interesting alloy and additional results will be published at a later date.

The extraordinary Hall coefficient has been found to vary by a factor of two and is correlated with the neutron diffraction data for the five Fe-Co samples. The resistivity, on the other hand, has been found to vary by only 15%. Apparently some source of variation other than a simple ρ^2 dependence influences the extraordinary Hall coefficient during the order-disorder transition. The Ni_3Mn samples show roughly the same trend; i.e., the larger values of R_1^* are associated with the greater degree of disorder. The results for samples 2, 3, and 4 do fit a ρ^2 dependence as shown in Fig. 8. For reasons discussed above, a reliable value for R_1^* could not be obtained for the disordered sample. Although R_1^* for Ni_3Mn shows a ρ^2 dependence (as would be expected for a change in impurity scattering due to ordering), too much significance should not be attached to this result in view of the failure of R_1^* for Fe-Co to follow a similar relation.

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Coulomb Interactions in the Uniform-Background Lattice Model*

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The uniform-background lattice model consists of a body-centered-cubic lattice of point charges of like sign embedded in a uniform background charge of the opposite sign. The method used by Fuchs to apply the Ewald sum formula to the case of static shear deformations is extended to apply to spatially periodic deformations. The dispersion relations (frequency as a function of wave number) are presented for propagation vectors in the [100], [110], [111], and [210] directions. Comparison is made with the dispersion relations for the same directions in a Born-von Kármán model of a body-centered cubic lattice in which only central interactions between nearest and next-nearest neighbors are considered. The values of the "Coulomb part" of the macroscopic elastic constants as calculated by Fuchs are used for this model. The problem of treating a model in which the background responds to the displacement of point charges is discussed.

INTRODUCTION

General Comments

THE uniform-background lattice model consists of point charges of like sign in a body-centered cubic (bcc) lattice arrangement embedded in a uniform background charge of the opposite sign. The net charge is zero.

In the study of the physical properties of metals, such as the specific heat or thermal and electrical conductivities, a knowledge of the behavior of elastic and thermal waves is essential. It has become apparent[1] that this behavior depends upon the interaction between the lattice of positively charged ions and the conduction electrons. An early attempt to treat this interaction was made by Staver,[2] who used an extension of the classical Bohm-Pines plasma treatment.[3] More recently Bardeen and Pines[4] have extended this type of approach. The present study of the uniform-background model forms a "first step" toward the quantitative application of the Bardeen and Pines results to a b.c.c. metal.

In much earlier work, Fuchs[5] has shown that simple shear disturbances in the bcc metal sodium do not affect the approximately uniform background of conduction electrons. Fuchs, however, considered only static shear deformations, whereas transverse thermal waves result in quite a different configuration. The work of Fuchs in treating the Coulomb interactions by Ewald sums will be reviewed briefly and the method extended to the case of deformations which are periodic in space.

Kohn[6] has also carried out some calculations of

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[1] J. de Launay, *Solid State Physics*, edited by F. Seitz and D. Turnbull (Academic Press, Inc., New York, 1956), first edition, Vol. II, Chap. 4.

[2] T. Staver, Ph.D. thesis, Princeton University, 1951 (unpublished); D. Bohm and T. Staver, Phys. Rev. 84, 836 (1952).

[3] D. Bohm and D. Pines, Phys. Rev. **85**, 338 (1952).

[4] J. Bardeen and D. Pines, Phys. Rev. **99**, 1140 (1955).

[5] K. Fuchs, Proc. Roy. Soc. (London) **A151**, 585 (1935); **A153**, 622 (1935); **A157**, 444 (1936).

[6] W. Kohn (private communications); see also footnote 19 of reference 4. Professor Kohn's numerical results provided a helpful comparison during the course of the present somewhat more extensive calculations, and the author is grateful to him for making them available.

dispersion relations for the purpose of studying the motion and energy of a b.c.c. lattice of electrons in a positive background (the minimum-energy configuration of a dilute electron plasma).

The secular equations will be obtained for the case in which the uniform background is assumed to remain undisturbed despite displacements of the point charges from their equilibrium positions. Solutions of the secular equation (circular frequency as a function of wave propagation vector) for special directions of the propagation vector will be given.

Some approaches to the treatment of the case when the background does not remain uniform will be discussed. It should be emphasized that useful information concerning the pure transverse modes in a metal like sodium may be obtained from the uniform-background model, but a truly representative model must allow for a response of the background.

Ewald Formula for the Coulomb Potential in a Perfect Lattice

Ewald[7] obtains the following formula for the Coulomb potential $\Psi(\mathbf{r})$ at a point $\mathbf{r}$ in a perfect lattice:

$$\Psi(\mathbf{r})=\frac{4\pi}{\Omega}\sum_{\mathbf{k}}{}'\left[\sum_t e_t \exp(-i\mathbf{k}\cdot\mathbf{x}^t)\frac{\exp(-k^2/4\eta+i\mathbf{k}\cdot\mathbf{r})}{k^2}\right]+\sum_l\sum_t e_t\frac{1-G(\eta^{\frac{1}{2}}R^{ltp})}{R^{ltp}}, \quad (1)$$

where Ω is the volume of a cellular polyhedron, $\mathbf{R}^l$ is a lattice vector, the $\mathbf{x}^t$ specify the basis relative to any $\mathbf{R}^l$, e_t is the charge at $\mathbf{x}^t$ and $\sum e_t=0$, the $\mathbf{k}$ are Fourier vectors, η is an arbitrary parameter, $\mathbf{R}^{ltp}$ is an abbreviation for $\mathbf{r}-\mathbf{R}^l-\mathbf{x}^t$, and $G(x)=(2/\sqrt{\pi})\int_0^x\exp(-z^2)dz$. This formula may be derived[8] by introducing two Gaussian distributions of charge of opposite sign centered at each lattice point. The sum over $\mathbf{k}$ is then the Fourier series for the potential at $\mathbf{r}$ due to all those Gaussian distributions of signs like the e_t. This sum will be referred to in the application to periodic deformations of the uniform-background model as $\Psi_a(\mathbf{r})$. The sum over l is the potential due to the point charges, each surrounded by a Gaussian distribution of charge of the opposite sign. This sum is referred to as $\Psi_b(\mathbf{r})$ in the application made in the next section. The parameter η is then the square of the half-width of each of the Gaussian distributions. The charge density $\rho_{lt}(\mathbf{r})$ due to the Gaussian distribution centered at $\mathbf{R}^l+\mathbf{x}^t$ and with sign like e_t is given by

$$\rho_{lt}(\mathbf{r})=e_t(\eta/\pi)^{\frac{3}{2}}\exp[-\eta(R^{ltp})^2]. \quad (2)$$

Because of the lattice periodicity the Fourier vectors $\mathbf{k}$ needed for the Fourier series are just the reciprocal lattice vectors multiplied by 2π.

The prime on the symbol for the sum over $\mathbf{k}$ denotes the omission of the value $k^2=0$ from the sum. Physically this omission arises from the charge neutrality requirement $\sum_t e_t=0$, since the zeroth Fourier coefficient must then be zero.

