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Momentum Transfer in Crystal Lattices with Vibrating Atoms

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Abstract

A momentum transfer equation previously used to describe non-elastic deformation in crystalline solids represented by point masses at fixed lattice positions is extended to take into account the existence of intrinsic (e.g. thermal) small amplitude vibrations of the masses about their mean positions in a lattice. Use of the time-dependent Schroedinger equation to describe momentum transfer and deformation is also discussed in terms of this vibrating point-mass lattice model. The result is that a modified and identical differential equation for momentum transfer is obtained from each approach; some solutions to this equation are presented. The previous particle momentum wave frequency dependence on wave vector and resulting applications to non-elastic deformation are unchanged, but these particle momentum waves can now be considered as modulating the usual high-frequency waves associated with the elastic modes of a crystalline solid.

1. *Introduction*

A connection between particle waves, momentum transfer, and non-elastic deformation in crystals has been presented in recent publications (Fitzgerald, 1966a, b). The differential equation used in this previous work assumes an equilibrium or undisturbed lattice which can be represented by regularly spaced point masses at fixed positions. The assumption of point masses is valid since linear momentum transfer between atoms is the process in question, and the mass of an atom is heavily concentrated in a nucleus of very small diameter compared to interatomic distances. On the other hand, the atoms of a real crystal are not stationary even at absolute zero, but instead vibrate with small amplitudes and high frequencies about regularly-spaced mean positions. The existence of such quantized vibrational modes for lattice atoms was, in fact, used in the original particle-wave description of deformation in order to account for hypervelocity phenomena and phonon fission (Fitzgerald, 1966b; Fitzgerald, 1964). It is clear that a more realistic lattice model will be one in which the existence of small-amplitude atomic vibrations at equilibrium is recognized at the outset. Such a 'vibrating lattice' model is considered in the present work and some of the necessary modifications and extensions of the particle-wave view of deformation are presented. The role of the time-dependent Schroedinger equation in momentum transfer and deformation (Fitzgerald & Tasi, 1967) is also discussed in terms of a vibrating lattice model.

2. *Momentum Transfer Between Vibrating Atoms in a One-dimensional Lattice*

Consider the infinitely long one-dimensional lattice of point masses, m, and spacing d as shown in Fig. 1(a). If the masses are assumed to be stationary in the absence of external forces, then the differential equation of motion for a particle *momentum* wave in the lattice produced by an applied force can be written in terms of a general nth mass as

$$m\frac{\partial v_n}{\partial t} = \mathbf{K}_p(v_{n+1} + v_{n-1} - 2v_n) \tag{2.1}$$

where v_n is the velocity of the nth mass, etc. and $\mathbf{K}_p$ is considered to be either a *momentum transfer constant* or a *velocity interaction constant* for the lattice as discussed in detail elsewhere (Fitzgerald, 1966b). For our

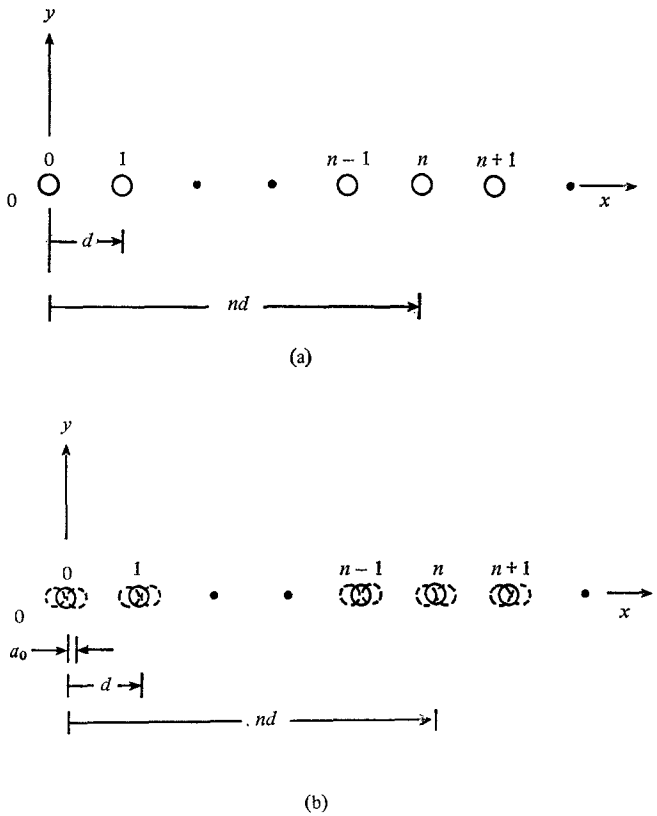

Figure 1.—Schematic drawing of an infinite one-dimensional (row) lattice of point masses. (a) Stationary masses, and (b) vibrating masses with amplitude of vibrations, a_0, much less than lattice spacing, d.

purpose here it is convenient to rewrite equation (2.1) in the form of a continuity equation for momentum transfer or flow along the lattice, namely,

$$\frac{\partial(mv_n)}{\partial t} = \mathbf{K}_p(v_{n-1} - v_n) - \mathbf{K}_p(v_n - v_{n+1}) \tag{2.2}$$

where now

$\frac{\partial(mv_n)}{\partial t}$	represents the net time rate of change of momentum of the nth lattice mass
$\mathbf{K}_p(v_{n-1} - v_n)$	is the rate of momentum transfer from mass $n-1$ to mass n
$\mathbf{K}_p(v_n - v_{n+1})$	is the rate of momentum transfer from mass n to mass $n+1$
$\mathbf{K}_p$	is the *momentum transfer constant* for the lattice

