gamma-rays alone nor Bohr orbit transitions alone will explain the observed spectra. This conclusion is based on the assumption that the residual thallium nuclei are not unstable with a lifetime short enough to be within the resolving time of the cloud chamber (~ 0.05 second). It is unlikely that there are such short lifetimes among the residual nuclei. If we take the experimental evidence on the emission of neutrons and protons from meson capture, then from a Segrè chart the most unfavorable lifetime is about three minutes.

Nothing definite can be said about the existence of a $2p-1s$ Bohr orbit transition. For if the $2p-1s$ transition is emitted from the assumed spectra the spectra which remain are consistent with the data. The data is consistent with the assumed spectra being totally due to bremsstrahlung photons from positrons and stray background photons. It is extremely unlikely, however, that the data could be accounted for by stray background photons alone, and the data could not be accounted for by bremsstrahlung photons alone because of the large numbers of electrons associated with negative mesons.

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The Acousto-Electric Effect*

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A new effect, the acousto-electric effect, is predicted on the basis of theoretical calculations. This effect deals with the generation of an electric current by a traveling longitudinal acoustic wave. The time-average of the generated current is found to depend on the sound power but not on the frequency of the acoustic wave. Illustrative calculations on a metal (sodium) and a semiconductor (n-type germanium) indicate that the effect should be experimentally measurable. An interesting analogy with the thermoelectric effect is pointed out.

I. INTRODUCTION

In this paper we discuss the effect on the conduction electrons of a crystal resulting from a single traveling longitudinal acoustic wave in the crystal. It is not difficult to see qualitatively how the electrons will be affected when the amplitude of the acoustic wave is small. The presence of a sinusoidal traveling acoustic wave gives rise to a sinusoidal electric field, this field traveling through the crystal with the same velocity as that of the acoustic wave. Consider the component of velocity of a conduction electron parallel to the velocity of the acoustic wave. For most of the conduction electrons, this component of velocity will be much larger in magnitude than the speed of the acoustic wave, so that these electrons are "out of phase" with respect to the traveling electric field. Thus, the time average of this field over their trajectories is zero, and these electrons are essentially unaffected by the presence of the acoustic wave. There are a few electrons, however, having components of velocity parallel to the wave which are comparable to the speed of the wave. These electrons are capable of being trapped by the moving electric field so that their time-averaged velocity in the direction of the field is exactly that of the field. Among these electrons, those having a maximum energy will be found to give rise to a net electric current. In a metal, these electrons are at the Fermi level. In an n-type semiconductor, these electrons are in the conduction band. Such a generation of an electric current by a traveling acoustic wave may be called the acousto-electric effect. It is interesting that the qualitative explanation of this effect which has just been given is analogous to the qualitative explanation of the operation of a linear accelerator.[1]

Let us consider a single traveling longitudinal acoustic wave moving along a long uniform rod of material, the ends of the rod being electrically insulated. The traveling acoustic wave could be induced by driving one end of the rod with a vibrator while matching the other end to the proper acoustic impedance to insure no reflection of the wave at the termination. The ends of the rod being electrically insulated, the acoustic wave would drag conduction electrons to one end of the rod, creating a deficiency of electrons at the other end. The resultant electric field along the rod will generate a conventional electric current which exactly cancels the current associated with the acousto-electric effect. The acousto-electric effect, therefore, may be measured by determining the electric potential difference between the two ends of the rod. An interesting comparison pointed out to the writer[2] is the striking analogy between this

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* This work was supported by the U. S. Office of Naval Research.

[1] J. C. Slater, Revs. Modern Phys. **20**, 473 (1948). See especially p. 483.

[2] H. Brooks, private communication.

potential difference and that occurring in the thermoelectric effect when the two ends of a metal rod are maintained at different temperatures. The net flow of phonons along a temperature gradient may be considered as a net flow of traveling acoustic waves along the gradient.

II. THE PERTURBATIVE POTENTIAL

In order to discuss the acousto-electric effect quantitatively, wave mechanics is necessary. We will use the one-electron approximation in solving Schrödinger's equation. Thus, a conduction electron of the crystal is assumed to move in an effective potential resulting from the nuclei plus all the other electrons of the crystal. We will assume that this potential $V(\mathbf{r}, t)$ may be written

$$V(\mathbf{r}, t)=V_0(\mathbf{r})+V_1(\mathbf{r}, t), \tag{1}$$

where $V_0(\mathbf{r})$ is the correct potential in the absence of the traveling acoustic wave and $V_1(\mathbf{r}, t)$, the perturbative potential, is an additional term resulting from the presence of the acoustic wave. We will make the approximation that V_1 is a slowly varying function of position (on the atomic scale).

The perturbative potential can be broken into two parts,

$$V_1=V_{1a}+V_{1b}, \tag{2}$$

where V_{1a} results from the charge unbalances set up by the acoustic wave, while V_{1b} results from the changes in interatomic spacing set up by the acoustic wave. We shall first determine V_{1a}.

Consider a simple longitudinal traveling acoustic wave

$$\mathbf{s}=\mathbf{S}\sin\boldsymbol{\sigma}\cdot(\mathbf{r}-\mathbf{C}t), \tag{3}$$

where the displacement $\mathbf{s}$, the amplitude $\mathbf{S}$, the acoustic wave vector $\boldsymbol{\sigma}$, and the wave velocity $\mathbf{C}$ all have the same direction. Let $\rho_+(\mathbf{r}, t)$ be the macroscopic charge density resulting from the ion cores of the crystal, an ion core being an atom of the crystal without its conduction electrons. If ρ_0 is the average value of ρ_+, then

$$(\rho_+-\rho_0)/\rho_0=-\nabla\cdot\mathbf{s}, \tag{4}$$

i.e., the fractional variation of the ion-core charge density equals the negative of the dilation $\nabla\cdot\mathbf{s}$. This variation of the ion-core charge density from its average value will be partially, but not completely, cancelled by a corresponding variation of the conduction-electronic macroscopic charge density $\rho_-(\mathbf{r}, t)$ from its mean value $-\rho_0$. This question has been discussed byBardeen,[3] who points out that for decreasing acoustic wavelength (increasing σ) the cancellation becomes less complete. We will assume that this effect may be expressed as

$$(-\rho_--\rho_0)/(\rho_+-\rho_0)=g(\boldsymbol{\sigma}). \tag{5}$$

We know that for infinite wavelength ($\sigma=0$) cancellation will be complete so that $g(0)=1$. For finite wavelength cancellation will be incomplete so that $g<1$. Since g should be independent of the orientation of $\boldsymbol{\sigma}$, it may be expanded as a power series in σ^2.

