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Transient Imperfections. The Propagation of Waves along a Line of Lattice Atoms†

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Motion of atoms along a close-packed row of atoms in a crystal is described. Each atom has a sinusoidal interaction with atoms not in the row. It also interacts by Hooke's law with its nearest neighbors in the row. For wavelike solutions, the displacements of the nearest neighbors are expanded in terms of time derivatives of the displacement of the atom in question. If this expansion converges, then solutions are obtained in both the classical and the quantum cases. In the classical case, seven different types of solutions are found. In the classical case, the conditions such that the atoms move over the potential barrier are carefully investigated. Conditions are given under which two waves give motion over the barrier when neither would separately. Similar considerations are given for combinations of three waves. Convergence does occur for reasonable potentials.

I. INTRODUCTION

There is a very great need for investigations both by theory and experiment of lattice motions which are large and hence anharmonic. In this paper we discuss the propagation of lattice waves along a line of atoms in a crystal. The motion will not be limited to small amplitude; in fact, the conditions under which atoms can move over the potential barriers which limit them to vibration in a given valley will be carefully examined.

II. FRENKEL-KONTOROVA MODEL

Consider a monatomic crystal composed of mass points m between which there are forces of interaction. Let us focus our attention on a line of atoms lying along some prominent crystallographic direction. The motions which will be described are undoubtedly of most importance for directions having closely spaced atoms and having neighboring rows which are not too near the line. The ⟨110⟩ directions in the fcc lattice represent such a case. Let the potential for motion along the line, i.e., along x, be composed of two parts. First an interaction of the jth atom on the line with the atoms of the lattice not on the line. This we write

$$V_{je} = \tfrac{1}{2} V_0 [1 - \cos(2\pi x_j / a)] , \qquad (1)$$

where V_0 is the amplitude of the off-axis potential, x_j is the displacement of the jth atom from equilibrium in a direction along the line and a is the period of this off-axis potential. There is also an interaction with atoms on the line of atoms. We assume that atoms on the line of atoms interact harmonically with their nearest neighbors on the line unless their nearest neighbor is at a distance greater than $\frac{3}{2}a$. If the separation is greater than $\frac{3}{2}a$ we assume zero interaction. In addition, we neglect the interaction between next-nearest neighbors. This model was first used by Frenkel and Kontorova[1] for discussing slip waves (i.e., waves in which the atoms move from one equilibrium position to the next along the line).

The Hamiltonian for the system is

$$H = T + V = \sum_{j=-\infty}^{+\infty} \left[\frac{p_j^2}{2m} + \tfrac{1}{4}\beta(x_{j+1} - x_j^2) + \tfrac{1}{4}\beta(x_j - x_{j-1})^2 + \frac{V_0}{2}\left(1 - \cos\frac{2\pi x_j}{a}\right)\right] . \quad (2)$$

III. CLASSICAL TREATMENT

From Eq. (2) one obtains the following equation of motion for the jth particle:

$$\frac{m\, d^2x_j}{dt^2} = \beta(x_{j-1} - 2x_j + x_{j+1}) - \frac{\pi V_0}{a}\sin\frac{2\pi x_j}{a} . \quad (3)$$

Solutions in the form of running waves can be found by setting

$$x_j(t+\delta) = x_{j-1}(t) , \quad x_j(t-\delta) = x_{j+1}(t) . \quad (4)$$

In Eq. (4) if δ is positive we are considering a wave moving towards increasing values of j. If δ is negative the wave is traveling towards decreasing j. If Eqs. (4) are inserted into the equation of motion (3) and if $x_{j-1}(t)$ and $x_{j+1}(t)$ are expressed in terms of $x_j(t)$ and time derivatives of $x_j(t)$ one finds that

$$(m - \beta\delta^2)\frac{d^2x_j}{dt^2} = -\frac{\pi V_0}{a}\sin\frac{2\pi x_j}{a} + \frac{\beta\delta^4}{12}\frac{d^4x_j}{dt^4} + \frac{\beta\delta^6}{360}\frac{d^6x_j}{dt^6} + \cdots . \quad (5)$$

If the displacement $x_j(t)$ does not vary too rapidly with time one can neglect the higher derivatives. Then we have

$$\alpha\frac{d^2x_j}{dt^2} = -\frac{\pi V_0}{a}\sin\frac{2\pi x_j}{a} + \frac{\beta\delta^4}{12}\frac{d^4x_j}{dt^4} + O\delta^6 , \quad (6)$$

where the effective mass α is

$$\alpha = m - \beta\delta^2 . \quad (7)$$

To integrate (6) multiply both sides by $\dot{x}_j$ (dots represent time derivatives) and integrate. One obtains

$$\alpha(\dot{x}_j)^2 = 2V_0\left(n^2 - \sin^2\frac{\pi x_j}{a}\right) + \tfrac{1}{6}\beta\delta^4(\dddot{x}_j\dot{x}_j - \tfrac{1}{2}\ddot{x}_j^2) , \quad (8)$$

where n is a constant of integration. x_j and $\dot{x}_j$ are, of course, real numbers. Therefore, from (8) the following kinds of solution can occur (where we have neglected the δ^4 term):

Type	Value of α	Value of n^2
A	$\alpha = 0$	$0 \le n^2 \le +1$
B	$\alpha > 0$	$0 < n^2 < +1$
C	$\alpha > 0$	$+1 < n^2 < +\infty$
D	$\alpha < 0$	$0 < n^2 < +1$
E	$\alpha < 0$	$n^2 = 0$
F	$\alpha < 0$	$-1 < n^2 < 0$
G	$\alpha < 0$	$-\infty < n^2 < -1$

It is helpful to define

$$\delta_0 = (m/\beta)^{1/2} . \quad (9)$$

Here δ_0 is the time required for a longitudinal sound wave to traverse one atomic distance along the line of atoms when the line of atoms is uncoupled from the rest of the lattice, i.e., when V_0 is 0. If c is the velocity of longitudinal sound waves along the uncoupled line of atoms, we have

$$c = a/\delta_0 = a(\beta/m)^{1/2} . \quad (10)$$

Let us consider various types of motion.