Fuchs's Application of the Ewald Formula

At first glance the requirement $\sum e_t=0$ seems to preclude the application to the present model in which the signs of all the point charges are the same. Fuchs, apparently at the suggestion of Bethe,[5] included formally the uniform background in the "basis." In the sum over t in Eq. (1) one value of t refers to this uniform background charge. Thus $\sum e_t=0$ may be satisfied for the proper density of the background charge. When the sum over t is performed, e_t is replaced, in the term where t refers to the background charge, by the constant charge density, and an integration is performed over a cellular polyhedron. As long as the Fourier functions $\exp(i\mathbf{k}\cdot\mathbf{x}^t)$ are orthogonal over the range of integration, this term contributes zero (for $k\neq 0$) in the Fourier series part of Eq. (1). Fuchs has shown it contributes a constant, which can be evaluated, in the direct lattice sum of Eq. (1).

Ewald's formula, Eq. (1), was derived for a perfect lattice with all ions in their equilibrium positions. If the lattice undergoes a static shear, the point charges may be regarded as forming a "new" lattice arrangement, for which, due to the lattice periodicity, the Fourier vectors are merely the vectors reciprocal to the "new" lattice (with the factor of 2π). For small shear, the "new" lattice and Fourier vectors may be expressed in terms of the old ones and the shear angle. The total Coulomb potential energy may be found from the potential, and the second derivative of the energy with respect to the shear angle related to the "Coulomb part" of the shear modulus.[5] By considering shears in different directions, Fuchs obtained expressions for the "Coulomb part" of the macroscopic elastic constant c_{44} and of the difference $c_{11}-c_{12}$. The individual values of c_{11} and c_{12} cannot be found since the method described here does not permit the calculation for a "Coulomb part" of a compressional modulus. Fuchs used empirical values of the latter for his calculations of c_{11} and c_{12}, and thus, did not obtain a value for their "Coulomb parts." His values for the "Coulomb parts" of c_{44} and $c_{11}-c_{12}$ will be obtained from the background model in the limit of infinite wavelength for the space periodicity.

EXTENSION TO PERIODIC DEFORMATIONS WITH THE BACKGROUND REMAINING CONSTANT

Calculation of the Potential $\Psi_a(\mathbf{r})$

Let the "point" charge at $\mathbf{R}^l+\mathbf{x}^t$ be displaced by $\mathbf{u}^{lt}=\mathbf{A}^t\sin(\boldsymbol{\kappa}\cdot\mathbf{R}^{lt})$, where $\mathbf{R}^{lt}=\mathbf{R}^l+\mathbf{x}^t$, and $\mathbf{A}^t$ is zero

[7] P. P. Ewald, Ann. Physik **64**, 253 (1921).

[8] P. P. Ewald, Nachr. Akad. Wiss. Göttingen, Math.-physik Kl. 3, 55 (1938); see also C. Kittel, *Introduction to Solid State Physics* (John Wiley and Sons, Inc., New York, 1953), first edition, Appendix B.

when t refers to the uniform background of charge. Then Eq. (2) becomes

$$\rho_{lt}=e_t(\eta/\pi)^{\frac{3}{2}}\exp[-\eta|\mathbf{r}-\mathbf{R}^{lt}|^2]\times[1+2\eta\mathbf{R}^{ltp}\cdot\mathbf{u}^{lt}-\eta(\mathbf{u}^{lt})^2+2\eta^2(\mathbf{R}^{ltp}\cdot\mathbf{u}^{lt})^2], \quad (3)$$

to second order in A^t. The Fourier-series expansion of the charge density at point $\mathbf{r}$ due to the Gaussian distributions having signs like the e_t can be written

$$\rho(\mathbf{r})=\sum_l\sum_t\rho_{lt}(\mathbf{r})=\sum_{\mathbf{k}}\rho_{\mathbf{k}}\exp(i\mathbf{k}\cdot\mathbf{r}). \quad (4)$$

Poisson's equation then yields the relation

$$\nabla^2\Psi_a(\mathbf{r})=-4\pi\rho(\mathbf{r}). \quad (5)$$

Expanding $\Psi_a(\mathbf{r})$ in a series similar to Eq. (4) with coefficients $b_{\mathbf{k}}$, there results from Eq. (5) the connection

$$b_{\mathbf{k}}=4\pi\rho_{\mathbf{k}}/k^2 \quad (6)$$

between the two sets of coefficients. From Eq. (4) by the usual methods of finding the inverse, and by use of Eq. (3), the coefficients $\rho_{\mathbf{k}}$ can be evaluated from the relation

$$\rho_{\mathbf{k}}=\frac{1}{V}\int\sum_l\sum_t e_t\exp[-i\mathbf{k}\cdot(\mathbf{R}^l+\mathbf{x}^t)]\times\exp[-(\eta R^2+i\mathbf{k}\cdot\mathbf{R})][1+2\eta\mathbf{R}\cdot\mathbf{u}^{lt}-\eta(\mathbf{u}^{lt})^2+2\eta^2(\mathbf{R}\cdot\mathbf{u}^{lt})^2]d^3\mathbf{R}, \quad (7)$$

where V is the entire volume of the lattice being considered, and the integration is over V. Regarding this as the sum of four terms, the values in the last three are zero when t refers to the background charge, since $A^t=0$. The first term is just the expression obtained by Fuchs, so that again the value is zero when t refers to the background charge. For simplicity of notation the rest of the basis (if any), now referring only to the point-charge positions, is absorbed into the $\mathbf{R}^l$ vectors and $\mathbf{u}^{lt}$ is replaced by

$$\mathbf{u}^l=\mathbf{A}\sin(\boldsymbol{\kappa}\cdot\mathbf{R}^l). \quad (8)$$

There results the expression

$$\rho_{\mathbf{k}}=\frac{q}{V}\int\sum_l\left(\frac{\eta}{\pi}\right)^{\frac{3}{2}}\exp(-i\mathbf{k}\cdot\mathbf{R}^l)\exp[-(\eta R^2+i\mathbf{k}\cdot\mathbf{R})]\times[1+2\eta\mathbf{R}\cdot\mathbf{u}^l-\eta(\mathbf{u}^l)^2+2\eta^2(\mathbf{R}\cdot\mathbf{u}^l)^2]d^3\mathbf{R}, \quad k\neq0, \quad (9)$$

where q is the charge on each of the point charges.

