Partial Derivatives of Eigenfrequencies of a Rectangular Parallelepiped and a Sphere of Elastically Anisotropic Solid

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Analytic expressions of partial derivatives of eigenfrequency with respect to elastic constants, density and size were derived for a rectangular parallelepiped and a sphere of elastically anisotropic solid, in order to provide an accurate inversion method for determining the elastic constants. The formulas were extended for determination of anisotropic dissipation constants from attenuation data of free oscillation of anelastic materials. A numerical example was given for an olivine specimen (orthorhombic) of rectangular parallelepiped.

1. Introduction

Elasticity measurement of Earth's materials is important for studies on constitution and structure of the Earth. Many methods have been devised for determination of elastic constants of the materials, most of which are macroscopically and microscopically anisotropic. The interferometry is excellent in accuracy (McSkimin, 1964), although a rather large specimen or plural ones are needed for measurements at different orientations, in particular, for low symmetry crystals. The Brillouin scattering method is also useful for very small specimens (Weidner and Carleton, 1977; Sawamoto *et al.*, 1984), but small defects in the materials often make the elasticity measurement difficult.

In the past decade, the resonance method was developed for accurate determination of elastic constants of a small specimen and it was applied to a sphere and a cube of isotropic solid (Soga and Anderson, 1967; Demarest, 1971), and also to a rectangular parallelepiped of anisotropic solids with orthorhombic crystal symmetry (Ohno, 1976) and with trigonal crystal symmetry (Ohno *et al.*, 1986). In the resonance method, we measure only the lowermost frequencies on one piece of small specimen, so that the applicability has been widely extended to the materials of geophysical interests. In fact, the rectangular parallelepiped resonance (RPR) method has been used to determine elastic constants of a number of rock-forming minerals of geophysical interest (Goto *et al.*, 1976; Sumino *et al.*, 1976; Sumino and Nishizawa, 1978; Babuska *et al.*, 1978;

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Suzuki *et al.*, 1983; Yamamoto *et al.*, 1987). The resonance method has merits in applicability to specimen with various shapes and sizes in principle, and also in measurements at low temperatures to 80 K (Sumino *et al.*, 1983) and at high temperatures even up to 1,800 K (Goto and Anderson, 1988). The resonant sphere technique (RST) used for elasticity measurement of isotropic material (Soga and Anderson, 1967) may also have potential in geophysics, if its applicability could be extended to anisotropic materials.

The resonance method is an indirect one to determine elastic constants of a specimen through an inversion procedure, and the basic data acquired by measurement are the resonant frequencies of many oscillatory modes. An angular eigenfrequency, ω , is dependent on all elastic constants $\{C_i\}$, mass M and shape of the specimen

$$\omega = \omega(C_i, M, s_j), \quad (1)$$

where s_j denotes the parameters specifying the shape and size of the specimen. In the resonance method, we measure resonant frequencies of many eigenmodes and sizes $\{s_j\}$ for a specimen with a mass M , and determine $\{C_i\}$ in order that the observed eigenfrequencies satisfy Eq. (1). This is a typical inversion problem to be solved with the least squares optimization. In the inversion calculation, the observation equations are expressed as

$$\delta\omega = \omega^o - \omega^c = (\partial\omega^c/\partial C_i^{(r)})\{C_i - C_i^{(r)}\} + (\partial\omega^c/\partial s_j^{(r)})\{s_j - s_j^{(r)}\} \quad (2)$$

where ω^o is the observed angular eigenfrequency, ω^c is the computed one by using the elastic constants $\{C_i^{(r)}\}$ and size $\{s_j^{(r)}\}$ at a reference state (r), and $\{C_i\}$ are elastic constants to be determined. The last term in Eq. (2) is a symbolic expression of correction for eigenfrequency due to the small changes of shape and size of the specimen. In Eq. (2), the summation convention is assumed for the repeated indices, hereafter unless stated. In order to determine the $\{C_i\}$ from a set of Eq. (2) for many oscillatory modes, we have to evaluate accurately the partial derivatives, $(\partial\omega^c/\partial C_i^{(r)})$ and $(\partial\omega^c/\partial s_j^{(r)})$, as well as the eigenfrequencies.

In the RPR method, the eigenfrequencies have been computed by the Rayleigh-Ritz method (variational method), in which the displacement eigenfunctions are expanded by the Legendre functions (cf., Demarest, 1971; Ohno, 1976). For computation of eigenfrequencies of an elastically anisotropic sphere by the Rayleigh-Ritz method, on the other hand, free oscillation eigenfunctions of a homogeneous and isotropic sphere are used as basis functions (Mochizuki, 1986, 1988). Thus, the numerical differentiation method is an easy way for evaluating the derivatives of eigenfrequency with respect to elastic constants. In the numerical method, a small change $\Delta\omega$ of eigenfrequency is computed for a small change ΔC_i of each elastic constant, and the derivative of eigenfrequency is numerically calculated by $\Delta\omega/\Delta C_i$. However, such derivatives may contain some errors due to nonlinearity between ω and C_i and computational errors (deficiency of significant figures). Particularly, computation of the derivatives by the numerical differentiation method is not practical for free vibration of anisotropic sphere, because it takes a very long time to compute the eigenfrequencies. Thus, formulas to compute directly the derivatives are desired to be expressed and programmed, so that the partial derivatives are computed as soon as the eigenfrequencies are obtained. Such

formulation has been known in seismology for isotropic or transversely isotropic Earth (Takeuchi and Saito, 1972), but it has not yet been obtained for general anisotropic materials with shape of sphere and rectangular parallelepiped.

The purpose of the present paper is to present theoretical background for computation of the derivatives, $\partial\omega/\partial C_i$ and $\partial\omega/\partial s_j$, for elastically anisotropic solids with general shape, and to obtain analytic expressions of the derivatives for a rectangular parallelepiped and a sphere. These formulas are also applied to description of anisotropic energy dissipation of material. A numerical example is given for an olivine of rectangular parallelepiped in shape.

2. Partial Derivatives of Free Oscillation Eigenfrequency

The free oscillation of an elastic body with volume V is described by a variational equation in the Cartesian coordinates

$$\delta \int L dV = 0, \quad (3)$$

where the L is Lagrangian defined by

$$L = \rho\omega^2 U_i^* U_i - \varepsilon_{ij}^* C_{ijkl} \varepsilon_{kl}. \quad (4)$$

The asterisk above denotes the complex conjugate, and C_{ijkl} is the fourth-order elastic tensor. The ε_{ij} is the strain tensor defined by $(U_{i,j} + U_{j,i})/2$, where $U_{i,j}$ is the spatial derivative of the i -th component U_i of displacement vector U with respect to x_j . The displacement vector U is expressed by a linear combination of known basis function vectors $v^{(p)}$ as follows:

$$U = \sum_{p=1}^N a_p v^{(p)}, \quad (5)$$

where N is the number of basis functions, a_p 's are the unknown constants to be determined, and the summation with respect to the index p or q is always explicitly shown through this paper to avoid confusion with the conventional expression. In order to determine the eigenfrequency ω as well as the unknown constants a_p , we substitute Eq. (5) into Eq. (3) with the aid of Eq. (4), and then obtain

$$\sum_{q=1}^N (\omega^2 \langle p | q \rangle - \langle p | C | q \rangle) a_q = 0, \quad (p = 1, 2, 3, \dots, N) \quad (6)$$

where

$$\langle p | q \rangle = \int v_i^{(p)*} \rho v_i^{(q)} dV \quad (7a)$$

$$\langle p | C | q \rangle = \int \varepsilon_{ij}^{(p)*} C_{ijkl} \varepsilon_{kl}^{(q)} dV \quad (7b)$$

and $\varepsilon_{ij}^{(p)}$ is strain tensor for $v^{(p)}$. When we adopt a condition of constraint for the coefficients a_p 's

$$\sum_{p=1}^N a_p^* a_p = 1, \quad (8)$$

Eq. (6) is an eigenvalue equation, where ω^2 is an eigenvalue and the a_p 's are the components of eigenvector corresponding to the eigenvalue. Once the eigenvalue and eigenvector are determined from Eq. (6), the angular eigenfrequency ω is obtained from the eigenvalue and the displacement vector U is computed by substituting the eigenvector into Eq. (5).

