

Mechanical Energy Flow in Crystal Lattices*†

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A detailed study of the mechanical energy transported through a completely general crystal lattice in the classical temperature range is presented. Both a mechanical "Poynting" vector and the corresponding mechanical "Poynting" theorem are established for an arbitrary, 3-dimensional, anisotropic, anharmonic crystal lattice, containing many atoms per cell, inclusive of substitutional impurities, and possessing an arbitrary range of atomic interactions. The extension of the energy-flow procedures to a quantum treatment is discussed, and the resulting quantum-mechanical form of the mechanical "Poynting" vector is given. In addition, a mechanical energy theorem, linking the average mechanical energy flow to the group velocity for the restricted case of a perfectly periodic and harmonic but otherwise completely general, crystal is derived for the classical temperature range.

INTRODUCTION

ALTHOUGH several workers have presented accounts of the mechanical energy flow within crystal lattices,^{1,2} previous studies have been somewhat restricted in scope. Peierls, in his classic paper on heat conduction in 1929 limited his work to anharmonic crystals having one atom per cell and near-neighbor coupling only. Brillouin's treatment included long-range atomic interactions but only for one-dimensional harmonic lattices containing only one atom per cell.³

The analysis presented here, however, removes these restrictions by covering a completely general 3-dimensional, anisotropic, anharmonic crystal inclusive of many atoms per cell and arbitrarily long-range atomic couplings. In addition, an unrestricted number of arbitrary substitutional atomic impurities are allowed in the lattice system.

Although classical mechanics is used here to simplify the analysis, similar results are obtainable for the quantized case by simply treating the dynamic variables as operators, and observing the necessary commutation properties.

The study of the mechanical energy flow in lattices presented here forms an integral part of an over-all analysis of the heat flow in crystal lattices by the author.⁴ It is shown there that the mechanical "Poynting" vector does indeed lead to the well-known

anharmonic, mass-fluctuation, and force-fluctuation components of the lattice thermal conductivity in the presence of an applied temperature gradient.

CLASSICAL CRYSTAL LATTICE MODEL

In this paper a general 3-dimensional lattice of a periodic structure containing many atoms per unit cell and having arbitrarily long-range atomic interactions will be assumed. The adiabatic approximation will be made in the classical temperature range of interest here (i.e., temperatures above the Debye temperature). The vibrating atoms will be treated as simple mass points, while the electronic contributions not of interest here, will be set aside.

Following the standard approach to lattice dynamics as detailed in the literature,⁵⁻⁸ we shall be interested in only relatively small displacements from equilibrium, as represented by $\mathbf{u}(i,n)$ for the i th atom in the n th unit cell. The basic classical equation of motion becomes (shown up to second order in anharmonic terms)

$$\begin{aligned}
 M(i,n) \frac{d^2 \mathbf{u}(i,n)}{dt^2} = & - \sum_{j,p} \mathbf{V}(ij,n) \cdot \mathbf{u}(j,p) \\
 & - \frac{1}{2} \sum_{j,p} \sum_{h,q} \mathbf{V}'(ijh,n) : \mathbf{u}(j,p) \mathbf{u}(h,q) \\
 & - \frac{1}{6} \sum_{j,p} \sum_{h,q} \sum_{c,w} \mathbf{V}''(ijhc,n) : \mathbf{u}(j,p) \mathbf{u}(h,q) \mathbf{u}(c,w) \\
 & + \dots \quad (1)
 \end{aligned}$$

The force tensors $\mathbf{V}(ij,n)$, $\mathbf{V}'(ijh,n)$, and $\mathbf{V}''(ijhc,n)$, as well as the atomic masses $M(i,n)$, in general may depend upon cell position n to allow for the presence of different coupling terms and masses near impurity sites. The summations over (j,p) , (h,q) , and (c,w) run over all of the atoms within the crystal, unless specified

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¹ R. E. Peierls, *Ann. Physik* **5**, 3, 1055 (1929).