According to equation (2.2) and the above remarks, we are postulating that as a result of an applied force some type of momentum transfer process occurs in the lattice for which the rate of momentum transfer depends on the velocity differences between adjacent masses. The exact nature and/or value of $\mathbf{K}_p$ is then of great importance. Fortunately it is possible to obtain an exact expression for $\mathbf{K}_p$ by writing a wave solution (Fitzgerald, 1966a, b) for v_n in equations (2.1) or (2.2) of the form

$$v_n = B\exp\left[-i(2\pi\nu_p t - knd)\right] \tag{2.3}$$

where $k = 2\pi/\lambda$ is the wave vector, d is the lattice spacing, B is a constant, and the frequency ν_p is given by

$$\nu_p = \frac{-i2\mathbf{K}_p}{\pi m}\sin^2\frac{kd}{2} \tag{2.4}$$

According to the particle-wave view of deformation (Fitzgerald, 1966a, b) equation (2.4) gives the frequency of a particle (momentum) wave in a lattice. In the limit of long wavelengths (small k) this frequency expression must therefore reduce to that for a free particle, i.e.,

$$\lim_{k\to 0}\frac{-i2\mathbf{K}_p}{\pi m}\sin^2\frac{kd}{2} = \frac{\hbar}{4\pi m}k^2 \tag{2.5}$$

where $\hbar k^2/4\pi m$ is the free-particle frequency. For small values of k the sine can be replaced by its argument in equation (2.5) so that

$$\mathbf{K}_p = i\hbar/2d^2 \tag{2.6}$$

and equation (2.1) becomes

$$m\frac{\partial v_n}{\partial t} = \frac{i\hbar}{2d^2}(v_{n+1} + v_{n-1} - 2v_n) \tag{2.1a}$$

Here an exact expression for $\mathbf{K}_p$ is obtained by imposition of the physical boundary condition that at long wavelengths the variation of frequency with wave vector for a particle wave in a lattice must be identical with that for a free particle (Fitzgerald, 1966a, b).

Now consider a lattice in which the point masses vibrate independently with small displacement amplitudes, a_0, about mean positions a distance d apart even in the absence of any external forces as shown schematically in Fig. 1(b). At a given temperature the intrinsic vibration frequency, ν_v, is assumed constant and the same for all atoms in the lattice in accordance with the Einstein model (Einstein, 1906, 1911) so that the displacement of a general nth mass from its mean position at any time, t, in the undisturbed lattice is given by

$$a_n = a_0 \exp\left[-i(2\pi\nu_v t + \theta_n)\right] \tag{2.7}$$

The displacement amplitude, a_0, is assumed to be so small compared to d that no changes in the lattice spacings are noticeable. The amplitude of the corresponding velocity oscillations, however, are not necessarily negligible since ν_v may be large (of the order of 10^{12} to 10^{14} cps). Thus if we differentiate equation (2.7) with respect to time to obtain the vibrational velocity of a general nth mass, the result is

$$v_n(\text{vibrational}) = -i2\pi\nu_v a_0 \exp\left[-i(2\pi\nu_v t + \theta_n)\right] \tag{2.8}$$

or

$$v_n(\text{vib.}) = b_0 \exp\left[-i(2\pi\nu_v t + \theta_n)\right] \tag{2.8'}$$

where $b_0 = -i2\pi\nu_v a_0$. Hence the amplitude of the velocity oscillation is $2\pi\nu_v$ times the displacement amplitude and not necessarily small for large values of ν_v. For interatomic distances, d, of the order of 3×10^{-8} cm values of vibrational displacement amplitude, a_0, up to 3×10^{-11} cm can be considered negligible, but these may result in vibrational *velocity* amplitudes of the order of 1800 cm/sec which cannot be neglected!

Consequently the general expression for the time rate of change of momentum for a general nth lattice mass given in equation (2.2) must be modified to take into account time variations of the equilibrium or self vibrational momentum as well as the rate of momentum transfer to and from the nth mass by adjacent masses which may result from external forces acting on the lattices. The continuity equation for momentum transfer through the nth mass then becomes

$$\frac{\partial(mv_n)}{\partial t} = \mathbf{K}_p(v_{n-1} - v_n) - \mathbf{K}_p(v_n - v_{n+1}) - i2\pi\nu_v(mv_n) \tag{2.9}$$

where the term $i2\pi\nu_v(mv_n)$ represents the time rate of change of momentum as a result of vibration, and the other terms have the same significance as in equation (2.2).

Equation (2.9) can be rewritten

$$m\frac{\partial v_n}{\partial t} = \mathbf{K}_p(v_{n+1} + v_{n-1} - 2v_n) - i2\pi\nu_v(mv_n) \tag{2.10}$$

As before, a wave solution for v_n can be assumed to be of the form

$$v_n = B\exp\left[-i(2\pi\nu t - knd)\right] \tag{2.11}$$

This turns out to be a valid solution provided the frequency ν is given by

$$\nu = \frac{-2i\mathbf{K}_p}{\pi m}\sin^2\frac{kd}{2} + \nu_v \tag{2.12}$$

$$= \nu_p + \nu_v \tag{2.13}$$

where ν_p is the frequency previously obtained [equation (2.4)] for a non-vibrating lattice. In order to evaluate $\mathbf{K}_p$ we again consider the limiting value of ν for long wavelengths (small values of the wave vector, k) and note that

$$\lim_{k\to 0}\nu = \frac{-2i\mathbf{K}_p}{\pi m}\frac{k^2d^2}{4} + \nu_v \tag{2.14}$$

We expect that the closely spaced potential variation within the lattice will have no influence on particles with long wavelengths ($k \to 0$) and the frequency expression given by equation (2.14) should be identical to that for a non-lattice particle of the same mass moving in an external field-free region, but with some kind of constant intrinsic or self energy U_v. A non-rigid or deformable particle, for example, could have a constant strain energy or even be deforming in an oscillatory manner as its center of mass moves with constant velocity, v. In any case, the general expression for the frequency of the de Broglie wave associated with such a particle of mass m is easily obtained from the expression for its total energy, E,

$$E = h\nu = \tfrac{1}{2}mv^2 + U_v$$

where $mv^2/2$ is the kinetic energy resulting from the translational velocity, v. Then

$$\nu = \frac{\hbar k^2}{4\pi m} + \frac{U_v}{h} \tag{2.15}$$

and by setting $U_v/h = \nu_v$ we again find from equations (2.14) and (2.15) that,

$$\mathbf{K}_p = i\hbar/2d^2 \tag{2.16}$$

The differential equation for momentum transfer in a lattice with vibrating point masses [equation (2.10)] therefore becomes

$$\frac{\partial(mv_n)}{\partial t} = i\left[\frac{\hbar}{2d^2}(v_{n+1} + v_{n-1} - 2v_n) - 2\pi\nu_v(mv_n)\right] \tag{2.17}$$

with a solution

$$v_n = B\{\exp -i[2\pi(\nu_p + \nu_v)\,t - knd]\} \tag{2.18}$$

where $\nu_p = (\hbar/\pi md^2)\sin^2 kd/2$ and $\nu_v =$ constant.