From Eqs. (3) and (5), the energy equation of free oscillation is expressed as

$$\sum_{p=1}^N \sum_{q=1}^N (\omega^2 \langle p | \varrho | q \rangle - \langle p | C | q \rangle) a_p^* a_q = 0. \quad (9)$$

Now let us consider change $\delta\omega$ of ω due to small changes of density and elastic constants, $\delta\varrho$ and δC_{ijkl} . Because the displacement vector U may also change into $U + \delta U$ owing to the $\delta\rho$ and δC_{ijkl}

$$U + \delta U = \sum_{p=1}^N (a_p + \delta a_p) v^{(p)}, \quad (10)$$

the energy Eq. (9) is written as

$$\sum_{p=1}^N \sum_{q=1}^N ((\omega + \delta\omega)^2 \langle p | \varrho + \delta\varrho | q \rangle - \langle p | C + \delta C | q \rangle) (a_p + \delta a_p)^* (a_q + \delta a_q) = 0. \quad (11)$$

When the higher-order terms of $\delta\varrho$, $\delta\omega$, δC_{ijkl} , and δa_p are ignored, the variational equation, i.e. the difference between Eqs. (9) and (11), is approximated as

$$\begin{aligned} & \sum_{p=1}^N \sum_{q=1}^N (\omega^2 \langle p | \varrho | q \rangle - \langle p | C | q \rangle) (a_p^* \delta a_q + a_q \delta a_p^*) \\ & + \sum_{p=1}^N \sum_{q=1}^N (\omega^2 \langle p | \delta\varrho | q \rangle + 2\omega\delta\omega \langle p | \varrho | q \rangle - \langle p | \delta C | q \rangle) a_p^* a_q = 0. \end{aligned} \quad (12)$$

The first summation vanishes on account of Eq. (6), and the variational equation is reduced to

$$\sum_{p=1}^N \sum_{q=1}^N (\omega^2 \langle p | \delta\varrho | q \rangle + 2\omega\delta\omega \langle p | \varrho | q \rangle - \langle p | \delta C | q \rangle) a_p^* a_q = 0, \quad (13)$$

where the first and the last terms, respectively, represent the changes in kinetic and strain energies due to the small changes, $\delta\varrho$ and δC_{ijkl} . For a homogeneous and anisotropic body, the elastic constants and density are independent of coordinates, and they are moved outside the brackets,

$$2\omega\delta\omega\varrho \sum_{p=1}^N \sum_{q=1}^N \langle p|q\rangle a_p^* a_q = -\omega^2\delta\varrho \sum_{p=1}^N \sum_{q=1}^N \langle p|q\rangle a_p^* a_q + \delta C_{ijkl} \sum_{p=1}^N \sum_{q=1}^N \langle p|q\rangle_{ijkl} a_p^* a_q, \quad (14)$$

where

$$\langle p|q\rangle = \int v_i^{(p)*} v_i^{(q)} dV \quad (15a)$$

$$\langle p|q\rangle_{ijkl} = \int \varepsilon_{ij}^{(p)*} \varepsilon_{kl}^{(q)} dV \quad (15b)$$

and the matrix elements, $\langle p|q\rangle_{ijkl}$, satisfy the following relationships

$$\langle q|p\rangle_{klij} = \langle p|q\rangle_{ijkl}^* \quad (16)$$

$$\langle p|q\rangle_{ijkl} = \langle p|q\rangle_{jikl} = \langle p|q\rangle_{ijlk} = \langle p|q\rangle_{jilk}.$$

It is convenient to represent the fourth-order elastic tensor C_{ijkl} by the Voigt notation C_{ij} ($i, j = 1, 2, \dots, 6$) based on the conversion rules: $11 \rightarrow 1, 23 \rightarrow 4$, etc. When using these conventional representations and rearranging Eq. (14) with respect to δC_{ij} ($1 \leq i \leq j \leq 6$) with the aid of symmetric relation $C_{ij} = C_{ji}$, the change $\delta\omega$ in eigenfrequency is expressed by

$$\delta\omega = \frac{\sum_{i=1}^6 \sum_{j=i}^6 \delta C_{ij} \sum_{p=1}^N \sum_{q=1}^N \langle p|q\rangle_{ij} a_p^* a_q - \omega^2 \delta\varrho \sum_{p=1}^N \sum_{q=1}^N \langle p|q\rangle a_p^* a_q}{2\omega\varrho \sum_{p=1}^N \sum_{q=1}^N \langle p|q\rangle a_p^* a_q}, \quad (17)$$

where the relationships between $\langle p|q\rangle_{ij}$ and $\langle p|q\rangle_{ijkl}$ are given in Appendix A. Since the $\delta\omega$ is expressed as a linear function of δC_{ij} and $\delta\varrho$, the partial derivatives of the eigenfrequency are easily written as

$$\partial\omega/\partial\varrho = -\omega/(2\varrho) \quad (18a)$$

$$\partial\omega/\partial C_{ij} = A_{ij}/2\omega\varrho \sum_{p=1}^N \sum_{q=1}^N \langle p|q\rangle a_p^* a_q, \quad (18b)$$

where

$$A_{ij} = \sum_{p=1}^N \sum_{q=1}^N \langle p|q\rangle_{ij} a_p^* a_q. \quad (19)$$

The eigenfrequency ω and the eigenvector a_p are determined by solving Eq. (6), and $\langle p|q\rangle$ and $\langle p|q\rangle_{ij}$ are also calculated by Eq. (15) with the aid of Appendix A. Then the partial derivatives can be calculated by Eqs. (18) and (19).

3. Analytic Expression of A_{ij}

In this section, analytic expression of A_{ij} in Eq. (19) is derived for rectangular parallelepiped and sphere of homogeneous and anisotropic materials.