² L. Brillouin, *Wave Propagation in Periodic Structures* (McGraw-Hill Book Company, Inc., New York, 1946).

³ A generalized mechanical energy-flux study has recently been published by R. J. Hardy [*Phys. Rev.* **132**, 1, 168 (1963)]. The application of his energy-flux operator to crystal lattices is limited to systems of only short-range interatomic coupling forces. The detailed internal-energy determination given here, however, shows that such a restriction is not necessary (i.e., for temperatures well enough below the melting point of the solid such that the number of atoms in a given macroscopic volume is constant).

⁴ L. M. Magid, *Phys. Rev.* **134**, 163 (1964), following paper.

⁵ M. Born and K. Huang, *Dynamical Theory of Crystal Lattices* (Oxford University Press, London, 1956).

⁶ J. M. Ziman, *Electrons and Phonons* (Oxford University Press, London, 1960).

⁷ R. E. Peierls, *Quantum Theory of Solids* (Oxford University Press, London, 1956).

⁸ P. G. Klemens, *Solid State Phys.* **7**, 1 (1958).

otherwise. For the completely general crystal treated here, no special assumptions need be made concerning the symmetry, form, nor range of interaction of the force tensors.

A MECHANICAL "POYNTING" THEOREM

The Poynting theorem of field theory relates the net flow of power through a closed surface to the net rate of increase of total energy within the volume enclosed by the surface. It is the purpose of this section to find the analogous relation for the mechanical system of vibrating atoms in a crystal lattice.

The problem here lies in finding the proper specification of the *total* mechanical energy (i.e., kinetic and potential) to attribute to an arbitrary volume, say ΔV , contained within the crystal. The assignment of the proper kinetic energy $T_{\Delta V}$ to ΔV , however, is straightforward,

$$T_{\Delta V} = \frac{1}{2} \sum_{\substack{i,n \\ \Delta V}} M(i,n) \mathbf{v}(i,n) \cdot \mathbf{v}(i,n), \quad (2)$$

where $\mathbf{v}(i,n) = \dot{\mathbf{u}}(i,n)$ is the particle velocity. The summation in Eq. (2) is limited to atoms within ΔV , as indicated by ΔV below the summation sign.

But because of the arbitrary long range of interaction assumed in the lattice, there is a difficulty with the potential energy, namely the splitting of the potential energy shared by two or more atoms (of which only

some are actually in ΔV) to be attributed to the potential energy $U_{\Delta V}$ of ΔV . By making the reasonable assumption that $\frac{1}{2}$ of the interaction energy between two atoms is contained in $U_{\Delta V}$ when only 1 of the 2 is actually in ΔV ; while, correspondingly, $\frac{1}{3}$ and $\frac{2}{3}$ of the interaction energy shared among 3 atoms is the $U_{\Delta V}$ when 1 or 2 atoms, respectively, are in ΔV , we find that

$$U_{\Delta V} = \frac{1}{2} \sum_{\substack{i,n \\ \Delta V}} \sum_{j,p} \mathbf{V}(ij,n) : \mathbf{u}(i,n) \mathbf{u}(j,p) \\ + \frac{1}{6} \sum_{\substack{i,n \\ \Delta V}} \sum_{j,p} \sum_{h,q} \mathbf{V}'(ijh,n) : \mathbf{u}(i,n) \mathbf{u}(j,p) \mathbf{u}(h,q) \\ + \dots \quad (3)$$

The summations in Eq. (3) on atoms (j,p) and (h,q) run over the entire crystal, while the sums on (i,n) are limited to atoms in ΔV . It can be shown that any other arbitrary splitting of shared potential energy would lead to expressions for $U_{\Delta V}$ that would violate the expected additivity property of energy contained in neighboring volumes.

