \int_{-\infty}^{+\infty} \left[ (L_{X'X}, (X,X')) - \frac{g}{\sqrt{4+g^2}} L_{X}, - \frac{1}{4+g^2} L \right. \\
- d(X-X') + \left( \frac{1-\cos 2\pi U}{4+g^2} \right) L \] dU dX' \tag{65}
\]

In order for first order error in \( U_v \) be zero for arbitrary variations in \( dU \) it follows

\[
L_{X'X}, (X,X') - \frac{g}{\sqrt{4+g^2}} L_{X}, - \frac{1}{4+g^2} L \tag{66}
\]

I rewrite Eq. (61) using integration by parts.

\[
U_v = U_t - \int_{-\infty}^{+\infty} \left[ (L_t, X', X') - \frac{g}{\sqrt{4+g^2}} L_t, X' - \frac{1}{4+g^2} L_t \right] U_t(X') \\
- L_t (\frac{\sin 2\pi U_t(X') - 2\pi U_t + f}{2\pi(4+g^2)}) \right] dX' \tag{67}
\]

Finally, using Eq. (66), the derivatives in the variational, Eq. (67), can be removed.

\[
U_v = \frac{1}{4+g^2} \int_{-\infty}^{+\infty} L_t(X,X') \left[ (\frac{\sin 2\pi U_t(X') - 2\pi U_t + f}{2\pi}) \right. \\
+ \left( 1-\cos 2\pi U_t \right) U_t \right] dX' \tag{68}
\]

Eq. (68) is a new identity like Eq. (61) except that for \( U_v[U]=U \) to be true in this case, \( L \) must satisfy Eq. (66).
No such restriction on $L$ is necessary for Eq. (61) to be an identity. To demonstrate Eq. (65) is such an identity directly, multiply Eq. (66) by $U(X)$ and integrate over all $X$. After integration by parts and use of the constraint, Eq. (68) will result with $U$ replacing $U_t$. So, the constraint on $L$ making the iteration a variational is Eq. (66) and this directly implies Eq. (68).

Eq. (68) should be reminiscent of the identity with the Green's function. In fact, if I choose

$$U_t(X) = H(X) \quad (69)$$

(the Heaviside function; also, see Eq. (41)) then the solution to Eq. (66) is exactly

$$L_t(X,X') = G_0(X-X') \quad (70)$$

and Eq. (68) reduces precisely to the iteration identity, Eq. (36d). But Eq. (69) does not have the correct boundary conditions for the solution. It is the boundary conditions when friction $\bar{g}$ is zero.

Suppose I choose Eq. (70) to be my permanent trial solution for the lagrangian multiplier. Then in Eq. (67) the first parenthesised term is exactly a delta function and it reduces exactly to my Green's function identity. But then Eq. (66) is not satisfied at the completion of iteration. If friction is zero, however, Eq. (70) will be a reasonable trial for reasons given above. Therefore, when friction is very small, the iteration with the Green's function is
nearly a variational. As \( g \) becomes large and Eq. (69) becomes unrealistic, first order error ought to become significant, slowing the convergence. In the previous section I observed more iterations are required when \( g \) is large.

This connection with a variational gives a rationale for the impressive convergence properties of an otherwise ad hoc method.
CHAPTER IV
FULL DISCRETE EQUATION

A. How the Discrete Problem Differs from the Continuum Approximation

Early in the last chapter it was assumed the continuum approximation is valid when the solution is smooth enough that higher derivatives than the second of the Taylor series expansion of the finite difference can be ignored. In this approximation the mass chain behaves like an elastic band. But I also indicated, purely on intuitive grounds, this might be somewhat drastic: Keeping discreteness could lead to solutions containing oscillatory behaviour as a consequence of particles successively falling into the bottom of the lattice potential minima. If these wiggles develop in $U$, this could have a marked influence on transport behavior. An oscillatory $U$ means larger values of $(U')^2$ and $f$ may increase because of the power balance formula, Eq. (31b).

I define discreteness $h$ as not negligible when

$$h = \sqrt{\frac{4+g^2}{K(1-V^2)}} \approx 1 \quad (71a)$$

Since

$$K = \frac{ka}{2\pi V_0} \quad (71b)$$
Figure 6 The above two diagrams indicate two possible static mass configurations with one vacancy. If these two configurations are the minimum and maximum potential energy arrangements, then the difference between these energies is the "pinning potential" for the vacancy. This potential must be overcome before transport of the vacancy is possible.
h will be non-negligible when the sinusoidal lattice force of amplitude $V_0$ is much stronger than the interactions between particles as quantified by $ka$. $U$ may still be smoothly varying when $h$ is large, so a continuum approximation would still be realistic. Until the solution to the discrete equation is known, we cannot a priori, by these arguments alone, know when such an assumption is possible.

In the continuum approximation there is only one static configuration of the particles (the masses are forever at rest). A geometric translation of a continuous string of masses does not change the configuration energy; i.e., the total potential energy of the particles. There are no empty positions in the string. This symmetry is broken with the advent of discreteness. In Fig. 6 are sketched two static mass configurations clearly having different configuration energies. Generally there are several static configurations for the same number of vacancies or interstitials in a given system. (The dynamical constraint for travelling waves may not sift out one static distribution of masses in the zero velocity limit of a solitary wave.) These static multikink solutions do not exist in the continuum approximation, the sine-Gordon equation. Because some static configurations of the discrete system are of higher energy than others, a vacancy or interstitial can be pinned to one configuration where energy is a local minima. (If the rigid background lattice potential had an impurity or some other irregularity, this could localize a vacancy
or interstitial at a site.) This complicated potential is sometimes referred to as a "pinning potential".

The force required to overcome the pinning potential acting as a barrier to the free translation of vacancies and interstitials is the Peierls stress at absolute zero. In one often cited calculation the one vacancy static equilibrium positions of the particles and the associated Peierls stress were determined analytically. A periodic lattice potential constructed of two smoothly connected parabolas with differing maximum curvature was used. The stress was found to be very sensitive to the relative maximum curvatures of the parabolas. As a function of this parameter the stress oscillated significantly and could even vanish.

So far my remarks have dealt with statics. The Peierls stress which appears when discreteness is introduced in computing static equilibrium configurations becomes a dynamical Peierls stress for solitary waves. Even if there is no phenomenological friction present, as in the case of the Frenkel-Kontorova equation, Eq. (5), an "intrinsic dynamical friction" develops. Waves are always damped for discrete lattices, contrasting with the continuum approximation of the same problem. That discreteness implies a dynamical friction can be made plausible with an elementary mathematical example. Consider
\( (h, v^2) \frac{\partial^2 U(X)}{\partial X^2} = \frac{1}{1 - v^2} \left( \frac{U(X+h) - 2U(X) + U(X-h)}{h^2} \right) = 0 \)

(72a)

In the continuum approximation this equation simplifies to

\( (0, v^2) \frac{\partial^2 U(X)}{\partial X^2} = U''(X) = 0 \)

(72b)

One solution of the continuum approximation is

\( U = \text{constant} \)

(72c)

But in the full discrete equation, Eq. (72a), a trial solution \( U = Ae^{ikX} \) leads to a transcendental equation for \( k \)

\( \left( \sin \frac{\pi k}{h} \right) = \pm v_k \)

(72d)

The solution to this indicial equation is a set of complex numbers, in general. A complex root means the solution is a damped oscillation. Even when there is no extrinsic dynamical friction, arbitrarily small forces need not sustain solitary wave motion in discrete lattices because of intrinsic dynamical friction. When oscillations arise in nonlinear systems of the kind suggested by the above example, it is classified as phonon radiation. Phenomenologically, an additional applied force is required to power these additional physical processes.

In Chapter III, Section E, I suggested this as the reason that as extrinsic friction, \( \bar{E} \), became smaller, the transport curves of Nakajima deviated more from the solution for the continuum approximation. Their use of finite
difference approximations introduces an intrinsic dynamical friction which does not lessen when phenomenological friction tends to zero.

As one last use of the above mathematical example, note that as $\bar{v}$ tends to zero, the inertial term $U''$ must increase to balance the finite difference particle interaction term. In turn, $U$ will oscillate more. This behavior also can be expected in the generalized Frenkel-Kontorova equation since the same operator, $(h, \bar{v}^2)_X$, is used. Consequently $f$ might be a strong function of velocity when the velocity is low, but become more regular for larger velocities.\(^{33}\)

Real systems are fundamentally atomic and the above considerations indicate the importance of discrete lattices for transport processes. When a Peierls potential exists, as I stated earlier, it acts as an additional barrier to the translation of vacancies or interstitials; however, this potential may still be less than that facing a single particle. That is, the collective dynamics leading to mass transport can still require less energy than single particle dynamics (diffusion-like) in the same lattice. It may not for the reasons given in the previous paragraph. It seems only realistic calculations can decide when this will be the case.
B. Applications Where Discreteness Must be Maintained

The previous section suggests physical criteria for deciding when discreteness is important. I deliberately used a terminology referring to the transport of vacancies and interstitials because much useful information on the role of "internal friction" has accumulated in the literature devoted to crystal dislocations.\textsuperscript{34} When crystal planes slide past one another due to an applied stress, a particular particle on one of the sliding planes would experience: its proximity to the nearest neighbors in its own crystal plane (approximately harmonic interactions); a periodic potential as each particle in the other crystal plane slides past (approximately sinusoidal); dissipative mechanisms (represented by some phenomenological friction term). Hence the Frenkel-Kontorova equation, Eq. (5), or some generalization of it. More complicated crystal defects move in a way that can be modeled by the same equation.\textsuperscript{35}

Application of mechanical stress to crystals causes defect transport. Experimental means are available to determine defect velocity as a function of stress,\textsuperscript{36} and for this reason it is well established that a continuum approximation is inadequate. An oscillatory wave follows the lattice defect and this "phonon wake" is interpreted as the emission of sound waves. The results to theoretical calculations are very sensitive to atomic force laws chosen.