3.1 Rectangular parallelepiped

In order to solve problem on free oscillation of a rectangular parallelepiped specimen with edge lengths $2L_i$ ($i=1, 2, 3$), Demarest (1971) and Ohno (1976) expanded the i -th component U_i of displacement vector in the Cartesian coordinates as follows:

$$U_i = \sum_{p=1}^N a_p^i v^{(p)} \quad (20)$$

with

$$v^{(p)} = P_l(x_1/L_1)P_m(x_2/L_2)P_n(x_3/L_3)/\sqrt{L_1L_2L_3}, \quad (21)$$

where $P_l(x)$ is the normalized Legendre polynomial of the l -th order. Thus the superscript “ p ” of $v^{(p)}$ is specified by a combination of indices (l, m, n). Because of the orthogonality of the basis functions and the condition given by Eq. (8), the denominator in Eq. (18b) is reduced to

$$\sum_{p=1}^N \sum_{q=1}^N \langle p|q \rangle a_p^* a_q = \sum_{i=1}^3 \sum_{p=1}^N (a_p^i)^* (a_p^i) = 1. \quad (22)$$

On the other hand, the change in strain energy due to small change of elastic constants δC_{ij} is written as

$$\sum_{p=1}^N \sum_{q=1}^N \langle p|\delta C|q \rangle a_p^* a_q = \sum_{s=1}^3 \sum_{t=1}^3 \sum_{p=1}^N \sum_{q=1}^N (\Gamma_{pq})^{st} (a_p^s)^* (a_q^t) = \sum_{i=1}^6 \sum_{j=i}^6 \delta C_{ij} A_{ij}, \quad (23)$$

where the matrix elements $(\Gamma_{pq})^{st}$ are given in Appendix B. Substituting the matrix elements into Eq. (23) and rearranging with respect to δC_{ij} , we obtain A_{ij} ($1 \leq i \leq j \leq 6$) as follows

$$\begin{aligned} A_{11} &= \sum_{p=1}^N \sum_{q=1}^N G_1(a_p^1)^* (a_q^1) \\ A_{12} &= \sum_{p=1}^N \sum_{q=1}^N \{G_8(a_p^2)^* (a_q^1) + G_9(a_p^1)^* (a_q^2)\} \\ A_{13} &= \sum_{p=1}^N \sum_{q=1}^N \{G_6(a_p^1)^* (a_q^3) + G_7(a_p^3)^* (a_q^1)\} \\ A_{14} &= \sum_{p=1}^N \sum_{q=1}^N \{G_6(a_p^1)^* (a_q^2) + G_7(a_p^2)^* (a_q^1) + G_8(a_p^3)^* (a_q^1) + G_9(a_p^1)^* (a_q^3)\} \\ A_{15} &= \sum_{p=1}^N \sum_{q=1}^N [G_1\{(a_p^1)^* (a_q^3) + (a_p^3)^* (a_q^1)\} + (G_6 + G_7)(a_p^1)^* (a_q^1)] \end{aligned}$$

$$\begin{aligned}
A_{16} &= \sum_{p=1}^N \sum_{q=1}^N [G_1\{(a_p^1)^*(a_q^2) + (a_p^2)^*(a_q^1)\} + (G_8 + G_9)(a_p^1)^*(a_q^1)] \\
A_{22} &= \sum_{p=1}^N \sum_{q=1}^N G_2(a_p^2)^*(a_q^2) \\
A_{23} &= \sum_{p=1}^N \sum_{q=1}^N \{G_4(a_p^3)^*(a_q^2) + G_5(a_p^2)^*(a_q^3)\} \\
A_{24} &= \sum_{p=1}^N \sum_{q=1}^N [G_2\{(a_p^2)^*(a_q^3) + (a_p^3)^*(a_q^2)\} + (G_4 + G_5)(a_p^2)^*(a_q^2)] \\
A_{25} &= \sum_{p=1}^N \sum_{q=1}^N \{G_4(a_p^1)^*(a_q^2) + G_5(a_p^2)^*(a_q^1) + G_8(a_p^2)^*(a_q^3) + G_9(a_p^3)^*(a_q^2)\} \\
A_{26} &= \sum_{p=1}^N \sum_{q=1}^N [G_2\{(a_p^1)^*(a_q^2) + (a_p^2)^*(a_q^1)\} + (G_8 + G_9)(a_p^2)^*(a_q^2)] \\
A_{33} &= \sum_{p=1}^N \sum_{q=1}^N G_3(a_p^3)^*(a_q^3) \\
A_{34} &= \sum_{p=1}^N \sum_{q=1}^N [G_3\{(a_p^2)^*(a_q^3) + (a_p^3)^*(a_q^2)\} + (G_4 + G_5)(a_p^3)^*(a_q^3)] \\
A_{35} &= \sum_{p=1}^N \sum_{q=1}^N [G_3\{(a_p^1)^*(a_q^3) + (a_p^3)^*(a_q^1)\} + (G_6 + G_7)(a_p^2)^*(a_q^2)] \\
A_{36} &= \sum_{p=1}^N \sum_{q=1}^N \{G_4(a_p^3)^*(a_q^1) + G_5(a_p^1)^*(a_q^3) + G_6(a_p^2)^*(a_q^3) + G_7(a_p^3)^*(a_q^2)\} \\
A_{44} &= \sum_{p=1}^N \sum_{q=1}^N \{G_2(a_p^3)^*(a_q^3) + G_3(a_p^2)^*(a_q^2) + G_4(a_p^2)^*(a_q^3) + G_5(a_p^3)^*(a_q^2)\} \\
A_{45} &= \sum_{p=1}^N \sum_{q=1}^N [G_3\{(a_p^1)^*(a_q^2) + (a_p^2)^*(a_q^1)\} + G_4(a_p^1)^*(a_q^3) + G_5(a_p^3)^*(a_q^1) \\
&\quad + G_6(a_p^3)^*(a_q^2) + G_7(a_p^2)^*(a_q^3) + (G_8 + G_9)(a_p^3)^*(a_q^3)] \\
A_{46} &= \sum_{p=1}^N \sum_{q=1}^N [G_2\{(a_p^3)^*(a_q^1) + (a_p^1)^*(a_q^3)\} + G_4(a_p^2)^*(a_q^1) + G_5(a_p^1)^*(a_q^2) \\
&\quad + (G_6 + G_7)(a_p^2)^*(a_q^2) + G_8(a_p^3)^*(a_q^2) + G_9(a_p^2)^*(a_q^3)] \\
A_{55} &= \sum_{p=1}^N \sum_{q=1}^N \{G_1(a_p^3)^*(a_q^3) + G_3(a_p^1)^*(a_q^1) + G_6(a_p^3)^*(a_q^1) + G_7(a_p^1)^*(a_q^3)\} \\
A_{56} &= \sum_{p=1}^N \sum_{q=1}^N [G_1\{(a_p^2)^*(a_q^3) + (a_p^3)^*(a_q^2)\} + (G_4 + G_5)(a_p^1)^*(a_q^1) + G_6(a_p^2)^*(a_q^1) \\
&\quad + G_7(a_p^1)^*(a_q^2) + G_8(a_p^1)^*(a_q^3) + G_9(a_p^3)^*(a_q^1)]
\end{aligned}$$

$$A_{66} = \sum_{p=1}^N \sum_{q=1}^N \{G_1(a_p^2)^*(a_q^2) + G_2(a_p^1)^*(a_q^1) + G_8(a_p^1)^*(a_q^2) + G_9(a_p^2)^*(a_q^1)\}, \quad (24)$$

where the coefficients G_i ($i=1, 2, \dots, 9$) are given by Ohno (1976).