$$g(\boldsymbol{\sigma})=1-\beta\sigma^2+\cdots. \tag{6}$$

Having determined the macroscopic charge density $(\rho_++\rho_-)$ resulting from the acoustic wave, we may now obtain V_{1a} from Poisson's equation[4]

$$(\rho_++\rho_-)=(\epsilon/8\pi)\nabla^2V_{1a}, \tag{7}$$

where ϵ is the dielectric constant. Equations (4), (5), (6), and (7) give

$$\mathbf{s}=-(\epsilon/8\pi\rho_0\beta\sigma^2)\nabla V_{1a}. \tag{8}$$

Substituting (3) into (8) gives

$$V_{1a}(\mathbf{r}, t)=\mathcal{V}_a\cos\boldsymbol{\sigma}\cdot(\mathbf{r}-\mathbf{C}t), \tag{9}$$

where

$$\mathcal{V}_a=(8\pi\beta\rho_0/\epsilon)(\boldsymbol{\sigma}\cdot\mathbf{S}). \tag{10}$$

In order to determine V_{1b}, we make use of the idea of a deformation potential as suggested by Bardeen and Shockley.[5] A uniform dilation or compression of a crystal will cause the bottom (or top) of some energy band of the crystal to shift its energy. For sufficiently small dilations the shift in energy of a given portion of the band will be directly proportional to the dilation. Starting with the potential acting on an electron in the undilated crystal, we can correctly express the effect of the dilation on a given portion of the band by adding to the original potential a constant perturbative potential equal to the shift in energy of that portion of the band. This perturbative potential is called a deformation potential. The assumption is now made that such a procedure is also valid for non-uniform dilations of the crystal, whereupon a non-uniform deformation potential is required. This assumption seems plausible provided that the dilation varies very slowly with position (on the atomic scale); i.e., the dilation results from a long wavelength acoustic wave. Taking V_{1b} proportional to the dilation, we have[6]

$$V_{1b}=A'\nabla\cdot\mathbf{s}. \tag{11}$$

Substituting (3) into (11), we obtain

$$V_{1b}(\mathbf{r}, t)=\mathcal{V}_b\cos\boldsymbol{\sigma}\cdot(\mathbf{r}-\mathbf{C}t), \tag{12}$$

where

$$\mathcal{V}_b=A'(\boldsymbol{\sigma}\cdot\mathbf{S}). \tag{13}$$

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[3] J. Bardeen, Phys. Rev. **52**, 688 (1937).

[4] Throughout this paper we will use atomic units; i.e. mass and charge are measured in units of the electronic mass and charge, respectively, energy is measured in Rydbergs (13.6 ev), distance in units of the Bohr radius, velocity in units of αc (the fine-structure constant multiplied by the velocity of light), time in units of $\hbar^3/me^4$, wave number in units of $me^4/2\pi\hbar^2$.

[5] J. Bardeen and W. Shockley, Phys. Rev. **80**, 72 (1950).

[6] We may disregard the fact that the constant of proportionality A' is a function of position in the band. It will later be shown that the acousto-electric effect results from conduction electrons lying in a very small energy range. Over such a small energy range A' may be assumed constant.

Equation (2) now gives

$$V_1(\mathbf{r}, t) = \mathcal{V} \cos \boldsymbol{\sigma} \cdot (\mathbf{r} - \mathbf{C}t), \tag{14}$$

and

$$\mathcal{V} = A(\boldsymbol{\sigma} \cdot \mathbf{S}), \tag{15}$$

where

$$A = A' + (8\pi\beta\rho_0/\epsilon). \tag{16}$$

III. THE WANNIER-SLATER THEOREM

Having determined $V(\mathbf{r}, t)$, we are in a position to write down Schrödinger's equation for the problem, namely

$$[-\nabla^2 + V(\mathbf{r}, t)]\psi(\mathbf{r}, t) = 2i\partial/\partial t\psi(\mathbf{r}, t). \tag{17}$$

The method we shall use in solving this equation was first used by Wannier[7] in studying excitons in crystals. The importance and generality of the method was first pointed out by Slater,[8] who showed that the motion of an electron in a periodic potential plus a slowly varying perturbative potential can be derived from the energy of the electron in the periodic potential alone. Slater restricted himself to time-independent perturbative potentials, but we can easily remove this restriction. In the absence of the traveling acoustic wave Schrödinger's equation is

$$[-\nabla^2 + V_0(\mathbf{r})]\psi_0(\mathbf{k}, \mathbf{r}, t) = 2i\partial/\partial t\psi_0(\mathbf{k}, \mathbf{r}, t), \tag{18}$$

where the wave vector $\mathbf{k}$ is a parameter determining the translational properties of the wave function; i.e.,

$$\psi_0(\mathbf{k}, \mathbf{r} + \mathbf{r}_n, t) = e^{i\mathbf{k}\cdot\mathbf{r}_n}\psi_0(\mathbf{k}, \mathbf{r}, t), \tag{19}$$

$\mathbf{r}_n$ being the position vector to the nth unit cell of the undeformed crystal. The wave function may be written in the form

$$\psi_0(\mathbf{k}, \mathbf{r}, t) = \sum\nolimits_n \Psi_0(\mathbf{k}, \mathbf{r}_n, t)a(\mathbf{r} - \mathbf{r}_n), \tag{20}$$

where

$$\Psi_0(\mathbf{k}, \mathbf{r}, t) = e^{i(\mathbf{k}\cdot\mathbf{r} - \frac{1}{2}E_0 t)}. \tag{21}$$

$a(\mathbf{r})$ is the Wannier function,[7] while $E_0(\mathbf{k})$ (a function of $\mathbf{k}$) is the energy of the electron. Following Slater, we assume that in the presence of the traveling acoustic wave, the wave function can be expanded in terms of the Wannier function, i.e.,

$$\psi(\mathbf{k}, \mathbf{r}, t) = \sum\nolimits_n \Psi(\mathbf{k}, \mathbf{r}_n, t)a(\mathbf{r} - \mathbf{r}_n), \tag{22}$$

ψ being the solution to Eq. (17). The Wannier-Slater theorem states that

$$[E_0(-i\nabla) + V_1(\mathbf{r} - \mathbf{C}t)]\Psi(\mathbf{r}, t) = 2i\partial/\partial t\Psi(\mathbf{r}, t). \tag{23}$$

This form of the theorem, including time explicitly, can be derived straightforwardly by the methods used in the appendix of reference 8. It is possible to determine the expectation values of the energy and the velocity of an electron in the deformed lattice from a knowledge of $\Psi(\mathbf{r}, t)$. In the appendix to this article it is shown that

$$E(\mathbf{k}) = 2i\int_\infty \Psi^* \frac{\partial}{\partial t}\Psi d\tau \bigg/ \int_\infty \Psi^*\Psi d\tau, \tag{24}$$

$$\mathbf{v}(\mathbf{k}) = \int_\infty \Psi^* \mathbf{v}_0(-i\nabla)\Psi d\tau \bigg/ \int_\infty \Psi^*\Psi d\tau. \tag{25}$$