The effect of discreteness on lattice defect transport
has been investigated for more than forty years and the need to maintain it in theoretical treatment is well established. More recently, in the past ten years, physicists have become more involved in research on "superionic conductors". In this class of materials, above a certain threshold temperature (characteristically several hundred degrees centigrade) their ionic conductivity is comparable to liquid electrolytes. One possible application of these solid electrolytes is the development of powerful, lightweight solid state batteries. One hindrance to technological development is a quantitative understanding of what makes these materials conduct ions so well. Beyond the threshold temperature the materials AgI, RbAg4I5 and CaF2, among others, have conductivities on the order of 1/2-cm. For comparison, NaCl at 200°C has a conductivity of about 10^-8/2-cm. Ultimately it is the transport properties of these materials, and thermodynamics, responsible for this behavior. At a high enough temperature, before the crystal actually melts, the carrier ions begin moving freely inside a crystal lattice formed by the remaining ions. Sometimes a structural phase transition occurs in the entire lattice at the onset of the high conductivity regime. This process is pictured as the melting of one ionic lattice inside another that remains rigid "on the average". This lattice forms a charged cage in which the mobile ions move.

The energy required to transport charge in these materials is termed the "activation energy". It is in
principle the same as the Peierls potential discussed earlier, with the added complication of the high temperature thermodynamics implied. The fixed ions execute large deviations about their lattice sites. Because of the small activation energies of superionic conductors, a few tenths electron volt, this is seen as evidence the ions help one another through the lattice. This "helping" is an example of correlated motion. The estimation of activation energies based on purely static configurations of the mobile ions on a rigid lattice using realistic lattice potentials clearly demonstrates how the low energy is a consequence of discreteness. The activation energies determined in this way are less than what can be explained by single particle calculations.

In some materials it is reasonable to use a model for superionic conductors where it is assumed the mobile ions travel down a crystal channel formed by the fixed ions. A generalized Frenkel-Kontorova equation is a natural equation to use in this circumstance for dynamical calculations. Statistical models exist in which the mobile ions rattle around in the rigid ion lattice in a diffusive or "hopping" fashion. While statistical treatments seem generally successful in prediction the behavior of ionic conductivity as a function of an applied electric field, there are possible exceptions. A peak in the microwave conductivity of silver iodide, AgI, has not been explained by purely statistical theories. It has been considered a candidate for
collective dynamics of the soliton type. Due to the experimental difficulty of performing an experiment of this kind, and a failure to confirm the results, this may not be a real discovery. The suggestion that the effect, if real, is a consequence of soliton-like waves has been criticized on theoretical grounds.\textsuperscript{42}

My final comment on superionic conductors is that it would be very surprising to me if the kinds of solitary wave calculations described in this work would be of any importance: The temperature of a superionic conductor is so high and the "rigid lattice" so dynamically active, that ideal assumptions implicit in the generalized Frenkel-Kontorova equation are likely no longer tenable. It would still be interesting to see how the activation energies determined using static calculations would be modified by adding dynamics of the solitary wave type. The calculations cited earlier gave terribly low activation energies, and whether this is because dynamics were lacking in the calculation or because the role of thermodynamics (i.e., large oscillations in the particles comprising the lattice) is considerable could perhaps be resolved. The calculational approach of this work could, I believe, be used for any sine-like lattice potential. A real lattice potential is quite sinusoidal in this application due to the summed Coulomb and Pauli repulsion (Born-Mayer) potentials.

I will not discuss the theory of Josephson junctions, but I would like to point out that the calculations of
Nakajima, et al., Marcus and Imry, and Büttiker and Thomas referred to in the chapter on the continuum approximation were devoted to fluxon (a quantum of magnetic flux) transport in such junctions. Some attention is currently being directed to the effects of discreteness.43

C. A Related Solvable Model

Exact solutions to a discrete lattice problem have recently been obtained so the continuum approximation can be readily compared with it.44 The differences in transport are qualitatively different in ways alluded to in the first section of this chapter. Recall the generalized Frnkel-Kontorova equation and the Green's function.

\[
\begin{align*}
(h,\overline{V}^2)\frac{d^2}{dx^2}U(X) + \frac{g}{\sqrt{4+g^2}} U' - (\frac{\sin \frac{2\pi U}{2} + f}{2\pi(4+g^2)}) &= 0 \quad (73a) \\
(h,\overline{V}^2)\frac{d^2}{dx^2}U(X) &= \frac{1}{1-\overline{V}^2} \left( \frac{U(X+h)-2U(X)+U(X-h)}{h^2} - \overline{V}^2 U'' \right) \quad (73b) \\
U(\pm\infty) &= 1 - \frac{\arcsin f}{2\pi} \quad (73c) \\
U(-\infty) &= -\frac{\arcsin f}{2\pi} \quad (73d)
\end{align*}
\]

\[G(X) = -\frac{1}{2\pi} \int_{-\infty}^{+\infty} \frac{e^{ikx} dk}{1-\overline{V}^2 \left( \left( \frac{\sin \frac{k}{2h} \sqrt{\frac{g}{4h}} \right)^2 - \overline{V}^2 k^2 \right) - \frac{g}{\sqrt{4+g^2}} ik + \frac{1}{4+g^2} } \quad (73e)\]

Instead of a sinusoidal potential, a lattice of parabolic sections is used. As a function of the displacement U, this potential is chosen to be
\[ V(U) = \frac{1}{2}(2\pi)U^2, \quad -\frac{1}{2} < U < \frac{1}{2} \quad (74) \]

We replace \( \sin 2\pi U \) in our equation like so:

\[ \sin 2\pi U(X) \implies 2\pi (U(X) - H(X)) \quad (75a) \]

By this clever device with a Heaviside function we see

\[ 2\pi (U(X) - H(X)) = \begin{cases} 2\pi U & X<0 \\ 2\pi (U-1) & X>0 \end{cases} \quad (75b) \]

This is the only segment needed in the single kink case.

We are assuming at \( X=X-vT-0 \), the solitary wave has carried the particle originally sitting in the first parabolic potential at \( \frac{1}{2}<U<1\frac{1}{2} \) to the location

\[ U(0) = \frac{1}{2} \quad (75c) \]

At this precise occurrence, the potential instantly switches to the parabolic potential appropriate for \( -\frac{1}{2}<U<\frac{1}{2} \). This assumes the dynamics of the particles are such that they will only pass the juncture between the parabolas once, at \( X=0 \). This possibility can be kept in mind when examining the final results. Because of Eq. (75a), the boundary conditions are

\[ U(+\infty) = 1 - \frac{f}{2\pi} \quad (76a) \]

\[ U(-\infty) = -\frac{f}{2\pi} \quad (76b) \]

and the modified equation of motion is
\((h, \mathbf{v})^2 U(X) + \frac{g}{\sqrt{4+g^2}} U' - \frac{1}{4+g^2} (U-H(X)+\frac{f}{2\pi}) = 0 \) \hspace{1cm} (76c)

By this device the equation is linear in \(U\) with an added inhomogeniety which includes the Heaviside function, Eq. (30b).

This can be solved using (suprise) the fourier transform with the inclusion of an additive factor of \(\frac{1}{2}\) so that \(U\) and \(H\) are zero on the average. In this way the transform will exist.

\[
U(X) + \frac{f}{2\pi} - \frac{1}{2} = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \bar{U}(k)e^{ikX}dk \hspace{1cm} (77a)
\]

\[
H(X) - \frac{1}{2} = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \frac{1}{\sqrt{2\pi}ik} e^{ikX}dk \hspace{1cm} (77b)
\]

In a straightforward way (compare with Eq. (22))

\[
\bar{U}(k) = \frac{1}{\sqrt{2\pi(4+g^2)}} \left( \frac{\bar{G}(k)}{k} \right) \hspace{1cm} (78)
\]

Here \(\bar{G}(k)\) is exactly Eq. (25), the fourier transform of the general Green's function, Eq. (73e). The apparent singularity at \(k=0\) is removable as the application of \(\bar{U}\) below will indicate. Therefore

\[
U(X) + \frac{f}{2\pi} - \frac{1}{2} = \frac{1}{2\pi(4+g^2)} \int_{-\infty}^{+\infty} \left( \frac{\bar{G}(k)}{k} \right)e^{ikX}dk \hspace{1cm} (79)
\]

Earlier, see Eqs. (26), I indicated how a phonon density of states for the general Green's function is related to the fourier transform of the Green's function. A more direct link to the solitary wave \(U\) is possible in this case. If we identify \(e^{ikX}/\sqrt{2\pi}\) in Eq. (79) as a phonon with wavevector \(k\), then \(\bar{G}(k)/k\) is essentially a phonon density of states.\(^{45}\)
That is, the relative number of phonons of wavevector $k$ comprising the solitary wave $U(X)$ is

$$dn(k) = \frac{\sqrt{2\pi}}{(4+g^2)^{\frac{3}{2}}} (\frac{G(k)}{k}) dk$$

(80a)

where

$$n = \int_{-\infty}^{+\infty} (\frac{dn(k)}{dk}) dk = 1$$

(80b)

by using Eqs. (75c) and (79).