We shall take the total mechanical energy within the arbitrary volume ΔV to be the sum of $T_{\Delta V}$ and $U_{\Delta V}$. Accordingly, by taking the derivative of $(T_{\Delta V} + U_{\Delta V})$ with respect to time, and applying the basic equation of motion for the system [i.e., Eq. (1)], we arrive at a mechanical "Poynting" theorem (up to second-order terms⁹)

$$\oint \mathbf{S} \cdot d\mathbf{a} = \frac{d}{dt} (T_{\Delta V} + U_{\Delta V}) = \frac{1}{2} \sum_{\substack{i,n \\ \Delta V}} \sum_{j,p} \mathbf{V}(ij,n) : [\mathbf{u}(i,n) \mathbf{v}(j,p) - \mathbf{u}(j,p) \mathbf{v}(i,n)] \\ + \frac{1}{3} \sum_{\substack{i,n \\ \Delta V}} \sum_{j,p} \sum_{h,q} \mathbf{V}'(ijh,n) : [\mathbf{u}(i,n) \mathbf{u}(h,q) \mathbf{v}(j,p) - \mathbf{u}(j,p) \mathbf{u}(h,q) \mathbf{v}(i,n)], \quad (4)$$

where \mathbf{S} is defined as the mechanical-power density entering the surface. The right side of Eq. (4) can be put into a more physically understandable form in terms of the various forces acting across the surface of ΔV , becoming

$$\oint \mathbf{S} \cdot d\mathbf{a} = \frac{1}{2} \left[\sum_{\substack{i,n \\ \Delta V}} \mathbf{f}^{\text{ext}}(i,n) \cdot \mathbf{v}(i,n) - \sum_{\substack{j,p \\ \text{not in } \Delta V}} \mathbf{f}^{\text{int}}(j,p) \cdot \mathbf{v}(j,p) \right] + \frac{2}{3} \left[\sum_{\substack{i,n \\ \Delta V}} \mathbf{F}^{\text{ext}}(i,n) \cdot \mathbf{v}(i,n) - \sum_{\substack{j,p \\ \text{not in } \Delta V}} \mathbf{F}^{\text{int}}(j,p) \cdot \mathbf{v}(j,p) \right] \\ + \frac{1}{3} \left[\sum_{\substack{i,n \\ \Delta V}} \mathbf{F}(i,n) \cdot \mathbf{v}(i,n) - \sum_{\substack{j,p \\ \text{not in } \Delta V}} \mathbf{F}(j,p) \cdot \mathbf{v}(j,p) \right], \quad (5)$$

where $\mathbf{f}^{\text{ext}}(i,n)$ and $\mathbf{f}^{\text{int}}(j,p)$ are, respectively, the net 2-atom interaction force on atom (i,n) in ΔV due to all of the atoms not in ΔV , and the net 2-atom force on atom (j,p) not in ΔV due to all of the atoms in ΔV . $\mathbf{F}^{\text{ext}}(i,n)$ and $\mathbf{F}^{\text{int}}(j,p)$ represent the corresponding

terms for the 3-atom interaction forces, while $\mathbf{F}(i,n)$ is the net 3-atom force on an atom within ΔV due to all other pairs of atoms (one in ΔV and one not in ΔV). $\mathbf{F}(j,p)$ is the corresponding force on an atom not in ΔV .

Physically, we see in Eq. (5) that only $\frac{1}{2}$ of the power acting on atom (i,n) actually flows into ΔV when only 1 of the 2 interacting atoms is in ΔV . Of course, when all of the interacting atoms are either in ΔV , or all outside, there can be no power flowing into ΔV . This is readily seen by the cancellation of such terms in Eq. (4). Furthermore, $\frac{2}{3}$ of the power enters ΔV when 2 of 3

⁹ The general form for the N th-order contribution to Eq. (4) is found to be

$$\frac{N}{(N+1)!} \sum_{\substack{i,n \\ \Delta V}} \sum_{j,p} \sum_{h,q} \dots \sum_{z,Z} \mathbf{v}^{N-N'}(ij\dots z,n) : \dots : \\ [\mathbf{u}(i,n) \mathbf{u}(h,q) \dots \mathbf{v}(j,p) - \mathbf{u}(j,p) \mathbf{u}(h,q) \dots \mathbf{v}(i,n)].$$

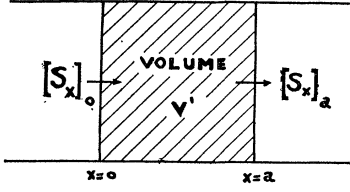


FIG. 1. Net x -directed power into volume $\Delta V'$.

interacting atoms act through the surface on 1 inside, and only $\frac{1}{3}$ of the power enters when 1 of 3 interacting atoms acts across the surface of ΔV on 1 of the other two. These results seem intuitively to be quite reasonable.