($\int_\infty d\tau$ denotes an integral over the entire crystal.) $\mathbf{v}_0(\mathbf{k})$, the velocity of an electron in the undeformed lattice, is given by

$$\mathbf{v}_0(\mathbf{k}) = \tfrac{1}{2}\nabla_k E_0(\mathbf{k}). \tag{26}$$

At this point we will introduce the effective-mass approximation, i.e., over the filled portion of the conduction band $E_0(\mathbf{k})$ will be approximated by

$$E_0(\mathbf{k}) = \alpha k^2. \tag{27}$$

Here the zero of energy is taken at the bottom of the band. Substituting (27) into (26), we get

$$\mathbf{v}_0(\mathbf{k}) = \alpha\mathbf{k}, \tag{28}$$

whereupon (25) becomes

$$\mathbf{v}(\mathbf{k}) = -i\alpha\int_\infty \Psi^*\nabla\Psi d\tau \bigg/ \int_\infty \Psi^*\Psi d\tau. \tag{29}$$

Substituting (27) into (23), we get

$$[-\alpha\nabla^2 + V_1(\mathbf{r} - \mathbf{C}t)]\Psi(\mathbf{r}, t) = 2i\partial/\partial t\Psi(\mathbf{r}, t). \tag{30}$$

The power of the Wannier-Slater method lies in the interpretation we may attach to Eq. (30). It is clear that (30) may be interpreted as Schrödinger's equation for a particle of mass m/α moving in the potential $V_1(\mathbf{r} - \mathbf{C}t)$. ($m$ is the mass of the electron.) $\Psi(\mathbf{r}, t)$ is thus the wave function determining the motion of the particle. A comparison of Eqs. (24) and (29) with Eqs. (39) and (34), respectively, of Sec. IV shows that this particle of mass m/α moving in the potential V_1 has the same energy and velocity as an electron moving in the potential $V_0 + V_1$. Henceforth we need concern ourselves only with the determination of Ψ rather than the true wave function ψ, since Ψ may be interpreted as a wave function for the purpose of determining expectation values of physical quantities.

IV. TRANSFORMATION OF SCHRÖDINGER'S EQUATION

In attempting to solve Eq. (30), we are faced with the problem that the equation is not separable since the Hamiltonian contains the time explicitly. The key to the method of attack is given by the observation that the time dependence of $V_1(\mathbf{r} - \mathbf{C}t)$ can be removed by the Galilean transformation

$$\mathbf{r}' = \mathbf{r} - \mathbf{C}t, \quad t' = t. \tag{31}$$

Let us therefore study the general properties of the

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[7] G. H. Wannier, Phys. Rev. **52**, 191 (1937).

[8] J. C. Slater, Phys. Rev. **76**, 1592 (1949).

wave function Ψ under such a transformation, this wave function being associated with a particle of mass m/α moving in the potential $V_1(\mathbf{r}-\mathbf{C}t)$. Equation (30), the Schrödinger's equation for such a particle, will transform into

$$[-\alpha\nabla'^2+V_1(\mathbf{r}')]\Psi'(\mathbf{r}',t')=2i\partial/\partial t'\Psi'(\mathbf{r}',t') \tag{32}$$

with the aid of (31). We now ask ourselves for the relation between $\Psi(\mathbf{r},t)$ and $\Psi'(\mathbf{r}',t')$. This relationship is determined by the following three conditions:

(1) Equations (30) and (32) must be equivalent.

(2) The velocity of the particle of mass m/α as measured in one coordinate system must be related to its velocity in the other system by the equation

$$\mathbf{v}'=\mathbf{v}-\mathbf{C}, \tag{33}$$

where the velocity of the particle is given by

$$\mathbf{v}=-i\alpha\int_\infty \Psi^*\boldsymbol{\nabla}\Psi d\tau \Big/ \int \Psi^*\Psi d\tau, \tag{34}$$

and similarly for $\mathbf{v}'$.

(3) Probability density must be invariant to coordinate transformations, i.e.,

$$\Psi'^*(\mathbf{r}',t')\Psi'(\mathbf{r}',t')=\Psi^*(\mathbf{r},t)\Psi(\mathbf{r},t). \tag{35}$$

These three conditions can be satisfied,[9] provided

$$\Psi'(\mathbf{r}',t')=\Psi(\mathbf{r},t)\exp[-i(\mathbf{C}\cdot\mathbf{r}-\tfrac{1}{2}C^2t)/\alpha]. \tag{36}$$

Condition (3) is obviously satisfied by Eq. (36). Condition (2) follows from (36) since

$$\begin{aligned}\mathbf{v}'&=-i\alpha\int_\infty \Psi'^*\boldsymbol{\nabla}'\Psi'd\tau' \Big/ \int_\infty \Psi'^*\Psi'd\tau'\\ &=-i\alpha(-i\mathbf{C}/\alpha)-i\alpha\int_\infty \Psi^*\boldsymbol{\nabla}\Psi d\tau \Big/ \int_\infty \Psi^*\Psi d\tau\\ &=\mathbf{v}-\mathbf{C}.\end{aligned}$$

Making use of the equations

$$\boldsymbol{\nabla}'=\boldsymbol{\nabla}, \tag{37}$$

$$\partial/\partial t'=\partial/\partial t+\mathbf{C}\cdot\boldsymbol{\nabla}, \tag{38}$$

we have

$$\begin{aligned}&[-\alpha\nabla'^2+V_1(\mathbf{r}')-2i\partial/\partial t']\Psi'(\mathbf{r}',t')\\ &\quad=[-\alpha\nabla^2+V_1(\mathbf{r}-\mathbf{C}t)-2i\mathbf{C}\cdot\boldsymbol{\nabla}-2i\partial/\partial t]\\ &\qquad\times\Psi(\mathbf{r},t)\exp[-i(\mathbf{C}\cdot\mathbf{r}-\tfrac{1}{2}C^2t)/\alpha]\\ &\quad=\exp[-i(\mathbf{C}\cdot\mathbf{r}-\tfrac{1}{2}C^2t)/\alpha][C^2/\alpha+2i\mathbf{C}\cdot\boldsymbol{\nabla}\\ &\qquad-\alpha\nabla^2+V_1(\mathbf{r}-\mathbf{C}t)-2i\mathbf{C}\cdot\boldsymbol{\nabla}-2C^2/\alpha\\ &\qquad+C^2/\alpha-2i\partial/\partial t]\Psi(\mathbf{r},t)\\ &\quad=\exp[-i(\mathbf{C}\cdot\mathbf{r}-\tfrac{1}{2}C^2t)/\alpha][-\alpha\nabla^2+V_1(\mathbf{r}-\mathbf{C}t)\\ &\qquad\qquad-2i\partial/\partial t]\Psi(\mathbf{r},t),\end{aligned}$$

so that condition (1) is satisfied by Eq. (36). The energy of a particle of mass m/α is given by

$$E=2i\int_\infty \Psi^*\frac{\partial}{\partial t}\Psi d\tau \Big/ \int_\infty \Psi^*\Psi d\tau. \tag{39}$$