3.2 Sphere

In order to describe free oscillation of an elastic sphere, it is convenient to use the contravariant canonical components, u^α , $\varepsilon^{\alpha\beta}$, and $K^{\alpha\beta\gamma\delta}$, of displacement vector, strain tensor and fourth-order elastic tensor in spherical coordinates (cf., Phinney and Burridge, 1973)

$$u^\alpha = C_{\alpha i}^+ u_i \quad (25a)$$

$$\varepsilon^{\alpha\beta} = C_{\alpha i}^+ C_{\beta j}^+ \varepsilon_{ij} \quad (25b)$$

$$K^{\alpha\beta\gamma\delta} = C_{\alpha i}^+ C_{\beta j}^+ C_{\gamma k}^+ C_{\delta l}^+ K_{ijkl}, \quad (25c)$$

where the Greek indices take one of indices $(-1, 0, 1)$ (abbreviated to $-, 0, +$), the subscripts i, j, k , and l take one of directional indices $(1, 2, 3)$ corresponding to (θ, ϕ, r) , and $C_{\alpha i}^+$ is the Hermitian conjugate of a unitary matrix

$$C_{i\alpha} = \begin{bmatrix} 1/\sqrt{2} & 0 & -1/\sqrt{2} \\ -i/\sqrt{2} & 0 & -i/\sqrt{2} \\ 0 & 1 & 0 \end{bmatrix}, \quad (26)$$

where $i = \sqrt{-1}$. The elastic tensor K_{ijkl} in spherical coordinates is related to that $C_{i'j'k'l'}$ in Cartesian coordinates by

$$K_{ijkl} = T_{ii'} T_{jj'} T_{kk'} T_{ll'} C_{i'j'k'l'}, \quad (27)$$

where i', j', k' , and l' take one of directional indices $(1, 2, 3)$ corresponding to (x, y, z) and $T_{ii'}$ is an element of the following matrix

$$T_{ii'} = \begin{bmatrix} \cos \theta \cos \phi & \cos \theta \sin \phi & -\sin \theta \\ -\sin \phi & \cos \phi & 0 \\ \sin \theta \cos \phi & \sin \theta \sin \phi & \cos \theta \end{bmatrix}. \quad (28)$$

Using Eqs. (25c) and (27), Mochizuki (1988) expanded the elastic tensor $K^{\alpha\beta\gamma\delta}$ by the generalized spherical harmonics $Y_s^{Mt}(\theta, \phi)$

$$K^{\alpha\beta\gamma\delta} = C_{ijkl} \sum_{s=(0,2,4)} \sum_{t=-s}^s W_{ijkl}^{\alpha\beta\gamma\delta}(s, t) Y_s^{Mt}(\theta, \phi), \quad (29)$$

where $M = \alpha + \beta + \gamma + \delta$ and

$$\begin{aligned}
W_{ijkl}^{\alpha\beta\gamma\delta}(s, t) = & \sum_{\alpha'=-1}^1 \sum_{\beta'=-1}^1 \sum_{\gamma'=-1}^1 \sum_{\delta'=-1}^1 C_{\alpha'i}^+ C_{\beta'j}^+ C_{\gamma'k}^+ C_{\delta'l}^+ (2s+1) \sum_{s_1=(0,2)} \sum_{s_2=(0,2)} \\
& (2s_1+1)(2s_2+1) \begin{pmatrix} s_1 & 1 & 1 \\ -(\alpha+\beta) & \alpha & \beta \end{pmatrix} \begin{pmatrix} s_1 & 1 & 1 \\ -(\alpha'+\beta') & \alpha' & \beta' \end{pmatrix} \begin{pmatrix} s_2 & 1 & 1 \\ -(\gamma+\delta) & \gamma & \delta \end{pmatrix} \\
& \times \begin{pmatrix} s_2 & 1 & 1 \\ -(\gamma'+\delta') & \gamma' & \delta' \end{pmatrix} \begin{pmatrix} s & s_1 & s_2 \\ -(\alpha+\beta+\gamma+\delta) & \alpha+\beta & \gamma+\delta \end{pmatrix} \\
& \times \begin{pmatrix} s & s_1 & s_2 \\ -t & \alpha'+\beta' & \gamma'+\delta' \end{pmatrix} \quad (30)
\end{aligned}$$

where

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix}$$

is Wigner's 3- j symbol (Edmonds, 1960), and its characteristics are shown in Appendix C.

When an elastic sphere with radius $\hat{a}$ vibrates, the energy equation is expressed as

$$\sum_{p=1}^N \sum_{q=1}^N (\rho\omega^2 \hat{a}^2 \langle p|q \rangle - C_{ijkl} \langle p|q \rangle_{ijkl}) a_p^* a_q = 0. \quad (31)$$

When using the contravariant canonical components of displacement vectors, strains and elastic constants, we obtain the matrix elements $\langle p|q \rangle$ and $\langle p|q \rangle_{ijkl}$ as follows

$$\langle p|q \rangle = \sum_{\alpha=-1}^1 \int v^{\alpha(p)*} v^{\alpha(q)} dV \quad (32a)$$

$$\begin{aligned}
\langle p|q \rangle_{ijkl} = & \sum_{\alpha=-1}^1 \sum_{\beta=-1}^1 \sum_{\gamma=-1}^1 \sum_{\delta=-1}^1 \sum_{s=(0,2,4)} \sum_{t=-s}^s W_{ijkl}^{\alpha\beta\gamma\delta}(s, t) \\
& \times \int \varepsilon^{\alpha\beta(p)*} Y_s^{M_t}(\theta, \phi) \varepsilon^{-\gamma-\delta(q)} (-1)^{\gamma+\delta} dV, \quad (32b)
\end{aligned}$$

where the volume integrations should be made on unit sphere.

As the basis functions in the Rayleigh-Ritz method, we adopted the eigenfunctions of free oscillation of a homogeneous and isotropic sphere, e.g., toroidal and spheroidal eigenfunctions, $|T, n, l, m\rangle$ and $|S, n, l, m\rangle$, where n, l , and m denote the radial, angular and azimuthal order numbers, respectively. Thus the superscript " p " of $v^{(p)}$ in Eq. (5) is determined by a combination of (O, n, l, m) , where O denotes S or T for spheroidal or toroidal eigenfunction, respectively. According to Woodhouse (1980), the contravariant canonical components of such eigenfunctions and strain tensor are generally expressed by

$$v^{\alpha(p)} = {}_n A_l^{\alpha}(r) Y_l^{\alpha m}(\theta, \phi) \quad (33)$$

$$\varepsilon^{\alpha\beta(p)} = {}_n B_l^{\alpha\beta}(r) Y_l^{(\alpha+\beta)m}(\theta, \phi), \quad (34)$$

where the summation convention is not applied to the repeated Greek indices and index “ l ,” and

$$\begin{aligned}
 {}_n A_l^0(r) &= {}_n U_l(r) \gamma_l \\
 {}_n A_l^\pm(r) &= \gamma_l \Omega_0^l \{ {}_n V_l(r) \pm i {}_n W_l(r) \} \\
 {}_n B_l^{00}(r) &= {}_n \dot{U}_l(r) \gamma_l \\
 {}_n B_l^{+-}(r) &= -(1/2) {}_n F_l(r) \gamma_l \\
 {}_n B_l^{0\pm}(r) &= (1/2) \gamma_l \Omega_0^l \{ {}_n X_l(r) \pm i {}_n Z_l(r) \} \\
 {}_n B_l^{\pm\pm}(r) &= \gamma_l \Omega_0^l \Omega_2^l \{ {}_n V_l(r) \pm i {}_n W_l(r) \} / r
 \end{aligned} \tag{35}$$

and

$$\begin{aligned}
 {}_n F_l(r) &= \{ 2 {}_n U_l(r) - l(l+1) {}_n V_l(r) \} / r \\
 {}_n X_l(r) &= {}_n \dot{V}_l(r) + \{ {}_n U_l(r) - {}_n V_l(r) \} / r \\
 {}_n Z_l(r) &= {}_n \dot{W}_l(r) - {}_n W_l(r) / r \\
 \gamma_l &= \sqrt{(2l+1)/4\pi} \\
 \Omega_N^l &= \sqrt{(l+N)(l-N+1)/2}.
 \end{aligned} \tag{36}$$

The overdot in Eqs. (35) and (36) denotes differentiation with respect to r , and the ${}_n U_l(r)$, ${}_n V_l(r)$, and ${}_n W_l(r)$ are radial eigenfunctions of free oscillation eigenfunctions of isotropic sphere. In the expressions of ${}_n A_l^\alpha(r)$ and ${}_n B_l^{\alpha\beta}(r)$, the spheroidal and toroidal eigenfunctions are gathered, and the real and imaginary parts of them come from spheroidal and toroidal basis functions, respectively.