A. Effective Mass Zero, Type $A\,(\alpha = 0)$

In this case one must integrate Eq. (5) with the term on the left-hand side of the equation set equal to zero. If the sixth derivative can be neglected we must integrate:

$$\frac{d^4x_j}{dt^4} = \frac{12\pi V_0\beta}{m^2a}\sin\frac{2\pi x_j}{a} . \quad (11)$$

We have only suceeded in integrating this once. One finds

$$\frac{dx_j}{dt}\frac{d^3x_j}{dt^3} - \frac{1}{2}\left(\frac{d^2x_j}{dt^2}\right)^2 = -\frac{6V_0\beta}{m^2}\cos\frac{2\pi x_j}{a} + K_3 . \quad (12)$$

B. Effective Mass Positive, Small Oscillations $(\alpha > 0,\ 0 < n^2 < 1)$

The following procedure will be adopted for all types of solutions: In Eq. (8) the terms in δ^4 will be neglected at first and a solution of the resulting approximate equation will be obtained. Using this solution the δ^4 terms will then be treated as a perturbation.

In Eq. (8) with the δ^4 term omitted $\dot{x}_j$ is zero when $\sin(\pi x_j/a) = n < 1$. Thus $x_j < \frac{1}{2}a$ so each atom in the line executes small oscillations about a given minimum. The velocity $|\dot{x}_j|$ decreases as x_j increases from zero to its limiting value. We introduce the new variables

$$z = \sin(\pi x_j/a) , \quad z_m = n . \quad (13)$$

The integral resulting from the approximate equation (8) is

$$\int_0^y \frac{dz}{(1-z^2)^{1/2}(z_m^2-z^2)^{1/2}} = \frac{\pi}{a}\left(\frac{2V_0}{\alpha}\right)^{1/2} t \, . \tag{14}$$

Since this is a standard elliptic integral[2] one finds

$$y = \sin\frac{\pi x_0}{a} = n \,\mathrm{sn}\; \frac{\pi}{a}\left(\frac{2V_0}{\alpha}\right)^{1/2} t \quad , \tag{15}$$

where sn is the elliptic function analogous to the sine. It is enough to treat the motion of the atom having $j = 0$ since the motion of all other atoms on the line is then given using Eqs. (4). The maximum amplitude x_0^m is

$$z_m = \sin(\pi x_0^m/a) = n \, . \tag{16}$$

The total energy of the system is a first integral of the equations of motion. From (2) and (4) the total energy E is

$$E = \textstyle\sum_j \{\frac{1}{2} m \dot{x}_j^2 + \frac{1}{2}\beta[\dot{x}_j^2\delta^2 + \delta^4(\frac{1}{3}\dot{x}_j \dddot{x}_j + \frac{1}{4}\ddot{x}_j^2) + O\delta^6]$$

$$+ \tfrac{1}{2} V_0[1 - \cos(2\pi x_j/a)]\} \, , \tag{17}$$

where the dots represent time derivatives. Note that only even powers of δ appear and that we have omitted terms in δ^6. The total energy can be written in terms of n, δ, δ_0, and x_j by using (4), (8), and (9) in Eq. (17). We find

$$E = Nn^2 V_0 \frac{\delta_0^2 + \delta^2}{\delta_0^2 - \delta^2} - \frac{2\delta^2 V_0}{\delta_0^2 - \delta^2} \sum_j \sin^2\frac{\pi x_j}{a} \, , \tag{18}$$

where N is the number of atoms in the chain and where δ^4 terms have been neglected.

Using the definitions for δ and δ_0 Eq. (7) is

$$\alpha = m(\delta_0^2 - \delta^2)/\delta_0^2 \, . \tag{19}$$

Since in case B one has $\alpha > 0$, Eq. (19) shows that $\delta < \delta_0$ so the phase velocity is greater than the velocity of sound in the uncoupled chain of atoms.

The dispersion relation can be obtained as follows: The period of oscillation T of the zeroth atom is four times the time required to go from zero displacement to the maximum displacement. So we have

$$\frac{1}{\nu} = T = \frac{4a}{\pi}\left(\frac{\alpha}{2V_0}\right)^{1/2} \int_0^{z_m} \frac{dz}{[(1-z^2)(z_m^2 - z^2)]^{1/2}}$$

$$= \frac{4a}{\pi}\left(\frac{\alpha}{2V_0}\right)^{1/2} K(n) \, , \tag{20}$$

where $K(n)$ is the complete elliptic integral of the first kind.[3] Using (4) and (15) the displacement of the jth atom is therefore

$$\sin(\pi x_j/a) = n \,\mathrm{sn}[(\pi/a)(2V_0/\alpha)^{1/2}(t - j\delta)] \, , \tag{21}$$

which can also be written

$$\sin(\pi x_j/a) = n \,\mathrm{sn}[4\nu K(n)(t - j\delta)] \, . \tag{22}$$

The phase velocity of the waves is

$$v = a/\delta = \nu\lambda = 2\pi\nu/q \, , \tag{23}$$

where $q = 2\pi/\lambda$ is the wave number. From (20) we obtain

$$\nu = \frac{qa}{2\pi\delta} = \frac{\pi}{4aK(n)}\left(\frac{2V_0}{\alpha}\right)^{1/2}$$

$$= \frac{\pi}{4aK(n)}\left(\frac{2V_0}{m - \beta(qa/2\pi\nu)^2}\right)^{1/2} \, .$$