The integrations in Eq. (9) are performed in Appendix A, under the assumption that the origin for the integration is far enough from the edge of the crystal that its effect is not felt (i.e., we are not concerned with surface effects). There results the expression

$$\rho_{\mathbf{k}}=(q/V)\sum_l[\exp(-i\mathbf{k}\cdot\mathbf{R}^l)\exp(-k^2/4\eta)]\times[1-i\mathbf{k}\cdot\mathbf{u}^l-\tfrac{1}{2}(\mathbf{k}\cdot\mathbf{u}^l)^2], \quad k\neq0, \quad (10)$$

For the value of $\rho_{\mathbf{k}}$ for $k=0$, the over-all charge-neutrality requirement must be considered. This may be expressed in the form $\int\rho(\mathbf{r})d^3\mathbf{r}=0$, which by Eq. (4) yields

$$\int\sum_{\mathbf{k}}\rho_{\mathbf{k}}\exp(i\mathbf{k}\cdot\mathbf{r})d^3\mathbf{r}=\sum_{\mathbf{k}}\rho_{\mathbf{k}}\int\exp(i\mathbf{k}\cdot\mathbf{r})d^3\mathbf{r}=\rho_0V=0. \quad (11)$$

The expression Eq. (10) is valid for $k\neq0$. Note, however, that all terms for $k=0$ are automatically zero except the first. This first term is just the expression obtained by Fuchs. The $\mathbf{k}$ values for that term are just the reciprocal lattice vectors (multiplied by 2π), $\mathbf{k}^h$. It is only necessary then in Eq. (10) to omit the reciprocal lattice vector corresponding to the origin of the reciprocal lattice in order to have this expression hold for all $\mathbf{k}$. This argument reveals then that a part of the Fourier vectors needed are the reciprocal lattice vectors (excluding the zero vector), which are needed also for the case of all $\mathbf{u}^l=0$. The remainder of the set of Fourier vectors will be identified in evaluating the total energy.

Let W_a be that part of the total Coulomb potential energy due to the potential Ψ_a; then we have

$$W_a=\tfrac{1}{2}q\sum_j\Psi_a(\mathbf{R}^j+\mathbf{u}^j). \quad (12)$$

For use in this equation, $\Psi_a(\mathbf{r})$ is evaluated at $\mathbf{r}=\mathbf{R}^j+\mathbf{u}^j$, using Eqs. (10) and (6). This is done by substituting $\mathbf{R}^j+\mathbf{u}^j$ for $\mathbf{r}$, and subtracting the potential due to the Gaussian distribution centered there. This latter quantity is a constant and will be denoted by d_a. Thus, one obtains

$$\Psi_a(\mathbf{R}^j+\mathbf{u}^j)=(4\pi q/V)\sum_{\mathbf{k}}\sum_l\{[\exp(-i\mathbf{k}\cdot\mathbf{R}^{lj})\times\exp(-k^2/4\eta)]/k^2\}\{1-i\mathbf{k}\cdot(\mathbf{u}^l-\mathbf{u}^j)-\tfrac{1}{2}[\mathbf{k}\cdot(\mathbf{u}^l-\mathbf{u}^j)]^2\}-d_a \quad (13)$$

where $\mathbf{R}^{lj}=\mathbf{R}^l-\mathbf{R}^j$. From the definition in Eq. (12), one obtains

$$W_a=(4\pi q^2/2V)\sum_{\mathbf{k}}\sum_l\sum_j\{[\exp(-i\mathbf{k}\cdot\mathbf{R}^{lj})\times\exp(-k^2/4\eta)]/k^2\}\{1+(\mathbf{k}\cdot\mathbf{u}^l)(\mathbf{k}\cdot\mathbf{u}^j)-\tfrac{1}{2}[(\mathbf{k}\cdot\mathbf{u}^l)^2+(\mathbf{k}\cdot\mathbf{u}^j)^2]\}-\tfrac{1}{2}Nqd_a, \quad (14)$$

where N is the total number of point charges in V. The sums of the terms of first order in $(\mathbf{k}\cdot\mathbf{u}^l)$ and $(\mathbf{k}\cdot\mathbf{u}^j)$ may be shown to be zero.

The lattice will at this point be specifically restricted to the b.c.c. lattice. The lattice vectors $\mathbf{R}^l$ thus have components along the principal axes of the cube (denoted as x, y, z, axes) given by $R_1{}^l=l_1a/2$, $R_2{}^l=l_2a/2$, and $R_3{}^l=l_3a/2$, where a is the cube edge length (about 4.22 A for sodium), and l as a superscript stands for the triad of integers l_1, l_2, l_3 which are either all odd or all even. In subsequent expressions the symbol l will appear not as a superscript, and will denote the square root of the sum of the squares of the three integers l_1, l_2, l_3. The components of the displacement $\mathbf{u}^l$ along the three principal axes will be denoted by u^l, v^l, and w^l,

respectively. The reciprocal lattice vectors $\mathbf{k}^h$ have components $k_1{}^h=h_1(2\pi/a)$, $k_2{}^h=h_2(2\pi/a)$, and $k_3{}^h=h_3(2\pi/a)$, where h and h_i play the same role that l and l_i play for the direct lattice vectors $\mathbf{R}^l$. The h_i are integers which are either all even or one even and two odd, corresponding to face-centered-cubic positions for a cube edge "length" of $4\pi/a$. The symbol $\mathbf{h}$ will be used for the vector whose components are the h_i. Other vectors will have components denoted by the subscripts 1, 2, and 3, also.

The x-component of the force on the jth ion will depend on $-\partial W_a/\partial u^j$. This derivative is found from Eq. (14) to be

$$-\partial W_a/\partial u^j=-(4\pi q^2/2V)\sum_{\mathbf{k}}\sum_l[\exp(-k^2/4\eta)]/k^2 \times[\exp i\mathbf{k}\cdot\mathbf{R}^{lj}+\exp -i\mathbf{k}\cdot\mathbf{R}^{lj}]k_1\mathbf{k}\cdot(\mathbf{u}^l-\mathbf{u}^j). \quad (15)$$

All those terms on the right side of Eq. (15) which depend on l may be expressed by use of Eq. (8) in the form of exponentials involving products of the form $\mathbf{k}\cdot\mathbf{R}^l$ and $(\mathbf{k}\pm\boldsymbol{\kappa})\cdot\mathbf{R}^l$. The sum over l is then performed, where use is made of the relation

$$\sum_l\exp(i\mathbf{k}'\cdot\mathbf{R}^l)=N\delta_{\mathbf{k}',\mathbf{k}^h}, \quad (16)$$

which involves the well-known Kronecker delta symbol. Since $\exp(i\mathbf{k}^h\cdot\mathbf{R}^j)=1$, and since certain terms for $+\mathbf{k}^h$ are the same as others for $-\mathbf{k}^h$, the resulting expression may be written

$$-\partial W_a/\partial u^j=-(4\pi q^2/\Omega)\sum_h\{[\exp-(\mathbf{k}^h+\boldsymbol{\kappa})^2/4\eta]/(\mathbf{k}^h+\boldsymbol{\kappa})^2 \times[(k_1{}^h+\kappa_1)(\mathbf{k}^h+\boldsymbol{\kappa})\cdot\mathbf{A}\sin\boldsymbol{\kappa}\cdot\mathbf{R}^j] -[(\exp-k^{h2}/4\eta)/k^{h2}]k_1{}^h\mathbf{k}^h\cdot\mathbf{A}\sin\boldsymbol{\kappa}\cdot\mathbf{R}^j\}, \quad (17)$$

where $N\Omega=V$.