It is not necessary to consider that a constant term appearing in the expression for the total energy of a field-free particle results from deformation of the particle, of course. A rigid particle moving in a region of *constant* potential will also possess a potential energy, $V = U_v$, although remaining field-free in the sense that no force is exerted on it by a constant potential (i.e., grad $V = 0$).

Equation (2.18) can be rewritten in the form

$$v_n = B\exp(-i2\pi\nu_v t).\exp[-i(2\pi\nu_p t - knd)] \tag{2.19}$$

The first term of equation (2.19) represents a time-dependent amplitude for the travelling particle wave which is itself described by the second term and has a frequency ν_p and wave vector k. Thus at a given time, $t = t_1$, equation (2.19) describes a wave of amplitude, $B_1 = B\exp(-i2\pi\nu_v t_1)$, and wavelength $\lambda = 2\pi/k$ extending along the row lattice of Fig. 1. At some later time, t_2, this wave will not only be shifted along the lattice, but will also have a different amplitude $B_2 = B\exp(-i2\pi\nu_v t_2)$. For $\nu_v \gg \nu_p$ the amplitude variation of the travelling particle wave will occur very rapidly compared to the period of the travelling particle (momentum) wave. Hence if the velocity variation along the row lattice of Fig. 1(b) is observed during some very short time interval, Δt, instead of instantaneously, then the amplitude will oscillate through its range ($-B$ to B) while the travelling velocity wave moves a negligible distance along the lattice. The result is that a kind of standing wave pattern will be observed (for the velocity) during the interval Δt as depicted in Fig. 2. That is, if

$$1/\nu_p \gg \Delta t \gg 1/\nu_v \tag{2.20}$$

the resulting velocity variation of the point masses (atoms) along an initially vibrating row lattice will appear as in Fig. 2(a). From Fig. 2 it is clear that during certain larger time intervals between the *observational* time intervals, the standing wave pattern will move along the row lattice with a propagation velocity, c_p, as depicted in Fig. 2(b). Hence equation (2.19) [and equation (2.18)] represents in this view a slowly moving, standing velocity wave in the row lattice. The translational or shift velocity along the row lattice of this (somewhat paradoxical) travelling standing wave is simply the propagation velocity of the particle momentum wave ($c_p = 2\pi\nu_p/k$) as previously discussed elsewhere (Fitzgerald, 1966b). The situation represented by equation (2.19) and Fig. 2 in which the amplitude of the propagating wave is modulated at a frequency much greater than that of the wave is, of course, quite the reverse of the usual amplitude modulation considered in which ν_v would be less than ν_p. We might, in fact, be tempted to rewrite equation (2.19) in a way such that the amplitude is modulated at the lower

frequency (ν_p) but since ν_v is a constant independent of the wave vector k, the expression $\exp[-i(2\pi\nu_v t - knd)]$ does *not* represent a travelling wave of frequency ν_v nor have any obvious physical meaning.

Instead of an infinite row lattice as depicted in Fig. 1, we next consider vibrating atoms in a one-dimensional lattice of finite length, $S = Nd$, with fixed ends as shown in Fig. 3. That is, we specify that $v_0(t) = v_N(t) = 0$ for all t. Because of the zero velocity conditions at the ends of this lattice

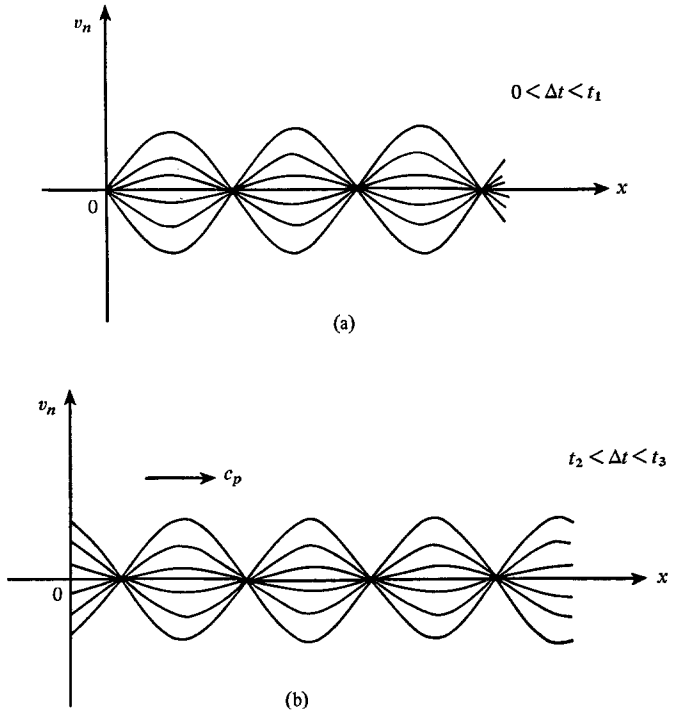

Figure 2.—Velocity v.s. distance x along the row lattice of Fig. 1(b) for a momentum wave [compare equation (2.19) of text] observed during a very short time interval Δt (a) between 0 and t_1, and (b) at a later time between t_2 and t_3.

