General, Closed-Form Expressions for Acoustic Waves in Cubic Crystals

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The Christoffel elastic equations are solved for long-wavelength elastic waves of arbitrary direction in cubic crystals, and exact explicit closed expressions are obtained for the phase and group velocities and displacement amplitudes. The velocity expressions that hold in the special directions are shown to follow from the general result. The problem of determining the elastic constants from the phase velocities in a general crystallographic direction is discussed with particular reference to Brillouin scattering.

The propagation of plane elastic waves in crystals is governed by a set of three simultaneous homogeneous equations, known as the Christoffel equations, for the components of the displacement amplitude $\vec{u}$:

$$(L_{\alpha\beta}-\rho v^2\delta_{\alpha\beta})u_\beta=0, \tag{1}$$

where $L_{\alpha\beta}$ are the Christoffel stiffness coefficients and ρ is the density of the material. The phase velocity v is determined by the vanishing of the determinant of the coefficients of this equation. Exact explicit closed expressions for v have, in the past, only been available for situations where symmetry conditions allow the secular determinant to be partially or completely factorized. Where factorization has not been possible, as is generally the case in cubic crystals except where the wave vector $\vec{k}$ happens to lie in a mirror plane,[1] investigators have resorted either to numerical procedures[2] or a variety of approximations such as Houston's method,[3] series expansions,[4] and approximations valid near to principal symmetry directions.[5] There has been particularly wide use made of these methods in cubic crystals for the purpose of calculating properties such as Debye specific heats,[6] second-sound velocities,[7] and phonon-focusing effects.[8] The exact velocity expressions which we derive below, while bearing some relation to formulas given by Philip and Viswanathan,[9] are much more compact and should, we believe, greatly facilitate calculations on many aspects of elastic waves in cubic crystals. It is also hoped that the results presented here will stimulate ultrasonics and Brillouin scattering experiments divorced from the special directions.

In the case of cubic symmetry the secular equation for elastic wave propagation takes on the form[2]

$$\begin{vmatrix}(C_{11}-C_{44})n_1^2-\mu & (C_{12}+C_{44})n_1n_2 & (C_{12}+C_{44})n_1n_3\\ (C_{12}+C_{44})n_2n_1 & (C_{11}-C_{44})n_2^2-\mu & (C_{12}+C_{44})n_2n_3\\ (C_{12}+C_{44})n_3n_1 & (C_{12}+C_{44})n_3n_2 & (C_{11}-C_{44})n_3^2-\mu\end{vmatrix}=0, \tag{2}$$

where C_{11}, C_{12}, and C_{44} are the conventional elastic constants, n_1, n_2, and n_3 are the direction cosines of $\vec{k}$, and $\mu=\rho v^2-C_{44}$. Expanding this determinant results in the following cubic equation for μ:

$$\mu^3-(C_{11}-C_{44})\mu^2+[(C_{11}+C_{12})KS]\mu-(C_{11}+2C_{12}+C_{44})K^2Q=0, \tag{3}$$

where $K=C_{11}-C_{12}-2C_{44}$, $S=n_1^2n_2^2+n_2^2n_3^2+n_3^2n_1^2$, and $Q=n_1^2n_2^2n_3^2$. In solving this equation we follow the standard method[10] of carrying out a linear transformation on μ to eliminate the quadratic term, and then expressing the roots in terms of trigonometric functions of the coefficients of the remaining terms. The results are conveniently expressed in terms of a redefined set of "elastic constants" $C_1=C_{11}+2C_{44}$, $C_2=C_{11}-C_{44}$, and $C_3=K/(C_{11}-C_{44})$:

$$\rho v_j^2=\tfrac{1}{3}C_1+\tfrac{2}{3}C_2(1-aS)^{1/2}\cos(\psi+\tfrac{2}{3}\pi j), \tag{4}$$

where $\psi=\frac{1}{3}\arccos[(1-\frac{3}{2}aS+bQ)/(1-aS)^{3/2}]$,

$a=3C_3(2-C_3)$,

$b=\frac{27}{2}C_3^2(3-2C_3)$.

Three velocities are generated as the polarization index j takes on the values 0, 1, and 2. One can visualize these solutions in terms of a geometrical construction consisting of three "phasors" displaced at 120° with respect to each other. This construction provides a vivid demonstration that as long as ψ remains small (or only slightly exceeds 120° or 240° since it is a multivalued function) there is a clear separation between, on the one hand, the quasilongitudinal velocity v_0, and on the other, the slow (v_1) and fast (v_2) quasitransverse velocities. In fact, ψ is confined to less than 30° in all but a few highly anisotropic crystals, notably RbBr, RbI, FeS_2, and KBr for which $\frac{2}{3} < C_3 < 1$. Even in these cases ψ only exceeds 30° when $\vec{k}$ lies in the close vicinity of a $\langle 110\rangle$ direction. In the $\langle 100\rangle$ and $\langle 111\rangle$ directions ψ vanishes whatever the value of C_3. For all known crystals $C_3 < 1$ while $C_3 = 0$ corresponds to elastic isotropy. If C_3 were to be greater than 1 the longitudinal velocity would, in certain directions, be less than one or both of the transverse velocities.