Using these same two equations we can finally write

$$f = \frac{1}{4+g^2} \int_{-\infty}^{+\infty} (\frac{G(k)}{k}) e^{ikx} dk$$

(81a)

$$= 2 \frac{g}{\sqrt{4+g^2}} \frac{1}{4+g^2} \int_{0}^{\infty} \frac{dk}{1-\frac{1}{2\hbar} [(\frac{\sin \frac{1}{2}hk}{\frac{1}{2}k})^2 - \frac{v^2k^2}{2}]} (\frac{1}{4+g^2})^2 + (\frac{g}{\sqrt{4+g^2}})^2$$

(81b)

Eq. (73a) can be solved in the continuum approximation with the result

$$U(X) = \frac{1}{2} + (-\frac{1}{2\pi} f + \frac{1}{2} \text{sgn}(X))(1-\exp(-\frac{1}{\frac{1}{2} \frac{g}{\sqrt{4+g^2}} + \text{sgn}(X)X}))$$

(82a)

$$= \frac{1}{2} + (-\frac{1}{2\pi} f + \frac{1}{2} \text{sgn}(X))(1-G_o(X))$$

(82b)

See Eq. (28). By matching derivatives $U'(+0)$ and $U'(-0)$, or alternatively, using Eq. (81b) in the continuum approximation, we find the transport relationship
Figure 7 Transport in the continuum approximation (dashed curve) and exact solution based on Eqs. (81b) and (83b) for a parabolic lattice potential. Here \( g = 0.1 \) and \( K = 4 \). See Eq. (15f). From the work of J.C. Kimball.
\[ f = \pi \frac{\xi}{\sqrt{4 + \xi^2}} \]  
\[ \overline{v} = \frac{\frac{f}{n}}{\sqrt{\left(\frac{f}{n}\right)^2 + \left(\frac{\xi}{\overline{\nu}}\right)^2 \left(1 - \left(\frac{f}{n}\right)^2\right)}} \]

The transport curves for the last two equations, the transport curves in the continuum approximation, are given in Figs. 3. This result more closely resembles my numerical solution to the continuum approximation of the generalized Frenkel-Kontorova equation, Figs. 4, than to the results of Figs. 2 because the friction is of the same type in both cases. The general solution to the transport problem is given by Eqs. (81) and the solution is unique for a given set of parameters. In Fig. 7 a solution is given as presented by Kimball for a select set of parameters. The dashed curve is the continuum approximation and the solid curve is the full discrete case.

For large velocities discreteness does not keep the solution from being soliton-like. This is not an acceptable description for low velocities. Below about \( \overline{\nu} = \frac{4}{\xi} \), strong resonances occur and there are times when a larger applied force means a smaller transport velocity. This may indicate the solitary wave becomes unstable. A threshold force is implied before single kink transport can occur. There is no reason to suspect these results are due to the kinky potential because the denominator of the integrand in
Eqs. (81) which produces these resonances also appears in the general Green's function where the same effects seem likely to occur.

D. Green's Function and Infinite Discreteness

The cases when \( h \) is taken to be zero or infinite would both seem to be physically uninteresting. But the case when \( h \) tends to zero gives meaningful results, namely the continuum approximation of Chapter III. Allowing \( h \) to be arbitrarily large gives a meaningful Green's function but an impossible transport problem. Setting \( h = \infty \) in the generalized Frenkel-Kontorova equation, Eq. (13b), gives

\[
-(\frac{-v^2}{1-v^2})u''(x) + \frac{\theta}{\sqrt{4+\theta^2}} u' - \left( \frac{\sin 2\pi \theta \theta + \theta}{2\pi(4+\theta^2)} \right) = \theta
\]  

(84a)

Or, when \( \theta = \theta = 0 \),

\[
-(\frac{-v^2}{1-v^2})u'' = \frac{\sin 2\pi \theta}{\theta}
\]

(84b)

There is no solution to this equation satisfying the boundary conditions.

The infinite discreteness case provides the opportunity to obtain the second analytical expression for \( G(X) \) which I gave earlier as Eqs. (29) and reproduce here for convenience.
\[ G_\infty(X) = \frac{1}{w} \left( \frac{1-v^2}{v^2} \right) \exp(eX) \sin(wX) H(-X) \quad (85a) \]
\[ e = \frac{1}{2} \left( \frac{1-v^2}{v^2} \right) \frac{g}{\sqrt{4+g^2}} \quad (85b) \]
\[ w = \frac{1}{2} \left( \frac{1-v^2}{v^2} \right) \frac{\sqrt{4+g^2}}{4+g^2} \quad (85c) \]

Note \( G_\infty(X) \) is zero for \( X \) greater than zero: There is no wavefront. For \( X \) less than zero there is a damped oscillatory tail (wake). The problem at \( \overline{v} = 0 \) is evident; I discussed this earlier. \( G_\infty \) and \( G_0 \) are compared in Fig. (8e). It is interesting to note that the number of wavelengths of the wake in which the amplitude drops by \( 1/e \approx 0.37 \) is independent of velocity.

\[ \frac{2\pi}{w} \left/ \left( \frac{1}{g} \right) \right. = \frac{2\pi g}{\sqrt{4-g^2}} = g + 0(g^3) \quad (86) \]

When discreteness is infinite, the interparticle interaction is zero compared to the lattice potential as can be seen from Eqs. (71). But some interparticle interaction must remain to maintain the cooperative effect of one particle helping the next particle down the line over a sinusoidal potential barrier. In this way the external force can remain less than that required to lift one particle over the sinusoidal potential in the absence of such a cooperative effect. But, roughly speaking, as \( h \to \infty, f \to 1 \). The Green's function \( G_\infty \) makes sense by itself because it is simply the trajectory of one particle in response to one impulse which comes along at velocity \( \overline{v} \). The oscillatory response is seen from a coordinate system moving along with the
Figure 8a Green's function for zero discreteness. The dashed line indicates the symmetric $g=0$ solution. See Eq. (36c). The remaining figures in this series show how the Green's function, Eq. (73e), changes as discreteness increases. In all cases $\tilde{v}=\tilde{g}=1/2$. 
A finite discreteness $h$ causes small oscillations to appear in the tail of the Green's function. However, "on the average", it is still very similar to the continuum approximation, Fig. 8a. Essentially no change occurs for $x > 0$. 

Figure 8b
G(X)

Figure 8c  As discreteness h increases the wake wavelength and amplitude of the Green's function increases.
Figure 8d. The tendencies which developed in Figs. (8b) and (8c) continue. The wavefront, $X > 0$, is beginning to decline and spurious numerical oscillations appear at the far right.
Figure 8e When discreteness $h$ is infinite, the wavefront vanishes and the oscillating tail reaches a limiting form.
See Eqs. (85). The dashed box indicates the size of the other drawings in this series. The dashed curve is the continuum approximation, Eq. (36c). Both curves have the same normalization. See Eq. (23).
impulse.

I have provided a series of graphs of the general Green's function for different values of discreteness $h$, Figs. 8. In Fig. 8a discreteness is zero and $G$ is the continuum approximation result with its asymmetric exponentially damped behavior. As soon as $h$ is finite, Fig. 8b, oscillations appear in the tail and the slope discontinuity changes character some. But, on the average, it still looks like the continuum approximation. Although the "elastic band" has become discrete, it is still "stiff". The remaining graphs show how the oscillations grow and the wavefront diminishes. The last of the series, Fig. 8e, shows the infinite discreteness limit. The dashed box shows the size of the preceding graphs of the series: A change of scale was made.

A series of similar graphs of $G(X)$ for increasing values of velocity $\bar{v}$ would show an originally highly oscillatory curve evolve into a smoother, longer wavelengthed curve. In Figs. 9 I provide a low and high velocity example. In the low velocity curve, Fig. 9a, it is very clear that oscillations appear in the wavefront and a substantial slope discontinuity exists at $X=0$. Entirely the opposite behavior in Fig. 9b, the higher velocity curve, is evident.

The limiting case of $\bar{v}$ tending to zero was described qualitatively in Section A of this chapter as being problematic. This is manifest in the Green's function in this limit. See Eq. (73e).
The smaller $\nu$ is, the spikier the Green's function is. Hence the spiky nature of Fig. 9a.

The Green's function $G(X)$ does not have the same asymptotic behavior as the solitary wave amplitude $U(X)$, even though the differential equations Eqs. (36a) and (36b) are similar. The Green's function resembles a nondispersive solitary wave because it is driven by impulse source terms. The solitary wave is a nondispersive solitary wave because the "source term" is a functional of itself: It maintains its own shape. We can learn something about the asymptotic behavior of $U$ by studying the asymptotic behavior of $G$ because of the similarity of the linearized equations. This statement is qualified because exactly how $G$ will be modified through the iteration identity, Eq. (31a), is not obvious. At the very least the wake of $U$ will be some modification of the wake of $G$ because of the applied force $f$. An additional observation is that while the Green's function is unique for a set of values of the parameters (i.e., Eq. (73e)), this does not mean $U$ is unique.
Figure 9a  This is the first of two graphs showing how the Green's function behaves as a function of velocity. In both cases $g=1/2$ and $h=1$. Here, for low velocity, the Green's function is very spiky. Note too the oscillations in the wavefront. The slope discontinuity at the origin is extremely large.