segment a standing wave solution to the differential equation for momentum transfer [equation (2.10)] through a general nth mass of the lattice seems appropriate,

$$v_n(t) = [B_1 \exp(iknd) + B_2 \exp(-iknd)] \exp(-i2\pi\nu t) \qquad (2.21)$$

and this does prove to be a solution. The condition that $v_n(0) = 0$ requires that $B_1 = -B_2$, so that the solution becomes

$$v_n(t) = 2iB_1 \exp(-i2\pi\nu t) \sin knd \qquad (2.22)$$

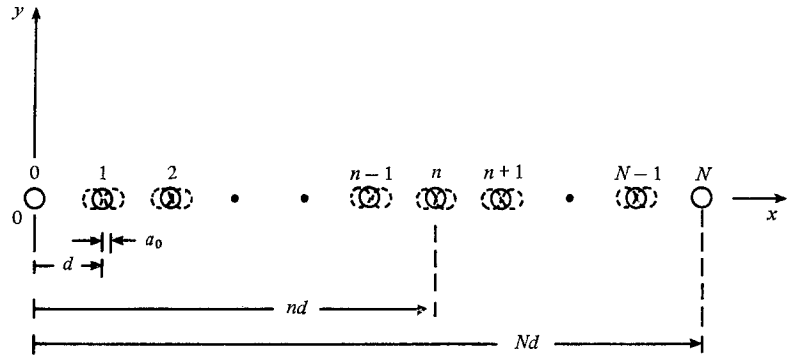

Figure 3.—Schematic drawing of a finite one-dimensional (row) lattice of vibrating point masses, m, with a length $S = Nd$ and fixed ends at 0 and N. Amplitude of vibration, a_0, is much less than the lattice spacing, d.

The condition that $v_N(0) = 0$ requires in addition that $\sin kNd = 0$ which follows if $kNd = q\pi$ where q is an integer, i.e., discrete values of the wave vector, k, are now demanded such that

$$k = q\pi/Nd \qquad \text{where } q = 1, 2, 3 \ldots (N-1) \tag{2.23}$$

The necessary frequency condition on ν again turns out to be,

$$\nu = \frac{-2i\mathbf{K}_p}{\pi m} \sin^2 \frac{kd}{2} + \nu_v \tag{2.24}$$

$$\tag{2.12}$$

$$= \nu_p + \nu_v \tag{2.25}$$

$$\tag{2.13}$$

where $\mathbf{K}_p = iK_p = i\hbar/2d^2$ as before and $\nu_v = \text{constant}$. Now, however, discrete values of k and therefore ν are necessary as given by equation (2.23). Minimum and maximum values of k are thus π/Nd and $(N-1)\pi/Nd \cong \pi/d$ corresponding to respective minimum and maximum values of ν_p

$$\nu_p(\min) \cong \frac{h}{8mS^2} \qquad (\text{for } S = Nd)$$

$$\nu_p(\max) \cong \frac{\hbar}{\pi m d^2} \qquad (\text{for } N \text{ large}) \tag{2.26}$$

The general prevalence of mosaic structures in real crystals indicates that finite lattice segments will generally be encountered in momentum transfer through crystals and a typical length of the order of a few microns is to be expected (Fitzgerald, 1966b; Hirsch, 1956). Thus characteristic values of ν_p may range from 10^2 to 10^{10} cps with accumulations of these particle wave modes near the ends of the frequency spectrum (Fitzgerald, 1966a, b). Hence the situation previously considered, $\nu_v \gg \nu_p$, is one which will generally prevail. For example, on the basis of the Einstein model (Einstein,

(1906, 1911) chosen to represent the vibrating crystal lattice, characteristic Einstein temperatures, θ_E, can be determined from experimental specific heat–temperature data where $\theta_E = h\nu_v/k$ or $\nu_v = k\theta_E/h = 0{\cdot}208 \times 10^{11}\,\theta_E$ (here k is Boltzman's constant). Values of θ_E obtained in this way are between 100 and 400 °K for many crystalline solids†; for aluminum $\theta_E \cong 350$ °K corresponding to a vibrational frequency of $7{\cdot}3 \times 10^{12}$ cps. On the other hand, the distance of closest approach, $d = 2{\cdot}86 \times 10^{-8}$ cm, for the aluminum lattice corresponds to a maximum particle wave frequency of $\nu_p(\max) = 8{\cdot}25 \times 10^9$ cps. Thus the condition that $\nu_v \gg \nu_p$ is easily met even for the highest particle wave modes in this case. For solids with larger interatomic spacings or heavier atoms values of $\nu_p(\max)$ will be even lower [compare equation (2.26)].

3. *The Schroedinger Equation for a Vibrating Atom in a One-dimensional Lattice*

A close connection between the momentum transfer equation [equations (2.2) and (2.6)] and the general time-dependent Schroedinger equation for stationary atoms in a row lattice has been demonstrated previously (Fitzgerald & Tasi, 1967). To show this it is only necessary to express the second derivative in terms of a second difference quotient and substitute the linear momentum, mv_n, for the wave property ψ_n to be associated with a general nth mass (atom) of the lattice. That is, the time-dependent Schroedinger equation for one of the masses, m, of the row lattice with stationary equilibrium positions shown in Fig. 1(a) is,

$$\frac{\partial^2 \psi_n}{\partial x^2} - \frac{2m}{\hbar^2} V_n \psi_n + \frac{2im}{\hbar} \frac{\partial \psi_n}{\partial t} = 0 \tag{3.1}$$

If ψ is a continuous function of x then the second differential operator has its common meaning that

$$\frac{\partial^2 \psi}{\partial x^2} = \lim_{\Delta x \to 0} \frac{\Delta^2 \psi}{\Delta x^2} = \lim_{\Delta x \to 0} \frac{\Delta \left(\lim\limits_{\Delta x \to 0} \dfrac{\Delta \psi}{\Delta x} \right)}{\Delta x}$$

since ψ is defined everywhere in the interval Δx. However if ψ is a real-property of the type that can be defined in the vicinity of the mass point in a lattice but not elsewhere, then a different meaning must be attached to the second derivative operator. Following Liebnitz (Fitzgerald & Tasi, 1967) the second derivative of the function ψ is therefore taken to be a second difference quotient such that

$$\left. \frac{\partial^2 \psi}{\partial x^2} \right|_{x = x_n} = \frac{\partial^2 \psi_n}{\partial x^2} = \frac{1}{d^2} (\psi_{n+1} + \psi_{n-1} - 2\psi_n) \tag{3.2}$$

where $\psi_n = \psi(x_n)$, etc., and d is the fixed lattice spacing shown in Fig. 1(a).

