Normal mode multiplet coupling on an aspherical, anelastic earth

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Accepted 1992 March 12. Received 1991 November 25

SUMMARY
Calculating the singlet eigenfrequencies and eigenfunctions of a non-rotating, aspherical, anelastic earth model is a computationally intensive procedure, particularly when the number of coupled multiplets incorporated in the basis set is large. Several methods of improving the computational efficiency of this task are developed and tested in this paper. By using a complex-to-real basis transformation and making some justifiable approximations, we reduce the original complex symmetric generalized eigenvalue problem for each target multiplet to a real symmetric ordinary eigenvalue problem. In addition, we improve the accuracy of the subspace projection method by extending the analysis to second order in the eigenfunctions and third order in the eigenfrequencies.

Key words: anelasticity, free oscillations, lateral heterogeneity, normal modes, surface waves, synthetic seismograms.

1 INTRODUCTION
To calculate accurate synthetic long-period seismograms by summation of the earth’s free oscillations, it is necessary to account for the coupling between multiplets \( \{ \ldots, nS_1, nS_0, nS_{-1}, \ldots \} \) or \( \{ \ldots, nT_{-1}, nT_0, nT_{+1}, \ldots \} \) produced by the earth’s anelasticity and lateral heterogeneity. This is commonly done using a Rayleigh–Ritz or Galerkin variational method: the singlet eigenfunctions of the perturbed earth are expressed as linear combinations of the eigenfunctions of an unperturbed spherical elastic earth model, and the expansion coefficients are found together with the singlet eigenfrequencies by solving a generalized matrix eigenvalue problem (Woodhouse 1980; Park & Gilbert 1986). The principal disadvantage of this method is that it is computationally very intensive, particularly when the number of multiplets incorporated in the basis set is large. This paper discusses a number of procedures which can be used to reduce the computational burden.

We begin by illustrating the theoretical and practical advantages of utilizing spherical earth basis eigenfunctions proportional to the real spherical harmonics \( \sqrt{2} X^m_n(\theta) \cos m\phi \), \( X^m_n(\theta) \), \( \sqrt{2} X^m_n(\theta) \sin m\phi \) rather than to the complex harmonics \( Y^m_n(\theta, \phi) = X^m_n(\theta) \exp (im\phi) \). The use of real basis functions reduces the time needed to calculate synthetic seismograms, because it eliminates the need to solve separately for the dual singlet eigenfunctions (Lognonnê & Romanowicz 1990). The complex symmetric generalized eigenvalue problem that must be solved can be reduced to a real symmetric ordinary eigenvalue problem by solving a generalized matrix eigenvalue problem (Woodhouse 1980; Park & Gilbert 1986). The principal disadvantage of this method is that it is computationally very intensive, particularly when the number of multiplets incorporated in the basis set is large. This paper discusses a number of procedures which can be used to reduce the computational burden.

We next discuss an alternative to the direct numerical solution of either the complex symmetric generalized eigenvalue problem or the real symmetric ordinary approximation, namely degenerate perturbation theory with the coupling strength treated as a small parameter. We consider a numerically stable version of this theory, the so-called subspace projection method (Park 1987; Dahlen 1987; Um, Dahlen & Park 1991). The resulting theory, when extended to second order in the eigenfunctions and third order in the eigenfrequencies, is extremely accurate and much less time consuming than brute-force diagonalization.

The principal type of coupling that we consider is that between multiplets of like type along a surface wave dispersion branch \( \{ \ldots, nS_{-1}, nS_0, nS_{+1}, \ldots \} \) or \( \{ \ldots, nT_{-1}, nT_0, nT_{+1}, \ldots \} \). Such along-branch coupling due to lateral velocity and density variations in the earth’s upper mantle is responsible for the observed phase, amplitude and path anomalies of long-period Love and Rayleigh waves (Lay & Kanamori 1985; Woodhouse & Wong 1986; Um, Dahlen & Park 1991). The principal limitation of our analysis is the neglect of rotational coupling between spheroidal and toroidal multiplets \( nS_i \) and \( nT_{i+1} \) (Masters, Park & Gilbert 1983).