Introducing Eq. (33) into Eq. (32a), and using orthogonality of the generalized spherical harmonics (see Appendix C), we have

$$\langle p | q \rangle = \langle O, n, l, m | O', n', l', m' \rangle = I \delta_{pq}, \tag{37}$$

where δ_{pq} is Kronecker's delta, and

$$I = \int [\{ {}_n U_l(r) \}^2 + l(l+1) \{ {}_n V_l(r) \}^2] r^2 dr \tag{38a}$$

for spheroidal eigenfunctions and

$$I = \int l(l+1) \{ {}_n W_l(r) \}^2 r^2 dr \tag{38b}$$

for toroidal eigenfunctions. In the matrix elements $\langle p | q \rangle_{ijkl}$ of strain energy obtained by substitution of Eq. (34) into Eq. (32b), on the other hand, a surface integral of triple products of the generalized spherical harmonics appears. Since this integral is analytically performed (see Appendix C), the matrix element of strain energy is expressed as

$$\begin{aligned}
\langle p|q\rangle_{ijkl} &= \langle O, n, l, m|O', n', l', m'\rangle_{ijkl} = \sum_{\alpha=-1}^1 \sum_{\beta=-1}^1 \sum_{\gamma=-1}^1 \sum_{\delta=-1}^1 \sum_{s=(0,2,4)} W_{ijkl}^{\alpha\beta\gamma\delta}(s, m-m') \\
&\times 4\pi(-1)^m(-1)^M \begin{pmatrix} l & s & l' \\ -m & m-m' & m' \end{pmatrix} \begin{pmatrix} l & s & l' \\ -(\alpha+\beta) & \alpha+\beta+\gamma+\delta & -(\gamma+\delta) \end{pmatrix} \\
&\times \int \{ {}_n B_l^{\alpha\beta}(r) \}^* {}_{n'} B_{l'}^{-\gamma-\delta}(r) r^2 dr. \quad (39)
\end{aligned}$$

The integrations with respect to radius in Eqs. (38) and (39) should be made in the range of $0 \leq r \leq 1$. Once the matrix elements $\langle p|q\rangle$ and $\langle p|q\rangle_{ijkl}$ are evaluated by Eqs. (37) and (39), the A_{ij} is obtained from Eq. (19) through the conversion rule between $\langle p|q\rangle_{ijkl}$ and $\langle p|q\rangle_{ij}$ in Appendix A, and the derivatives of eigenfrequency with respect to C_{ij} are computed by

$$\partial\omega/\partial C_{ij} = A_{ij}/2\omega\hat{a}^2 \sum_{p=1}^N \sum_{q=1}^N \langle p|q\rangle a_p^* a_q. \quad (40)$$

4. Partial Derivatives with Respect to Size of Specimen

The eigenfrequencies depend not only on elastic constants but also on sample size, as seen in Eq. (1). Both sample size and density change with the change of physical condition such as temperature, but mass M of the sample is usually constant. Thus it is convenient to take density as dependent parameter. When the eigenfrequency is considered to be a function of elastic constants, mass, and size, the partial derivatives of eigenfrequency with respect to half edge lengths L_i ($i=1, 2, 3$) of a rectangular parallelepiped are given by

$$(\partial\omega/\partial L_i)_{M,C,L} = (\partial\omega/\partial L_i)_{q,C,L} + (\partial\omega/\partial q)_C (\partial q/\partial L_i)_{M,L}, \quad (41a)$$

where the L and C are symbolic expression of size (except i -th edge length) and elastic constants. For a sphere with radius $\hat{a}$, on the other hand, we have

$$(\partial\omega/\partial \hat{a})_{M,C} = (\partial\omega/\partial \hat{a})_{q,C} + (\partial\omega/\partial q)_C (\partial q/\partial \hat{a})_M. \quad (41b)$$

Since the $(\partial q/\partial L_i)_{M,L}$ and $(\partial q/\partial \hat{a})_M$ are written as

$$(\partial q/\partial L_i)_{M,L} = -q/L_i \quad (42a)$$

$$(\partial q/\partial \hat{a})_M = -3q/\hat{a}, \quad (42b)$$

Eqs. (41a) and (41b) are reduced to

$$(\partial\omega/\partial L_i)_{M,C,L} = (\partial\omega/\partial L_i)_{q,C,L} + (1/2)(\omega/L_i) \quad (43a)$$

$$(\partial\omega/\partial \hat{a})_{M,C} = (\partial\omega/\partial \hat{a})_{q,C} + (3/2)(\omega/\hat{a}). \quad (43b)$$

Thus the derivatives, $(\partial\omega/\partial L_i)_{q,C,L}$ and $(\partial\omega/\partial \hat{a})_{q,C}$, should be evaluated.

4.1 Rectangular parallelepiped

Suppose that a half edge length L_i ($i=1, 2, 3$) of the specimen changes by δL_i ,

keeping density ρ and elastic moduli C_{ij} constant. When the higher-order terms of $\delta L_i/L_i$ are ignored, the changes of coefficients G_i in Eq. (24) due to δL_i are approximated as follows

$$\begin{aligned}\delta G_1 &= -2G_1\delta L_1/L_1, \quad \delta G_2 = -2G_2\delta L_2/L_2, \quad \delta G_3 = -2G_3\delta L_3/L_3 \\ \delta G_4 &= -G_4\{(\delta L_2/L_2) + (\delta L_3/L_3)\}, \quad \delta G_5 = -G_5\{(\delta L_2/L_2) + (\delta L_3/L_3)\} \\ \delta G_6 &= -G_6\{(\delta L_1/L_1) + (\delta L_3/L_3)\}, \quad \delta G_7 = -G_7\{(\delta L_1/L_1) + (\delta L_3/L_3)\} \\ \delta G_8 &= -G_8\{(\delta L_1/L_1) + (\delta L_2/L_2)\}, \quad \delta G_9 = -G_9\{(\delta L_1/L_1) + (\delta L_2/L_2)\}.\end{aligned}\quad (44)$$

Replacing δC_{ij} and G_i in Eq. (23) with C_{ij} and δG_i , respectively, and considering Eq. (22), we have a variation of energy equation

$$2\rho\omega\delta\omega + \sum_{i=1}^3 (\delta L_i/L_i)\Phi_i = 0 \quad (45)$$

where

$$\begin{aligned}\Phi_i &= \sum_{p=1}^N \sum_{q=1}^N \{[p|q]_{11i}(a_p^1)*a_q^1 + [p|q]_{12i}(a_p^1)*a_q^2 + [p|q]_{13i}(a_p^1)*a_q^3 \\ &\quad + [p|q]_{21i}(a_p^2)*a_q^1 + [p|q]_{22i}(a_p^2)*a_q^2 + [p|q]_{23i}(a_p^2)*a_q^3 \\ &\quad + [p|q]_{31i}(a_p^3)*a_q^1 + [p|q]_{32i}(a_p^3)*a_q^2 + [p|q]_{33i}(a_p^3)*a_q^3\}.\end{aligned}\quad (46)$$

The coefficients $[p|q]_{ijk}$ are given in Appendix D. Therefore we simply obtain

$$(\partial\omega/\partial L_i)_{\theta,C,L} = -\Phi_i/(2\rho\omega L_i). \quad (47)$$

Substituting this into Eq. (43a), we have

$$(\partial\omega/\partial L_i)_{M,C,L} = -\Phi_i/(2\rho\omega L_i) + (1/2)(\omega/L_i), \quad (48)$$

where the summation convention is not applied to the repeated index "i."