Equation (16) determines the Fourier vectors $\mathbf{k}$ since it is found that the $\mathbf{k}'$ in that equation are given by $\mathbf{k}$, $(\mathbf{k}+\boldsymbol{\kappa})$, or $(\mathbf{k}-\boldsymbol{\kappa})$, when the sum over l is performed in Eq. (15). These Fourier vectors correspond to the reciprocal lattice points (except the origin) and to two "satellite" points for each reciprocal lattice point at $\pm\boldsymbol{\kappa}$ from the latter. The origin of the reciprocal lattice was excluded by the charge-neutrality requirement, but its "satellites" are not excluded. As will be seen, these latter contribute an effect of special significance to the dispersion relations. To emphasize their particular contributions, the sum over the reciprocal lattice space will be rewritten with the origin's satellite contributions written as a separate term, and the others included in $\sum_h'$, where the prime denotes the omission of $\mathbf{k}^h=0$. In addition certain of the terms vanish because of lattice symmetry; these will not be written. The result then, in component form, can be written

$$-\partial W_a/\partial u^j=-(4\pi q^2/\Omega)\{[S_{11}'-\textstyle\sum_h'(F'(\mathbf{k}^h))(k_1{}^h)^2 +\sum_h'(F'(\mathbf{k}^h+\boldsymbol{\kappa}))(k_1{}^h+\kappa_1)^2]u^j +[S_{12}'+\sum_h'(F'(\mathbf{k}^h+\boldsymbol{\kappa}))(k_1{}^h+\kappa_1)(k_2{}^h+\kappa_2)]v^j +[S_{13}'+\sum_h'(F'(\mathbf{k}^h+\boldsymbol{\kappa}))(k_1{}^h+\kappa_1)(k_3{}^h+\kappa_3)]w^j\}, \quad (18)$$

where $S_{ij}'=[\exp(-\kappa^2/4\eta)](\kappa_i\kappa_j)/\kappa^2$, $F'(\mathbf{x})=[\exp(-x^2/4\eta)]/x^2$. The terms S_{ij}' contain the effect of the satellite points of the origin of reciprocal lattice space. The first of the sums of type $\sum_h'$ in the coefficient of u^j contains the effect of the reciprocal lattice points, and all of the other $\sum_h'$ sums in the equation contain the effect of all the other satellite points.

Calculation of the Potential $\Psi_b(\mathbf{r})$

As indicated in Eq. (1), Ewald finds for the case of all $\mathbf{u}_l=0$, the expression

$$\Psi_b(\mathbf{r})=\sum_l\sum_t e_t[1-G(\eta^{\frac{1}{2}}R^{ltp})]/R^{ltp}. \quad (19)$$

The situation for the present considerations yields a similar expression in which R^{ltp} stands for $|\mathbf{r}-\mathbf{R}^l-\mathbf{x}^t-\mathbf{u}^{lt}|$, instead of $|\mathbf{r}-\mathbf{R}^l-\mathbf{x}^t|$ which was indicated for the case considered by Ewald. The expression Eq. (19) may be derived[8] by adding three potentials at $\mathbf{r}$. These are the sums over l and t of the potentials due to (1) the point charge e_t at the point $\mathbf{R}^l+\mathbf{x}^t+\mathbf{u}^{lt}$, (2) that part of the Gaussian distribution (with sign opposite to e_t) which lies inside a sphere centered at $\mathbf{R}^l+\mathbf{x}^t+\mathbf{u}^{lt}$ and has $\mathbf{r}$ as a point on the surface, and (3) the rest of the Gaussian distribution of charge.

When the value of t refers to the uniform background charge, the $\mathbf{u}^{lt}$ are zero, and the resulting term is identical to the corresponding term treated by Fuchs. The value of this term will be denoted by d_b, and is, of course, independent of $\mathbf{u}^l$. The total potential energy W_b due to the potential Ψ_b is given by

$$W_b=\tfrac{1}{2}q\sum_j\Psi_b(\mathbf{R}^j+\mathbf{u}^j). \quad (20)$$

W_b is evaluated to second order in A, where $\mathbf{R}^j+\mathbf{u}^j$ is substituted for $\mathbf{r}$ in Eq. (19) and in the sum over l the value of $l=j$ is omitted. The expression is

$$W_b=\tfrac{1}{2}q^2\sum_{l,j}\left\{\frac{1-G(\eta^{\frac{1}{2}}R^{lj})}{(R^{lj})^3} \times\left[-\frac{(\mathbf{u}^l-\mathbf{u}^j)^2}{2}+\frac{3}{2(R^{lj})^2}[\mathbf{R}^{lj}\cdot(\mathbf{u}^l-\mathbf{u}^j)]^2\right] +2\left(\frac{\eta}{\pi}\right)^{\frac{1}{2}}\frac{\exp[-\eta(R^{lj})^2]}{(R^{lj})^2}\left[-\frac{(\mathbf{u}^l-\mathbf{u}^j)^2}{2} +\left(\frac{3}{2(R^{lj})^2}+\eta\right)[\mathbf{R}^{lj}\cdot(\mathbf{u}^l-\mathbf{u}^j)]^2\right]\right\}+\tfrac{1}{2}Ned_b. \quad (21)$$

The first-order terms in $(\mathbf{u}^l-\mathbf{u}^j)$ vanish.

The force on the jth ion depends in part on $-\partial W_b/\partial u^j$. This is evaluated from Eq. (21) by use of Eq. (8) and the trigonometric identity

$$\sin(\boldsymbol{\kappa}\cdot\mathbf{R}^l)-\sin(\boldsymbol{\kappa}\cdot\mathbf{R}^j)=\sin(\boldsymbol{\kappa}\cdot\mathbf{R}^{lj})\cos(\boldsymbol{\kappa}\cdot\mathbf{R}^j) -2\sin^2(\tfrac{1}{2}\boldsymbol{\kappa}\cdot\mathbf{R}^{lj})\sin(\boldsymbol{\kappa}\cdot\mathbf{R}^j).$$

The resulting expression for $-\partial W_b/\partial u^j$ may be written

$$-\partial W_b/\partial u^j=-q^2\sum_l{}'\{[G_l'(6R_1{}^{lj}\mathbf{R}^{lj}\cdot\mathbf{u}^j-2u^j)+H_l'(6/(R^{lj})^2+4\eta)(R_1{}^{lj}\mathbf{R}^{lj}\cdot\mathbf{u}^j-2u^j)]\times\sin^2(\tfrac{1}{2}\boldsymbol{\kappa}\cdot\mathbf{R}^{lj})\},\quad(22)$$

where

$$G_l'=[1-G(\eta^{\frac{1}{2}}R^{lj})]/(R^{lj})^3,$$

and

$$H_l'=2(\eta/\pi)^{\frac{1}{2}}\{\exp[-\eta(R^{lj})^2]\}/(R^{lj})^2.$$

Secular Equation

The total Coulomb potential energy is W_a+W_b. The equations of motion of the jth ion have the form $M\ddot{u}^j=-\partial W_a/\partial u^j-\partial W_b/\partial u^j$, where M is the mass associated with each of the point charges. The equations of motion will be written in the matrix form

$$\mathbf{F}_u\mathbf{A}=\lambda^2\mathbf{A},\quad(23)$$

where the subscript u indicates the matrix operator was derived from the uniform background model. The elements of $\mathbf{F}_u$ are given by

$$F_{u,ii}=S_{ii}+\sum_h{}'\{[F(\mathbf{h}+\mathcal{K})](h_i+\mathcal{K}_i)^2-F(\mathbf{h})h_i^2\}+(1/2\pi)\sum_l{}'\{G_l(6l_i^2/l^2-2)+H_l[(3/l^2+a^2\eta/2)l_i^2-1]\}(1-C_1C_2C_3),\quad(24)$$