We can now determine the transformation properties of E under a Galilean transformation. Thus,

$$\begin{aligned}E'&=2i\int_\infty \Psi'^*\frac{\partial}{\partial t'}\Psi'd\tau' \Big/ \int_\infty \Psi'^*\Psi'd\tau'\\ &=2i\int \Psi^*\frac{\partial}{\partial t}\Psi d\tau \Big/ \int_\infty \Psi^*\Psi d\tau\\ &\qquad+2i\mathbf{C}\cdot\int_\infty \Psi^*\boldsymbol{\nabla}\Psi d\tau \Big/ \int_\infty \Psi^*\Psi d\tau+C^2/\alpha\\ &=E-2\mathbf{C}\cdot\mathbf{v}/\alpha+C^2/\alpha.\end{aligned} \tag{40}$$

In analogy with Eq. (19), we may define the wave vector $\mathbf{k}'$ in the transformed system by

$$\psi_0'(\mathbf{k}',\mathbf{r}'+\mathbf{r}_n,t')=e^{i\mathbf{k}'\cdot\mathbf{r}_n}\psi_0'(\mathbf{k}',\mathbf{r}',t'). \tag{41}$$

We may now apply Eqs. (19) and (41) to the case of a particle of mass m/α. Making use of Eq. (36), we get

$$\mathbf{k}'=\mathbf{k}-\mathbf{C}/\alpha, \tag{42}$$

so that $\mathbf{k}$ has the transformation properties of momentum.

V. SOLUTION OF SCHRÖDINGER'S EQUATION

Having transformed Eq. (30) into (32), we may separate variables in the wave function Ψ',

$$\Psi'(\mathbf{k}',\mathbf{r}',t')=e^{-\frac{1}{2}iE't'}\Phi'(\mathbf{k}',\mathbf{r}'). \tag{43}$$

Φ' satisfies the time-independent Schrödinger equation

$$[-\alpha\nabla'^2+V_1(\mathbf{r}')]\Phi'=E'\Phi'. \tag{44}$$

Let us orient our coordinate system such that the acoustic wave is moving along the x axis. Then we may write

$$\Phi'(\mathbf{r}')=\varphi_x'(x')\varphi_y'(y')\varphi_z'(z'), \tag{45}$$

$$E'=E_x'+E_y'+E_z', \tag{46}$$

where

$$[-\alpha\partial^2/\partial x'^2+V_1(x')]\varphi_x'=E_x'\varphi_x', \tag{47}$$

$$-\alpha\partial^2\varphi_y'/\partial y'^2=E_y'\varphi_y', \tag{48}$$

$$-\alpha\partial^2\varphi_z'/\partial z'^2=E_z'\varphi_z'. \tag{49}$$

Equations (48) and (49) give

$$\varphi_y'=\exp(ik_y'y'), \tag{50}$$

$$\varphi_z'=\exp(ik_z'z'), \tag{51}$$

$$E_y'=\alpha k_y'^2, \tag{52}$$

$$E_z'=\alpha k_z'^2. \tag{53}$$

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[9] W. Pauli, *Handbuch der Physik* (Springer, Berlin, 1933), Vol. 24, Chap. 2, p. 100.

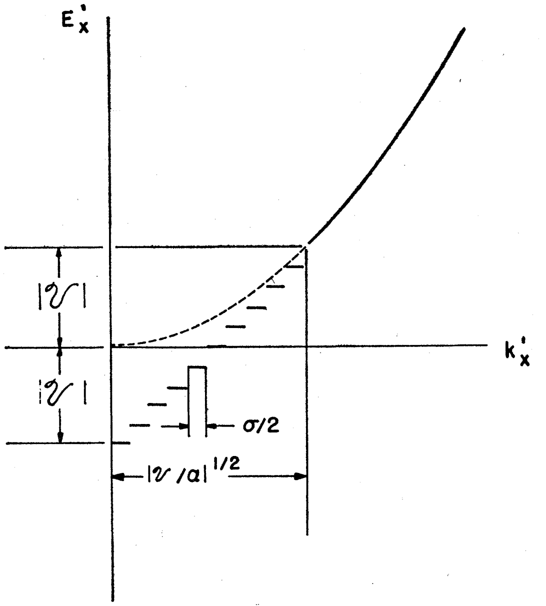

FIG. 1. E_x' *versus* k_x'.

Substituting Eq. (14) into (47), we get

$$[-\alpha\partial^2/\partial x'^2+\mathcal{V}\cos(\sigma x')]\varphi_x'=E_x'\varphi_x'. \tag{54}$$

Dividing Eq. (54) by α, we obtain an equation mathematically equivalent to Schrödinger's equation for an electron traveling in a one-dimensional sinusoidal potential (Mathieu's equation). This problem has recently been exhaustively studied by Slater,[10] whose results indicate that the following approximate conclusions may be drawn concerning the energy levels associated with Eq. (54). For energies larger (in absolute value) than the amplitude $|\mathcal{V}|$, the curve of E_x' *versus* k_x' is essentially unchanged from its form in the absence of the acoustic wave; i.e., $E_x'=\alpha k_x'^2$. For energies smaller (in absolute value) than the amplitude $|\mathcal{V}|$, the curve of E_x' *versus* k_x' resembles a staircase function, E_x' being independent of k_x' throughout a given Brillouin zone associated with the deformed lattice. These discrete allowed values of E_x' correspond to the energy levels of the harmonic oscillator formed by each trough of the perturbative potential. We will assume that the staircase function rises uniformly from the energy $-|\mathcal{V}|$ to the energy $+|\mathcal{V}|$. Each step will have a width $\sigma/2$. The curve of E_x' *versus* k_x' is shown in Fig. 1.

Equation (44), like (18), is Schrödinger's equation for a periodic potential, so that, like Eq. (26), we have

$$\mathbf{v}'(\mathbf{k}')=\tfrac{1}{2}\nabla_{k}'E'(\mathbf{k}'), \tag{55}$$

so that for $k_x'^2>|\mathcal{V}/\alpha|$,

$$v_x'=\alpha k_x', \tag{56}$$

while for $k_x'^2<|\mathcal{V}/\alpha|$,

$$v_x'=0. \tag{57}$$

Making use of the transformation properties of energy and velocity previously given, we can now determine these quantities in the unprimed coordinate system. For $(k_x-C/\alpha)^2>|\mathcal{V}/\alpha|$,

$$\begin{aligned}E&=E'+2\mathbf{C}\cdot\mathbf{v}'/\alpha+C^2/\alpha\\&=\alpha(\mathbf{k}'+\mathbf{C}/\alpha)^2\\&=\alpha k^2,\end{aligned} \tag{58}$$

$$\begin{aligned}v_x&=\alpha k_x'+C\\&=\alpha k_x.\end{aligned} \tag{59}$$

For $(k_x-C/\alpha)^2<|\mathcal{V}/\alpha|$,

$$\begin{aligned}E&=E'+C^2/\alpha\\&=E_x'+\alpha(k_y^2+k_z^2)+C^2/\alpha,\end{aligned} \tag{60}$$

$$v_x=C. \tag{61}$$

Because of Eq. (60), surfaces of constant E do not have inversion symmetry in k space, as can be seen from Fig. 2, showing the surface of $E=E_F$ (the Fermi level).