$G(X)$

$\overline{V} = 0.3$
Figure 9b For large velocities the Green's function is very smooth in contrast to Fig. 9a. The slope discontinuity at $X=0$ is barely visible.
In order to explain my last statement regarding the uniqueness of $U(X)$, let us examine the small amplitude solutions (phonon-like) of the generalized Frenkel-Kontorova equation.

\[ (h, v^2) \frac{d^2}{dx^2} U(X) + \frac{g}{\sqrt{4 + g^2}} U' - (\frac{\sin 2\pi U}{2 (4 + g^2)}) + f = 0 \quad (88) \]

I specify

\[ U(X) = \begin{cases} 1 - \frac{\arcsin f}{2\pi} + s(X), & X \gg 0 \\ - \frac{\arcsin f}{2\pi} + s(X), & X \ll 0 \end{cases} \quad (89a) \]

where $s(X)$ is small. Substitution into Eq. (88) and linearizing gives

\[ (h, v^2) \frac{d^2}{dx^2} s(X) + \frac{g}{\sqrt{4 + g^2}} s' - \frac{\sqrt{1 - f^2}}{4 + g^2} s = 0 \quad (89b) \]

As a trial solution let

\[ s(X) = A e^{ikX} \quad (89c) \]

so substitution gives an indicial equation for $k$.

\[ \frac{1}{1 - v^2} \left[ (\sin \frac{\pi k}{2h})^2 - \frac{g}{\sqrt{4 + g^2}} \right] - \frac{g}{\sqrt{4 + g^2}} ik + \frac{\sqrt{1 - f^2}}{4 + g^2} = 0 \quad (89d) \]

In the continuum approximation this reduces to

\[ k^2 - \frac{g}{\sqrt{4 + g^2}} ik + \frac{\sqrt{1 - f^2}}{4 + g^2} = 0 \quad (90a) \]

where there are only two roots to the indicial equation, namely
\[ k_\pm = \frac{1}{2} \left( -\frac{E}{\sqrt{4+g^2}} \pm \sqrt{\frac{4}{4+g^2}} \right) i \]  

(90b)

These are the exponents in the trial solution of \( U \), Eq. (42), for the continuum approximation. \( k_+ \) is the exponent for \( X>0 \), \( k_- \) is the exponent for \( X<0 \). Therefore, the asymptotic solution of \( U \) is, in the continuum approximation, unique. Whatever the behavior of \( U \) when \( U=0 \), even if this behavior is not unique, it only has one asymptotic behavior available to it for large magnitude \( X \).

There is no such unambiguity in the discrete case. The solution to Eq. (89d) is not generally unique. This may indicate the transport curves will not be unique. While this indicates \( U \) is not unique given \( g \), \( \overline{V} \) and \( h \), at least it offers the promise of providing a way of labelling the various possibilities.

When \( f=0 \), the left side of Eq. (89c) is the denominator of the fourier transform of the Green's function, Eq. (25).

\[ -\frac{1}{\sqrt{2\pi} \overline{G}(k)} = \frac{1}{1-V^2} \left[ \left( \frac{\sin \frac{1}{2}hk}{\chi h} \right)^2 - V^2 k^2 \right] - \frac{E}{\sqrt{4+g^2}} ik + \frac{1}{4+g^2} \]  

(91a)

The Green's function only depends on the modulus of Eq. (91a), appearing as a denominator in \( \overline{G}(k) \) when expressed in real and imaginary parts. This denominator is
\[
\frac{1}{1 - \nu^2} \left[ \left( \frac{\sin \frac{\theta h}{\hbar} k^2}{\hbar} - \nu^2 k^2 \right) + \frac{1}{4 + \gamma^2} \right]^2 + \left( \frac{\gamma}{\sqrt{4 + \gamma^2}} k^2 \right)^2 \quad (91b)
\]

This denominator also appears in Eq. (81b), the exact solution to a discrete lattice transport problem. When this denominator is minimized, the expressions it appears in will peak. Peaking will appear near those values of \( k \) satisfying

\[
\frac{1}{1 - \nu^2} \left[ \left( \frac{\sin \frac{\theta h}{\hbar} k^2}{\hbar} - \nu^2 k^2 \right) + \frac{1}{4 + \gamma^2} \right] = 0 \quad (92a)
\]

as can be seen from Eq. (91b). But this is merely an unusual form of the phonon dispersion relationship. Since a phonon in my notation appears essentially as

\[
e^{i k x} = e^{i (k \bar{x} - \nu T)} \quad (92b)
\]

the frequency of such a phonon participating in the solitary wave is

\[
\Omega(k) = k \nu \quad (92c)
\]
or

\[
\nu = \frac{\Omega(k)}{k} \quad (92d)
\]

If a phonon of wavevector \( k \) in our dynamical system has a phase velocity \( \frac{\Omega(k)}{k} \) which matches the velocity of the solitary wave, as indicated in Eq. (92d), then it will couple strongly to the solitary wave. That is, in satisfying the dispersion relation Eq. (92a), a large number of such
phonons contribute to the Green's function. Saying this in reverse, if a discernable periodic oscillation in the Green's function appears, it must be due to a particularly large contribution by phonons of a wavevector satisfying Eq. (92a).

The transport solution Eq. (81b) is interpretable in this phonon phenomenology. Oscillations in the velocity of a solitary wave as a function of applied force is due to instances where the kink and phonons strongly couple. Whether this carries over in such a straightforward way for the generalized Frenkel-Kontorova equation is not obvious, but this is reasonable and not a suggestion original with me.47

E. Some Results

Those parameters constant for a transport curve in a full discrete calculation will be the friction parameter $\bar{g}$ and the relative spring constant $K$. See Eq. (15f). The parameter $h$ is convenient for the purpose of quantifying "discreteness", but for a given transport curve it is a function of velocity. In fact

$$\lim_{V \to 0} h = \frac{2}{\sqrt{K}}$$  \hspace{1cm} (93a)

$$\lim_{V \to 1} h = \lim_{V \to 1} \frac{\bar{g}}{K} = \infty$$  \hspace{1cm} (93b)

The only substantive difference between the computer program I wrote to perform calculations in the discrete
case and the program in Appendix I for the continuum approximation is the subroutine computing the Green's function. In Appendix II is a copy of the subroutine used to compute the Green's function as well as the final iterations of the solitary wave solution. The two limiting expressions of the Green's function, Eqs. (28) and (29), were used to test the subroutine. Determination of the Green's function is about 75% of the total time needed for the computations.

A global trial solution for the full discrete model solitary wave does not seem feasible without considerable numerical work. Reasonable estimates of the asymptotic solitary wave damping and wake wavelengths can probably be obtained by calculating the roots to the linearized differential equation, Eq. (89d). However, an estimate of wake amplitudes cannot be made easily. The invariants, Eqs. (17), can be used to connect asymptotic solutions and obtain such an estimate, but this appears to be more trouble than it is worth. Consequently a good trial solution for the transport relation

\[ f = f(\bar{v}, \bar{g}, K) \]  

(94)

is not available. My choice is to stick with the trial solutions used in the continuum approximation, Eqs. (42) and (44b). The convergence properties of the iteration are so well behaved that trial solutions do not need to be accurate.
Figure 10 The points in a full discrete calculation are for $g = \frac{1}{2}$ and $K = 1$. The smooth curve passing through the origin is the continuum approximation. Note the scale at the far right indicating discreteness $h$ for a given velocity $\bar{v}$. This result is preliminary.
Remember the iteration identity does not have a unique solution. My major difficulty after beginning calculations in the discrete case was that the iterations converged to a peculiar solution where a single kink "feeds" on an exponentially growing oscillation (an anti-wake?) preceding it. I obtained the desired solution by simply changing the boundary conditions to

\[ \begin{align*}
U(\pm \infty) &= -\frac{\arcsin f}{2\pi} \\
U(-\infty) &= -1 - \frac{\arcsin f}{2\pi}
\end{align*} \]  

All this does is shift \( U(X) \) down by 1, but the numerical iteration evolves differently none the less. I believe the reason for this is that if the oscillating Green's function multiplies a number of order unity in the iteration, these oscillations will tend to grow in successive iterations.

In Eqs. (95) I insure the oscillations grow on the trailing side of the kink because then \( U(-\infty) = 1 \). See Appendix II for such an iteration.

I find \( K=1 \) gives a mass chain loose enough so discreteness is evident but not overwhelming. A choice of \( \tilde{g} = \frac{1}{2} \) gives a wake on the Green's function not excessively long for computer calculations. A commonly used value for \( \tilde{g} \) in the literature is 0.1. In Fig. 10 is a preliminary transport curve computed for \( K=1 \) and \( \tilde{g} = \frac{1}{2} \). The solid curve passing through the origin is the continuum approximation and the points are my results. There are two distinct regions
Figure 11  Solitary wave profile from the series used to construct the transport curve of Fig. 10. Here $\bar{v}=0.82$ and the wavelength of the oscillating wake is about 8 units.
on this curve: In one, increasing the force increases the velocity and so solitary waves are indicated. In the other the existence of solitary waves is problematic because increasing the force decreases the velocity.

The presence of discreteness generally increases the force required to achieve transport. For \( \bar{v} > 0.3 \) the force increases monotonically with velocity like the continuum approximation but has staircase like undulations of a kind predicted by Ishioka. More computational time is needed to establish whether resonance peaks exist for velocities smaller than 0.3.