Solving for ν^2 one finds

$$\nu^2 = \pi^2 V_0/8ma^2K^2(n) + (qa/2\pi\delta_0)^2 \, . \tag{24}$$

Because δ^4 terms were neglected, this dispersion relation does not contain terms in q^4. The constant term is associated with $q = 0$ ($\lambda = \infty$) when all atoms of the chain move together. As n increases the amplitude of oscillation increases but the first term in (24) decreases since[3]

$$K(n) = \tfrac{1}{2}\pi\,[1 + 2(\tfrac{1}{8}n^2) + 9(\tfrac{1}{8}n^2)^2 + 50(\tfrac{1}{8}n^2)^3 + \cdots] \, . \tag{25}$$

When q is zero, ν^2 approaches $V_0/8m\pi^2a^2$ as n approaches zero. We call this limit ν_0^2.

Let us treat the δ^4 term in Eq. (8). If we substitute from Eqs. (6) and (8) into the δ^4 term we obtain

$$\alpha\dot{x}^2 = n^2\left[2V_0 - \frac{2\beta\delta^4}{3}\left(\frac{\pi V_0}{\alpha a}\right)^2\right]$$

$$- \sin^2\frac{\pi x}{a}\left[2V_0 - \frac{\beta\delta^4}{3}\left(\frac{\pi V_0}{\alpha a}\right)^2(4n^2+1)\right]$$

$$- \beta\delta^4\left(\frac{\pi V_0}{\alpha a}\right)^2 \sin^4\frac{\pi x}{a} \, .$$

If we define a dimensionless variable h where

$$h = (\beta\delta^4/3V_0)(\pi V_0/\alpha a)^2 \, , \tag{26}$$

then the above equation is

$$\dot{x}^2 = (2V_0/\alpha)\{n^2(1-h) - \sin^2(\pi x/a)$$

$$\times [1 - \tfrac{1}{2}(4n^2+1)h] - \tfrac{3}{2}h\sin^4(\pi x/a)\} \, , \tag{27}$$

where h is a small quantity compared with unity. If $V_0 = 1$ eV, $\beta = 10^5$ dyn/cm, and $a = 2.86$ Å, then $h = 0.065\,28$, where we took $\alpha = \frac{1}{2}m$. Note that m cancels out in h. Thus the first effect of the δ^4 terms is to alter slightly the values of n^2, the amplitude, and of ν, the frequency associated with the motion. The $\sin^4(\pi x/a)$ term must however be considered further.

Actually Eq. (27) can be written as

$$\dot{x}^2=\frac{2V_0}{\alpha}\left[n^2(1-h)-[1-(4n^2+1)\tfrac{1}{2}h]\sin^2\frac{\pi x}{a}-\tfrac{3}{2}h\sin^2\frac{\pi x}{a}\left(n^2-\frac{\alpha}{2V_0}\dot{x}^2\right)\right],$$

which gives

$$\frac{dx[1-\tfrac{3}{4}h\sin^2(\pi x/a)]}{\{n^2(1-h)-[1-(n^2+1)\tfrac{1}{2}h]\sin^2(\pi x/a)\}^{1/2}}=dt\left(\frac{2V_0}{\alpha}\right)^{1/2}. \quad (28)$$

This integrates, giving

$$\operatorname{sn}^{-1}(\sin\phi,k)-\frac{\tfrac{3}{4}h}{1-\tfrac{3}{4}h}E(\phi k)=\frac{\pi t}{a(1-\tfrac{3}{4}h)}\left(\frac{2V_0}{\alpha}[1-(n^2+1)\tfrac{1}{2}h]\right)^{1/2}, \quad (29)$$

where

$$k^2=n^2(1-h)/[1-(n^2+1)\tfrac{1}{2}h], \quad (30)$$

$$\sin\phi=\sin(\pi x/a)/k, \quad (31)$$

and where $\operatorname{sn}^{-1}(\phi,k)$ is an elliptic integral of the first kind, and $E(\phi,k)$ is an elliptic integral of the second kind.[4] The lowest order of approximation gives

$$\sin\frac{\pi x}{a}=k\operatorname{sn}\left[\frac{\pi t}{a(1-\tfrac{3}{4}h)}\left(\frac{2V_0}{\alpha}[1-(n^2+1)\tfrac{1}{2}h]\right)^{1/2}\right]. \quad (32)$$

But $E(\phi,k)$ is

$$E(\phi k)=\tfrac{1}{2}(1+n^2)\sin\phi+\tfrac{1}{2}(1-n^2)\times\ln[(1+\sin\phi)/\cos\phi]+\cdots. \quad (33)$$

Thus, if we take only the first term to use in Eq. (29) and carry out the inversion we find that

$$\sin\frac{\pi x}{a}\left(1-\frac{3h}{8}\frac{(n^2+1)}{k}\cos\frac{\pi x}{a}\left(1+4e^{-\pi K(k')/K(k)}\right)\right)=k\operatorname{sn}\left(\frac{\pi t(2V_0/\alpha)[1-(n^2+1)\tfrac{1}{2}h]}{a(1-\tfrac{3}{4}h)}\right), \quad (34)$$

where $K(k)$ is the complete elliptic integral of the first kind and where $k'^2=1-k^2$. Note that Eq. (34) is correct to first order in h; terms in h^2 were neglected.