VI. APPLICATION TO A METAL

In this section we shall apply our previous results to the calculation of the electronic current density in a metal. The average value of velocity in the direction of the acoustic wave for the conduction electrons is given by

$$\langle v_x\rangle=\textstyle\sum_{\mathbf{k}}{}'\,v_x(\mathbf{k})/\sum_{\mathbf{k}}{}'\,1, \tag{62}$$

the prime denoting a summation over the occupied states. We will assume that the energy levels below a certain energy E_F (the Fermi energy) are all filled, while those above this energy are all empty. Since the levels are very closely spaced, we can replace the sums in Eq. (62) by the equivalent integrals over k space, i.e.,

$$\langle v_x\rangle=\int' v_x(\mathbf{k})d\tau_k\Big/\int' d\tau_k. \tag{63}$$

Because of the reflection symmetry of $\mathbf{v}(\mathbf{k})$ and of the Fermi surface (surface in k space for which $E=E_F$) with respect to k_y and k_z, it follows that

$$\langle v_y\rangle=\langle v_z\rangle=0. \tag{64}$$

Thus the electronic current density J is

$$J=n\langle v_x\rangle, \tag{65}$$

where n, the number of conduction electrons per unit volume, is given by

$$n=2/(2\pi)^3\int' d\tau_k. \tag{66}$$

For metals, n can be expressed in the form

$$n=n_e n_a/\Omega, \tag{67}$$

where n_e is the number of conduction electrons per atom, n_a is the number of atoms per unit cell of the

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[10] J. C. Slater, Phys. Rev. 87, 807 (1952). See especially Fig. 3, p. 813.

crystal, and Ω is the volume of the unit cell. It will be necessary to compute $\langle v_x\rangle$ separately for the following three ranges of the variable $|\mathcal{V}/\alpha|^{\frac{1}{2}}$.

Range I $|\mathcal{V}/\alpha|^{\frac{1}{2}}<|E_F/\alpha|^{\frac{1}{2}}-C/\alpha$;
range II $|E_F/\alpha|^{\frac{1}{2}}+C/\alpha>|\mathcal{V}/\alpha|^{\frac{1}{2}}>|E_F/\alpha|^{\frac{1}{2}}-C/\alpha$;
range III $|\mathcal{V}/\alpha|^{\frac{1}{2}}>|E_F/\alpha|^{\frac{1}{2}}+C/\alpha$.

First we consider range I.

$$\int' d\tau_k=\frac{4}{3}\pi\left(\frac{E_F}{\alpha}\right)^{\frac{3}{2}}+\frac{\pi}{\alpha}\int_{C/\alpha-|v/\alpha|^{\frac{1}{2}}}^{C/\alpha+|v/\alpha|^{\frac{1}{2}}}\left\{\left[E_F-E_x'\left(k_x-\frac{C}{\alpha}\right)-\frac{C^2}{\alpha}\right]-[E_F-\alpha k_x^2]\right\}dk_x$$
$$=\frac{4\pi}{3}\left(\frac{E_F}{\alpha}\right)^{\frac{3}{2}}+\frac{2\pi}{3}\left|\frac{\mathcal{V}}{\alpha}\right|^{\frac{3}{2}}. \tag{68}$$

$$\int' v_x(\mathbf{k})d\tau_k=\frac{\pi}{\alpha}\int_{C/\alpha-|v/\alpha|^{\frac{1}{2}}}^{C/\alpha+|v/\alpha|^{\frac{1}{2}}}\left\{\left[E_F-E_x'\left(k_x-\frac{C}{\alpha}\right)-\frac{C^2}{\alpha}\right]C-[E_F-\alpha k_x^2]\alpha k_x\right\}dk_x$$
$$=2\pi C|\mathcal{V}/\alpha|^{\frac{3}{2}}. \tag{69}$$

In obtaining (68) and (69), we have made use of the fact that

$$\int_0^{\pm|v/\alpha|^{\frac{1}{2}}} E_x'(k_x')dk_x'=0. \tag{70}$$

Combining (63), (68), and (69), we get

$$\langle v_x\rangle=3C[1+2|E_F/\mathcal{V}|^{\frac{3}{2}}]^{-1}. \tag{71}$$

Combining (63), (65), (66), and (69), we get

$$J=(C/2\pi^2)|\mathcal{V}/\alpha|^{\frac{3}{2}}. \tag{72}$$

It should be pointed out that $\langle v_x\rangle$ fails to vanish in range I not because of the form of $v_x(\mathbf{k})$ but rather because of the shape of the Fermi surface (see Fig. 2). For example, if the Fermi surface were cylindrical in shape with the axis of the cylinder parallel to the k_x axis, then $\langle v_x\rangle$ would vanish in spite of Eqs. (59) and (61). The net average velocity results entirely from a thin ring of electrons in k space—this ring being those electrons lying near the Fermi surface which have $\mathbf{v}_x=\mathbf{C}$, the velocity of the acoustic wave.

In range III, however, all the electrons contribute equally to the net electronic current. This follows from the fact that all the occupied states are associated with a value of k_x such that $(k_x-C/\alpha)^2<|\mathcal{V}/\alpha|$, so that each electron moves with an average value of v_x equal to C. It immediately follows that in range III

$$\langle v_x\rangle=C. \tag{73}$$

Combining Eqs. (65), (67), and (73), we get

$$J=(n_en_a/\Omega)C \tag{74}$$

for the current density in range III.

We shall not bother to determine $\langle v_x\rangle$ in range II since this intermediate range covers only a very small variation in the variable $|\mathcal{V}/\alpha|$. This can be seen from the fact that $|E_F/\alpha|^{\frac{1}{2}}$ is about 300 times the size of C/α in a typical metal. Henceforth we will assume

range I $|\mathcal{V}/\alpha|^{\frac{1}{2}}<|E_F/\alpha|^{\frac{1}{2}}$,
range II $|\mathcal{V}/\alpha|^{\frac{1}{2}}>|E_F/\alpha|^{\frac{1}{2}}$.

It can be seen that at the upper limit of range I, Eq. (71) goes into Eq. (73).