In Fig. 11 is a selected solitary wave profile for a large velocity where the wake is prominent. Although very small amplitude oscillations in the asymptotic regions occur even in the example for \( \bar{v} = \frac{1}{2} \) of Appendix II, a significant wake is not evident except at large velocities. The wake amplitude and wavelength decrease as solitary wave velocity decreases. The transport curve moves closer to the continuum approximation curve as this occurs. This is because less energy is needed to power a diminishing wake. Below a velocity of 0.3 the wake seems to continue diminishing, but I do not trust the results below this point other than their indicating the end of the solitary wave regime.

There is no doubt about the convergence of the iterations. It is just as definite as in the continuum approximation although more iterations are necessary. In the continuum approximation I described how a large number of
TABLE II

Comparison of Exact Solution to the Problem Solved in Sec. C With the Iteration of This Work

<table>
<thead>
<tr>
<th>( \bar{v} )</th>
<th>Present Work</th>
<th>Ref. 32</th>
<th>300 pts.</th>
<th>500 pts.</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.75</td>
<td>0.407</td>
<td>0.405</td>
<td>0.46</td>
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</tr>
<tr>
<td>0.50</td>
<td>0.191</td>
<td>0.188</td>
<td>0.22</td>
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<td>0.193</td>
<td>0.18</td>
<td>0.18</td>
<td></td>
</tr>
</tbody>
</table>

The 500 point column most closely corresponds to the calculations of Fig. 10. The results of my calculations could be systematically too small because wakes are by necessity truncated resulting in an underestimation of the force. This should not be important in the calculations of Fig. 10 because the friction parameter chosen is large and the wake is strongly damped. Eq. 74 was used to replace the sinusoidal potential with parabolic segments.
iterations is required when \( g \) is large; i.e., when \( \bar{v}=1 \). This also carries over to the discrete case. A large number of points is not necessary to represent \( G \) for large velocity because the wake wavelength is large. But the number of iterations required is larger than what is required for moderate velocities and so more points are used anyhow. In contrast, calculations for small velocities require a larger number of points to represent the Green's function adequately because it is more oscillatory. The number of iterations and points needed ranged from 10 for moderate velocities at 200 points to 50 iterations at 300 points for extreme velocities, large and small. Running time per solitary wave ranged from about 2 minutes to almost 5 minutes on an IBM 3033 computer.

Even though I emphasize these results are preliminary, and probably not accurate, I believe the qualitative structure of the computed curve is correct. An easy way to confirm the precision of the calculation is to increase the number of points used to represent the solitary wave. Having done this I believe the precision is better than 3\%. In order to gauge the accuracy of the calculations, the results of the solvable model given in Section C can be used. The results are in Table II, and were obtained by replacing the sinusoidal potential by the appropriate parabolas. Because of the larger value of \( K \), the oscillations in the Green's function have smaller wavelengths so this test constitutes a more difficult calculation. A more comprehensive
Figure 12 The intersection between parabolas and a sinusoidal curve indicates the graphical solution to the phonon dispersion equation, Eqs. (96a). The value of $K=1$ used here corresponds to the value used in the transport curve Fig. (10). Numbers labelling the parabolas are velocities $V$. Note the first possible instance where the slopes of the two functions match in addition to simple crossing is somewhere between the velocities 0.3 and 0.2 near $k=3\pi/2$. This is consistent with Fig. 10 when interpreting such a match as the condition for a resonance in the transport curve.
comparison still needs to be made.

The phonon dispersion relation, Eq. (92a), can be re-written as

\[ \sin^2 \kappa = (\kappa)^2 - \frac{1}{4\kappa} \]  

(96a)

where

\[ \kappa = \frac{1}{2} \hbar k \]  

(96b)

When the sinusoidal function on the left side of Eq. (96a) equals the parabolic function of the right side, a phonon will strongly couple to the kink as suggested in the last section. When such a match occurs and in addition the slopes of these two functions agree, an especially strong coupling can be predicted. See Fig. 12 where it is demonstrated graphically for \( K=1 \) that the first such strong coupling will occur between velocities 0.3 and 0.2, and this is the place on the transport curve of Fig. 10 where the beginning of a resonance is suggested. The smaller the velocity is, the more frequent such matches occur. In this limit matches of this kind occur close to the maxima and minima of the sinusoidal for a normalized phonon wavevector

\[ \kappa = \frac{1}{2} N \pi \]  

(97a)

where \( N \) is an integer. Substitution of this into Eq. (96a) gives
For \(N=3\), the first possible matching of this kind for \(K=1\)
(see Fig. 12 and Eq. (97a)), then

\[
\bar{v}_N = \begin{cases} 
\frac{1}{N\pi \sqrt{K}} & \text{N even} \\
\frac{1}{N\pi} \sqrt{4 + \frac{1}{K}} & \text{N odd}
\end{cases} \quad (97b)
\]

This is consistent with Fig. 12 and the actual onset of resonant behavior in Fig. 10. The next such resonance should occur approximately at

\[
\bar{v}_3 = \frac{\sqrt{5}}{3\pi} \approx 0.24 \quad (98a)
\]

and so on. Using Eq. (97b), the peaks and the shoulder between them in Fig. 7 can be predicted with an error of less than 10%. As \(N\) becomes larger, Eq. (97b) will become better and better for predicting such matching. A similar analysis is possible for matching which includes second derivatives.
CHAPTER V
CONCLUSION

The numerical scheme I have presented is a straightforward method for solving a difficult numerical problem of mathematical physics. It is based on a Green's function making physical sense and there are no simplifying assumptions. In this approach, familiar linear analytical techniques are used to help penetrate a nonlinear problem.

In the continuum approximation of the transport problem posed herein, I have shown how to avoid finite difference approximations in the numerical analysis which would reintroduce exactly what has been assumed not to exist. A good global trial solution to the single kink transport problem is a natural consequence of the methodology and is aided by a choice of dimensionless parameters making the transport problem a one parameter problem. My calculations indicate the presence of friction limits the velocity obtainable by the solitary waves. It would be useful to find a simple potential (inverted parabolas?) having an exact solution with this property. The work presented here has been recently published.49

Without assuming the continuum approximation, I have preliminary results confirming what simpler models have
predicted. Discreteness generally increases the force necessary to transport a kink. Above a critical velocity the transport curve is much like the continuum approximation with undulations added. Below this critical velocity an opposite behavior is indicated where increasing the applied force slows the solitary wave. This critical velocity is predictable in the phonon phenomenology and I give a simple approximate formula which does predict it. These results are naturally more important than a continuum approximation because real systems are atomic and there are times when this cannot be ignored in transport problems.

A much more interesting generalization of the work presented here would allow situations where we are not constrained to only consider travelling wave solutions to the generalized Frenkel-Kontorova equation. A Green's function depending on X and T can be derived in principle for

$$U_{XX}(X,T) - U_{TT} - g U_T - U = \left(\frac{\sin 2\pi U}{2\pi} - 2\pi U + f(T)\right) = S(X,T)$$

(99)

where \(f(T)\) might be a time dependent force field, so

$$U(X,T) = \iint G(X-X',T-T')S[U(X',T')]dX'dT'$$

(100)

When \(f\) is a constant, \(G\) is simply related to a Bessel function of zero order. This is too general of a problem, and a first step in using something more general than travelling waves would be to try to find "persistant" solu-
tions when a sinusoidal time dependent field is present. Perhaps the time dependence of the solution could be averaged or factored out so the problem is reduced to that of one variable. In any event, this would be especially pertinent to the A.C. conductivity of ionic materials, Josephson junctions, or any other A.C. process.

Work is in progress to use the canonical ensemble formalism of classical thermodynamics to treat nonlinear modes as system excitations having their own effective masses, momenta and lifetimes. Statistical and dynamical theories ought to be consistent. A statistical theory which assumes a solitary wave in a discrete system can move arbitrarily slow is incorrect as is one which assumes solitary waves (always) can move arbitrarily close to the speed of sound.
REFERENCES

1. A.R. Bishop, in *Solitons in Action*, edited by K. Lonn- 
2. Ibid.
3. R.D. Parmentier, in *Solitons in Action*.
   61, 1443 (1973).
5. Ibid.
6. A. Seege and P. Schiller, in *Physical Acoustics, Prin-
7. Parmentier.
8. A. Barone, F. Esposito, C.J. Magee and A.C. Scott, Nuvo 
   cimento 1, 227 (1971).
9. Ibid.
10. J.A. Krumhansl, in *Solitons and Condensed Matter Phy-
    sics*, edited by A.R. Bishop and T. Schneider (Springer-
    Verlag, New York, 1978).
13. T. Schneider and E. Stoll, in *Solitons and Condensed 
    Matter Physics*.
15. D.W. McLaughlin and A.C. Scott, in *Solitons in Action*.
17. E. Ben Jacob and Y. Imry, in *Solitons and Condensed Matter Physics*.
20. Seeger.
25. Marcus.
27. R. Landauer, unpublished notes entitled "Nucleation Theory of Overdamped Soliton Motion" as courteously supplied to me by M. Büttiker.
30. Ibid.
33. Flytzanis.
34. Seeger.
35. Flytzanis.
36. Ibid.
38. Ibid.
41. K. Funke and A. Jost, Berichte der Bunsen-Gesellschaft, Bd. 75, Nr. 5, 436 (1971); see also Ref. 40.
42. Pietronero and Strassler.
43. Bishop.
44. Kimball.
45. Flytzanis.
47. Ibid.; see also Kimball.
48. Ishioka.
APPENDIX I