and

$$F_{u,ij}=S_{ij}+\sum_h{}'\{[F(\mathbf{h}+\mathcal{K})](h_i+\mathcal{K}_i)(h_j+\mathcal{K}_j)\}+(1/2\pi)\sum_l{}'\{[G_l6l_il_j/l^2+H_l(3/l^2+a^2\eta/2)l_il_j]S_iS_jS_m\},\quad(i,j,m\text{ unequal})\quad(25)$$

where

$$\boldsymbol{\kappa}=\mathcal{K}2\pi/a,\quad F(\mathbf{x})=\exp(-\pi^2x^2/a^2\eta)/x^2,$$

$$S_{ij}=F(\mathcal{K})\mathcal{K}_i\mathcal{K}_j,\quad G_l=[1-G(\tfrac{1}{2}\eta^{\frac{1}{2}}al)]/l^3,$$

$$G(x)=(2/\sqrt{\pi})\int_0^x\exp(-z^2)dz,$$

$$H_l=(2\eta^{\frac{1}{2}}a/\sqrt{\pi})\exp(-\tfrac{1}{4}\eta a^2l^2)/l^2,\quad C_i=\cos(\mathcal{K}_il_i\pi),$$

and

$$S_i=\sin(\mathcal{K}_il_i\pi).$$

(Note that the index j on u^j does not enter the expressions.) The $\mathcal{K}$ and $\mathcal{K}_i$ play the same role for $\boldsymbol{\kappa}$ that $\mathbf{h}$ and h_i play for $\mathbf{k}^h$, except that the h_i are all integers.

The dimensionless "frequency" λ used here is related to the actual circular frequency ω by

$$\lambda^2=\omega^2/\omega_M{}^2,\quad\omega_M{}^2=4\pi nq^2/M.\quad(26)$$

The constant $\omega_M{}^2$ is the square of the plasma frequency for particles of charge q, mass M, and numerical density n. For the b.c.c. lattice, $n=N/V=1/\Omega=2/a^3$. The secular equation is readily obtained from Eq. (23), and is a cubic equation in λ^2.

As previously mentioned, Kohn has worked with this type of model in which the point charges were electrons. Bardeen and Pines[4] mention that Kohn obtained a "sum rule" for the three solutions of the secular equation. This rule is that the sum of the three values of λ^2, corresponding to any $\boldsymbol{\kappa}$, is unity. The derivation is given in Appendix B. Another interesting feature, also derived in Appendix B, is that if one plots the three solutions for λ^2 corresponding to any direction of $\boldsymbol{\kappa}$, as a function of the magnitude of the propagation vector, one solution approaches unity and the other two approach zero as κ goes to zero. It is easily seen from the derivation that the satellite points of the origin of reciprocal lattice space are responsible for both these occurrences.

The dispersion curves have been obtained by solving the secular equation for the three values of λ^2 for several values of $\mathcal{K}$ when $\boldsymbol{\kappa}$ is in each of the directions [100], [110], [111], and [210]. The solutions were obtained for two values of η, agreement serving as a check on the numerical calculations. (The last figures shown in each entry of the first column of Tables I, II, III, and IV are the first figures which did not agree exactly for the two values of η.)

It seemed desirable to make some comparison between the uniform background model and the results of the static-strain considerations of Fuchs. This comparison has been made in terms of the dispersion relations. To obtain dispersion relations based upon the claculations of Fuchs, one may consider a Born-von Kármán model in which only nearest and next-nearest neighbors interact, and then only by central forces. There are then two force constants of this model, α_1 and α_2. The secular equation may be derived in terms of these force constants [see, for instance, Eq. (11.5) of reference 1]. By considering only pure shear modes in the directions [100] and [110], one may relate α_1 and α_2 to c_{44} and $c_{11}-c_{12}$ [see Eqs. (11.11) and (11.12) of reference 1]. Thus, the force constants of the Born-von Kármán model are determined by the shear moduli alone. Solutions for longitudinal modes may be determined in terms of α_1 and α_2. Of course, the dispersion relations determined in this manner do not reduce to the elasticity expressions in the limit of long wavelengths, unless the Cauchy relations apply.[1] For the purpose of making comparisons with the uniform background relations, "Coulomb parts" of α_1 and α_2 were determined from Fuchs' "Coulomb parts" of c_{44} and $c_{11}-c_{12}$. The results of the calculations are presented in Tables I, II, III, and IV. The quantity $\Lambda_u{}^2$ is defined by $\Lambda_u{}^2=2\pi\lambda^2$. The corresponding solutions for the Born-von Kármán model are denoted by $\Lambda_B{}^2$. The additional subscripts 1, 2, and 3 arbitrarily identify the three branches. In the directions [100], [110], and [111], branches 1 and 2 are pure transverse, while branch 3 is pure longitudinal. In the direction [210], the branches are mixed longitudinal and transverse, except for cases of elastic isotropy[1] ($c_{11}-c_{12}=2c_{44}$), which does not hold for either model. Kohn's results agreed with those given in Tables I, II, and III.

Some sample plots of the dispersion relations are

TABLE I. Values of Λ for the [100] direction. ($\mathcal{K}_2=\mathcal{K}_3=0$; $\Lambda_1=\Lambda_2$.)

Λ_{u1}	Λ_{B1}	$\mathcal{K}$
0.0000	0.000	0.00
0.1912	0.191	0.10
0.3828	0.377	0.20
0.5735	0.554	0.30
0.7611	0.717	0.40
0.9400	0.862	0.50
1.1041	0.988	0.60
1.2451	1.09	0.70
1.3542	1.16	0.80
1.4234	1.22	0.90
1.4472	1.22	1.00
Λ_{u3}	Λ_{B3}	$\mathcal{K}$
2.50663	0.000	0.00
2.49196	0.210	0.10
2.44740	0.420	0.20
2.37171	0.610	0.30
2.26393	0.777	0.40
2.12512	0.919	0.50
1.96071	1.03	0.60
1.78381	1.11	0.70
1.61704	1.17	0.80
1.49351	1.21	0.90
1.44719	1.22	0.90

given in Figs. 1, 2, 3, and 4. It will be seen from Fig. 2 that the branch which does not approach zero at zero κ exhibits a behavior similar to that of the "optical modes" for lattices with an irreducible basis. If the lattice with irreducible basis is regarded as two interpenetrating simple lattices, optical modes may be described as due to one lattice "moving against" the other. There is always an accompanying "acoustical mode" in which the two lattices "move together." The uniform background model provides an optical-type behavior in which the point charges may be regarded as "moving against" the (fixed) uniform background. Since the latter is fixed, there is no accompanying acoustical behavior. In a pure shear mode, the density of the point charges is not changed, and there is consequently no change in the interaction with the uniform background; hence, the optical-type behavior does not arise. It might then seem surprising that in a nonsymmetry direction, such as [210], only one branch does not have zero frequency for zero κ. However, for the optical-type mode, as the wavelength becomes infinite, the points become fixed in their lattice positions (relative to one another), and the whole lattice moves back and forth through the uniform background parallel

TABLE II. Values of Λ for the [110] direction. ($\mathcal{K}_1=\mathcal{K}_2$, $\mathcal{K}_3=0$.)