† A value of $\theta_E \cong 1300$°K is used to fit the experimental specific heat–temperature variation for diamond (C).

Then if the property ψ_n to be associated with the motion of the nth mass is taken to be a real-property, and in particular the linear momentum, $\psi_n = mv_n$, we have from equations (3.1) and (3.2),

$$\frac{1}{d^2}(\psi_{n+1} + \psi_{n-1} - 2\psi_n) - \frac{2m}{\hbar^2} V_n \psi_n + \frac{2im}{\hbar} \frac{\partial \psi_n}{\partial t} = 0$$

rearranging and substituting $\psi_n = mv_n$,

$$\frac{\partial(mv_n)}{\partial t} = \frac{i\hbar}{2d^2}(v_{n+1} + v_{n-1} - 2v_n) - \frac{i}{\hbar} V_n mv_n \tag{3.3}$$

Equation (3.3) above can be considered as an alternative form of the Schroedinger equation for a single (but completely general) atom of a row lattice. Stationary point masses (atoms) in such a lattice are assumed to be in equilibrium at the lattice points as a result of the existence of a periodic potential energy $V(x) = V(x + d)$ as shown in Fig. 4(a). The absolute value of such a potential is arbitrary and is selected in this figure to be zero at the lattice points, $n - 2$, $n - 1$, n, $n + 1$, $n + 2$, etc. Then

$$\ldots V_{n-2} = V_{n-1} = V_n = V_{n+1} = V_{n+2} \ldots = 0$$

where $V_n = V(x_n)$, etc. Equation (3.3) therefore reduces to

$$\frac{\partial(mv_n)}{\partial t} = \frac{i\hbar}{2d^2}(v_{n+1} + v_{n-1} - 2v_n) \tag{3.4}$$

for fixed or stationary atoms in a row lattice. This is identical to the momentum transfer equation [equation (2.1a)] obtained in Section 2 on the basis of linear momentum conservation between adjacent masses in the lattice.

If the lattice masses are now considered to be vibrating with small amplitudes, a_0, about their mean positions in the lattice as shown in Fig. 1(b), their equilibrium energies are no longer zero. Instead, even at equilibrium each mass possesses a constant vibrational energy U_v. This can be considered as equivalent to the situation depicted in Fig. 4(b) where the periodic lattice potential has a plateau of width $2a_0$ and height $V_0 = U_v$ above zero at each lattice site. In this case

$$\ldots V_{n-2} = V_{n-1} = V_n = V_{n+1} = V_{n+2} \ldots = V_0$$

and equation (3.3) becomes

$$\frac{\partial(mv_n)}{\partial t} = \frac{i\hbar}{2d^2}(v_{n+1} + v_{n-1} - 2v_n) - i2\pi \frac{V_0}{h}(mv_n) \tag{3.5}$$

which is seen to be identical to equation (2.17) previously obtained if V_0/h is set equal to ν_v. The differential equations (2.1a) and (2.17) are thus seen to be forms of the general (non-relativistic) time-dependent Schroedinger equation for a stationary or vibrating atom, respectively, in a periodic row lattice. In order to put the Schroedinger equation into the forms presented in equations (2.1a) and (2.17) it was necessary, first, to extend

the usual meaning of the second derivative operator in order to allow its use in a discontinuous (but regular) medium such as a crystal lattice; and, second, to consider that momentum waves can be associated with moving particles in place of (or in addition to) the usual probability waves of contemporary wave mechanics. Further, although a given mass may move from one lattice site to another, the differential equation used to describe its velocity is valid only in the immediate vicinity of a lattice point and

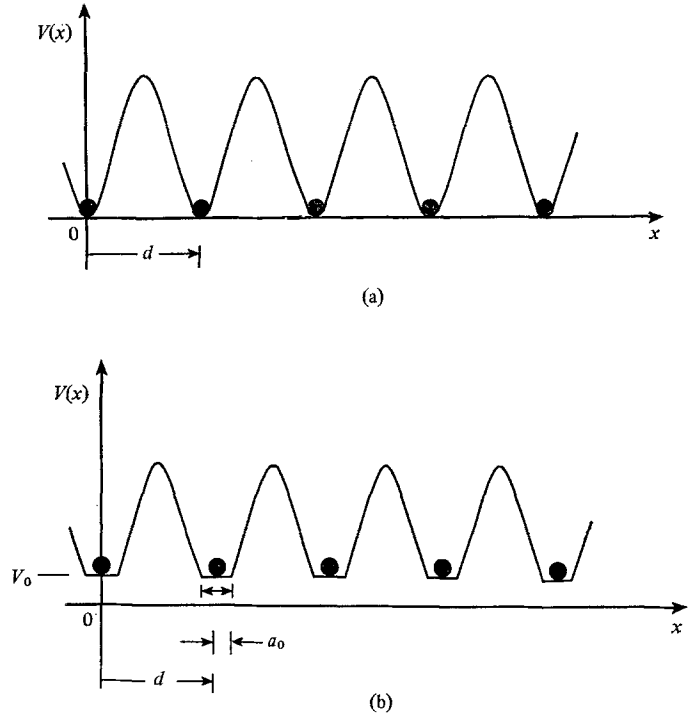

Figure 4.—Schematic representation of periodic potential energy variation $V(x) = V(x + d)$ in row lattice of Fig. 1(a) for stationary point masses at zero equilibrium potential [compare Fig. 1(a)], and (b) for vibrating point masses at equilibrium potential of V_0 [compare Fig. 1(b)].

hence does not provide a description of exactly what happens to a migrating mass (atom) *between* lattice points. This, of course, follows from the idea that a real-property (momentum) wave is to be associated with a moving mass or particle and that the property in question can be defined only in the vicinity of a particle and not elsewhere (Fitzgerald, 1966a, b). Most of the atoms in a crystal lattice at any given time are certainly in the vicinity of regular lattice points and therefore a general equation for lattice-site atoms as opposed to interstitial or irregularly located atoms is of interest.