In addition, it can be shown that the mechanical "Poynting" theorem of Eqs. (4) and (5), reduces to the established Poynting theorem of elastic continuum theory when this system is limited to short-range "surface-contact" forces and harmonic (i.e., linear) force terms only.

$$S_x = (1/A_x) \left\{ \frac{1}{2} \sum_{\substack{i,n \\ n_x > 0}} \sum_{\substack{j,p \\ p_x < 0}} \mathbf{V}(ij,n) : [\mathbf{u}(i,n)\mathbf{v}(j,p) - \mathbf{u}(j,p)\mathbf{v}(i,n)] + \frac{1}{3} \sum_{\substack{i,n \\ n_x > 0}} \sum_{\substack{(j,p,h,q) \\ p_x, q_x < 0}} \mathbf{V}'(ijh,n) : \cdot [\mathbf{u}(i,n)\mathbf{u}(h,q)\mathbf{v}(j,p) - \mathbf{u}(j,p)\mathbf{u}(h,q)\mathbf{v}(i,n)] + \frac{1}{3} \sum_{\substack{(i,n,h,q) \\ n_x, q_x > 0}} \sum_{\substack{j,p \\ p_x < 0}} \mathbf{V}'(ijh,n) : \cdot [\mathbf{u}(i,n)\mathbf{u}(h,q)\mathbf{v}(j,p) - \mathbf{u}(j,p)\mathbf{u}(h,q)\mathbf{v}(i,n)] \right\}, \quad (6)$$

where A_x = surface normal to S_x . The validity of Eq. (6) can be checked by using it to determine the energy flow across a second surface at plane $x=a$ (cf. Fig. 1). One then will find that the net energy flow into the volume $\Delta V'$ formed between the planes at $x=0$ and $x=a$, and given by the difference in S_x at $x=0$ and $x=a$, satisfies the integral form of the Poynting theorem, as it must.

QUANTUM OPERATOR FORM OF ENERGY-FLOW DENSITY

Results similar to those given above for the mechanical "Poynting" theorem and "Poynting" vector can readily be obtained using quantum-mechanical procedures, thereby eliminating the high-temperature restriction. One needs only to treat the dynamic variables as time-dependent operators, express the system Hamiltonian in symmetric form, and then replace Newton's law as the basic equation of motion

$$S_x = (1/A_x) \left\{ \frac{1}{2} \sum_{\substack{i,n \\ n_x > 0}} \sum_{\substack{j,p \\ p_x < 0}} \mathbf{V}(ij,n) : [\mathbf{u}(i,n)\mathbf{v}(j,p) - \mathbf{u}(j,p)\mathbf{v}(i,n)] + \frac{1}{3} \sum_{\substack{i,n \\ n_x > 0}} \sum_{\substack{(j,p,h,q) \\ p_x, q_x < 0}} \mathbf{V}'(ijh,n) : \cdot \left[\mathbf{u}(i,n) \left(\frac{\mathbf{u}(h,q)\mathbf{v}(j,p) + \mathbf{v}(j,p)\mathbf{u}(h,q)}{2} \right) - \mathbf{u}(j,p)\mathbf{u}(h,q)\mathbf{v}(i,n) \right] + \frac{1}{3} \sum_{\substack{(i,n,h,q) \\ n_x, q_x > 0}} \sum_{\substack{j,p \\ p_x < 0}} \mathbf{V}'(ijh,n) : \cdot \left[\mathbf{u}(i,n)\mathbf{u}(h,q)\mathbf{v}(j,p) - \mathbf{u}(j,p) \left(\frac{\mathbf{u}(h,q)\mathbf{v}(i,n) + \mathbf{v}(i,n)\mathbf{u}(h,q)}{2} \right) \right] \right\}, \quad (8)$$