Λ_{u1}	Λ_{B1}	$\mathcal{K}$
0.0000	0.000	0.000
0.2665	0.266	0.141
0.5080	0.506	0.282
0.6120	0.609	0.354
0.7012	0.697	0.424
0.8264	0.819	0.566
0.8694	0.862	0.707
Λ_{u2}	Λ_{B2}	$\mathcal{K}$
0.0000	0.000	0.000
0.0975	0.098	0.141
0.1881	0.186	0.282
0.2277	0.223	0.354
0.2624	0.256	0.424
0.3118	0.301	0.566
0.3292	0.316	0.707
Λ_{u3}	Λ_{B3}	$\mathcal{K}$
2.60663	0.000	0.000
2.49050	0.403	0.141
2.44737	0.759	0.282
2.42002	0.919	0.354
2.39215	1.05	0.424
2.34588	1.23	0.566
2.32779	1.30	0.707

TABLE III. Values of Λ for the [111] direction. ($\mathcal{K}_1=\mathcal{K}_2=\mathcal{K}_3$; $\Lambda_1=\Lambda_2$.)

Λ_{u1}	Λ_{B1}	$\mathcal{K}$
0.00000	0.000	0.000
0.2232	0.214	0.173
0.48590	0.420	0.347
0.63678	0.517	0.433
0.79867	0.609	0.520
1.13705	0.777	0.693
1.44718	0.918	0.866
Λ_{u3}	Λ_{B3}	$\mathcal{K}$
2.50663	0.000	0.000
2.48664	0.500	0.173
2.41053	0.892	0.347
2.33921	1.03	0.433
2.23766	1.11	0.520
1.92281	1.11	0.693
1.44718	0.918	0.866

TABLE IV. Values of Λ for the [210] direction. ($\mathcal{K}_1=2\mathcal{K}_2$, $\mathcal{K}_3=0$.)

Λ_{u1}	Λ_{B1}	$\mathcal{K}$
0.00000	0.000	0.000
0.2127	0.212	0.112
0.66461	0.649	0.373
0.77171	0.746	0.447
0.90526	0.862	0.559
0.99998	0.936	0.671
1.03875	0.963	0.745
Λ_{u2}	Λ_{B2}	$\mathcal{K}$
0.000	0.000	0.000
0.14	0.124	0.112
0.468	0.389	0.373
0.555	0.455	0.447
0.682	0.544	0.559
0.797	0.611	0.671
0.863	0.672	0.745
Λ_{u3}	Λ_{B3}	$\mathcal{K}$
2.507	0.000	0.000
2.493	0.294	0.112
2.371	0.889	0.373
2.319	1.015	0.447
2.236	1.157	0.559
2.156	1.227	0.671
2.111	1.247	0.745

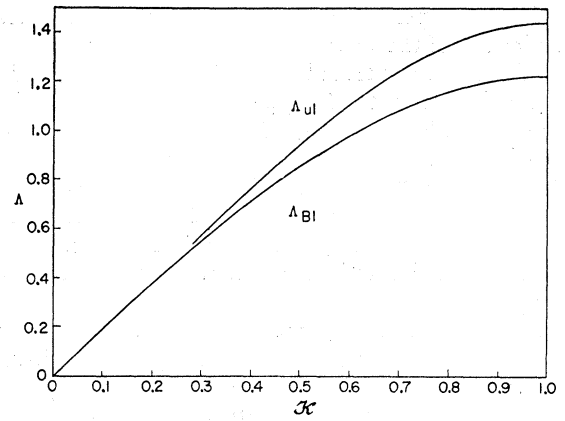

FIG. 1. Dispersion for transverse waves in the [100] direction. This is typical of the results obtained for the acoustical-type modes. Near the origin the two models agree, while the uniform background yields values rising above those for the other model as the zone boundary is approached. In this direction the abscissa has the value unity at the boundary of the first Brillouin zone.

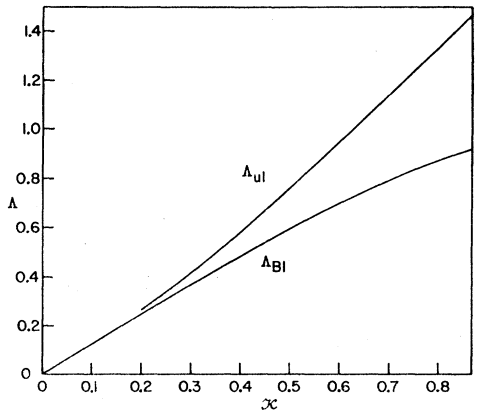

FIG. 3. Dispersion for transverse waves in the [111] direction. The greatest difference in the behavior of acoustical-type modes for the two models occurs in this direction. Notice that even for the Born-von Kármán model the frequency does not reach a relative maximum until well into the second zone. In this direction the abscissa value is $3\frac{1}{2}/2$ at the zone boundary.

to $\boldsymbol{\kappa}$. Since the background is isotropic, the direction of $\boldsymbol{\kappa}$ becomes immaterial.

In a separate calculation, the solutions for the square of the circular frequency were obtained for the uniform background model and expanded to order κ^2, for the pure transverse modes corresponding to $\boldsymbol{\kappa}$ in the [100] direction and in the [110] direction. These expressions were compared to those for the same directions according to the theory of elasticity, in which the coefficients of κ^2 depend upon the combinations of macroscopic elastic constants c_{44} and $c_{11}-c_{12}$. The Ewald sum expressions deduced for these elastic constants are, of course, exactly the same as those obtained by Fuchs.

COMMENTS ON THE CASE OF A RESPONDING BACKGROUND

A model in which the background does not remain uniform but responds to the motion of the point charges should provide a more realistic picture of the behavior of sodium metal. Accordingly in this section the point charges will be considered to be positive ions, and the background charge as due to electrons. As a first step in "freeing" the uniform background, the application of Fermi-Thomas statistics[9] is suggested. The use of Fermi-Thomas statistics yields the Yukawa equation

$$(\nabla^2-K^2)\phi=-4\pi q\rho^+, \tag{27}$$

where

$$K^2=4\pi nq^2\left(\frac{3}{2\zeta_0}\right), \tag{28}$$

ζ_0 is the (maximum) Fermi energy per electron at absolute zero, ρ^+ is the change in the numerical density of point charges, and ϕ is the change of electrostatic potential due to the motion of both ions and electrons.

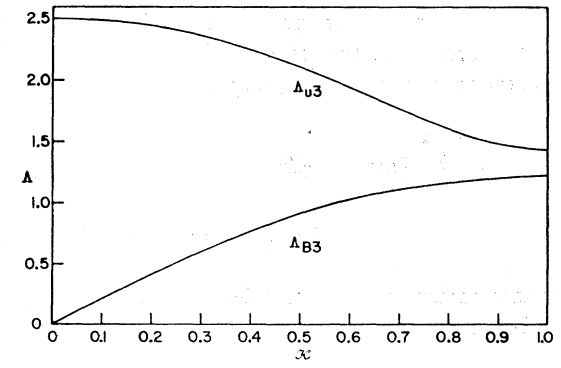

FIG. 2. Dispersion for longitudinal waves in the [100] direction. The optical-type behavior for the uniform background model contrasts with the acoustical-type behavior for the other model. Similar results are obtained for one branch in each of the other three directions for which the calculations were made. In this direction the abscissa has the value unity at the zone boundary.