C. Continuous Motion over Barriers ($\alpha>0$, $1\leq n^2<\infty$)

In this case if the δ^4 terms are omitted in Eq. (8) one sees that $\dot{x}^2$ is greater than zero, no matter what x is. Hence, in one type of such a motion the particles move continuously in the plus-x direction. We obtain the solution by integrating Eq. (28). Let us at first omit terms in h. We take

$$k^2=1/n^2 \quad (35)$$

and on integrating and inverting one obtains

$$\sin\frac{\pi x}{a}=\operatorname{sn}\left[\frac{n\pi t}{a}\left(\frac{2V_0}{\alpha}\right)^{1/2}\right]. \quad (36)$$

We can still use Eq. (18) for the energy of the system. This dispersion relation is found as before, i.e.,

$$\frac{1}{\nu}=T=\frac{4a}{\pi}\left(\frac{\alpha}{2V_0}\right)^{1/2}\int_0^{\pi/2}\frac{d\phi}{(n^2-\sin^2\phi)^{1/2}}; \quad (37)$$

therefore,

$$\frac{1}{\nu}=T=\frac{4a}{\pi}\left(\frac{\alpha}{2V_0}\right)^{1/2}\left(\frac{1}{n}\right)K\left(\frac{1}{n}\right),$$

$$\nu=\frac{qa}{2\pi\delta}=\frac{\pi n}{4aK(1/n)}\left(\frac{2V_0}{\alpha}\right)^{1/2}=\frac{\pi n}{4aK(1/n)}\left(\frac{2V_0}{m-\beta(qa/2\pi\nu)^2}\right)^{1/2}. \quad (38)$$

Solving for ν^2 one finds

$$\nu^2=\frac{\pi^2n^2V_0}{8ma^2K^2(1/n)}+\left(\frac{qa}{2\pi\delta_0}\right)^2, \quad (39)$$

where terms q^4 have been neglected. When n approaches unity $K(1/n)$ approaches infinity giving a zero first term in (39). When n approaches infinity $K(1/n)$ approaches $\tfrac{1}{2}\pi$ and the first term goes to infinity.

D. Small Oscillations near Top of Barrier ($\alpha<0$, $0<n^2<+1$)

In this case, in (8) one achieves imaginary quantities on both sides if $\sin^2(\pi x_0/a)>n^2$. After integration inversion and rearrangement one obtains:

$$\sin\frac{\pi x_0}{a}=n\left\{1-(1-n^2)\operatorname{sn}^2\left[\frac{\pi t}{a}\left(\frac{2V_0}{|\alpha|}\right)^{1/2}\right]\right\}^{-1/2}=n\left\{n^2+(1-n^2)\operatorname{cn}^2\left[\frac{\pi t}{a}\left(\frac{2V_0}{|\alpha|}\right)^{1/2}\right]\right\}^{-1/2}, \quad (40)$$

where cn is the elliptic function analogous to the cosine. Thus $\sin(\pi x/a)$ is unity when sn is unity and is n when sn is zero. The dispersion relation is obtained in the usual way, i.e.,

$$\frac{1}{\nu}=\frac{4a}{\pi}\left(\frac{|\alpha|}{2V_0}\right)^{1/2}\int_{\sin^{-1}(n)}^{\pi/2}\frac{d\phi}{(\sin^2\phi-n^2)^{1/2}}=(4a/\pi)(|\alpha|/2V_0)^{1/2}\times[K((1-n^2)^{1/2})-F(\sin^{-1}(n),(1-n^2)^{1/2})],$$

where $F(\sin^{-1}(n), k^2)$ is the incomplete elliptic integral of the first kind. Solving for ν^2, we have

$$\nu^2 = \frac{-\pi^2 V_0}{8ma^2[K((1-n^2)^{1/2}) - F(\sin^{-1}(n), (1-n^2)^{1/2})]^2} + \left(\frac{qa}{2\pi\delta_0}\right)^2 [K((1-n^2)^{1/2} - F(\sin^{-1}(n), (1-n^2)^{1/2})] , \quad (41)$$

This shows that in the present case there is a limiting wave number q_c. Only larger wave numbers give positive values of ν^2.

E. Transient Motion near Top of Barrier ($a<0, n^2=0$)

This is a special case associated with a particular energy of the system. The integration is elementary and one finds

$$\tan\frac{\pi x}{2a} = A \exp\left[+\frac{\pi t}{a}\left(\frac{2V_0}{|\alpha|}\right)^{1/2}\right], \quad (42)$$

where the constant A gives the initial value of x. Note that

$$\dot{x} = \sin(\pi x/a)\,(2V_0/|\alpha|)^{1/2} ,$$

so the velocity reaches a maximum at the top of the barrier, i.e., at $\frac{1}{2}a$. If $A=1$ the atom in question starts at $\frac{1}{2}a$ with maximum velocity and ends at infinite time at $x=a$ with zero velocity.

F. Small Oscillations near Bottom ($a<0, -1<n^2<0$)

The equation for integration in this case is

$$\frac{(\pi/a)\,dx}{[\,|n^2| + \sin 2(\pi x/a)]^{1/2}} = \frac{\pi}{a}\,dt\left(\frac{2V_0}{|\alpha|}\right)^{1/2} ,$$

which integrates to give

$$\sin\frac{\pi x}{a} = |n| \operatorname{sn}\left[\frac{\pi t}{a}\left(\frac{2V_0}{|\alpha|}(1+|n^2|)\right)^{1/2}\right]\left\{1+|n^2| \operatorname{cn}^2\left[\frac{\pi t}{a}\left(\frac{2V_0}{|\alpha|}(1+|n^2|)\right)^{1/2}\right]\right\}^{-1/2} . \quad (43)$$

Thus $\sin(\pi x/a)$ varies between $+|n|$ and $-|n|$ as time increases. The dispersion relation is

$$\nu^2 = \frac{-\pi^2 V_0(1+|n^2|)}{8ma^2F^2(\sin^{-1}|n|, (1+|n^2|)^{-1/2})} + \left(\frac{qa}{2\pi\delta_0}\right)^2 . \quad (44)$$

Again there is a critical q and only larger wave numbers give physically meaningful solutions.