We wish to express the current density J in terms of the acoustic intensity Υ (the acoustic energy crossing unit area in unit time). Υ may be expressed in terms of U, the acoustic energy per atom, by

$$\Upsilon=(n_aCU/\Omega). \tag{75}$$

If M is the mass of the atom, then from Eq. (3) we get

$$U=M\dot{s}_{\text{max}}^2=M(\sigma SC)^2. \tag{76}$$

Combining Eqs. (15), (75), and (76), we get

$$|\mathcal{V}/\alpha|=|A/\alpha|(\Omega\Upsilon/n_aMC^3)^{\frac{1}{2}}. \tag{77}$$

Combining Eqs. (72), (74), and (77), we get

$$J=B\Upsilon^{\frac{3}{4}},\quad \Upsilon\leqslant\Upsilon_M; \tag{78}$$
$$J=J_M,\quad \Upsilon\geqslant\Upsilon_M; \tag{79}$$

where

$$B=\frac{2}{(2\pi C)^2}\left|\frac{A}{\alpha}\right|^{\frac{3}{2}}\left(\frac{\Omega C}{n_aM}\right)^{\frac{3}{4}}, \tag{80}$$
$$J_M=(n_en_aC/\Omega), \tag{81}$$
$$\Upsilon_M=(J_M/B)^{4/3}. \tag{82}$$

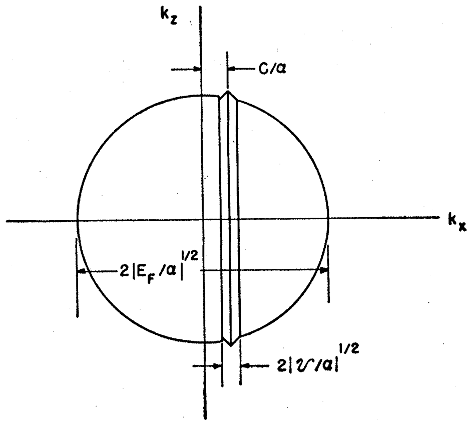

FIG. 2. The Fermi surface in k space.

As an example, let us compute the current density in sodium, where $\Omega = 257.5$, $|A| = 0.161$, $M = 4.22\times 10^4$, $n_e = 1$, $n_a = 1$, $C = 1.75\times 10^{-3}$, and $\alpha = 1$. (As is noted in Appendix B of reference 5, $\frac{3}{2}|A|$ is equal to the "interaction constant" of Sommerfeld and Bethe, a constant which may be determined from high-temperature conductivity data. The value of the interaction constant for sodium quoted by Sommerfeld and Bethe[11] has been used to determine the above value of $|A|$.) Using the above values, we obtain $B = 0.199$, $\Upsilon_M = 1.11\times 10^{-6}$, and $J_M = 6.80\times 10^{-6}$. If, in place of atomic units, we wish to express Υ in units of ergs/cm² sec and J in units of microamperes/cm², then $B = 601$, $\Upsilon_M = 3.60 \times 10^{16}$ ergs/cm² sec, and $J_M = 1.60\times 10^{15}$ μa/cm² $= 1600 \times 10^6$ amperes/cm². The above values of Υ_M and J_M show that it would be experimentally impossible to ever reach saturation, so that range I is the only range of interest. The above value of B indicates that it should be possible to detect the acousto-electric effect experimentally. For example, if $\Upsilon = 10^{-4}$ ergs/cm² sec (equivalent to an intensity level of 50 db), then $J = 0.601$ μa/cm².

VII. APPLICATION TO AN *N*-TYPE SEMICONDUCTOR

We wish to calculate the current density resulting from the electrons in the conduction band of an n-type semiconductor. It is assumed that, in the conduction band, the Fermi factor can be approximated by the Boltzmann factor

$$\exp-[E(\mathbf{k})-E_F]/\kappa T,$$

where E_F is the Fermi energy and κ is Boltzmann's constant. Thus

$$\langle v_x\rangle = \frac{\int_\infty v_x(\mathbf{k})e^{-[E(\mathbf{k})-E_F]/\kappa T}d\tau_k}{\int_\infty e^{-[E(\mathbf{k})-E_F]/\kappa T}d\tau_k}. \tag{83}$$

Since $E(\mathbf{k})$ differs from αk^2 only over a very small region of k space, we may make the approximation

$$\int_\infty e^{-E(\mathbf{k})/\kappa T}d\tau_k \cong \int_\infty e^{-(\alpha/\kappa T)k^2}d\tau_k = \left(\frac{\pi\kappa T}{\alpha}\right)^{\frac{3}{2}}. \tag{84}$$

This approximation is not sufficient for the numerator of (83), however, since the total nonvanishing contribution to $\langle v_x\rangle$ comes from this small region where $E(\mathbf{k})\neq\alpha k^2$.

$$\int_\infty v_x(\mathbf{k})e^{-E(\mathbf{k})/\kappa T}d\tau_k = \frac{\pi\kappa T}{\alpha}\int_{C/\alpha-|\Upsilon/\alpha|^{\frac{1}{2}}}^{C/\alpha+|\Upsilon/\alpha|^{\frac{1}{2}}} \times[C\exp\{-(1/\kappa T)[E_x'(k_x-C/\alpha)+C^2/\alpha]\} - \alpha k_x\exp\{-(\alpha/\kappa T)k_x^2\}]dk_x. \tag{85}$$

For the purpose of evaluating the above integral, we may take

$$E_x'(k_x-C/\alpha) = 2\alpha|\Upsilon/\alpha|^{\frac{1}{2}}(|k_x-C/\alpha|-\tfrac{1}{2}|\Upsilon/\alpha|^{\frac{1}{2}}). \tag{86}$$

We will also assume the temperature is large enough such that

$$C^2/\alpha \ll \kappa T, \tag{87}$$

$$|\Upsilon| \ll \kappa T. \tag{88}$$

It will later be shown that these two conditions are satisfied under almost all practical experimental conditions. After some manipulation (85) becomes

$$\int_\infty v_x(\mathbf{k})e^{-E(\mathbf{k})/\kappa T}d\tau_k = 2\pi C|\Upsilon/\alpha|^{\frac{3}{2}}, \tag{89}$$

so that

$$\langle v_x\rangle = (2C/\sqrt{\pi})|\Upsilon/\kappa T|^{\frac{3}{2}}. \tag{90}$$