By substituting for ρv_j^2 in Eq. (1) one readily obtains that the components of the displacement amplitude $\vec{u}_j$ are in the proportion

$$u_{jx} : u_{jy} : u_{jz} = \frac{n_1}{T_j - 3n_1^2 C_3} : \frac{n_2}{T_j - 3n_2^2 C_3} : \frac{n_3}{T_j - 3n_3^2 C_3}, \tag{5}$$

$$T_j = 1 + 2(1 - aS)^{1/2} \cos(\psi + \tfrac{2}{3}\pi j).$$

The group velocity $\vec{V}_j$ can be calculated from the tensor elastic constants $C_{\alpha\beta\gamma\delta}$ and the normalized amplitudes $e_{j\alpha}$ by means of the equation[11]

$$V_{j\alpha} = (\rho v_j)^{-1} C_{\alpha\beta\gamma\delta}\, e_{j\beta} e_{j\gamma} n_\delta. \tag{6}$$

In the case of cubic symmetry this formula reduces to the expression given by Miller and Musgrave[2]:

$$V_{j\alpha} = \frac{n_\alpha C_{44}}{\rho v_j} + \frac{e_{j\alpha}^2(\rho v_j^2 - C_{44})}{n_\alpha \rho v_j}. \tag{7}$$

Alternatively one can obtain $\vec{V}_j$ directly from Eq. (4) by differentiating the frequency $\omega_j = kv_j$ with respect to the wave vector:

$$\vec{V}_j = \partial\omega_j/\partial\vec{k}, \quad V_{j\alpha} = \partial\omega_j/\partial k_\alpha, \tag{8}$$

which yields the following expression for the x component of $\vec{V}_j$

$$V_{jx} = n_1[v_j + A_j(1 - 2S - n_1^2) + B_j n_2^2 n_3^2 (1 - 3n_1^2)], \tag{9}$$

where

$$A_j = \frac{C_2 C_3 (2 - C_3)}{\rho v_j} \cdot \left\{ \frac{(bQ - \frac{1}{2}aS)\sin(\psi + \frac{2}{3}\pi j)}{(1 - aS)^2 \sin(3\psi)} - \frac{\cos(\psi + \frac{2}{3}\pi j)}{(1 - aS)^{1/2}} \right\}$$

and

$$B_j = \frac{3 C_2 C_3^2 (3 - 2C_3)}{\rho v_j} \cdot \frac{\sin(\psi + \frac{2}{3}\pi j)}{(1 - aS)\sin(3\psi)}.$$

Corresponding expressions for the y and z components of $\vec{V}_j$ are obtained by cyclic interchange of n_1, n_2, and n_3.

The well-known phase velocity expressions that apply when $\vec{k}$ lies in one of the symmetry planes can be obtained from Eq. (4) by inserting the particular constraints on S and Q that apply in these planes. When $\vec{k}$ lies in the (001) plane at an angle θ to the x axis, $S = \cos^2\theta \sin^2\theta$ and $Q = 0$. It follows from the definition of ψ that

$$\cos 3\psi = 4\cos^3\psi - 3\cos\psi = (1 - \tfrac{3}{2}aS)/(1 - aS)^{3/2}. \tag{10}$$

Equation (10) factorizes as follows:

$$[\cos\psi - \epsilon][\cos(\psi + 2\pi/3) - \epsilon][\cos(\psi + 4\pi/3) - \epsilon] = 0, \tag{11}$$

$$\epsilon = -\tfrac{1}{2}(1 - aS)^{-1/2}.$$

Any one of the roots of Eq. (11) determines the three values of $\cos(\psi + \frac{2}{3}\pi j)$, and hence from Eq. (4) the three velocities. Taking the second root, one obtains

$$\rho v_0^2, \rho v_2^2 = \tfrac{1}{2}\{(C_{11}+C_{44}) \pm [(C_{11}-C_{44}) - 4K(C_{11}+C_{12})\cos^2\theta \sin^2\theta]^{1/2}\},$$
$$\rho v_1^2 = C_{44}. \tag{12}$$

Either of the other two roots of Eq. (11) would lead to the same three values of ρv^2 but in a different order.