G. Motion over Barriers ($a<0, -\infty<n^2<-1$)

On integration and inversion one obtains

$$\sin\frac{\pi x}{a} = |n| \operatorname{sn}\left[\frac{\pi t}{a}\left(\frac{2V_0}{|\alpha|}(1+|n^2|)\right)^{1/2}\right]\left\{|n^2| + \operatorname{cn}^2\left[\frac{\pi t}{a}\left(\frac{2V_0}{|\alpha|}(1+|n^2|)\right)^{1/2}\right]\right\}^{-1/2} . \quad (45)$$

Hence in case G the atoms go over the barriers since from (8) the velocity never goes to zero. The dispersion relation is

$$\nu^2 = -\frac{\pi^2 V_0(1+|n^2|)}{8ma^2K^2((1+|n^2|)^{-1/2})} + \left(\frac{qa}{2\pi\delta_0}\right)^2 . \quad (46)$$

Again only large wave numbers are physically allowed.

IV. TOTAL ENERGY

To evaluate the partition function so that the thermal behavior of the model can be studied, it is necessary to find E and ν for all the normal modes of the system.

Case B. Small Oscillations ($\alpha>0,\ 0<n^2<+1$). Since we are especially interested in cases in which the particles are near the tops of the barriers we attempt to use expressions appropriate for that limit. From Eqs. (18) and (22) one finds

$$E_B = Nn^2V_0 + \frac{16n^2ma^2K^2(n)}{\pi^2}\left(\frac{qa}{2\pi\delta_0}\right)^2 \times [N - \textstyle\sum_j \operatorname{sn}^2 4\nu K(n)(t-j\delta)] . \quad (47)$$

As n approaches unity, $K(n)$ approaches infinity. In fact, we have

$$K(n) = \ln\left(\frac{4}{(1-n^2)^{1/2}}\right) + \frac{1}{4}\left\{\ln\left(\frac{4}{(1-n^2)^{1/2}}\right) - 1\right\}(1-n^2) + \cdots . \quad (48)$$

Therefore, since E is finite one must require that q approach zero. This also requires that ν approach zero as n^2 approaches unity [see Eq. (24)]. Then $E=Nn^2V_0$, which implies that all atoms are sitting on top of the barrier.

Case C ($\alpha>0,\ +1<n^2<+\infty$). Again from (18), but using this time Eq. (36), one finds

$$E_c = Nn^2 V_0 + \frac{16ma^2K^2(1/n)(qa/2\pi\delta_0)^2}{\pi^2} \times\left[N - \frac{1}{n^2}\sum_j \mathrm{sn}^2 4\nu K\left(\frac{1}{n}\right)(t-j\delta)\right]. \quad (49)$$

Thus when n^2 approaches unity from larger values $K(1/n)$ approaches infinity, and again q and ν must both approach zero. Hence, in this limit also all particles sit simultaneously on the tops of the barriers with no kinetic energy.

Case D ($\alpha < 0$, $0 < n^2 < 1$). From Eq. (40) it is clear that $\sin(\pi x_0/a)$ is unity when sn is unity, but x_0^2 is positive and approaches 0 as n^2 approaches 1. x_0^2 is zero when $\sin^2(\pi x_0/a) = n^2$. Thus, the particles oscillate near the top of the barrier but do not travel along the chain. As n^2 approaches unity the amplitude of oscillation decreases. When n^2 approaches unity $K((1-n^2)^{1/2})$ approaches $\frac{1}{2}\pi$ and $F(\sin^{-1}(n),\ (1-n^2)^{1/2})$ approaches $K((1-n^2)^{1/2})$; thus, the denominator of (41) goes to zero and q must approach infinity to keep ν^2 positive. The appropriate expansions for $K((1-n^2)^{1/2})$ and $F(\sin^{-1}(n),\ (1-n^2)^{1/2})$ are

$$K((1-n^2)^{1/2}) = \tfrac{1}{2}\pi\left[1 + 2\left(\frac{1-n^2}{8}\right) + 9\left(\frac{1-n^2}{8}\right)^2 + \cdots\right], \quad (50)$$

$$F(\sin^{-1}(n),\ (1-n^2)^{1/2}) = \tfrac{1}{2}\pi - (1-n^2)^{1/2} - \frac{\pi}{2}\left(\frac{1-n^2}{8}\right) - \frac{(1-n^2)^{3/2}}{24} - \cdots . \quad (51)$$

In case D the energy is

$$E = Nn^2V_0 - 16ma^2n^2\left(\frac{qa}{2\pi\delta_0}\right)^2 \{K((1-n^2)^{1/2}) - F(\sin^{-1}n, (1-n^2)^{1/2})\}\left(N - \sum_j n[1-(1-n^2)\,\mathrm{sn}^2 4\nu\{K-F\}(t-j\delta)]^{-1/2}\right). \quad (52)$$

Since q approaches at most $2\pi/a$ and since the two { } brackets both approach zero again, E approaches $Nn^2V_0 = NV_0$ when n^2 approaches unity.