4.2 Sphere

When the eigenfrequency of an elastic sphere changes from ω to $\omega + \delta\omega$ owing to small change $\delta\hat{a}$ of radius in keeping density and elastic moduli constant, the variation of energy equation expressed by Eq. (31) is reduced to

$$2\rho\omega\hat{a}(\omega\delta\hat{a} + \delta\omega\hat{a}) \sum_{p=1}^N \sum_{q=1}^N \langle p|q \rangle a_p^* a_q = 0 \quad (49)$$

and we easily obtain

$$(\partial\omega/\partial\hat{a})_{\theta,C} = -\omega/\hat{a}. \quad (50)$$

Thus Eq. (43b) for a sphere is expressed as

$$(\partial\omega/\partial\hat{a})_{M,C} = \omega/(2\hat{a}). \quad (51)$$

This is an analytic expression of derivative of eigenfrequency with respect to radius of a sphere.

5. Numerical Example

A numerical example is given for a rectangular parallelepiped olivine, whose elastic constants, density, and edge lengths are listed in Table 1. The derivatives of eigenfrequencies with respect to elastic constants are computed by using the analytic expression, Eq. (18), and they are compared in Table 2 with those calculated by the numerical differentiation method, where the derivatives of eigenfrequency are numerically calculated by using change in eigenfrequency for small change of elastic constants. Small differences are found between the derivatives computed by the analytical and numerical methods. When dependence of eigenfrequency on the elastic constants is represented by quadratic form of elastic moduli, the values of the derivatives computed by numerical and analytical methods have to agree with each other. Thus the small differences between the derivatives may come from the third- or higher-order effect of elastic constants on the eigenfrequencies. Because the derivatives can be obtained as soon as the eigenfrequency is computed, the analytic expression is also useful for iterative inversion to determine elastic constants from observed resonant frequencies.

Elastic constants of the olivine specimen are redetermined by using the derivatives computed analytically, and the determined elastic constants are compared in Table 1 with those obtained by Ohno (1976), who used the derivatives computed by the numerical method for determination of elastic constants. Although slight differences are found between the present and previous values of the elastic constants, they are within the uncertainty of elastic constants. Thus agreement between both elastic constants is good. This suggests that the derivatives of eigenfrequencies are correctly evaluated by the analytical formula.

In elasticity measurements of elastically anisotropic spheres, the analytic expression has been successfully used for rutile, periclase, CaO and olivine spheres (Suzuki *et al.*,

Table 1. List of physical parameters of the specimen, olivine-1.*

Edge length (mm, $l_i = 2L_i$)	$l_1 = 2.745$ $l_2 = 2.832$ $l_3 = 2.015$
Density (g/cm ³)	$\rho = 3.316$
Elastic constants (GPa)	
Ohno, (1976)	Present results
$C_{11} = 324 \pm 3$	$C_{11} = 322.8 \pm 2.3$
$C_{22} = 196 \pm 3$	$C_{22} = 197.0 \pm 1.5$
$C_{33} = 232 \pm 2$	$C_{33} = 232.9 \pm 1.1$
$C_{44} = 63.9 \pm 0.3$	$C_{44} = 63.92 \pm 0.18$
$C_{55} = 77.9 \pm 0.3$	$C_{55} = 77.91 \pm 0.26$
$C_{66} = 78.8 \pm 0.4$	$C_{66} = 79.00 \pm 0.25$
$C_{23} = 68.8 \pm 1.4$	$C_{23} = 70.3 \pm 1.6$
$C_{31} = 71.5 \pm 1.5$	$C_{31} = 71.1 \pm 1.9$
$C_{12} = 71.5 \pm 1.8$	$C_{12} = 71.8 \pm 2.2$

* A natural olivine with approximate composition ($\text{Mg}_{1.8}\text{Fe}_{0.2}\text{SiO}_4$).

Table 2. Comparison of values of the derivatives, $\partial f/\partial C_{ij}$ (kHz/GPa), computed for olivine-1 by analytical and numerical methods.

No.	Mode	$\partial f/\partial C_{11}$	$\partial f/\partial C_{22}$	$\partial f/\partial C_{33}$	$\partial f/\partial C_{23}$	$\partial f/\partial C_{31}$	$\partial f/\partial C_{12}$	$\partial f/\partial C_{44}$	$\partial f/\partial C_{55}$	$\partial f/\partial C_{66}$
1	A _u -1	0.003	0.007	0.010	-0.012	-0.008	0.002	1.274	0.468	2.859
	EV-1	0.01	0.02	0.02	-0.03	-0.01	-0.01	1.30	0.50	2.90
2	B _{1u} -1	0.145	2.063	0.091	-0.828	0.214	-1.055	1.658	0.044	0.003
	EZ-1	0.12	2.11	0.08	-0.89	0.17	-1.04	1.65	0.12	0.11
3	A _u -2	0.027	0.090	0.007	-0.033	0.011	-0.087	3.766	3.104	0.153
	EV-2	0.04	0.10	0.01	-0.05	0.00	-0.10	3.81	3.13	0.18
4	B _{3u} -1	0.056	2.512	0.274	-1.645	0.218	-0.647	0.003	0.012	1.147
	EX-1	0.07	2.57	0.30	-1.76	0.20	-0.74	0.00	0.01	1.07
5	B _{1g} -1	0.025	0.124	0.020	-0.086	-0.022	0.002	0.001	0.000	6.536
	OZ-1	0.03	0.13	0.02	-0.10	-0.04	0.00	0.02	0.04	6.58
6	B _{3g} -1	0.027	0.268	0.018	-0.047	-0.003	-0.148	8.249	0.004	0.007
	OX-1	0.01	0.29	0.02	-0.04	-0.01	-0.14	8.33	-0.01	0.00
7	A _g -1	0.259	3.481	0.348	-2.172	0.569	-1.868	0.000	0.000	0.000
	OD-1	0.24	3.57	0.39	-2.34	0.50	-1.86	0.00	0.00	0.00
8	B _{2g} -1	0.092	1.693	0.113	-0.788	0.160	-0.749	0.764	2.634	0.857
	OY-1	0.10	1.77	0.13	-0.88	0.14	-0.81	0.70	2.72	0.89
9	B _{1u} -2	1.159	0.070	0.123	-0.057	-0.606	-0.058	0.313	2.919	0.027
	EZ-2	1.21	0.06	0.12	-0.08	-0.69	-0.13	0.33	2.94	0.13
10	B _{2u} -1	1.284	0.158	0.248	0.122	-1.090	-0.431	0.056	0.004	3.147
	EY-1	1.34	0.21	0.32	-0.04	-1.23	-0.55	0.06	0.05	3.08
11	B _{2g} -2	0.064	0.087	0.022	-0.007	-0.042	0.066	0.181	7.644	0.095
	OY-2	0.07	0.11	0.03	-0.03	-0.05	0.05	0.20	7.73	0.13
12	A _g -2	1.229	1.905	0.652	-1.251	-0.901	-1.271	0.034	0.002	0.281
	OD-2	1.24	1.88	0.68	-1.26	-0.97	-1.37	0.03	0.00	0.28

In the upper row, the derivative values by the present study and mode name by Mochizuki's nomenclature (1988) are indicated. In the lower row, the derivative values by the numerical differentiation method by Ohno (1976) and mode name by Ohno's nomenclature are indicated. Values of the parameters needed for calculating the derivatives are listed in Table 1.