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Throughout this paper, we use lower case and upper case bold letters, respectively, to denote real vectors and tensors in ordinary three-dimensional space \( \mathbf{u}, \mathbf{M}, \text{etc.} \). We use lower case and upper case sans serif letters, respectively, to denote \( \infty \)-dimensional vectors and matrices that arise in the variational analysis \( \mathbf{r}, \mathbf{s}, \mathbf{E}, \mathbf{A}, \mathbf{T}, \text{etc.} \).

2 VARIATIONAL METHOD

Let \( \rho, \kappa \) and \( \mu \) be the density, incompressibility and rigidity of the unperturbed spherical elastic earth model. These parameters are perturbed by the earth’s lateral heterogeneity and anelasticity:

\[
\begin{align*}
\rho &\rightarrow \rho + \delta \rho, \\
\kappa &\rightarrow \kappa + i \kappa Q_\kappa^{-1} \text{sgn } \sigma, \\
\mu &\rightarrow \mu + i \mu Q_\mu^{-1} \text{sgn } \sigma,
\end{align*}
\]

where \( \sigma \) is the complex frequency and

\[
\text{sgn } \sigma = \begin{cases} 
1, & \text{if } \Re \sigma > 0; \\
\text{sgn } B, & \text{if } \Re \sigma < 0.
\end{cases}
\]

Anelasticity is accounted for by the dimensionless bulk and shear in situ quality factors \( Q_\kappa \) and \( Q_\mu \); physical dispersion can be justifiably ignored in calculating the singlet eigenfrequencies and eigenfunctions, because the calculations are performed one target multiplet at a time, and the frequency range over which the coupling is significant is quite narrow.

2.1 Eigenfrequencies and eigenfunctions

We denote the degenerate eigenfrequencies and associated basis eigenfunctions of the spherical elastic earth model by \( \omega_k, \mathbf{e}_k \). As noted above, the eigenfunctions are chosen to be real: \( \mathbf{e}_k = \mathbf{e}_k^* \), where an asterisk denotes complex conjugation. In addition, they are assumed to be orthonormal in the sense

\[
\int_V \rho \mathbf{e}_k \cdot \mathbf{e}_{k'} \, dV = \delta_{kk'},
\]

where the integration is over the volume \( V \) of the earth model. We write the perturbed complex eigenfunctions \( \mathbf{u} \) of the aspherical anelastic earth in the form

\[
\mathbf{u} = \sum_k u_k \mathbf{e}_k.
\]

To find the complex eigenfrequencies \( \sigma \) and the associated complex eigenvectors of coefficients

\[
\mathbf{u} = \begin{pmatrix} u_1 \\ \vdots \\ u_m \end{pmatrix},
\]

we must solve the \( \infty \times \infty \) generalized matrix eigenvalue problem

\[
(\Omega^2 + \mathbf{E} + i \mathbf{A} \text{sgn } \sigma) \cdot \mathbf{u} = \sigma^2 (I + \mathbf{T}) \cdot \mathbf{u}.
\]

The quantities \( I, \Omega, \mathbf{E}, \mathbf{A} \) and \( \mathbf{T} \) are, respectively, the identity matrix, the diagonal matrix of degenerate eigenfrequencies, and the elastic, anelastic and kinetic energy perturbation matrices, with elements

\[
I_{kk'} = \delta_{kk'},
\]

\[
\Omega_{kk'} = \omega_k \delta_{kk'},
\]

\[
E_{kk'} = \int_V [\delta \mathbf{k} (\nabla \cdot \mathbf{s}_k)(\nabla \cdot \mathbf{s}_{k'}) + 2 \delta \mu (\mathbf{F}_k : \mathbf{F}_{k'})] \, dV,
\]

\[
+ \int_V \rho [s_k \cdot \nabla \phi_{k'} + s_{k'} \cdot \nabla \phi_k + s_k \cdot \nabla \Phi \cdot s_{k'}] \, dV + \int_V \rho [s_k \cdot \nabla \Phi \cdot s_{k'}] \, dV
\]