If the semiconductor is doped with impurity atoms having a valence one unit greater than that of the semiconducting atoms, then for sufficiently high temperatures the number of conduction electrons per unit volume is $n_a f/\Omega$, f being the fraction of atoms which are impurity atoms, while n_a and Ω have the same meaning as in Sec. VI. For low temperatures, however, most of the excess electrons will be trapped in donor levels lying below the bottom of the conduction band, so that there will be very few conduction electrons. We will assume that there are two donor levels (one for each spin) for each impurity atom, these levels lying below the bottom of the conduction band. The energy of these levels will be denoted by E_D. (Taking the zero of energy at the bottom of the conduction band will make E_D negative.) The number of conduction electrons per unit volume can now be written in two forms:

$$n = [2/(2\pi)^3]\int_\infty e^{-[E(\mathbf{k})-E_F]/\kappa T}d\tau_k, \tag{91}$$

$$n = (n_a f/\Omega)[1-2\{e^{(E_D-E_F)/\kappa T}+1\}^{-1}]. \tag{92}$$

It should be noted that the Fermi factor *cannot* be approximated by the Boltzmann factor in Eq. (92), since the Fermi level may lie very close to the donor levels. Combining Eqs. (84), (91), and (92), we may

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[11] A. Sommerfeld and H. Bethe, *Handbuch der Physik* (Springer, Berlin, 1933), Vol. 24, Chap. 2, p. 524.

solve for n in terms of E_D. Defining the quantity

$$\eta=(\Omega/4n_af)(\kappa T/\pi\alpha)^{\frac{3}{2}}e^{-|E_D|/\kappa T}, \tag{93}$$

we may consider the two limiting cases of $\eta\gg1$ (high temperature) and $\eta\ll1$ (low temperature). For $\eta\gg1$,

$$n=n_af/\Omega, \tag{94}$$

while for $\eta\ll1$,

$$n=\tfrac{1}{4}(\kappa T/\pi\alpha)^{\frac{3}{2}}e^{-|E_D|/\kappa T}. \tag{95}$$

Combining Eqs. (65), (77), (90), (94), and (95), we get, for $\eta\gg1$,

$$J=\mathcal{B}f(\Upsilon/T^2)^{\frac{3}{4}}, \tag{96}$$

where

$$\mathcal{B}=\frac{2}{(\pi)^{\frac{1}{2}}MC}\left(\frac{n_aM}{\Omega C}\right)^{\frac{1}{4}}\left(\frac{A}{\kappa}\right)^{\frac{3}{2}}, \tag{97}$$

while for $\eta\ll1$,

$$J=Be^{-|E_D|/\kappa T}\Upsilon^{\frac{3}{4}}, \tag{98}$$

B being given by Eq. (80). From (96) and (98), it can be seen that J vanishes both at very low and at very high temperatures.

As an example, we take germanium, where $\Omega=306.4$, $|A|=0.125$, $M=1.335\times10^5$, $n_a=2$, $C=2.46\times10^{-3}$, $\alpha=1$, and $|E_D|=2.94\times10^{-3}$. (The above value of $|A|$ was obtained from reference 5.) Expressing J in units of microamperes/cm², T in degrees Kelvin, and Υ in ergs/cm² sec, we have

$$\mathcal{B}=7.10\times10^8,$$
$$Be^{-|E_D|/\kappa T}=78.4\times10^{-(202/T)},$$
$$\eta=1.10(T^{\frac{3}{2}}/f)\times10^{-(7+202/T)}.$$

Condition (87) for germanium is

$$T\gg0.955,$$

while condition (88) is

$$T\gg3.06\times10^{-5}\sqrt{\Upsilon},$$

so that these two conditions are completely satisfied under most experimental conditions. The above values of B and $\mathcal{B}$ indicate that it should be possible to detect the acousto-electric effect in germanium. For example, if $f=10^{-5}$, $T=273$°K, and $\Upsilon=1$ erg/cm² sec (90 db), then $\eta=9.05$, and $J=1.57$ μa/cm². If $f=10^{-5}$, $T=100$°K, and $\Upsilon=1$ erg/cm² sec, then $\eta=0.105$, and $J=0.75$ μa/cm².

The writer is indebted to Professors J. C. Slater, J. Bardeen, and H. Brooks and to Dr. E. P. Gross for discussion and correspondence.

APPENDIX

In order to prove Eq. (24), we start with the definition of the expectation value of energy,

$$E(\mathbf{k})=2i\int_\infty\psi^*\frac{\partial}{\partial t}\psi d\tau\bigg/\int_\infty\psi^*\psi d\tau. \tag{1a}$$

Making use of Eq. (22), we get

$$E(\mathbf{k})=2i\frac{\sum_{n,n'}\Psi^*(\mathbf{k},\mathbf{r}_{n'},t)(\partial/\partial t)\Psi(\mathbf{k},\mathbf{r}_n,t)\int_\infty a^*(\mathbf{r}-\mathbf{r}_{n'})a(\mathbf{r}-\mathbf{r}_n)d\tau}{\sum_{n,n'}\Psi^*(\mathbf{k},\mathbf{r}_{n'},t)\Psi(\mathbf{k},\mathbf{r}_n,t)\int_\infty a^*(\mathbf{r}-\mathbf{r}_{n'})a(\mathbf{r}-\mathbf{r}_n)d\tau}. \tag{2a}$$

In reference 7, it is shown that

$$\int_\infty a^*(\mathbf{r}-\mathbf{r}_{n'})a(\mathbf{r}-\mathbf{r}_n)d\tau=\delta_{n,n'}, \tag{3a}$$

so that

$$E(\mathbf{k})=2i\frac{\sum_n\Psi^*(\mathbf{k},\mathbf{r}_n,t)(\partial/\partial t)\Psi(\mathbf{k},\mathbf{r}_n,t)}{\sum_n\Psi^*(\mathbf{k},\mathbf{r}_n,t)\Psi(\mathbf{k},\mathbf{r}_n,t)}. \tag{4a}$$

Since the perturbative potential is slowly varying on the atomic scale, Ψ will also be slowly varying, and the crystal sums in (4a) may be replaced by the corresponding integrals, i.e.,

$$E(\mathbf{k})=2i\int_\infty\Psi^*\frac{\partial}{\partial t}\Psi d\tau\bigg/\int_\infty\Psi^*\Psi d\tau. \tag{5a}$$

The proof of Eq. (25) is somewhat more involved. The method to be used is similar to that used by Slater in the appendix of reference 8. The Wannier function may be written

$$a(\mathbf{r}-\mathbf{r}_n)=N^{-1}\sum_{\mathbf{k}'}e^{-i[\mathbf{k}'\cdot\mathbf{r}_n-\frac{1}{2}E_0(\mathbf{k}')t]}\psi_0(\mathbf{k}',\mathbf{r},t), \tag{6a}$$

where N is the number of unit cells in the crystal. The sum is over all the allowed values of $\mathbf{k}$ in the first Brillouin zone of reciprocal space. To check the correctness of (6a), we multiply both sides of the equation by $\exp i[\mathbf{k}\cdot\mathbf{r}_n-\frac{1}{2}E_0(\mathbf{k})t]$ and sum over n. Using the fact that

$$\begin{aligned}\sum_n e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}_n}&=N\quad\text{if}\quad\mathbf{k}=\mathbf{k}'\\&=0\quad\text{if}\quad\mathbf{k}\neq\mathbf{k}',\end{aligned} \tag{7a}$$