MECHANICAL ENERGY-FLOW DENSITY

Consideration of energy conservation has led to the equating of the net rate of increase of total mechanical energy within an arbitrary volume to the surface integral of the power density \mathbf{S} into the volume across its outer surface [i.e., Eq. (4)]. Note that \mathbf{S} is not actually determined by Eq. (4), but only its divergence or surface integral is fixed. Therefore, we shall not be able to obtain a unique result for \mathbf{S} , but only one which has the right surface integral in all cases.

A simple way to determine one such suitable, precise expression for the component energy flow along a given direction (the $+x$ axis, for example), is to expand ΔV into the entire half-space to the right of the plane at $x=0$, leaving the other half-space with $x < 0$ as the volume "not in ΔV ." If we examine Eq. (4), one finds that

by the dynamical properties of the atomic displacement and momentum operators. However, it is well known that the equations governing the time dependence of the operators $\mathbf{u}(i,n)$ and $\mathbf{p}(i,n)$ are identical in form to the classical equations of motion. That is,

$$\mathbf{v}(i,n) = \dot{\mathbf{u}}(i,n) = -i\hbar^{-1}[\mathbf{u}(i,n), H] = M(i,n)^{-1}\mathbf{p}(i,n), \quad (7a)$$

and

$$\dot{\mathbf{p}}(i,n) = -i\hbar^{-1}[\mathbf{p}(i,n), H] = \mathbf{F}(i,n) = M(i,n) \frac{d^2\mathbf{u}(i,n)}{dt^2}, \quad (7b)$$

where $\mathbf{F}(i,n)$ is the net force acting on atom (i,n) .

Following the same procedures as in the classical case, one then finds for the mechanical "Poynting" vector operator (shown up to first order in anharmonic terms) that

where the usual commutation properties between $\mathbf{u}(i,n)$ and $\mathbf{p}(i,n) = M(i,n)\mathbf{v}(i,n)$ are to be applied.

**PROOF OF THE MECHANICAL
"ENERGY THEOREM"**

The expected relation between the average energy flow and the group velocity can now be established for a general crystal lattice as long as we restrict our scope to systems that are perfectly periodic (in the direction of energy flow, at least) and limit ourselves to harmonic (i.e., linear) force terms only. To simplify the analysis, we will limit our discussion to the classical temperature region. Similar results, however, can be obtained for the quantum case.

Under these restrictions, the random atomic vibrations may be analyzed in terms of uniform traveling-wave normal mode solutions. That is, the instantaneous atomic displacement from equilibrium can be described as

$$\mathbf{u}(i,n) = \frac{2 \operatorname{Re}}{[2Nm_i]^{1/2}} \sum_{k,s} \mathbf{A}_i(k,s) Q_{k,s} \times \exp[i(\mathbf{k} \cdot \mathbf{X}_n - \omega t)], \quad (9)$$

where \mathbf{k} is the wave vector, ω is the radian frequency, and $\mathbf{A}_i(k,s)$ is the polarization vector for the mode (k,s) . The symbol s indicates the particular polarization branch. The details of these well-known normal mode solutions can be found readily in the literature.⁵⁻⁸

One necessary relation, however, to be useful later, is the dispersion relation defining the value of $\omega^2(k,s)$ as

$$\omega^2(k,s) = \sum_{i,j,L} [m_i m_j]^{-1/2} \times \mathbf{V}(ij) : \mathbf{A}_i^*(k,s) \mathbf{A}_j(k,s) \exp(i\mathbf{k} \cdot \mathbf{X}_L), \quad (10)$$

where

$$\mathbf{X}_L = \mathbf{X}_p - \mathbf{X}_n.$$

To avoid problems with boundary effects, it is convenient to consider an infinite crystal.¹⁰ N is then taken as the number of unit cells per unit volume, and the values m_i and m_j are the masses of unit-cell atoms in the perfectly periodic lattice.