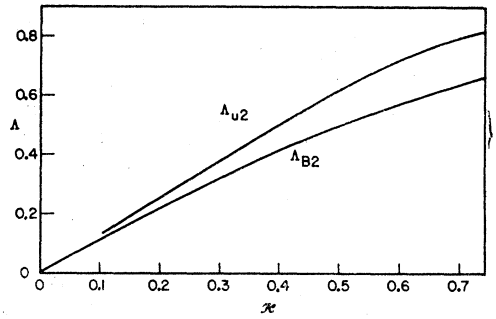

FIG. 4. Dispersion for Branch 1 in the [210] direction. The branches are mixed transverse and longitudinal in this direction. The behavior of Branch 2 was similar to that of Branch 1. Branch 3 exhibited the optical-type mode for the uniform background model. In this direction the abscissa value is $5\frac{1}{2}/3$ at the zone boundary.

[9] N. F. Mott and H. Jones, *The Theory of the Properties of Metals and Alloys* (Oxford University Press, Oxford, 1936), first edition, p. 48. See also reference 4.

The solution to Eq. (27) has the form

$$\phi(\mathbf{r})=q\int[\exp(-K|\mathbf{r}-\mathbf{x}|)/|\mathbf{r}-\mathbf{x}|]\rho^{+}(\mathbf{x})d^{3}\mathbf{x}. \quad (29)$$

By using the Dirac delta function, one may write the change in ion density as

$$\rho^{+}(\mathbf{x})=\sum_{l}[\delta(\mathbf{x}-\mathbf{R}^{l}-\mathbf{u}^{l})-\delta(\mathbf{x}-\mathbf{R}^{l})]. \quad (30)$$

The use of Eq. (30) in Eq. (29) yields to second order in $|\mathbf{u}^{l}|$ the expression

$$\phi(\mathbf{r})=q\sum_{l}\frac{\exp(-K|\mathbf{r}-\mathbf{R}^{l}|)}{(\mathbf{r}-\mathbf{R}^{l})^{2}}\times\left\{[K+|\mathbf{r}-\mathbf{R}^{l}|^{-1}][(\mathbf{r}-\mathbf{R}^{l})\cdot\mathbf{u}^{l}-(\mathbf{u}^{l})^{2}/2]+\left[\frac{3}{2(\mathbf{r}-\mathbf{R}^{l})^{2}}+\frac{3K}{|\mathbf{r}-\mathbf{R}^{l}|}+K^{2}\right]\frac{((\mathbf{r}-\mathbf{R}^{l})\cdot(\mathbf{u}^{l}))^{2}}{(\mathbf{r}-\mathbf{R}^{l})^{2}}\right\}. \quad (31)$$

The quantity K^{-1} is called the screening radius. For sodium on the basis of "free" electron theory, this turns out to be $(1.00)a/2\pi$, to three significant figures. This is an extremely short screening radius.

When the procedure discussed in the previous section was followed, the equations of motion for a representative ion yielded a dispersion relation, from which an expression for the macroscopic elastic constants c_{ij} may be found. In particular the expression for c_{44} was found to be

$$c_{44}=(q^{2}/a^{4})\sum_{l}{}'\{[(\exp(-\tfrac{1}{2}Kal))/l^{3}](3Kal+6+\tfrac{1}{2}K^{2}a^{2}l^{2})(l_{2}^{2}l_{1}^{2}/l^{2})-2(\tfrac{1}{2}Kal+1)l_{1}^{2}\}. \quad (32)$$

A calculation for c_{44} was made for sodium. The above "free-electron" theory value for K was used. The value of a was taken to be 4.22 A, as quoted by Fuchs.[5] The resulting value of the electrostatic part of c_{44} was only 0.155 times the value calculated by Fuchs.[5] Another calculation was made using a screening radius due to Pines[10] rather than the free-electron value. From this calculation the value of the electrostatic part of c_{44} was found to be 0.528 times the value obtained by Fuchs.

These calculations may be taken as one piece of evidence of the failure of the statistical treatment of interionic forces, since the values calculated by Fuchs check well with experiment. As indicated by White,[11] the Fermi-Thomas statistics do not yield a change of electron density which is satisfactory for this purpose. Evidently the most satisfactory results would come from a treatment similar to White's in which the change in electron density is found from the variation in electron wave functions. Such an approach would involve first performing the complicated numerical calculations of the wave functions.

It should be mentioned that White's calculations for the elastic constants of copper[11] yield $c_{11}=13.5\times10^{11}$, $c_{44}=-5.6\times10^{11}$, and $c_{12}=18.7\times10^{11}$, in units of dynes/cm^2. He compares these with the experimental values $c_{11}=17.0\times10^{11}$, $c_{44}=7.5\times10^{11}$, and $c_{12}=12.3\times10^{11}$, in the same units. The values calculated by Fuchs are all in better agreement with the experimental values. In particular Fuchs obtained a positive value for c_{44}.

For any satisfactory theory for treating the responding background, the optical-type mode found from the uniform background model must not appear. It will then be possible, by extending the method by which Fuchs's values for c_{44} and $c_{11}-c_{12}$ were found from the uniform background model, for one to calculate a "Coulomb part" of c_{11}, and hence of c_{12}.

The author wishes to express his gratitude to Dr. R. Ferrell, who suggested the problem and directed the work on it. The contributions to the work from many long conversations with Dr. J. de Launay are gratefully acknowledged.

APPENDIX A

There are four integrals to be evaluated in Eq. (9) for $\rho_{\mathbf{k}}$. In the evaluation $\mathbf{u}^{l}$ will be replaced by $\mathbf{A}\sin(\boldsymbol{\kappa}\cdot\mathbf{R}^{l})$, and certain constants having no effect on the integration will be factored out (these will not be explicitly written in this Appendix). The first of the integrals, then is

$$I_{1}=\int\exp[-(\eta R^{2}+i\mathbf{k}\cdot\mathbf{R})]d^{3}R. \quad (A\text{-}1)$$

Polar coordinates will be chosen with the polar axis along $\mathbf{k}$. The point whose position vector is $\mathbf{R}$, has polar coordinates (R,θ,ϕ).

The integration is over the volume V of the lattice. The assumption will be made that surface effects are not of interest, and the range of R will be taken to be from zero to infinity. Thus I_1 may be written in the form

$$I_{1}=\int_{0}^{\infty}\int_{0}^{\pi}\int_{0}^{2\pi}\{\exp[-(\eta R^{2}+ikR\cos\theta)]\}R^{2}\sin\theta d\phi d\theta dR. \quad (A\text{-}2)$$

The integration over ϕ yields 2π. The integration over θ is also straightforward, resulting in

$$I_{1}=(4\pi/k)\int_{0}^{\infty}[\exp(-\eta R^{2})]\sin kRRdR. \quad (A\text{-}3)$$

[10] D. Pines, *Solid State Physics*, edited by F. Seitz and D. Turnbull (Academic Press, Inc., New York, 1955), first edition, Vol. 1, p. 394.