The case of $\vec{k}$ lying in the $(0\bar{1}1)$ plane at an angle θ to the x axis follows a similar treatment with

$$\epsilon = (C_{11} - 3C_{12} - 4C_{44} - 3K\cos^2\theta)/4(C_{11}-C_{44})(1-aS)^{1/2},$$

and the three velocities are

$$\rho v_0^2, \rho v_1^2 = \tfrac{1}{4}\{(C_{11}+C_{12}+4C_{44}) + K\cos^2\theta \pm [(C_{11}+C_{12})^2 - K(6C_{11}+14C_{12}+8C_{44})\cos^2\theta + K(9C_{11}+15C_{12}+6C_{44})\cos^4\theta]^{1/2}\},$$
$$\rho v_2^2 = \tfrac{1}{2}\{(C_{11}-C_{12}) - K\cos^2\theta\}. \tag{13}$$

The converse problem of determining, in a systematic way, the elastic constants from a single set of measured velocities in a general direction is an important one particularly with regard to Brillouin scattering in cubic crystals. In the past, experimental investigations have been hampered by the lack of a relatively simple general method for obtaining the elastic constants, and as a result have, with few exceptions,[12] been confined to the special directions. This entails less flexibility in sample preparation and also means that measurements have to be done in at least two directions since one or more of the Brillouin doublets are invariably absent[13] when the scattering vector lies in a special direction. Both of these disadvantages are, in principle, overcome by avoiding the usual geometry and locating the scattering vector in a general direction, preferably far from one of the special directions.

In general one could approach this problem by noting that the coefficients in Eq. (3) are related to the three velocities in a particular direction by

$$(C_{11}-C_{44}) = \mu_0 + \mu_1 + \mu_2, \tag{14}$$

$$(C_{11}+C_{12})KS = \mu_0\mu_1 + \mu_1\mu_2 + \mu_2\mu_0, \tag{15}$$

$$(C_{11}+2C_{12}+C_{44})K^2Q = \mu_0\mu_1\mu_2, \tag{16}$$

$$\mu_j = \rho v_j^2 - C_{44}.$$

The first two equations, which are linear and quadratic, respectively, in the C's, can be used to eliminate two of these elastic constants. Substituting into the third equation leads one to an equation of degree 6 in the third elastic constant. This equation would then have to be solved numerically or otherwise and spurious roots eliminated.

However, it is to be expected that in many cases such as, for instance, where the variation of elastic constants with temperature is being studied,[14] approximate values $C_1^{(0)}, C_2^{(0)}, C_3^{(0)}$ will be known. Here the following iteration procedure for numerically arriving at the actual elastic constants would probably be more convenient.[15] An improved set of values $C_1^{(1)}, C_2^{(1)}, C_3^{(1)}$ is obtained by solving the simultaneous linear equations

$$v_j^{(0)} + \sum_{i=1}^{3}(C_i^{(1)} - C_i^{(0)})\partial v_i^{(0)}/\partial C_i = v_j, \tag{17}$$

where $v_j^{(0)}$ and its derivatives are evaluated from Eq. (4) using the original set of elastic constants and v_j are the three observed velocities. The process is repeated until the desired accuracy is obtained. This latter method can also be tailored to the calculation of the elastic constants from a measurement of the group velocities in an arbitrary direction. In this case there are nine velocity components to match and nine unknowns: three elastic constants and the directions of the three wave vectors. Special care has, of course, to be exercised where the wave surface exhibits cuspidal features.

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Spin Polarons in Two-Dimensional Quantum Crystals of Fermions: Application to ^{3}He in Confined Geometries

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We study the magnetic polarization induced around vacancies in two-dimensional quantum crystals of fermions. A vacancy creates a ferromagnetic spin polaron in an alternate lattice, but does not in a triangular (nonalternate) lattice. The situation of ^{3}He in confined geometries is discussed, in particular with respect to the observed tendency to ferromagnetism.

Two recent papers[1,2] have proposed, independently, that a vacancy in bulk bcc ^{3}He induces a ferromagnetic polarization of the surrounding spins over a volume limited by exchange and entropy. The purpose of this Letter is to extend this study to two-dimensional (2D) systems, in the limit of $J/t \ll 1$, where J is the strength of exchange interactions and t is a characteristic tunneling frequency. It was recently suggested[3] that vacancies could induce ferromagnetism in the registered phase of ^{3}He on Grafoil,[4] or in the incommensurate monolayers of ^{3}He adsorbed on various substrates.[5] Such a mechanism, derived from Nagaoka's theorem,[6] was first proposed[7] for bulk bcc ^{3}He. Our main result is that, while vacancies still favor ferromagnetism in 2D alternative lattices, they favor a magnetic vortex ordering in a triangular lattice, a case of experimental interest.

Case of an alternate lattice.—First, we deal with the case of a simple quadratic lattice, with one fermion localized on each lattice site, and one vacancy which can tunnel to a nearest neighbor with a tunneling frequency t. Throughout this paper we write $t = |\tau|$, where τ is the tunneling matrix element.

In the limit of vanishing exchange interactions, Nagaoka's theorem can be entirely reproduced: The ground state, in the presence of one vacancy, is ferromagnetic (with the same difficulty about the thermodynamic limit). In the same limit, the single-particle density of states can be calculated.[8]

The nth moment of the density of states is given by the number of vacancy paths returning to the origin after n steps, with the condition that the initial spin configuration is restored. In this case, all the odd moments vanish. The density of states is symmetric with respect to the origin, for any spin configuration. In the fully ferromag-