Thus for each of the various kinds of motions considered if we treat one mode of motion only then all of the atoms achieve the top of the barrier together. It is necessary to combine several of such modes to make a wave packet if one is to achieve barrier crossing in a limited region. Since summations of elliptic functions are intricate the resulting wave-packet theory will not be simple.

V. SUPERPOSITION

It is necessary to know the resultant displacement when two or more waves are simultaneously present in the chain. Consider to be specific the case in which two waves g and h are present. Suppose that g represents a wave traveling in the positive direction and h represents a wave traveling in the negative direction. Then we have

$$x_j = g(t - j\delta_+) \pm h(t + j\delta_-) . \quad (53)$$

To be more specific, assume first that both waves are of type B ($\alpha > 0$, $0 < n^2 < +1$). Then we have

$$\sin\frac{\pi x_{j+}}{a} = n_+\,\mathrm{sn}\left[\frac{\pi}{a}\left(\frac{2V_0}{\alpha_+}\right)^{1/2}\{t - \delta_+ j\}\right], \quad (54)$$

$$\sin\frac{\pi x_{j-}}{a} = n_-\,\mathrm{sn}\left[\frac{\pi}{a}\left(\frac{2V_0}{\alpha_-}\right)^{1/2}\{t - \delta_- j\}\right]. \quad (55)$$

But we have

$$\sin(A+B) = \sin A\cos B + \cos A \sin B$$

and

$$\cos B = (1-\sin^2 B)^{1/2} = \left\{1 - n_-^2\,\mathrm{sn}^2\left[\frac{\pi}{a}\left(\frac{2V_0}{\alpha_-}\right)^{1/2}\{t+\delta_- j\}\right]\right\}^{1/2} = \mathrm{dn}\left[\frac{\pi}{a}\left(\frac{2V_0}{\alpha_-}\right)^{1/2}\{t+\delta_- j\}\right],$$

where $\mathrm{dn}^2(u) = 1 - k^2\,\mathrm{sn}^2(u)$ is an elliptic function and where we have used both trigonometric and elliptic identities. Thus, we have

$$\sin\frac{\pi}{a}(x_{j+} + x_{j-}) = n_+\,\mathrm{sn}\left[\frac{\pi}{a}\left(\frac{2V_0}{\alpha_+}\right)^{1/2}\{t - \delta_{+j}\}\right]\mathrm{dn}\left[\frac{\pi}{a}\left(\frac{2V_0}{\alpha_-}\right)^{1/2}\{t+\delta_- j\}\right] + n_-\,\mathrm{dn}\left[\frac{\pi}{a}\left(\frac{2V_0}{\alpha_+}\right)^{1/2}\{t - \delta_+ j\}\right]\mathrm{sn}\left[\frac{\pi}{a}\left(\frac{2V_0}{\alpha_-}\right)^{1/2}\{t+\delta_- j\}\right]. \quad (56)$$

In order to decide whether particles go over the barrier in this case one needs to know the velocity of a particle when it is atop a barrier. Consider the $j = 0$ particle. From (8) we have

$$\dot{x}_j = (2V_0/\alpha)^{1/2}[n^2 - \sin^2(\pi x_j/a)]^{1/2} .$$

Thus, we have

$$\dot{x}_{0+} + \dot{x}_{0-} = \left(\frac{2V_0}{\alpha_+}\right)^{1/2} n_+ \operatorname{cn}\left[\frac{\pi}{a}\left(\frac{2V_0}{\alpha_+}\right)^{1/2} t\right] + \left(\frac{2V_0}{\alpha_-}\right)^{1/2} n_- \operatorname{cn}\left[\frac{\pi}{a}\left(\frac{2V_0}{\alpha_-}\right)^{1/2} t\right]. \tag{57}$$

From (56) we have

$$\sin\frac{\pi}{a}(x_{0+} + x_{0-}) = n_+ \operatorname{sn}\left[\frac{\pi}{a}\left(\frac{2V_0}{\alpha_+}\right)^{1/2} t\right] \operatorname{dn}\left[\frac{\pi}{a}\left(\frac{2V_0}{\alpha_-}\right)^{1/2} t\right] + n_- \operatorname{dn}\left[\frac{\pi}{a}\left(\frac{2V_0}{\alpha_+}\right)^{1/2} t\right] \operatorname{sn}\left[\frac{\pi}{a}\left(\frac{2V_0}{\alpha_-}\right)^{1/2} t\right]. \tag{58}$$

We want $(\dot{x}_{0+} + \dot{x}_{0-}) > 0$ when $(x_{0+} + x_{0-}) = \frac{1}{2}$. This can be achieved. Consider the motion of the $j = 0$ particle. Figure 1 shows the two waves with the correct arrangement at about the critical moment. The $j = 0$ particle still has some forward velocity. If $n_+ = n_-$, then one finds that the particle goes over the barrier if

$$n_+ > 0.524 . \tag{59}$$

When n_+ differs from n_- the $j = 0$ particle goes over the barrier if

$$n_+ + n_- > 1.048 . \tag{60}$$

If three type-B waves are combined the resultant displacement is found from

$$\begin{aligned}\sin(\pi/a)(x_1 + x_2 + x_3) = {} & n_1 \operatorname{sn}[4\nu_1 K(n_1)(t - j\delta_1)] \operatorname{dn}[4\nu_2 K(n_2)(t - j\delta_2)] \operatorname{dn}[4\nu_3 K(n_3)(t + j\delta_3)] \\ & + n_2 \operatorname{sn}[4\nu_2 K(n_2)(t - j\delta_2)] \operatorname{dn}[4\nu_3 K(n_3)(t + j\delta_3)] \operatorname{dn}[4\nu_1 K(n_1)(t - j\delta_1)] \\ & + n_3 \operatorname{sn}[4\nu_3 K(n_3)(t + j\delta_3)] \operatorname{dn}[4\nu_1 K(n_1)(t - j\delta_1)] \operatorname{dn}[4\nu_2 K(n_2)(t - j\delta_2)] \\ & - n_1 n_2 n_3 \operatorname{sn}[4\nu_1 K_1(n_1)(t - j\delta_1)] \operatorname{sn}[4\nu_2 K(n_2)(t - j\delta_2)] \operatorname{sn}[4\nu_3 K(n_3)(t + j\delta_3)] .\end{aligned} \tag{61}$$