4. *Extension of the Results to Three Dimensions*

The momentum transfer equation for a one-dimensional lattice with vibrating atoms can be readily extended to three dimensions. This extension has been described in detail elsewhere (Fitzgerald, 1966a, b) for stationary atoms and therefore the procedure is only briefly sketched here. Consider for convenience an infinitely large, cubic lattice with spacing d and vibrating point masses, m. Momentum transfer may then occur between adjacent

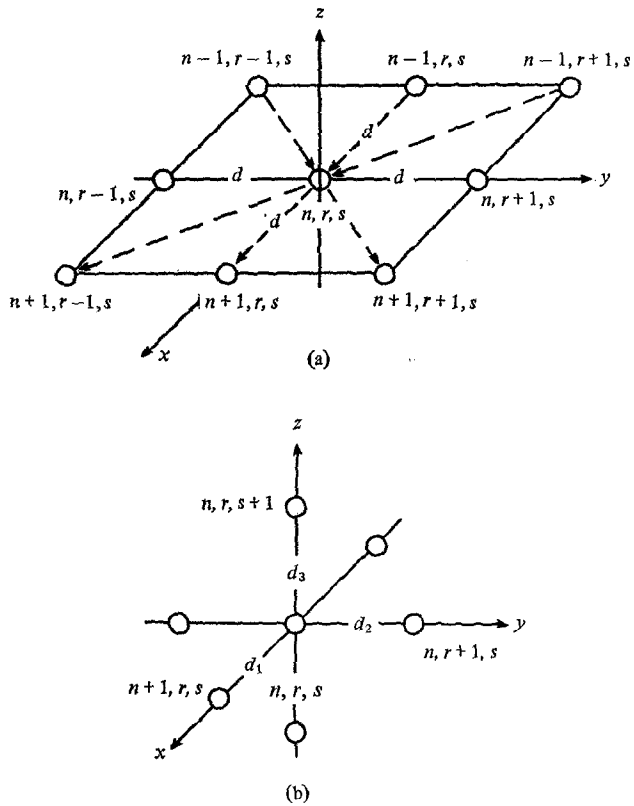

Figure 5.—(a) Schematic drawing showing location and designation of nearest and next-nearest neighbors in the xy plane only for a point mass at n, r, s in a cubic lattice. Here simultaneous multiple momentum transfer to and from the mass at n, r, s is assumed as indicated for the x-direction by arrows between atoms. Momentum transfer in the x-direction to the mass at n, r, s is not considered to take place from the two masses $(n, r-1, s$ and $n, r+1, s)$ along the y axis, however. Similar designations and diagrams apply to the additional nearest and next-nearest neighbor masses and for momentum transfer in the y and z directions (compare text). In fact, multiple momentum transfer apparently does not occur since its assumption leads to contradictions as discussed in the text. (b) Diagram and designation of adjacent masses along the x, y, z axes for a point mass at n, r, s in a lattice with spacings d_1, d_2, d_3 in the x, y, z directions as shown.

masses in various directions within the lattice, but in particular we investigate the possibility of simultaneous momentum transfer occurring to and from a general mass located at (n,r,s) and its nearest and next-nearest neighbors in the lattice as indicated in Fig. 5(a). Three differential equations for the velocity components u, v, w in the x, y, z directions can then be set up for a general mass point at n, r, s in terms of a nearest-neighbor momentum transfer constant $\mathbf{K}_p$ and a next-nearest neighbor momentum transfer constant $\mathbf{L}_p$. Since these three equations represent statements of conservation of momentum in the three directions, x, y, z, they are uncoupled. That is, momentum is independently conserved in each direction and the differential equation for the velocity $u_{n,r,s}$ contains no terms in v or w, etc. The absence of coupling makes solutions to these equations relatively simple; they are of the form,

$$\begin{aligned} u_{n,r,s} &= A\exp\left[-i(2\pi\nu t - k_1 nd - k_2 rd - k_3 sd)\right] \\ v_{n,r,s} &= B\exp\left[-i(2\pi\nu t - k_1 nd - k_2 rd - k_3 sd)\right] \\ w_{n,r,s} &= C\exp\left[-i(2\pi\nu t - k_1 nd - k_2 rd - k_3 sd)\right] \end{aligned} \tag{4.1}$$

and lead to *three* different ν versus k characteristics for any general direction (k_1,k_2,k_3) in $\mathbf{k}$ space. The occurrence of three $\nu - k$ curves for particle waves in the lattice raises a fundamental difficulty which indicates that the original assumption of simultaneous momentum transfer through a mass from and to multiple lattice masses is incorrect. That is, three $\nu - k$ curves will result generally in three different values of group velocity $v_g = 2\pi\, d\nu/dk$ for a given value of k and thus require one mass to have three different particle velocities ($v_g = v_{\text{particle}}$ at small values of k). This is in violation of what has been termed (Fitzgerald, 1966b) the 'Supreme court' condition of 'one mass, one velocity' and hence leads to the conclusion that momentum transfer occurs from a lattice mass to only *one* other mass at a time. Only in this way can a single $\nu - k$ curve be assured for any direction in the lattice. Therefore the one-dimensional momentum transfer equations apply directly to three-dimensional lattices where the spacing, d_j, between lattice masses in a particular direction, $\mathbf{k}$, is used. In particular, for a lattice with spacings d_1, d_2, d_3 in the x, y, z directions as shown in Fig. 5(b) we can write three *independent* momentum transfer equations,

$$\begin{aligned} \frac{\partial(mu_{n,r,s})}{\partial t} &= \frac{i\hbar}{2d_1^2}(u_{n+1,r,s} + u_{n-1,r,s} - 2u_{n,r,s}) - i2\pi\nu_v(mu_{n,r,s}) \\ \frac{\partial(mv_{n,r,s})}{\partial t} &= \frac{i\hbar}{2d_2^2}(v_{n,r+1,s} + v_{n,r-1,s} - 2v_{n,r,s}) - i2\pi\nu_v(mv_{n,r,s}) \\ \frac{\partial(mw_{n,r,s})}{\partial t} &= \frac{i\hbar}{2d_3^2}(w_{n,r,s+1} + w_{n,r,s-1} - 2w_{n,r,s}) - i2\pi\nu_v(mw_{n,r,s}) \end{aligned} \tag{4.2}$$

It also can be argued from this type of analysis *that momentum transfer in any particular direction in a lattice takes place only between masses (atoms) aligned in that direction.* Then transverse momentum transfer of the type

indicated in Fig. 6 would be ruled out. These restrictions on the type of momentum transfer that can take place between lattice masses are in agreement with a macroscopic 'collision' process for momentum transfer. We might, for instance, allow simultaneous multiple momentum transfer from a number of masses *to* a single mass, but certainly do not expect simultaneous motion of the mass in several different directions in order to transfer momentum *from* itself to other masses! (Such multiple transfer could result only from a breaking-up or fissioning of the mass into smaller fragments.)