\[
+ \frac{1}{2} \int_V [\delta \sigma \nabla \Phi + \rho \nabla \delta \Phi \cdot [s_k \cdot \nabla s_{k'} + s_{k'} \cdot \nabla s_k - s_k (\nabla \cdot s_{k'}) - s_{k'} (\nabla \cdot s_k)] \, dV,
\]

\[
A_{kk'} = \int_V \kappa Q_\kappa^{-1} (\nabla \cdot s_k)(\nabla \cdot s_{k'}) + 2 \mu Q_\mu^{-1} (\mathbf{F}_k : \mathbf{F}_{k'}) \, dV,
\]

\[
T_{kk'} = \int_V \rho (s_k \cdot s_{k'} \cdot s_{k'}) \, dV.
\]
The quantity $\delta \Phi$ is the perturbation in the gravitational potential due to the density perturbation $\delta \rho$, $\phi_k$ is the incremental gravitational potential associated with the displacement $s_k$, and $\Gamma_k = \frac{1}{2}[\nabla s_k + (\nabla s_k)^T] - \frac{1}{2}(\nabla \cdot s_k)I$ is the associated deviatoric strain. The expressions for $E$, $A$ and $T$ must be augmented by additional terms (Woodhouse & Dahlen 1978) if there are perturbations in the locations of any internal or external boundaries in addition to the volumetric perturbations $\delta \rho$, $\delta x + i k Q^{-1} \sigma \delta \Gamma \text{sgn} \sigma$ and $\delta u + i u Q^{-1} \delta \Gamma \text{sgn} \sigma$. The only boundary perturbations considered here are those associated with the earth's hydrostatic ellipticity; the required modifications to $E$ and $T$ are calculated using the formulae of Henson (1989).

The perturbation matrices $E$, $A$ and $T$ are all real and symmetric as a consequence of the reality of the basis eigenfunctions $s_k$:

$$E^T = E, \quad (14)$$
$$A^T = A, \quad (15)$$
$$T^T = T, \quad (16)$$

where $T$ denotes the transpose. It suffices to calculate the eigensolutions with right half-plane ($\Re \sigma > 0$) eigenfrequencies, since $-\sigma^*$, $u^*$ is a solution of (8) if $\sigma$, $u$ is. To find $\sigma$, $u$ we must solve a complex symmetric generalized eigenvalue problem

$$\left(\Omega^2 + V\right) \cdot u = \sigma^2 \left(I + T\right) \cdot u, \quad (17)$$

where $V$ is the total potential energy perturbation matrix

$$V = E + iA. \quad (18)$$

The matrix $V$ is complex symmetric, $V^T = V$, because of the explicit factor of $i$ in (18).

Accidental degeneracies may render the problem (17) defective; in that case it is not possible to represent the response to an earthquake as a sum of normal modes. We ignore that possibility and assume that the eigenfrequencies $\sigma$ are all distinct; in that case, there exists a complex congruent transformation $U$ that simultaneously diagonalizes $\Omega^2 + V$ and $I + T$ (Horn & Johnson 1985):

$$U^T \cdot \left(\Omega^2 + V\right) \cdot U = \Sigma^2, \quad (19)$$
$$U^T \cdot \left(I + T\right) \cdot U = I, \quad (20)$$

where $\Sigma$ is the diagonal matrix of right half-plane eigenfrequencies $\sigma$. Equations (19) and (20) together imply that

$$\Omega^2 + V \cdot U = \left(I + T\right) \cdot U \cdot \Sigma^2, \quad (21)$$

so that $U$ is the matrix whose columns are the associated complex eigenvectors $u$. Equation (20) stipulates that the left half-plane and right half-plane eigenfunctions $u^*$ and $u$ are dual biorthonormal bases in the sense

$$\int_{\nu'} \left(\rho + \delta \rho\right)(u_k \cdot u_k) \, dV = \delta_{kk}. \quad (22)$$