Substituting the uniform plane-wave solutions of

Eq. (9) into the power density expression of Eq. (6) (with the anharmonic terms deleted), and taking the time average of the result, one finds

$$\langle S_x \rangle_{\text{av}} = \frac{\operatorname{Re}}{2A_x N} \sum_{k,s} \sum_{k',s'} Q_{k,s}^* Q_{k',s'} (-2i\omega) \delta_{\omega,\omega'} \times \sum_{\substack{i,n \\ n_x > 0}} \sum_{\substack{j,L \\ L_x < -n_x}} (m_i m_j)^{-1/2} \mathbf{V}(ij) : \mathbf{A}_i^*(k,s) \mathbf{A}_j(k',s') \times \exp\{i[\mathbf{k}' \cdot \mathbf{X}_L + \mathbf{X}_n \cdot (\mathbf{k}' - \mathbf{k})]\}. \quad (11)$$

Although in Eq. (11), $\omega = \omega'$ (for nonzero time average), \mathbf{k} does not apparently at this point have to be equivalent to \mathbf{k}' .¹¹ It can be shown, however, that for the lossless system considered here, the value of $\langle S_x \rangle_{\text{av}}$ would vary with position x unless $\mathbf{k} = \mathbf{k}' + \mathbf{K}$ (\mathbf{K} is any reciprocal lattice vector). The Poynting theorem disallows such variation in a homogeneous lossless system. Accordingly, setting $\mathbf{k} = \mathbf{k}' + \mathbf{K}$, Eq. (11) can be reduced to

$$\langle S_x \rangle_{\text{av}} = \frac{\operatorname{Im}}{|\mathbf{a}_2 \times \mathbf{a}_3| N} \sum_{k,s} \omega Q_{k,s} Q_{k,s}^* \times \sum_{\substack{n_x \\ n_x > 0}} \sum_{\substack{i,j,L \\ L_x < -n_x}} (m_i m_j)^{-1/2} \mathbf{V}(ij) : \mathbf{A}_i^*(k,s) \mathbf{A}_j(k,s) \times \exp[i(\mathbf{k} \cdot \mathbf{X}_L)]. \quad (12)$$

To reduce Eq. (12) to a more familiar form requires a counting argument as indicated in Fig. 2. By inspection of Fig. 2, it is seen that the double sum on n_x (for $n_x > 0$) and L_x (for $-L_x > n_x$) can be reduced to the single sum on L_x (from $-L_x = 1$ to ∞) as¹²

$$\sum_{\substack{n_x \\ n_x > 0}} \sum_{\substack{L \\ L_x < -n_x}} [\dots] = \sum_{\substack{L \\ L_x < 0}} |l_1| [\dots], \quad (13)$$

where l_1 is the integer associated with the \mathbf{a}_1 component of the lattice vector \mathbf{X}_L , and \mathbf{b}_1 is chosen as the x direction, as

$$\mathbf{X}_L = (l_1 \mathbf{a}_1 + l_2 \mathbf{a}_2 + l_3 \mathbf{a}_3). \quad (14)$$

As a result of Eq. (13), Eq. (12) finally becomes

$$\langle S_x \rangle_{\text{av}} = \frac{-\operatorname{Im}}{|\mathbf{a}_2 \times \mathbf{a}_3| N} \sum_{k,s} \omega Q_{k,s}^* Q_{k,s} \sum_{\substack{i,j,L \\ L_x < 0}} (m_i m_j)^{-1/2} \mathbf{V}(ij) : \mathbf{A}_i^*(k,s) \mathbf{A}_j(k,s) l_1 \exp[i(\mathbf{k} \cdot \mathbf{X}_L)] = \frac{\operatorname{Im}}{|\mathbf{a}_2 \times \mathbf{a}_3| N} \sum_{k,s} \omega Q_{k,s}^* Q_{k,s} i \frac{\partial}{\partial k_1} [\frac{1}{2} \omega^2(k,s)] = \frac{1}{V} \sum_{k,s} (\omega^2 Q_{k,s}^* Q_{k,s}) \frac{1}{b_1} \frac{\partial \omega}{\partial k_1}, \quad (15)$$

¹⁰ Although \mathbf{k} is then continuous, the summation sign will be maintained for use later in finite crystals.