we immediately obtain Eqs. (20) and (21). Applying (6a) to (22), we get

$$\psi(\mathbf{k},\mathbf{r},t)=N^{-1}\sum_{n,\mathbf{k}'}e^{-i[\mathbf{k}'\cdot\mathbf{r}_n-\frac{1}{2}E_0(\mathbf{k}')t]}\times\Psi(\mathbf{k},\mathbf{r}_n,t)\psi_0(\mathbf{k}',\mathbf{r},t), \tag{8a}$$

so that the ψ's are expanded in terms of the ψ_0's. The proof of Eq. (25) starts with the definition of the expectation value of velocity,

$$\mathbf{v}(\mathbf{k})=-i\frac{\int_\infty \psi^*(\mathbf{k},\mathbf{r},t)\nabla\psi(\mathbf{k},\mathbf{r},t)d\tau}{\int_\infty \psi^*(\mathbf{k},\mathbf{r},t)\psi(\mathbf{k},\mathbf{r},t)d\tau}. \tag{9a}$$

We will have occasion to use the orthogonality property of the ψ_0's,

$$\int_\infty \psi_0^*(\mathbf{k}',\mathbf{r},t)\psi_0(\mathbf{k},\mathbf{r},t)d\tau=I\delta(\mathbf{k},\mathbf{k}'), \tag{10a}$$

where $\delta(\mathbf{k},\mathbf{k}')$ is the Kronecker delta, and I is some normalization constant independent of $\mathbf{k}$. Another useful property is the fact that

$$-i\int_\infty \psi_0^*(\mathbf{k}',\mathbf{r},t)\nabla\psi_0(\mathbf{k},\mathbf{r},t)d\tau=I\mathbf{v}_0(\mathbf{k})\delta(\mathbf{k},\mathbf{k}'). \tag{11a}$$

(11a) follows from (9a) and (10a) when $\mathbf{k}=\mathbf{k}'$. The fact that the integral vanishes when $\mathbf{k}\neq\mathbf{k}'$ is mathematically equivalent to the well-known fact that optical transitions between two energy levels in the same band are forbidden. If we now substitute (8a) into (9a) and simplify with the help of (10a) and (11a), we obtain

$$\mathbf{v}(\mathbf{k})=\frac{\sum_{n,n',\mathbf{k}'}\Psi^*(\mathbf{k},\mathbf{r}_n,t)\mathbf{v}_0(\mathbf{k}')e^{-i\mathbf{k}'\cdot(\mathbf{r}_{n'}-\mathbf{r}_n)}\Psi(\mathbf{k},\mathbf{r}_{n'},t)}{\sum_{n,n',k'}\Psi^*(\mathbf{k},\mathbf{r}_n,t)e^{-i\mathbf{k}'\cdot(\mathbf{r}_{n'}-\mathbf{r}_n)}\Psi(\mathbf{k},\mathbf{r}_{n'},t)}. \tag{12a}$$

The denominator of the right-hand side of (12a) may be simplified by the relation

$$\delta_{n,n'}=N^{-1}\textstyle\sum_{\mathbf{k}'}e^{-i\mathbf{k}'\cdot(\mathbf{r}_{n'}-\mathbf{r}_n)}. \tag{13a}$$

(13a) may be checked by multiplying both sides of the equation by $\exp[i\mathbf{k}\cdot(\mathbf{r}_{n'}-\mathbf{r}_n)]$ and summing over n'. Using (7a), we obtain the obviously correct relation

$$1=\textstyle\sum_{n'}\delta_{n,n'}e^{i\mathbf{k}\cdot(\mathbf{r}_{n'}-\mathbf{r}_n)}.$$

Since $\mathbf{v}_0(\mathbf{k})$, as a function of $\mathbf{k}$, has the periodicity of the reciprocal lattice, we may expand $\mathbf{v}_0$ as a Fourier series,

$$\mathbf{v}_0(\mathbf{k})=\textstyle\sum_{n'}\mathbf{A}_{n,n'}e^{i\mathbf{k}\cdot(\mathbf{r}_{n'}-\mathbf{r}_n)}, \tag{14a}$$

where

$$\mathbf{A}_{n,n'}=N^{-1}\textstyle\sum_{\mathbf{k}'}\mathbf{v}_0(\mathbf{k}')e^{-i\mathbf{k}'\cdot(\mathbf{r}_{n'}-\mathbf{r}_n)}. \tag{15a}$$

(15a) may be checked by multiplying both sides of the equation by $\exp[i\mathbf{k}\cdot(\mathbf{r}_{n'}-\mathbf{r}_n)]$ and summing over n', whence, with the aid of (7a), Eq. (14a) is obtained. Combining (14a) and (15a), we may write the operator equation

$$\mathbf{v}_0(-i\nabla)=\textstyle\sum_{n',\mathbf{k}'}\mathbf{v}_0(\mathbf{k}')e^{-i\mathbf{k}'\cdot(\mathbf{r}_{n'}-\mathbf{r}_n)}\exp[(\mathbf{r}_{n'}-\mathbf{r}_n)\cdot\nabla]. \tag{16a}$$

We have need of the relation

$$\Psi(\mathbf{k},\mathbf{r}_{n'},t)=\exp[(\mathbf{r}_{n'}-\mathbf{r}_n)\cdot\nabla]\Psi(\mathbf{k},\mathbf{r}_n,t), \tag{17a}$$

which is Taylor's expansion in a vector form. Combining (16a) and (17a) gives

$$N\mathbf{v}_0(-i\nabla)\Psi(\mathbf{k},\mathbf{r}_n,t)=\textstyle\sum_{n',k'}\mathbf{v}_0(\mathbf{k}')e^{-i\mathbf{k}'\cdot(\mathbf{r}_{n'}-\mathbf{r}_n)}\Psi(\mathbf{k},\mathbf{r}_{n'},t). \tag{18a}$$

The numerator of the right-hand side of (12a) may be simplified with the aid of (18a). Substituting (13a) and (18a) into (12a) gives

$$\mathbf{v}(\mathbf{k})=\frac{\sum_n\Psi^*(\mathbf{k},\mathbf{r}_n,t)\mathbf{v}_0(-i\nabla)\Psi(\mathbf{k},\mathbf{r}_n,t)}{\sum_n\Psi^*(\mathbf{k},\mathbf{r}_n,t)\Psi(\mathbf{k},\mathbf{r}_n,t)}. \tag{19a}$$

Since Ψ is slowly varying on the atomic scale, the crystal sums in (19a) may be replaced by the corresponding integrals; i.e.,

$$\mathbf{v}(\mathbf{k})=\int_\infty\Psi^*\mathbf{v}_0(-i\nabla)\Psi d\tau\bigg/\int_\infty\Psi^*\Psi d\tau. \tag{20a}$$