1992a; Oda *et al.*, 1989; Oda *et al.*, 1992; Suzuki *et al.*, 1992b). Thus, report on results of actual computation for spherical specimens is omitted here.

6. Extension to the Determination of Anisotropic Dissipation Constants

The resonant oscillation of actual Earth's materials is dissipative in energy due to

anelasticity. Because of energy dissipation the oscillation shows not only shift in resonant frequency but also broadening of peak width on spectrum. This dissipation phenomenon has been observed on normal modes of the solid Earth and provides us with an important information in constructing its rheological model. Anelasticity of a single-crystal is not as large as that of the Earth and the shift in eigenfrequencies due to dissipation is negligibly small for attenuating oscillation of the single-crystal, but the accurate measurement of attenuation is useful to clarify the mechanisms of physical dissipation. The anelastic properties of dissipative materials are represented by complex elastic constants, $C_{ij}(1 + iQ_{ij}^{-1})$, where the Q_{ij}^{-1} are intrinsic dissipation constants of the material, and the summation convention is not applied for repeated indices. Responding to the introduction of complex elastic constants, the eigenfrequency is expressed as complex quantity, $\omega(1 + iq/2)$, where the real part is eigenfrequency calculated from real parts of the complex elastic constants and the q denotes dimensionless parameter representing degree of attenuation of oscillation. Because the imaginary part of the complex elastic constants is so small that the small change of $\delta\omega$ and δC_{ij} in Eq. (17) are replaced by $\delta\omega = i\omega q/2$ and $\delta C_{ij} = iC_{ij}Q_{ij}^{-1}$, the vibrational attenuation, q , is expressed by

$$q = \frac{\sum_{i=1}^6 \sum_{j=i}^6 A_{ij} C_{ij} Q_{ij}^{-1}}{Q\omega^2 \sum_{p=1}^N \sum_{q=1}^N \langle p|q \rangle a_p^* a_q}. \quad (52)$$

This means that the q is expressed by a linear combination of Q_{ij}^{-1} .

It was demonstrated that the resonance method is applicable to determination of anisotropic dissipation constants Q_{ij}^{-1} from vibrational attenuation data of many oscillation modes through an inversion calculation (Sumino *et al.*, 1976). In the right-hand side of Eq. (52), the parameters other than Q_{ij}^{-1} are already evaluated in determining the real parts of the complex elastic constants from observed resonant frequencies. When the vibrational attenuation, q , is measured for a number of oscillation modes, the unknown parameters Q_{ij}^{-1} may be determined from the observed attenuation data by the inversion technique similar to that used to determine the elastic constants. This method has successfully applied to determination of anisotropic dissipation constants of CaO and olivine single-crystals (Oda *et al.*, 1991; Suzuki *et al.*, 1992 b).

7. Conclusions

The analytic expression for computation of the partial derivatives of eigenfrequency with respect to elastic constants was derived for the isotropic Earth by Takeuchi and Saito (1972), and the algorithm has been used to determine Earth's structure from seismic data on surface wave dispersions and on eigenperiods of Earth's free oscillation (e.g., Jordan and Anderson, 1974). The present work has extended their study to the free oscillation of a finite anisotropic body for the purpose of accurate determination of elastic constants by resonance method.

The present analytical method gives the following advantages: 1) the partial

derivatives of eigenfrequencies are accurately and quickly computed, in comparison with the numerical differentiation method, and 2) iterative inversion to determine elastic constants from data of eigenfrequencies is possible, because the derivatives are calculated as soon as the eigenfrequencies are obtained.

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APPENDIX A

The relationships between $\langle p | q \rangle_{ijkl}$ and $\langle p | q \rangle_{ij}$ are given as follows:

$$\begin{aligned}
 \langle p | q \rangle_{11} &= \langle p | q \rangle_{1111} & \langle p | q \rangle_{12} &= \langle p | q \rangle_{1122} + \langle p | q \rangle_{2211} \\
 \langle p | q \rangle_{13} &= \langle p | q \rangle_{1133} + \langle p | q \rangle_{3311} & \langle p | q \rangle_{14} &= 2(\langle p | q \rangle_{1132} + \langle p | q \rangle_{3211}) \\
 \langle p | q \rangle_{15} &= 2(\langle p | q \rangle_{1113} + \langle p | q \rangle_{1311}) & \langle p | q \rangle_{16} &= 2(\langle p | q \rangle_{1112} + \langle p | q \rangle_{1211}) \\
 \langle p | q \rangle_{22} &= \langle p | q \rangle_{2222} & \langle p | q \rangle_{23} &= \langle p | q \rangle_{2233} + \langle p | q \rangle_{3322} \\
 \langle p | q \rangle_{24} &= 2(\langle p | q \rangle_{2232} + \langle p | q \rangle_{3222}) & \langle p | q \rangle_{25} &= 2(\langle p | q \rangle_{2213} + \langle p | q \rangle_{1322}) \\
 \langle p | q \rangle_{26} &= 2(\langle p | q \rangle_{2212} + \langle p | q \rangle_{1222}) & \langle p | q \rangle_{33} &= \langle p | q \rangle_{3333} \\
 \langle p | q \rangle_{34} &= 2(\langle p | q \rangle_{3332} + \langle p | q \rangle_{3233}) & \langle p | q \rangle_{35} &= 2(\langle p | q \rangle_{3313} + \langle p | q \rangle_{1333}) \\
 \langle p | q \rangle_{36} &= 2(\langle p | q \rangle_{3312} + \langle p | q \rangle_{1233}) & \langle p | q \rangle_{44} &= 4\langle p | q \rangle_{2323} \\
 \langle p | q \rangle_{45} &= 4(\langle p | q \rangle_{2313} + \langle p | q \rangle_{1323}) & \langle p | q \rangle_{46} &= 4(\langle p | q \rangle_{2312} + \langle p | q \rangle_{1223}) \\
 \langle p | q \rangle_{55} &= 4\langle p | q \rangle_{1313} & \langle p | q \rangle_{56} &= 4(\langle p | q \rangle_{1312} + \langle p | q \rangle_{1213}) \\
 \langle p | q \rangle_{66} &= 4\langle p | q \rangle_{1212}
 \end{aligned}$$