The restriction to 'central' or in-line momentum transfer between lattice masses allows the three-dimensional Schroedinger equation to be easily

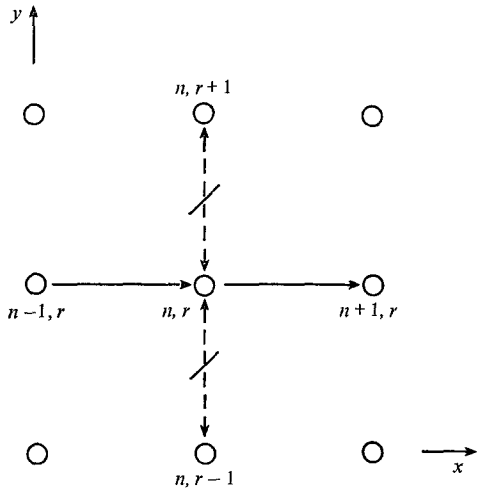

Figure 6.—Representation of $x-y$ plane of a cubic lattice showing non-occurrence (dashed arrows) of transverse x-momentum transfer between masses such as n, $r+1$; n, r; and n, $r-1$. Instead, in-line or 'central' momentum transfer takes place from one atom to another as shown by solid arrows.

applied to obtain results identical to those in equation (4.2). The Schroedinger equation for an atom of mass, m, at a lattice site n, r, s in a three-dimensional crystal may be written as,

$$\frac{\partial^2 \psi_{n,r,s}}{\partial x^2} + \frac{\partial^2 \psi_{n,r,s}}{\partial y^2} + \frac{\partial^2 \psi_{n,r,s}}{\partial z^2} - \frac{2m}{\hbar^2} V_{n,r,s} \psi_{n,r,s} + \frac{2im}{\hbar} \frac{\partial \psi_{n,r,s}}{\partial t} = 0 \quad (4.3)$$

If the momentum vector $\mathbf{P}$ is now substituted for ψ the Schroedinger equation becomes

$$\frac{\partial^2(\mathbf{P}_{n,r,s})}{\partial x^2} + \frac{\partial^2(\mathbf{P}_{n,r,s})}{\partial y^2} + \frac{\partial^2(\mathbf{P}_{n,r,s})}{\partial z^2} - \frac{2m}{\hbar^2} V_{n,r,s} \mathbf{P}_{n,r,s} + \frac{2im}{\hbar} \frac{\partial \mathbf{P}_{n,r,s}}{\partial t} = 0 \quad (4.4)$$

which results directly in three independent scalar equations of the same form for the x, y, z components of momentum; $P_x = mu$, $P_y = mv$, $P_z = mw$,

$$\begin{aligned}
&\frac{\partial^2(mu_{n,r,s})}{\partial x^2} + \frac{\partial^2(mu_{n,r,s})}{\partial y^2} + \frac{\partial^2(mu_{n,r,s})}{\partial z^2} \\
&\qquad - \frac{2m}{\hbar^2} V_{n,r,s}(mu_{n,r,s}) + \frac{2im}{\hbar} \frac{\partial(mu_{n,r,s})}{\partial t} = 0 \\
&\frac{\partial^2(mv_{n,r,s})}{\partial x^2} + \frac{\partial^2(mv_{n,r,s})}{\partial y^2} + \frac{\partial^2(mv_{n,r,s})}{\partial z^2} \\
&\qquad - \frac{2m}{\hbar^2} V_{n,r,s}(mv_{n,r,s}) + \frac{2im}{\hbar} \frac{\partial(mv_{n,r,s})}{\partial t} = 0 \qquad (4.5) \\
&\frac{\partial^2(mw_{n,r,s})}{\partial x^2} + \frac{\partial^2(mw_{n,r,s})}{\partial y^2} + \frac{\partial^2(mw_{n,r,s})}{\partial z^2} \\
&\qquad - \frac{2m}{\hbar^2} V_{n,r,s}(mw_{n,r,s}) + \frac{2im}{\hbar} \frac{\partial(mw_{n,r,s})}{\partial t} = 0
\end{aligned}$$

Replacing the second derivative operators by second difference quotients in the same manner as previously done for one-dimensional lattices, we note that for the x-component of velocity, for example, these become [compare Fig. 4(b)]:

$$\begin{aligned}
\left.\frac{\partial^2(mu_{n,r,s})}{\partial x^2}\right|_{x=x_{n,r,s}} &= \frac{m}{d_1^2}(u_{n+1,r,s} + u_{n-1,r,s} - 2u_{n,r,s}) \\
\left.\frac{\partial^2(mu_{n,r,s})}{\partial y^2}\right|_{y=y_{n,r,s}} &= \frac{m}{d_2^2}(u_{n,r+1,s} + u_{n,r-1,s} - 2u_{n,r,s}) \qquad (4.6) \\
\left.\frac{\partial^2(mu_{n,r,s})}{\partial z^2}\right|_{z=z_{n,r,s}} &= \frac{m}{d_3^2}(u_{n,r,s+1} + u_{n,r,s-1} - 2u_{n,r,s})
\end{aligned}$$