COMPUTER PROGRAM FOR
THE CONTINUUM APPROXIMATION
WITH SAMPLE OUTPUT
FRENKEL-KONTOROVA MODEL WITH FRICTION AND EXTERNAL FIELD
CONTINUUM APPROXIMATION

PARAMETERS

G  FRICTION
N  NUMBER OF MESH POINTS—LESS THAN OR EQUAL TO 500
NI  NUMBER OF ITERATIONS
NIS  NUMBER OF ITERATIONS SKIPPED BEFORE ENERGY INVARIANT IS
      USED TO INCREMENT THE EXTERNAL FIELD VALUE F

VALUES OF PARAMETERS SUPPLIED BY USER

G=0.2D0
N=50
NI=5
NIS=1

DERIVED CONSTANTS

PI=3.141592654D0
G0=4.D0*G**2
X0=IDINT(15.D0/(1.D0-G0))
X1=IDINT(15.D0/(1.D0+G0))
DX=(X1-X0)/(N-1)
NP=N-1
NIP=NI+1
NIS=NI-9

MAIN PROGRAM

CALL PPRINT
CALL PTRIAL
CALL UTRIAL
CALL GRNFCN
CALL GPRINT
EACH PASS THROUGH THE NEXT DO LOOP ITERATES \( u \) ONCE. (ALL OF THE \( j \) INDEXES ARE USED TO STORE ONLY THOSE VALUES OF THE SUCCESSIVE ITERATIONS OF \( u, F, Du \) AND ERROR NEEDED FOR THE OUTPUT. SEE THE DESCRIPTION GIVEN IN SUBROUTINE \( UPRINT \).)

\begin{verbatim}
21 DO 1000 JI=1,NIP
22 JIP=JI+1
23 JIM=JI-1
24 IF (NI.LE.10) GO TO 500
25 JI8 =JI-NI+11
26 JI8M =JI8-1
27 JI8MM=JI8M-1
28 500 CONTINUE
29 CALL FITER
30 CALL UITER
31 IF (JL.EQ.NIP) GO TO 1000
32 1000 CONTINUE
33 CALL HEAD
34 CALL UPRINT
35 CALL FIPRINT
36 CALL ERRDE
37 STOP
38 END
\end{verbatim}
SUBROUTINE UTRIAL
IMPLICIT REAL*8 (A-H,O-Z)
DIMENSION UT(500), GREEN(1000), U(500,11), PI(11,2)
COMMON PI,G,GO,F,UINF,X0,X,DX,UT,PI, GREEN,N,WP,NIP,NIP,NIS,J,
* JIP,JIP,JIP,JIP,JIP,JIP
THE COMPUTATION OF THE TRIAL SOLUTION FOR U(X) USES THE FORMULAS

\[
U(X) = \frac{(\arcsin F)}{2\pi} + \frac{(2/\pi) \arctan E}{(G + G0 \cdot \text{SGN}(X)) X/2}
\]

\[
G0 = G / \sqrt{(4G^2)}
\]
\[
G1 = \sqrt{\left(\frac{4\sqrt{1-F^2} + G^2}{4+G^2}\right)}
\]

DO 100 I=1,N
X=X0+DX*(I-1)
IF (X.EQ.0.DO) GO TO 50
\[
G1 = \sqrt{\left(\frac{4D0 \cdot \sqrt{1-F^2} + G^2}{4D0 + G^2}\right)}
\]
\[
U(I,1) = UINF + 2.D0/PI*DATA(DEXP((G1+GO*DABS(X)/X)*X/2.D0))
\]
UT(I) = U(I,1)
GO TO 100
50 U(I,1) = UINF+0.5D0
UT(I) = U(I,1)
100 CONTINUE
RETURN
END
SUBROUTINE UPRINT
IMPLICIT REAL*8(A-H,O-Z)
DIMENSION UT(500), GREEN(1000), U(500,11), FI(11,2)
COMMON PI,G,GO,FINF,XO,X1,DX,UT,FI, GREEN,N, MP,NI,NIP,NIS,J
   *1,JIP,J18,J1M,J1MM

IF NI IS LESS THAN 10, ALL ITERATIONS OF U(X) ARE PRINTED.
IF NI IS GREATER THAN 10, ONLY THE FINAL TEN ITERATIONS OF U(X)
ARE PRINTED.

DO 200 I=1,N
   X=X0+DX* (I-1)
   WRITE (6,100) X,I,I
   100 FORMAT (5X,*X ( •  ,I3
   ,')=
   ,F10.6,3X,'U ( •  ,I3, •  )='
   IF (NI.GT.10) GO TO 160
   WRITE (6,125) (U(I,IP),IP=1,NIP)
   125 FORMAT (*+»,31X,T1 F9.6)
   GO TO 200
   160 WRITE (6,170) (U(I,IP),IP=1,11)
   170 FORMAT (*+»,31X,T1 F9.6)
   CONTINUE
200 CONTINUE
RETURN
END
SUBROUTINE FTRIAL
IMPLICIT REAL*8(A-H,O-Z)
DIMENSION UT(500), GREEN(1000), U(500, 11), PI(11, 2)
COMMON PI, G, G0, F, UINF, X0, X1, DX, UT, PI, GREEN, N, NP, NI, NIP, NIS, J
*I, JIP, JII, JIM, JIBM, JIBMM

COMPUTATION OF A TRIAL VALUE FOR F DETERMINED BY SUBSTITUTION OF
THE FORMULA FOR THE TRIAL FUNCTION OF U(X) INTO THE ENERGY INVAR-
IANT WITH THE RESULT GIVEN BELOW.

F = (2/PI)*G SQRT(G**2+4SQRT(1-F**2))
F = 4.0*G/PI
C1 = (PI/8.0)**2
F = F*DSQRT(DSQRT(1.0+(.25D0-C1)*F**4)-(.5D0-C1)*F**2)
IF (F.GT.1.0) DO)
UINF = -DARSIN (FJ/2.0/PI
WRITE (6,100) F, UINF
100 FORMAT (5X, 'F-TRIAL=', F8.6, 3X, 'UINF-TRIAL=', F9.6)
RETURN
END
SUBROUTINE PPRINT
IMPLICIT REAL*8 (A-H,O-Z)
DIMENSION UT(500),GREEN(1000),U(500,11),FI(11,2)
COMMON PI,G,G0,F,INF,X3,X1,DX,U,UT,FI,GREEN,N,NI,NP,NIP,NME,NIS,J
*1,JIP,JIB,JIM,JIBM,JIBM

THIS SUBROUTINE PRINTS THE VALUES OF THE PROGRAM PARAMETERS AND
SELECTED DERIVED PROGRAM CONSTANTS.

WRITE (6,100)
100 FORMAT ('PARAMETERS')
WRITE (6,105) G
105 FORMAT ('G=',F6.3,'(FRICTION)')
WRITE (6,110) N
110 FORMAT ('N= ',13,8X,'(NUMBER OF MESH POINTS)')
WRITE (6,115) NI
115 FORMAT ('NI=',13,6X,'(ITERATIONS BEFORE INCREMENTING F')
WRITE (6,200) NO
200 FORMAT ('NO= ',13,8X,'(NUMBER OF ITERATIONS)')
WRITE (6,205) G0
205 FORMAT ('G0=G/SQRT(4+G**2) = ',F9.6)
WRITE (6,220) X0
220 FORMAT ('X0= ',13,8X,'(NUMBER OF MESH POINTS)')
WRITE (6,215) X1
215 FORMAT ('X1= ',13,8X,'(NUMBER OF MESH POINTS)')
WRITE (6,220) DX
220 FORMAT ('DX= ',13,8X,'(NUMBER OF MESH POINTS)')
RETURN
END
SUBROUTINE UITER
IMPLICIT REAL*8 (A-H,O-Z)
DIMENSION UT(500), GREEN(1000), U(500,11), FI(11,2)
COMMON PI,G,GO,P, UINF, XO, X1, DX, U, UT, FI, GREEN, N, NP, NI, NIP, NI8, NIS, J
* , JIP, JIR, JIM, JI8M, JI8MM

THIS SUBROUTINE ITERATES U(X) ONCE.

ITERATION FORMULAS
U(X) = -F/2PI + (SUM + U0 - U1) / (4 + G**2)
X1 = (GO + SGN(X-XP)) (X-XP) / 2
SUM = \sum (U(XP) - SIN(2PI U(XP))/2PI) DXP
X0

THE SIMPLE TRAPEZOIDAL RULE IS USED TO NUMERICALLY COMPUTE THE INTEGRAL.

U0 = (0 + (F-ARSIN(F))/2PI) [EXP(-((GO+1) (X-X0))/2)/((GO+1)/2)
U1 = (1 + (F-ARSIN(F))/2PI) [EXP(-((GO-1) (X-X1))/2)/((GO-1)/2)
U(X) = U(I,J) U(XP) = U(IP,J) J = ITERATION INDEX

THE U MATRIX HAS ALL ELEVEN COLUMNS FILLED WHEN MI IS GREATER THAN TEN.