### 2.2 Synthetic seismograms

The $\infty \times \infty$ Green's matrix $G(\sigma)$ in the right half-plane is (Tromp & Dahlen 1990a)

$$G(\sigma) = \left[\Omega^2 + V - \sigma^2 \left(I + T\right)\right]^{-1} = U \cdot (\Sigma^2 - \sigma^2 I)^{-1} \cdot U^T, \quad \Re \sigma > 0. \quad (23)$$

The corresponding time-domain impulse response $G(t)$ is obtained by a straightforward application of Cauchy's theorem, invoking the symmetry $G(-\sigma^*) = G^*(\sigma)$:

$$G(t) = \Re \left[U \cdot \left(\Sigma\right)^{-1} \cdot \exp \left(i \Sigma t\right) \cdot U^T\right]H(t), \quad (24)$$

where $H(t)$ is the Heaviside function. Source–receiver reciprocity is guaranteed by the relation $G^T(t) = G(t)$. The response of an accelerometer polarized in the $i$ direction at $x$, to a step-function moment tensor source $MH(t)$ situated at $x$, is

$$a(t) = r^T \cdot \partial_t G(t) \cdot s, \quad (25)$$

where $r$ and $s$ are the real unperturbed source and receiver vectors:

$$r_k = \hat{v} \cdot e_k(x), \quad (26)$$
$$s_k = M \cdot \nabla e_k(x). \quad (27)$$

This can be rewritten in the form

$$a(t) = \Re \left[r^T \cdot \exp \left(i \Sigma t\right) \cdot s^*\right]H(t), \quad (28)$$
where \( r' \) and \( s' \) are complex transformed source and receiver vectors:

\[
\begin{align*}
    r' &= U^T \cdot r, \\
    s' &= U^T \cdot s.
\end{align*}
\]

2.3 Numerical procedure

To find the matrix \( U \) we first calculate the Cholesky decomposition

\[
I + T = L \cdot L^T,
\]

where \( L \) is real and lower triangular with inverse \( L^{-1} \). The generalized eigenvalue problem (17) can be rewritten as an ordinary eigenvalue problem:

\[
C \cdot w = \sigma^2 w,
\]

where

\[
\begin{align*}
    w &= L^T \cdot u, \\
    C &= L^{-1} \cdot (\Omega^2 + V) \cdot L^{-T}.
\end{align*}
\]

The matrix \( C \) that must be diagonalized is complex symmetric: \( C^T = C \). If \( C \) is diagonalizable (this is guaranteed if there are no accidental degeneracies) then it is complex orthogonally diagonalizable (Horn & Johnson 1985):

\[
\begin{align*}
    W^T \cdot C \cdot W &= \Sigma^2, \\
    W^T \cdot W &= I.
\end{align*}
\]

The complex orthogonal matrix \( W \) is the matrix whose columns are the eigenvectors \( w \); the matrix \( U \) is found by back transformation:

\[
U = L^{-T} \cdot W.
\]

It is noteworthy that it is unnecessary to solve separately for the dual eigenvectors of the complex conjugate matrix \( C^* \). The Green’s matrix (24) and the response to an earthquake (28) can both be calculated only in terms of the matrix \( U \) of eigenvectors \( u \) (Lognonné 1991; Tromp & Dahlen 1990b).

In practice, the \( \infty \times \infty \) matrices \( E, A \) and \( T \) must be truncated to perform numerical calculations. The coupling strengths are roughly comparable on either side of a target multiplet along a dispersion branch \( \{ \ldots, nS_{j-1}, nS_0, nS_{j+1}, \ldots \} \) or \( \{ \ldots, nT_{j-1}, nT_0, nT_{j+1}, \ldots \} \). For this reason, we always incorporate the same number of basis multiplets on either side. Adopting a slightly modified notation in which the index \( k \) is used to label multiplets rather than singlets, we write \( \Sigma, U \) and \( U^T \) in the form

\[
\Sigma = \begin{pmatrix}
    \Sigma_{-1} & \Sigma_{-2} & \cdots & \Sigma_0 & \Sigma_1 & \cdots
\end{pmatrix},
\]

\[
U = \begin{pmatrix}
    U_{-10} & U_{-11} & \cdots & U_{00} & U_{01} & \cdots \\
    U_{-20} & U_{-21} & \cdots & U_{10} & U_{11} & \cdots \\
    \vdots & \vdots & \ddots & \vdots & \vdots & \ddots
\end{pmatrix},
\]

\[
U^T = \begin{pmatrix}
    U_{-10}^T & U_{-11}^T & \cdots & U_{00}^T & U_{01}^T & \cdots \\
    U_{-20}^T & U_{-21}^T & \cdots & U_{10}^T & U_{11}^T & \cdots \\
    \vdots & \vdots & \ddots & \vdots & \vdots & \ddots
\end{pmatrix}.
\]