APPENDIX B

$$\begin{aligned}
(\Gamma_{pq})^{11} &= \delta C_{11} G_1 + \delta C_{66} G_2 + \delta C_{55} G_3 + \delta C_{56} G_4 + \delta C_{56} G_5 + \delta C_{15} G_6 + \delta C_{15} G_7 + \delta C_{16} G_8 + \delta C_{16} G_9 \\
(\Gamma_{pq})^{22} &= \delta C_{66} G_1 + \delta C_{22} G_2 + \delta C_{44} G_3 + \delta C_{24} G_4 + \delta C_{24} G_5 + \delta C_{46} G_6 + \delta C_{46} G_7 + \delta C_{26} G_8 + \delta C_{26} G_9 \\
(\Gamma_{pq})^{33} &= \delta C_{55} G_1 + \delta C_{44} G_2 + \delta C_{33} G_3 + \delta C_{34} G_4 + \delta C_{34} G_5 + \delta C_{35} G_6 + \delta C_{35} G_7 + \delta C_{45} G_8 + \delta C_{45} G_9 \\
(\Gamma_{pq})^{23} &= \delta C_{56} G_1 + \delta C_{24} G_2 + \delta C_{34} G_3 + \delta C_{44} G_4 + \delta C_{23} G_5 + \delta C_{36} G_6 + \delta C_{45} G_7 + \delta C_{25} G_8 + \delta C_{46} G_9 \\
(\Gamma_{pq})^{32} &= \delta C_{56} G_1 + \delta C_{24} G_2 + \delta C_{34} G_3 + \delta C_{23} G_4 + \delta C_{44} G_5 + \delta C_{45} G_6 + \delta C_{36} G_7 + \delta C_{46} G_8 + \delta C_{25} G_9 \\
(\Gamma_{pq})^{31} &= \delta C_{15} G_1 + \delta C_{46} G_2 + \delta C_{35} G_3 + \delta C_{36} G_4 + \delta C_{45} G_5 + \delta C_{55} G_6 + \delta C_{13} G_7 + \delta C_{14} G_8 + \delta C_{56} G_9 \\
(\Gamma_{pq})^{13} &= \delta C_{15} G_1 + \delta C_{46} G_2 + \delta C_{35} G_3 + \delta C_{45} G_4 + \delta C_{36} G_5 + \delta C_{13} G_6 + \delta C_{55} G_7 + \delta C_{56} G_8 + \delta C_{14} G_9 \\
(\Gamma_{pq})^{12} &= \delta C_{16} G_1 + \delta C_{26} G_2 + \delta C_{45} G_3 + \delta C_{25} G_4 + \delta C_{46} G_5 + \delta C_{14} G_6 + \delta C_{56} G_7 + \delta C_{66} G_8 + \delta C_{12} G_9 \\
(\Gamma_{pq})^{21} &= \delta C_{16} G_1 + \delta C_{26} G_2 + \delta C_{45} G_3 + \delta C_{46} G_4 + \delta C_{25} G_5 + \delta C_{56} G_6 + \delta C_{14} G_7 + \delta C_{12} G_8 + \delta C_{66} G_9
\end{aligned}$$

APPENDIX C

Orthogonality of the generalized spherical harmonics is expressed by

$$\int (Y_s^{Ml})^* Y_{s'}^{M'l'} d\Omega = \frac{4\pi \delta_{ss'} \delta_{ll'}}{(2s+1)}, \quad (C1)$$

where the integral is made on the surface of unit sphere. The integration of triple product of generalized spherical harmonics is given by

$$\begin{aligned}
\int (Y_s^{Ml})^* Y_{s'}^{(M-M'')l'} Y_{s''}^{M''l''} d\Omega &= 4\pi (-1)^{M+l} \\
&\times \begin{pmatrix} s & s' & s'' \\ -M & M-M'' & M'' \end{pmatrix} \begin{pmatrix} s & s' & s'' \\ -l & l' & l'' \end{pmatrix}, \quad (C2)
\end{aligned}$$

where Wigner's 3-*j* symbol

$$\begin{pmatrix} l_1 & l_2 & l_3 \\ -m_1 & m_2 & m_3 \end{pmatrix}$$

is zero unless the following selection rules are satisfied

$$|m_i| \leq l_i \quad (C3a)$$

$$|l_1 - l_2| \leq l_3 \leq l_1 + l_2 \quad (C3b)$$

$$m_1 = m_2 + m_3 \quad (C3c)$$

APPENDIX D

$$\begin{aligned}
[p|q]_{111} &= 2C_{11}G_1 + C_{15}G_6 + C_{15}G_7 + C_{16}G_8 + C_{16}G_9 \\
[p|q]_{221} &= 2C_{66}G_1 + C_{46}G_6 + C_{46}G_7 + C_{26}G_8 + C_{26}G_9 \\
[p|q]_{331} &= 2C_{55}G_1 + C_{35}G_6 + C_{35}G_7 + C_{54}G_8 + C_{54}G_9 \\
[p|q]_{231} &= 2C_{56}G_1 + C_{36}G_6 + C_{54}G_7 + C_{25}G_8 + C_{46}G_9 \\
[p|q]_{321} &= 2C_{56}G_1 + C_{45}G_6 + C_{36}G_7 + C_{46}G_8 + C_{25}G_9 \\
[p|q]_{311} &= 2C_{15}G_1 + C_{55}G_6 + C_{13}G_7 + C_{14}G_8 + C_{56}G_9 \\
[p|q]_{131} &= 2C_{15}G_1 + C_{13}G_6 + C_{55}G_7 + C_{56}G_8 + C_{14}G_9 \\
[p|q]_{121} &= 2C_{16}G_1 + C_{14}G_6 + C_{56}G_7 + C_{66}G_8 + C_{12}G_9 \\
[p|q]_{211} &= 2C_{16}G_1 + C_{56}G_6 + C_{14}G_7 + C_{12}G_8 + C_{66}G_9
\end{aligned}$$

$$\begin{aligned}
[p|q]_{112} &= 2C_{66}G_2 + C_{56}G_4 + C_{56}G_5 + C_{16}G_8 + C_{16}G_9 \\
[p|q]_{222} &= 2C_{22}G_2 + C_{24}G_4 + C_{24}G_5 + C_{26}G_8 + C_{26}G_9 \\
[p|q]_{332} &= 2C_{44}G_2 + C_{34}G_4 + C_{34}G_5 + C_{45}G_8 + C_{45}G_9 \\
[p|q]_{232} &= 2C_{24}G_2 + C_{44}G_4 + C_{23}G_5 + C_{25}G_8 + C_{46}G_9 \\
[p|q]_{322} &= 2C_{24}G_2 + C_{23}G_4 + C_{44}G_5 + C_{46}G_8 + C_{25}G_9 \\
[p|q]_{312} &= 2C_{46}G_2 + C_{36}G_4 + C_{45}G_5 + C_{14}G_8 + C_{56}G_9 \\
[p|q]_{132} &= 2C_{46}G_2 + C_{45}G_4 + C_{36}G_5 + C_{56}G_8 + C_{14}G_9 \\
[p|q]_{122} &= 2C_{26}G_2 + C_{25}G_4 + C_{46}G_5 + C_{66}G_8 + C_{12}G_9 \\
[p|q]_{212} &= 2C_{26}G_2 + C_{46}G_4 + C_{25}G_5 + C_{12}G_8 + C_{66}G_9
\end{aligned}$$

$$\begin{aligned}
[p|q]_{113} &= 2C_{55}G_3 + C_{56}G_4 + C_{56}G_5 + C_{15}G_6 + C_{15}G_7 \\
[p|q]_{223} &= 2C_{44}G_3 + C_{24}G_4 + C_{24}G_5 + C_{46}G_6 + C_{46}G_7 \\
[p|q]_{333} &= 2C_{33}G_3 + C_{34}G_4 + C_{34}G_5 + C_{35}G_6 + C_{35}G_7 \\
[p|q]_{233} &= 2C_{34}G_3 + C_{44}G_4 + C_{23}G_5 + C_{36}G_6 + C_{45}G_7 \\
[p|q]_{323} &= 2C_{34}G_3 + C_{23}G_4 + C_{44}G_5 + C_{45}G_6 + C_{36}G_7 \\
[p|q]_{313} &= 2C_{35}G_3 + C_{36}G_4 + C_{45}G_5 + C_{55}G_6 + C_{13}G_7 \\
[p|q]_{133} &= 2C_{35}G_3 + C_{45}G_4 + C_{36}G_5 + C_{13}G_6 + C_{55}G_7 \\
[p|q]_{123} &= 2C_{45}G_3 + C_{25}G_4 + C_{46}G_5 + C_{14}G_6 + C_{56}G_7 \\
[p|q]_{213} &= 2C_{45}G_3 + C_{46}G_4 + C_{25}G_5 + C_{56}G_6 + C_{14}G_7
\end{aligned}$$