A(U,G) = (DSIN(2*DO*PI*U)/(2*DO*PI) - U) * G

THE NEXT STATEMENT IS PROTECTION IN CASE SUBROUTINE PITER PRODUCES AN F LARGER THAN 1.

IF (F.GT.1.D0) F=1.D0
UINF=-DARSIN(F)/2.D0/PI
I INDEXES THE VALUE OF X FOR WHICH \( U(X) \) IS TO BE ITERATED.

INTEGRATION IS OVER XP IS INDEXED BY IP.

```fortran
DO 1000 I=2,NP

IIP=I-1+N+1
SUM=A*UT(I),GREEN(IIP)/2.DO
DO 500 IP=2,NP
IIP=I-IP+N+1
SUM=SUM+A*UT(IP),GREEN(IIP)
CONTINUE

500 CONTINUE
IIP=I-N+N+1
SUM=(SUM+A*UT(N),GREEN(IIP))/2.DO*DX
C
C=UI*NFPF/(2.DO*PI)
U0=(0.DO+C)*(DEXP(-(GO+1.DO)*DX*(I-1)/2.DO))/(GO+1.DO)*2.DO
U1={(1.DO+C)*(DEXP(-(GO-1.DO)*DX*(I-N)/2.DO))/(GO-1.DO)*2.DO
UT(I)=-F/2.DO/PI+(SUM+U0-U1)/(4.DO+G**2)
IF (NI.GT.10) GO TO 750
U(I,JIP)=UT(I)
GO TO 1000
750 IF (JI.GE.NI8) U(I,JIP)=UT(I)
1000 CONTINUE

THE NEXT BLOCK OF STEPS FREES THE ENDPOINTS U(X0) AND U(X1) IN THE
ITERATIONS. THAT IS, HOW THE ITERATION PROCEDS DETERMINES THEIR
VALUES.

IF (NI.GT.10) GO TO 1500
U(I,JIP)=U(2,JIP)
U(N,JIP)=U(NP,JIP)
GO TO 2000
1500 IF (JI.GE.NI8) GO TO 1600
GO TO 2000
1600 U(I,JIP)=U(2,JIP)
U(N,JIP)=U(NP,JIP)
2000 CONTINUE
RETURN
END
```
SUBROUTINE FITES
IMPLICIT REAL*8 (A-H, O-Z)
DIMENSION UT (500), GREEN (1000), U (500, 11), FI (11, 2)
COMMON PI, G, GO, P, UNF, XO, XI, UX, UT, FI, GREEN, N, NP, NI, NIP, NIS, J
*1, JIP, JIB, JIM, JIBM, JISHM

THE ENERGY INVARIANT IS USED TO COMPUTE A NEW F CALLED FP BASED ON
THE CURRENT U(X). IF THE NUMBER OF INCREMENTS COMPUTED, JI, IS
GREATER THAN THE NUMBER OF ITERATIONS TO BE SKIPPED BEFORE ALLOW­
ING THE ITERATED F TO ENTER INTO THE ITERATION PROCESS, NIS, THEN
F = FP IN ALL REMAINING ITERATIONS.

\[ F = 2 \pi G \sqrt{4G^2 \int_{X_0}^{X_1} \left( \frac{\partial U}{\partial X} \right)^2 \, dx} \]

THE DX IN THE INTEGRATION LIMITS MEANS THE ENDPOINTS OF THE NUMER­
ICAL FIELD ARE NOT USED.

A FINITE DIFFERENCE IS USED FOR THE DERIVATIVE AND A MIDPOINT
FORMULA IS USED TO APPROXIMATE THE INTEGRAL.

THE MAGNITUDE OF THE LARGEST DIFFERENCE BETWEEN CORRESPONDING SUC­
CESSIVE ELEMENTS OF THE CURRENT U AND THE PREVIOUS ITERATION OF U
IS ALSO COMPUTED. THIS IS INDICATED AS DU ON THE OUTPUT.

\[ DU = \max (|U(I-NEW) - U(I-OLD)|), \quad I=1,N \]

IF NI IS LESS THAN 10, ALL ITERATIONS ARE SAVED FOR PRINTING.
IF NI IS GREATER THAN 10, ONLY THE LAST TEN ITERATIONS ARE SAVED
FOR PRINTING.

THE ARRAY FI HOLDS BOTH THE DU AND FP VALUES. THE FIRST ROW
HOLDS THE FP VALUES AND THE SECOND ROW HOLDS THE DU VALUES.

COMPUTATION OF DU

\[ DU = 0.0 \]

IF (JI .EQ. 1) GO TO 3000
IF (NI.GT.10) GO TO 1500
DO 1000 I=1,N
DUP=DABS(U(I, JIM)-U(I,JI))
DU=DMAX1(DU,DUP)
1000 CONTINUE
FI(JI, 2)=DU
GO TO 3000

1500 IF (JIM.I.T.NI8) GO TO 3000
DO 1700 I=1,N
DUP=DABS(U(I, JI8M)-U(I,JI8MM))
DU=DMAX1(DU,DUP)
1700 CONTINUE
FI(JI8M, 2)=DU
3000 CONTINUE

COMPUTATION OF F
SUM=0.DO
NM=N-1
DO 4000 I=3,NM
IM=I-1
SUM=SUM+(UT(I)-UT(IM))**2
4000 CONTINUE
FP=2.DO*PI*G*DSQRT(4.DO+G**2)*SUM/DX
IF (JI.EQ.1) FI(JI,1)=FP
IF (NI.GT.10) GO TO 4500
FI(JI,1)=FP
GO TO 5000
4500 IF (JI.GE.NI8) FI(JI8M,1)=FP
5000 CONTINUE
IF (JI.GT.NI8) F=FP
RETURN
END
SUBROUTINE FIPRINT
IMPLICIT REAL*8(A-H,O-Z)
DIMENSION UT(500),GREEN(1000),U(500,11),FI(11,2)
COMMON PI, G, GO, F, JINF, XO, X1, DX, U, UT, FI, GREEN, H, NP, NI, NIP, NIS, J
*1, JIP, J18, JIN, J18M, J18N

ARRAY FI IS PRINTED, ALONG WITH LABELS, WHEN FIPRINT IS CALLED.

WRITE (6,100)
100 FORMAT (5X)
IF (NI.GT.10) GO TO 500
WRITE (6,200) (FI(I,1),I=1,NIP)
200 FORMAT (21X,'ITERATED F=',11F9.6)
WRITE (6,300)
300 FORMAT (5X)
WRITE (6,400) (FI(I,2),I=2,NIP)
400 FORMAT (29X,*DU=*,16X,10F9.6)
GO TO 900
500 WRITE (6,500) (FI(I,1),I=1,11)
500 FORMAT (21X,'ITERATED F=',11F9.6)
WRITE (6,600)
600 FORMAT (5X)
WRITE (6,700) (FI(I,2),I=3,11)
700 FORMAT (29X,*DU=*,18X,10F9.6)
GO TO 900
800 CONTINUE
900 CONTINUE
RETURN
END
SUBROUTINE ERRDE
IMPLICIT REAL*8 (A-H, O-Z)
DIMENSION UT (500), GREEN (1000), U (500, 11), FI (11, 2)
COMMON PI, G, G0, UINF, X0, X1, DX, U, UT, FI, GREEN, U, NP, NI, NIP, N18, NIS, J
*I, JIP, J18, JIN, J18M, J18MM

ALL GROUPS OF 3 SUCCESSIVE POINTS OF THE FINAL ITERATION OF U ARE
SUBSTITUTED INTO THE DIFFERENTIAL EQUATION FOR U TO ESTABLISH HOW
WELL IT IS SOLVED. FINITE DIFFERENCES ARE USED TO APPROXIMATE THE
DERIVATIVES. THIS RESIDUAL IS COMPUTED AT THE ENDPOINTS OF U AND
THE MAXIMUM RESIDUAL AT POINTS IN BETWEEN IS ALSO DETERMINED.
THESE THREE NUMBERS ARE IDENTIFIED AS ERROR ON THE OUTPUT.

U'' + (G/SQRT(4+G**2)) U' - (SIN (2PI*U) + F) / (2PI (4+G**2)) = 0

ERROR0 = E(2)
ERROR1 = MAX (E(N), I=2, N-1)
ERROR = E(N-1)

E(N) = (U(N-1) - 2U(N) + U(N+1)) / DX**2
+ (G/SQRT(4+G**2)) (U(N+1) - U(N-1)) / 2DX
- {1/2PI (4+G**2)} (SIN 2PI U(N) + F)

NM = N - 1
ERROR0 = 0. DO
DO 1000 I = 2, NM
ERROR = UT(I-1) - 2 * UT(I) + UT(I+1) / (DX**2)
ERROR = ERROR + G0 * (UT(I+1) - UT(I-1)) / (2 * DX)

IF (I.EQ.2) ERROR0 = DABS (ERROR)
IF (I.EQ. NM) ERROR1 = DABS (ERROR)
IF (I.NE.2 .AND. I.NE.NM) ERROR = DMAX1 (ERROR, ERROR)

1000 CONTINUE
WRITE (6, 1500)
1500 FORMAT (6, 1500)
1500 WRITE (6, 2000) ERROR0, ERROR, ERROR1
1500 FORMAT (26X, 'ERROR=', 13X, 3F9.6)
RETURN
END
SUBROUTINE HEAD
IMPLICIT REAL*8 (A-H, O-Z)
DIMENSION UT(500), GREEN(1000), U(500,11), PI(11,2)
COMMON PI, G, G0, F, G0F, X0, X1, DX, UT, PI, GREEN, N, NP, NI, NIP, NI8, NIS, J
*1, JIP, JIS, JIM, J18H, J18M

C
C THIS SUBROUTINE PROVIDES THE TABLE HEADING FOR THE PRINTED ITERATIONS OF U.