If the motion of the $j = 0$ atom is investigated, Fig. 2 shows the waves at about the critical moment. In this case one finds that the particle goes over the barrier if

$$n_1 + n_2 + n_3 > 1.072 . \tag{62}$$

We therefore conclude that several waves which individually could not give rise to motion over the barrier can nevertheless combine in such a way that particles subject to their combined action will move over the barriers.

Consider combinations of F-type waves. The resulting displacements at $j = 0$ from two F-type waves are given by

$$\sin\frac{\pi}{a}(x_1 + x_2) = \frac{k_1' \operatorname{sn}(1)}{[2 - \operatorname{dn}^2(1)]^{1/2}}\left(\frac{1 + (2k_2^2 - 1)\operatorname{sn}^2(2)}{2 - \operatorname{dn}^2(2)}\right)^{1/2} + \frac{k_2' \operatorname{sn}(2)}{[2 - \operatorname{dn}^2(2)]^{1/2}}\left(\frac{1 + (2k_1^2 - 1)\operatorname{sn}^2(1)}{2 - \operatorname{dn}^2(1)}\right)^{1/2}, \tag{63}$$

where we have

$$(1) = 2\pi\nu_1(t + t_1), \quad (2) = 2\pi\nu_2(t + t_2) . \tag{64}$$

The frequencies are given by Eq. (44). t_1 and t_2 are constants and

$$k_1^2 = \frac{1}{1 + |n_1|^2}, \quad k_1'^2 = 1 - k_1^2, \qquad k_2^2 = \frac{1}{1 + |n_2|^2}, \quad k_2'^2 = 1 - k_2^2 . \tag{65}$$

An examination shows that motion over the barriers occurs if $k_1 + k_2 \geq 1.089\,278$.

Next consider the combination of a B-type and an

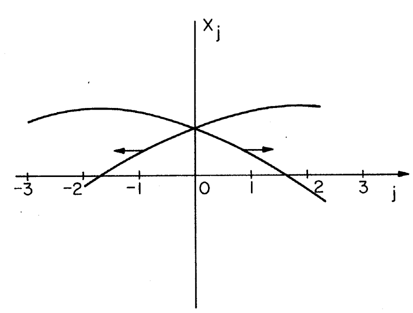

FIG. 1. Combination of two type-B waves to give motion over the barrier.

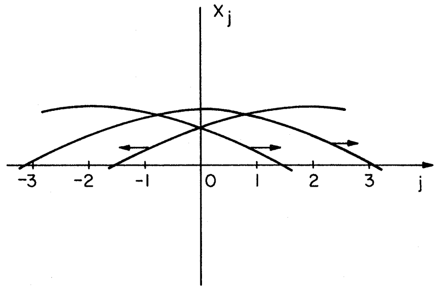

FIG. 2. Combination of three type-B waves to give motion over the barrier.

F-type wave. The displacement at $j = 0$ of the combination is

$$\sin\frac{\pi}{a}(x_1 + x_2) = n_1 \,\mathrm{sn}(1)\left(\frac{1 + (2k_2^2 - 1)\,\mathrm{sn}^2(2)}{2 - \mathrm{dn}^2(2)}\right)^{1/2} + \frac{k_2'\,\mathrm{sn}(2)\mathrm{dn}(1)}{(2 - \mathrm{dn}^2(2))^{1/2}} \quad . \tag{66}$$

In this case one can also get motion over the barrier, but the conditions necessary are not obvious. The combination $n_1 = \sin 36°$ and $k_2 = \sin 27°$ will suffice, but both larger and smaller values of n_1 will not do.

The well-established combination laws for the elliptic functions can be used to ensure a stress-free surface at one or at both ends of a row of atoms just as one sets up standing waves using plane harmonic waves. However since one can count densities of normal modes using periodic boundary conditions we shall not give the results.

VI. QUANTIZED TREATMENT

The problem can be treated quantum mechanically as follows: If the wavelike solutions given in Eq. (4) are inserted into the Hamiltonian of Eq. (2) one finds

$$H = \sum_j H_j = \sum_j \left[\frac{p_j^2}{2m}\left(1 + \frac{\beta\delta^2}{m}\right) + \frac{\beta\delta^4}{2}\left(\ddot{x}_j^2 + \frac{\dot{x}_j \dddot{x}_j}{6}\right) + \cdots + \frac{V_0}{2}\left(1 - \cos\frac{2\pi x_j}{a}\right)\right]. \tag{67}$$

The problem therefore splits into single-particle problems for which

$$H_j \psi_j = E_j \psi_j \ . \tag{68}$$

The total wave function is either a product or a determinant of the ψ_j's depending on the symmetry requirements.