Each submatrix \( \Sigma_k \) contains the complex perturbed eigenfrequencies \( \sigma \) associated with the \( k \)th multiplet; the target multiplet is denoted by \( k = 0 \), and we use positive and negative values of \( k \), respectively, to denote the neighbouring multiplets with \( \omega_k > \omega_0 \) or \( \omega_k < \omega_0 \). Note that \( U_{kk} \) denotes the \( kk \)’ submatrix of the truncated matrix \( U^T \), not the transpose of the submatrix \( U_{kk} \). The acceleration response of the target multiplet in this notation is

\[
a_0(t) = \Re [r_0^T \cdot \exp (i\Sigma_k^T) \cdot s_0]H(t),
\]
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where

\[ r'_0 = \sum_k U^T_{0k} \cdot r_k, \]  
\[ s'_k = \sum_k U^T_{lk} \cdot s_k. \]

To insure a minimal loss in accuracy due to the truncation, we select each multiplet \( n \), \( n \), or \( n \), as the target in turn, compute and diagonalize a new matrix \( C \) to find \( \Sigma_n \) and \( U^T_{lk} \), and sum the target responses \( \sigma_n(t) \) to form a complete single-branch seismogram. Much of the computational burden is associated with the need to update the basis multiplets for each new target.

2.4 Real symmetric approximation

The anelastic perturbation matrix \( A \) is diagonal if the quality factors \( Q_\alpha \) and \( Q_\omega \) are spherically symmetric. Variations in the spherical earth decay rate along a dispersion branch are slight; this suggests that it may be permissible to approximate \( A \) by a multiple of the identity:

\[ A = 2\omega_0 \alpha_k, \]  
where \( \alpha_k \) is the decay rate of the target multiplet. Perturbations \( \delta \rho \) to the earth’s density are also slight; this motivates the additional approximation

\[ \sigma^2(I + T) = \omega_0^2(I + T) + 2\omega_0(\delta \omega + i\alpha_k) I, \]

where \( \delta \omega \) is the real perturbation to the degenerate frequency \( \omega_0 \). Inserting both (43) and (44) into (17) leads to a real symmetric eigenvalue problem for \( \delta \omega \) and \( u \):

\[ D \cdot u = \delta \omega u, \]

where

\[ 2\omega_0 D = \Omega^2 - \omega_0^2 I + E - \omega_0^2 T. \]

Since \( D \) is real and symmetric, it can be diagonalized by a real orthogonal transformation \( U \):

\[ U^T \cdot D \cdot U = \Delta, \]

\[ U^T \cdot U = I, \]

where \( \Delta \) is the diagonal matrix of real perturbations \( \delta \omega \). The acceleration response of the target multiplet in this approximation is

\[ a_n(t) = [r'_0 \cdot \cos (\omega_0 t + \Delta), t \cdot s'_k] \exp (-\alpha_k t) H(t), \]

where \( r'_0 \) and \( s'_k \) are the real transformed source and receiver vectors, given as before by (41) and (42). The approximate eigenfunctions \( u \) are real and orthonormal with respect to the unperturbed density:

\[ \int_V \rho u_k \cdot u_k \cdot dV = \delta_{kk}. \]

Algebraically, the above approximation is equivalent to that employed by Um, Dahlen & Park (1991); however, it is numerically more efficient because the matrix \( D \) is real symmetric rather than complex Hermitian.