Therefore the expression for the time rate of change of the x-component of momentum at n, r, s becomes, according to equation (4.5),

$$\begin{aligned}
\frac{\partial(mu_{n,r,s})}{\partial t} &= \frac{i\hbar}{2d_1^2}(u_{n+1,r,s} + u_{n-1,r,s} - 2u_{n,r,s}) \\
&\quad + \frac{i\hbar}{2d_2^2}(u_{n,r+1,s} + u_{n,r-1,s} - 2u_{n,r,s}) \\
&\quad + \frac{i\hbar}{2d_3^2}(u_{n,r,s+1} + u_{n,r,s-1} - 2u_{n,r,s}) \\
&\quad - i\frac{2\pi}{\hbar} V_{n,r,s}(mu_{n,r,s}) \qquad (4.7)
\end{aligned}$$

The first term on the right-hand side of this equation represents the net transfer of the x-component of momentum from masses at $n+1, r, s$ and $n-1, r, s$ along the x axis to the lattice mass at the n, r, s. The second and third terms, however, represent a *transverse* net transfer of x-component momentum from masses at $n, r+1, s$; $n, r-1, s$ and masses at $n, r, s+1$; $n, r, s-1$ along the y and z axes respectively. Such transverse or sideways momentum transfer is not possible according to our previous remarks (compare Fig. 6) and hence these terms must be zero. Entirely similar results are obtained for the y and z component equations of equation (4.5) so that these three component equations become identical to those of equation (4.2) where $V_{n,r,s} = V_0$ and $\nu_v = V_0/h$ as before.

The same result can be obtained using the three-dimensional Schroedinger equation if we restrict our attention to plane momentum waves at the outset. However, the physical reasons leading to the final equations are quite different in the two cases. In the case originally discussed here we allow variations in $P_x = mu$ with y and z, but rule out *transfer* of this momentum in directions perpendicular to x; this results in $\partial^2 P_x/\partial z^2 = \partial^2 P_x/\partial y^2 = 0$, according to the second difference quotient expressions for these derivatives and the resulting terms which appear in the momentum transfer equation as exemplified by equation (4.7). For plane waves we specify that P_x is a function of x only and therefore constant in y and z directions; $\partial^2 P_x/\partial y^2$ and $\partial^2 P_x/\partial z^2$ can therefore be set equal to zero at the outset or their equivalent second difference quotients [equation (4.6)] set equal to zero since now $u_{n,r+1,s} = u_{n,r-1,s} = u_{n,r,s}$ etc.

5. *Conclusions*

Consideration of crystal lattices with point masses vibrating at a common frequency, ν_v, about mean lattice sites requires the addition of a term, $i2\pi m\nu_v(mv_n)$, to the differential momentum transfer equation previously adduced for particle momentum waves in a lattice. The modified equation [equation (2.17)] also results (in both one and three dimensions) from application of the time-dependent Schroedinger equation to describe the behavior of a general nth mass within the vicinity of a lattice site. A particuar solution to this momentum transfer equation has been presented in which traveling particle momentum waves of frequency ν_p have their amplitudes modulated at a higher frequency, ν_v, to produce a type of drifting standing wave pattern as shown in Fig. 2. For convenience an 'Einstein' model of the crystal lattice was used in which the masses vibrate independently, but with a common frequency, ν_v, about their mean lattice positions. Such independent vibrations of each mass can be expected in general to have random phase relations even though they may have identical velocity amplitudes, B_0. However, if we imagine that by some happy accident all of the independent vibrations of the atoms in a particular crystal are in

phase ($\ldots\theta_{n-1} = \theta_n = \theta_{n+1} \ldots = \theta$) then it is possible to write a solution for the velocity, v_n, of a general nth mass of the form

$$v_n(t) = B_0 \exp\left[-i(2\pi\nu_v t + \theta)\right] + B_1 \exp\left\{-i\left[2\pi(\nu_p + \nu_v)t + \theta - knd\right]\right\}$$

$$= \left(1 + \frac{B_1}{B_0}\exp\left[-i(2\pi\nu_p t - knd)\right]\right) B_0 \exp\left[-i(2\pi\nu_v t + \theta)\right] \qquad (5.1)$$

'modulating' wave 'carrier' wave

Of course, this happy accident seems quite improbable, since it would correspond to an intrinsic oscillatory translation of an entire crystal sample. On the other hand, if we recall the mosaic structure of real crystals which are broken up into fragments of micron size, it could be imagined that such crystalline substructures vibrate randomly with respect to other substructures, but that the masses (atoms) of each substructure are in phase. Then equation (5.1) above could apply to the velocity of a general nth mass within a finite lattice segment with discrete values of the wave vector, k, required.

Another alternative is to consider that the intrinsic vibrations of the lattice masses result from vibrational modes of the lattice as a whole (Debye or Born-von Karman models) instead of independent vibrations (Einstein model). Then a regular, periodic variation of the intrinsic vibration velocity will occur along a one-dimensional lattice for example,

$$v_n(\text{vib.}) = B_0 \exp\left[-i(2\pi\nu_v t - k_v x)\right] \qquad (5.2)$$

where $\nu_v = c_s/\lambda$; c_s is the velocity of sound in the lattice considered as a continuum (Debye model)

or,
$$v_n(\text{vib.}) = B_0 \exp\left[-i(2\pi\nu_v t - k_v nd)\right] \qquad (5.3)$$

where, for a one-dimensional lattice and nearest neighbor interactions only, $\nu_v = 1/\pi\sqrt{(K_e/m)}\sin k_v d/2$; K_e is an elastic interaction constant between adjacent lattice masses (Born-von Karman model).

In these latter cases it is no longer possible to characterize the intrinsic lattice vibration by a single frequency, ν_v; rather a collection of vibrational modes of different frequencies is supposed to be present. The Debye model does lead to an accumulation of vibrational modes at the highest frequency, ν_D, however. Similarly, it is often found on the basis of the Born-von Karman model that a high preponderance or accumulation of modes about one very high frequency does occur (Fitzgerald, 1966b). Thus the use of a single frequency, ν_v, to characterize the vibrational modes of a lattice remains a fairly good approximation in many cases.

A study of additional solutions of the type given by equation (5.1) promises to provide the basis for a more detailed description of the propagation of particle momentum waves produced by the application of a unidirectional force or load on a crystal, and the interaction of such waves with the intrinsic vibrational modes of the crystal leading to a release of lattice binding energy (Fitzgerald, 1966b; Fitzgerald & Wright, 1967).

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