[11] H. C. White, Ph.D. thesis, Massachusetts Institute of Technology, 1955 (unpublished); Phys. Rev. 98, 1552(A) (1954).

Integration once by parts yields

$$I_1=(2\pi/\eta)\int_0^\infty[\exp(-\eta R^2)]\cos kR dR. \quad \text{(A-4)}$$

This last integral can be evaluated by integration in the complex plane as suggested by Franklin.[12] The result is given by

$$\int^\infty[\exp(-\eta R^2)]\cos kR dR = (\pi/4\eta)^{\frac{1}{2}}\exp(-k^2/4\eta). \quad \text{(A-5)}$$

The value of I_1 can now be found by using Eq. (A-5) in Eq. (A-4).

The second integral in the expression for ρ_k has the form

$$I_2=\int\{\exp[-(\eta R^2+i\mathbf{k}\cdot\mathbf{R})]\}\mathbf{R}\cdot\mathbf{A}d^3R. \quad \text{(A-6)}$$

The point whose position vector is $\mathbf{A}$ has polar coordinates (A, θ_A, ϕ_A). The scalar product $\mathbf{R}\cdot\mathbf{A}$ will be written as $RA\cos\alpha$. It is readily established that $\int_0^{2\pi}\cos\alpha d\phi=2\pi\cos\theta\cos\theta_A$. The integration over θ reduces upon one integration by parts to the same as that encountered in evaluating I_1. Repeated integration by parts reduces the integral over R to the form Eq. (A-5). There results the expression

$$I_2=-i(\pi/\eta)^{\frac{3}{2}}(\mathbf{k}\cdot\mathbf{A}/2\eta)\exp(-k^2/4\eta). \quad \text{(A-7)}$$

The third integral in the expression for ρ_k is of the same form as I_1.

The fourth integral in the expression for ρ_k has the form

$$I_3=\int\{\exp[-(\eta R^2+i\mathbf{k}\cdot\mathbf{R})]\}(\mathbf{R}\cdot\mathbf{A})^2d^3R. \quad \text{(A-8)}$$

The expression $(\mathbf{R}\cdot\mathbf{A})^2$ is written $(RA)^2\cos^2\alpha$. It is found that

$$\int_0^{2\pi}\cos^2\alpha d\phi=2\pi\cos^2\theta_A+\pi\sin^2\theta(1-3\cos^2\theta_A).$$

The use of integration by parts reduces the integral over θ to the same one met in evaluating I_1 and I_2. The resulting expression may be repeatedly integrated by parts until the form Eq. (A-5) is obtained for the integration over R. The expression for I_3 is given by

$$I_3=(1/\eta)(\pi/\eta)^{\frac{3}{2}}[\exp(-k^2/4\eta)][A^2/2-(\mathbf{k}\cdot\mathbf{A})^2/4\eta]. \quad \text{(A-9)}$$

APPENDIX B

The secular equation (a cubic in λ^2) is obtained from the matrix equation Eq. (23). If the coefficient of $(\lambda^2)^3$ is -1, then the coefficient of $(\lambda^2)^2$ is $\sum_i F_{u,ii}$, $i=1, 2, 3$.

[12] P. Franklin, *Methods of Advanced Calculus* (McGraw-Hill Book Company, Inc., New York, 1944), first edition, p. 248.

Let λ_j^2 be the jth root of the secular equation for a value of κ. The secular equation may also be written in the form

$$(\lambda_1^2-\lambda^2)(\lambda_2^2-\lambda^2)(\lambda_3^2-\lambda^2)=0. \quad \text{(B-1)}$$

In this way of expressing the secular equation the coefficient of $(\lambda^2)^2$ is $\sum_j\lambda_j^2$. It is thus established that

$$\sum_j\lambda_j^2=\sum_i F_{u,ii}, \quad \text{(B-2)}$$

where $F_{u,ii}$ is given in Eq. (24). The use of Eq. (24) yields

$$\sum_j\lambda_j^2=\sum_i S_{ii}+\sum_h'\{[F(\mathbf{h}+\mathfrak{K})](\mathbf{h}+\mathfrak{K})^2-[F(\mathbf{h})]h^2\}+(1/2\pi)\sum_l'[4G_l+H_l(a^2\eta l^2/2)]\times(1-C_1C_2C_3). \quad \text{(B-3)}$$

[The symbols in Eq. (B-3) are defined following Eq. (25).] Since the right side of Eq. (B-3) must be independent of η, it will be evaluated in the limit as $\eta\to\infty$. In this limit, $G_l\to 0$ and $H_l\to 0$, so in Eq. (B-3) the entire $\sum_l'\to 0$, also. Since

$$[F(\mathbf{h}+\mathfrak{K})](\mathbf{h}+\mathfrak{K})^2=\exp[-(\mathbf{h}+\mathfrak{K})^2\pi^2/a^2\eta],$$

the $\sum_h'\to 0$ in Eq. (B-3). Thus, Eq. (B-3) becomes

$$\sum_j\lambda_j^2=\lim_{\eta\to\infty}\sum_i S_{ii}=\lim_{\eta\to\infty}\exp(-\mathfrak{K}^2\pi^2/a^2\eta)=1. \quad \text{(B-4)}$$

Equation (B-4) is just the mathematical statement of the sum rule.

It can also be shown that at $\kappa=0$ one of the λ_j^2 is unity and the other two are zero.

From Eq. (B-1) and the secular equation obtained from Eq. (23), in the manner used to find Eq. (B-2), it is found that

$$\sum_{i>j}\lambda_i^2\lambda_j^2=\sum_{i>j}(F_{u,ii}F_{u,ij}-F_{u,ij}^2), \quad \text{(B-5)}$$

and

$$\lambda_1^2\lambda_2^2\lambda_3^2=\prod_i F_{u,ii}+2\prod_{i>j}F_{u,ij}-\sum_{i>j>m}F_{u,ii}F_{u,jm}. \quad \text{(B-6)}$$

[$F_{u,ij}$ is given in Eq. (25).]

Let $p_i=\kappa_i/\kappa$ be the ith direction cosine of κ. It can then be shown that

$$\lim_{\kappa\to 0}F_{u,ij}=p_ip_j,$$

and

$$\lim_{\kappa\to 0}F_{u,ii}=p_i^2. \quad \text{(B-7)}$$

When Eq. (B-7) is used in Eq. (B-6), it is found that $\lim\lambda_1^2\lambda_2^2\lambda_3^2=0$. Thus, at least one of the λ_i^2 must be zero, say $\lambda_1^2=0$. When this value and Eq. (B-7) are used in Eq. (B-5), it is found that $\lim\lambda_2^2\lambda_3^2=0$, hence either λ_2^2 or λ_3^2 is zero, say $\lambda_2^2=0$. Finally, then, from the sum rule Eq. (B-4), $\lim\lambda_3^2=1$. Note that the result is independent of p_i, and hence of the direction of propagation.