If one omits δ^4 terms and higher powers of δ the Schrödinger equation obtained from (68) is

$$\frac{\partial^2 \psi_j}{\partial x_j^2} + \frac{2m}{\hbar^2[1 + (\beta/m)\delta^2]}\left[E_j - \frac{V_0}{2}\left(1 - \cos\frac{2\pi x_j}{2}\right)\right]\psi_j = 0 \ . \tag{69}$$

The ψ_j are therefore the Mathieu functions. Equation (69) can be put in more standard form by introducing[5]

$$z - \frac{\pi}{2} = \frac{\pi x_j}{a} \quad , \quad r = \frac{2ma^2}{\hbar^2\pi^2}\left(\frac{E_j - \frac{1}{2}V}{1 + \beta\delta^2/m}\right) \quad , \tag{70}$$

with

$$s = ma^2 V_0 / \hbar^2\pi^2(1 + \beta\delta^2/m) \ .$$

One finds that

$$\frac{d^2\psi_j}{dz^2} + (r - 2s\cos 2z)\psi_j = 0 \ . \tag{71}$$

The appropriate boundary condition for a periodic potential is that the probability of the atom being found in each minima is equal. Thus we have

$$\psi_j(x_j + a) = e^{i\mu\pi}\psi_j(x_j) \quad \text{or} \quad \psi_j(z + \pi) = e^{i\mu\pi}\psi_j(z) \ . \tag{72}$$

If one adopts periodic boundary conditions

$$\mu N \pi = 2\pi h \ ,$$

where h is an integer, we thus have

$$\mu = 2h/N \ , \tag{73}$$

i.e., μ is a rational fraction.

The allowed energies E_j occur in energy bands which spread over a larger energy range the larger the energy and the smaller the energy barrier V_0. The states at the top and bottom of each band are periodic with period a or $2a$. The energies for such states and their wave functions are well known. For states far below the top of the barrier one has

$$E_j^n = (2n + 1)\pi\hbar\left(\frac{V_0(1 + \beta\delta^2/m)}{2ma^2}\right)^{1/2} - \frac{(2n+1)^2 + 1}{32}\,\frac{2\pi^2\hbar^2(1 + \beta\delta^2/m)}{ma^2} + O(V_0)^{-1/2} \ , \tag{74}$$

where $n = 0, 1, 2$, etc. We have assumed that these states are not appreciably broadened by tunneling. Inserting $\delta = ka/\nu$ and $E_j = 2\pi\nu\hbar$, one can solve for ν^2 to obtain

$$\nu^2_{\text{bound}} = \frac{(2n+1)^2 V_0}{ma^2} + \frac{\beta}{m}k^2a^2 - \frac{(2n+1)^2 + 1}{32}\,\frac{2\pi^2\hbar^2}{ma^2} \times \left(1 + \frac{\beta k^2 a^4}{(2n+1)^2 V_0}\right) + O(V_0)^{-1/2} \ . \tag{75}$$

For states far above the top of the barrier the energies associated with the top and bottom of the various bands are given by

$$E_j^n=\frac{V_0}{2}+\frac{\pi^2\hbar^2[1+(\beta/m)\delta^2]}{2ma^2}n^2+\frac{ma^2V_0^2}{16\pi^2\hbar^2(1+\beta\delta^2/m)(n^2-1)}+OV_0^4\,. \quad (76)$$

Substituting for E and δ one finds

$$h\nu_{\text{free}}=\frac{V_0}{2}+\frac{\pi^2\hbar^2n^2}{2ma^2}+\frac{8\beta k^2a^2}{n^2}+OV_0^2\,. \quad (77)$$

This last equation is not very helpful since it gives the energies or frequencies associated with the band edges (i.e., the tops and bottoms of the bands), but for energies much larger than V_0 the bands are very wide.

The wave functions described have equal probabilities for the jth atom to be in any valley. To describe localized particles it would be necessary to construct wave packets made up of Mathieu functions. We will leave such treatments for a later paper.

The treatment given depends in a very important way on our ability to make a convergent expansion of the displacement in terms of time derivatives. It is not enough to say that x_{j+1} is the same as x_j except for a phase factor. Such a procedure does not allow the harmonic forces to be described in terms of an effective mass. Such a procedure generates separable but complicated equations of motion.

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Lattice Dynamics of Transition Metals—Application to Paramagnetic Nickel

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The problem of lattice dynamics of transition metals is investigated. For the case of paramagnetic nickel, the isotropic two-band model is used to evaluate the static dielectric function in the Hartree approximation. The bare-ion potential is represented by a two-parameter model potential. The phonon frequencies are calculated for the configurations $(3d)^9(4s)^1$ and $(3d)^{9.4}(4s)^{0.6}$, and compared with the experimental measurements along the three principal symmetry directions [100], [110], and [111]. A fairly good agreement is obtained for both configurations.

I. INTRODUCTION

A good deal of work has been done on the lattice dynamics of normal metals and we have a fairly satisfactory understanding of phonons in these metals.[1-4] The problem of lattice dynamics of transition metals is interesting but characteristically difficult. In these metals the distinction between the core and the conduction electron is not clear. The outermost d shell is not completely filled and the electronic-band-structure calculations[5] show that the wave functions of the conduction electrons have a strong d character. Thus the d states are not sufficiently tightly bound and it is not valid to treat them in the same way as in the case of free atoms. Harrison[6] approached this problem by generalizing the pseudopotential formulation to include the d states in the transition metals. The pseudopotential obtained by him includes the effects of s-d hybridization but is nevertheless weak. The pseudopotential approach for transition metals has not yet been utilized for developing a theory of lattice vibrations in these metals. Sinha[7] and Golibersuch[8] have independently studied the electron-phonon interaction in transition metals using the augmented-plane-wave method. Because of the complexities of these approaches, actual calculations for any metal have not been attempted as yet.

Recently, the authors[9] proposed a noninteracting band model to calculate the static dielectric function of the transition metals (hereafter we refer to this paper as I). The free-electron approximation is used for the electrons in the s band, while