WRITE (6,50)
50 FORMAT (5X)
WRITE (6,60)
60 FORMAT (78X, 'ITERATION NUMBER'*
WRITE (6,65)
65 FORMAT (35X, 'TRIAL')
IF (NI.GT.10) GO TO 75
WRITE (6,70) (I, I=1, NI)
70 FORMAT (38X, 10I9)
GO TO 79
WRITE (6,76) (I, I=NI8, NI)
76 FORMAT (38X, 10I9)
WRITE (6,80)
80 FORMAT (5X)
RETURN
END
SUBROUTINE GRNFCN
!
IMPLICIT REAL*8(A-H,O-Z)
!
DIMENSION UT(500),GREEN(1000),U(500,11),FI(11,2)
!
COMMON PI,G,GO,F,FINP,X0,X1,DX,U,UT,FI,GREEN,N,NI,NIP,NIP,NIS,JI

THE GREEN'S FUNCTION IS COMPUTED AND STORED IN ARRAY GREEN(I), I=2,2N. THIS CORRESPONDS TO X=M*DX, M=-(N-1), (N-1). THE INDEX I IS CONNECTED TO X BY X=(I-(N+1))*DX.

THE GREEN'S FUNCTION FOR THE CONTINUUM APPROXIMATION IS

\[ G(x) = -\frac{(G_0 + \text{SGN}(x))}{2} \times x \]

NPLS=N+1
NTWO=2*N
DO 1000 I=2,NTWO
IF (I.GT.NPLS) GO TO 500
GREEN(I)=-DEXP(-G0/(1.D0)*DX*(I-N-1)/2.DO)
GO TO 1000
500 GREEN(I)=-DEXP(-G0+1.DO)*DX*(I-N-1)/2.DO)
1000 CONTINUE
RETURN
END
SUBROUTINE GPRINT

IMPLICIT REAL*8(A-H,O-Z)

DIMENSION UT(500), GREEN(1000), U(500,11), FI(11,2)

COMMON PI, G, G0, P, DINF, X0, X1, DX, U, FI, GREEN, N, NP, NIP, NIS, J
* I, JIP, JI8, JIM, JIPM, JIPMM

THIS SUBROUTINE PRINTS THE GREEN'S FUNCTION AS GIVEN BY THE ARRAY GREEN(I).

WRITE (6,200)
200 FORMAT (5X)

WRITE (6, 250)
250 FORMAT (5X,'GREEN'S FUNCTION')

NTWO=2*N
DO 1000 I=2, NTWO
   X=(I-(N+1))*DX
   WRITE (6,500) X, I, GREEN(I)
500 FORMAT (1X, 'X=', F10.6, 3X, 'G(',I3,')=', E15.6)

CONTINUE

WRITE (6,600)
600 FORMAT (5X)

RETURN

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**ITERATED F** = 0.251152 0.258870 0.260224 0.260311 0.260259 0.260229
**DU** = 0.011806 0.006935 0.005503 0.005109 0.005018
**ERROR** = 0.003952 0.002223 0.009628
APPENDIX II

SAMPLE COMPUTER OUTPUT FOR
A FULL DISCRETE CALCULATION
SUBROUTINE GRNFCN
IMPLICIT REAL*8 (A-H,O-Z)
DIMENSION U(900),U(900,11),PI(11,2),GREEN(2000,2)
COMMON PI,H,V,S,GBAK,G,G0,P,UNF,X0,X1,DX,U,UT,FI,GROUND,N,NP,NI,NK

THE GREEN'S FUNCTION IS COMPUTED AND STORED IN ARRAY GREEN(I,1),
I=2,2N. THIS CORRESPONDS TO X=M*DX, M=-(N-1), (N-1). THE INDEX
I IS CONNECTED TO X BY X= (I-(N+1) )*DX.

THE GREEN'S FUNCTION FOR THE DISCRETE MODEL IS

\[
G(X) = \left(-\frac{1}{\pi}\right) \int_{0}^{\infty} \left( A(K) \cos(KX) + B(K) \sin(KX) \right) \, dK \\
\]

\[
D1 = \left( \frac{\sin(KH/2)}{KH/2} \right)^2 - (VK)^2 / (1-V^2) + 1 / (4+G^2)
\]

\[
D2 = G*K/SQRT(4+G^2)
\]

\[
D3 = D1*2+D2*2
\]

\[
A(K) = D1/D3
\]

\[
B(K) = -D2/D3
\]

THE INTEGRATION IS ACCOMPLISHED VIA THE MIDPOINT FORMULA.

\[
DK = \min(\pi/X/MSC, KMAX/MSCMIN, PI/H/MSC)
\]

MSC=THERE ARE TWO TRIGONOMETRIC FUNCTIONS IN THE INTEGRAND HAVING
DIFFERENT PERIODS. ONE HAS PERIOD 2PI/X AND THE OTHER 4PI/H. MSC
IS THE NUMBER OF SUBDIVISIONS OF ONE HALF OF THE SMALLEST OF THESE
PERIODS USED IN DEFINING DK FOR THE NUMERICAL INTEGRATION.

MSCMIN=MINIMUM NUMBER OF TOTAL NUMBER OF INTERVALS FOR INTEGRATION
OVER K.
USER CHOICES

RKMAX=100.DO
MSC=4
MSCMIN=500

WRITE (6,100)
100 FORMAT (5X)
WRITE (6,110) RKMAX, MSC
110 FORMAT (5X, 'RKMAX=', F9.3, 5X, 'MSC=', I4)

H2=H/2.DO
V2=1.DO-V**2
G1=1.DO/(4.DO+G**2)
NPLS=N+1
NTWO=2*N

LOOP FOR GREEN (I,1).

DO 1000 I=2, NTWO
  X=(I-N-1)*DX
  DK1=PI/(DABS(X)+0.001DO)/MSC
  DK2=RKMAX/MSCMIN

1000 CONTINUE
DK3 = PI /((H+0.001)*D)/M
DK = DMIN1(DK1,DK2)
DK = DMIN1(DK3,DK)

LOOP FOR INTEGRATION OVER K.

IKP = IDINT(RKMAX/DK+0.5)

(IKP IS THE NUMBER OF INTEGRATION INTERVALS AND IS STORED IN THE ARRAY GREEN(I,2) LATER IN THIS SUBROUTINE.)

SUM = 0.0
DO 500 IK = 1, IKP
   RK = (IK-0.5)*DK
   D1 = ((DSIN(RK*H2)/H2)**2-(V*RK)**2)/V2+G1
   D2 = G0*RK
   D3 = D1**2+D2**2
   A = D1/D3
   B = -D2/D3
   SUM = SUM + A*DCOS(RK*X) + B*DSIN(RK*X)
500 CONTINUE

GREEN(I,1) = SUM*DK/PI
GREEN(I,2) = IKP

TEST NORMALIZATION OF GREEN(I,1)
SUM = 0.0
DO 2000 I = 2, NTWO
2000 CONTINUE
SUM = SUM + GREEN(I,1)
WRITE (6,2010) SUM
2010 FORMAT (5X,'NORMALIZATION OF -G(X)/(4+G**2) = ',F9.6)
RETURN
END
PARAMETERS
GBA = 0.500  (FRICTION)
V = 0.500  (VELOCITY)
S = 1.000  (HARMONIC CONSTANT)
N = 200  (NUMBER OF MESH POINTS)
NI = 10  (NUMBER OF ITERATIONS)
NIS = 1  (ITERATIONS SKIPPED BEFORE INCREMENTING F)

DERIVED CONSTANTS
G = GBA * V / SQRT(1 - V**2) = 0.288675
G0 = G / SQRT(4 + G**2) = 0.142857
μ = SQRT((4 + G**2) / (S * (1 - V**2))) = 2.333333  (DISCRETENESS)
X0 = -17.0
X1 = 17.0
DX = 0.170854
F_TRIAL = 0.359029  UINF_TRIAL = 0.058446

KMAX = 100.000  MSC = 4
NORMALIZATION OF -G(X)/(4 + G**2) = 1.005276
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Note: The table continues with similar entries but is truncated for brevity.
VITA

The author was born in Youngstown, Ohio, May 1, 1951, the oldest child of Mary Ann and Louis Adams. He has two brothers, Michael and Philip, and one sister, Mary Lou. He graduated from the first class of Oakton High School in Vienna, Virginia, in 1969, after attending the W.T. Woodson High School in Fairfax, Virginia, for almost three years. After spending one year at Cleveland State University, Ohio, in an engineering physics curriculum, he transferred to Youngstown State University where he became a member and officer of The Society of Physics Students and a chapter charter member of the Sigma Pi Sigma Physics Honor Society. Upon graduating in 1973 with a B.S. in a combined program of physics and mathematics, he was awarded the Frank M. Clark Memorial Award. In 1975 he graduated from New Mexico State University with a M.S. in physics.
Candidate: Louis William Adams, Jr.

Major Field: Theoretical Solid State Physics


Approved:

[Signatures]

Major Professor and Chairman

Dean of the Graduate School

EXAMINING COMMITTEE:

[Signatures]

Date of Examination: July 9, 1980