¹¹ The usual orthogonality relations do not apply here because of the limited sums involved.

¹² The counting argument used here for a general 3-dimensional crystal is similar to that used by Brillouin (cf. Ref. 2) for the power flow in a one-dimensional lattice with one atom per cell.

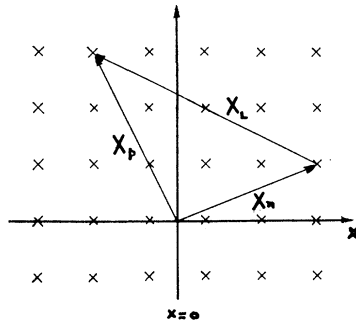


FIG. 2. Unit-cell locations near plane $x=0$.

where

$$\frac{\partial}{\partial k_1} \left[\sum_{i,j} (m_i m_j)^{-1/2} \mathbf{V}(ij) : \mathbf{A}_i^*(k,s) \mathbf{A}_j(k,s) \right] = 0,$$

$$V = N(\mathbf{a}_1 \cdot \mathbf{a}_2 \times \mathbf{a}_3); \quad \mathbf{k} = k_1 \mathbf{b}_1 + k_2 \mathbf{b}_2 + k_3 \mathbf{b}_3,$$

$$b_1 = \frac{|\mathbf{a}_2 \times \mathbf{a}_3|}{\mathbf{a}_1 \cdot \mathbf{a}_2 \times \mathbf{a}_3}; \quad \mathbf{a}_i \cdot \mathbf{b}_j = \delta_{ij}.$$

In like fashion, the other components of $\langle \mathbf{S} \rangle_{av}$ can be found, yielding for the vector time-average mechanical-power density,

$$\langle \mathbf{S} \rangle_{av} = \sum_{k,s} \langle w(k,s) \rangle \mathbf{v}(k,s), \quad (16)$$

where $\langle w(k,s) \rangle_{av}$ is the time-average stored mechanical-energy density per mode, given by

$$\langle w(k,s) \rangle_{av} = (1/V) [\omega^2 Q_{k,s}^* Q_{k,s}], \quad (17a)$$

and $\mathbf{v}(k,s)$ is the group velocity of the (k,s) mode

$$\mathbf{v}(k,s) = \left[\frac{\partial \omega}{\partial k_1} \mathbf{e}_1 + \frac{\partial \omega}{\partial k_2} \mathbf{e}_2 + \frac{\partial \omega}{\partial k_3} \mathbf{e}_3 \right]. \quad (17b)$$

That is, the time-average mechanical-energy density (per mode) is equated to the product of the average mechanical (i.e., kinetic and potential) energy and the group velocity of that mode.

CONCLUSIONS

We have now shown that for any 3-dimensional perfect harmonic lattice, the average mechanical energy does indeed flow with the group velocity (on a per-mode basis), independent of any restrictions whatsoever upon the nearness of interacting neighbors.¹³ The only restriction that was found necessary was to limit the proof to perfect harmonic lattices. But since the normal modes used are only approximate solutions for any other case, an exact proof of the energy theorem would not be expected to be possible.

For the imperfect anharmonic lattice (i.e., inclusive of nonlinearities and point defects), however, we were able to determine a useful expression for the instantaneous mechanical-power density, in terms of atomic displacements and velocities. From this expression, a determination of the lattice components of thermal conductivity has been made by the author,⁴ (cf. following article).

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¹³ That is, for temperatures sufficiently below the melting point of the crystal such that the number of atoms within the elemental volume ΔV remains constant.