2.5 Complex-to-real basis transformation

Smooth models of the earth’s lateral heterogeneity are commonly expanded in spherical harmonics. The above development in terms of real basis eigenfunctions is of course applicable in this case; however, it is then advantageous to employ complex basis eigenfunctions proportional to \( Y_n^m(\theta, \phi) \) at the outset, since this enables the elastic, anelastic and kinetic energy perturbation matrices to be calculated analytically in terms of Wigner 3-j symbols (Woodhouse & Dahlen 1978; Woodhouse 1980). In this section we show how to transform the resulting complex generalized eigenvalue problem into the complex symmetric generalized eigenvalue problem considered here; the analysis generalizes the elastic self-coupling transformation considered by Luh (1973).

Let \( \{ \epsilon_1, \ldots, \epsilon^0, \ldots, \epsilon \} \) denote the real basis eigenfunctions proportional, respectively, to \( \{ \sqrt{2} X^l_\ell(\theta) \cos \phi, \ldots, X^l_\ell, \ldots, \sqrt{2} X^\ell_\ell(\phi) \sin \phi \} \), and let \( \{ \epsilon^{-1}, \ldots, \epsilon^0, \ldots, \epsilon^1 \} \) denote the complex eigenfunctions proportional, respectively, to \( \{ Y^l_\ell(\theta, \phi), \ldots, Y^l_\ell(\theta, \phi), \ldots, Y^l_\ell(\theta, \phi) \} \). We adopt the complex harmonic normalization convention of Edmonds (1960), and define the real associated Legendre functions \( X^m_\ell(\theta) \) by \( X^m_\ell(\theta, \phi) = X^m_\ell(\theta) \exp (im\phi) \). Let \( Z \) denote any of the real
symmetric matrices $E, A$ or $T$, and let $\tilde{Z}$ be the corresponding complex Hermitian matrix $\tilde{E}, \tilde{A}$ or $\tilde{T}$ defined using $(\tilde{e}_1, \ldots, \tilde{e}_i, \ldots, \tilde{e}_n)$ rather than $(\epsilon_1, \ldots, \epsilon_i, \ldots, \epsilon_n)$ in the defining equations (11)-(13). The reality of the perturbations $\delta \rho, \delta \kappa, \delta \mu, \kappa Q_{z-1}$ and $\mu Q_{z-1}$ and the symmetry $Y_{r_m} = (-1)^{r_m+n}(\tilde{Z}_{r_m} - m \cdot m')^*$ give rise to two symmetries of $\tilde{Z}$:

$$\tilde{Z}_{r_m}^m = (\tilde{Z}_{r_m}^{m'})^* = (-1)^{r_m+n}(\tilde{Z}_{r_m} - m \cdot m')^*.$$  

(51)

The first of the two conditions (51) is simply the statement that $\tilde{Z}$ is Hermitian: $\tilde{Z}^* = \tilde{Z}$. The perturbed eigenfunctions $u$ can be expanded in terms of either the real or the complex basis functions:

$$u = \sum_i \sum_m u_i^m e_i = \sum_i \sum_m \bar{u}_i^m \bar{e}_i.$$  

(52)

The coefficient vectors $u_i^m$ and $\bar{u}_i^m$ are related by

$$u_i^m = \frac{1}{\sqrt{2}} [\bar{u}_i^m + (-1)^m \bar{u}_i^{-m}],$$  

(53)

$$u_i^0 = \bar{u}_i^0,$$  

(54)

$$u_i^m = \frac{i}{\sqrt{2}} [\bar{u}_i^m - (-1)^m \bar{u}_i^{-m}].$$  

(55)

A change of basis from $(\tilde{e}_1, \ldots, \tilde{e}_i, \ldots, \tilde{e}_n)$ to $(\epsilon_1, \ldots, \epsilon_i, \ldots, \epsilon_n)$ transforms a complex Hermitian matrix-times-vector product of the form $\tilde{Z} \cdot \bar{u}$ to $Z \cdot u$, where $Z$ is real symmetric. Every real submatrix $Z_{kk}$ is of the form

$$Z_{kk} = \begin{pmatrix} z_{-} & z_0 & Z_{+} \\ z_{-} & z_0 & z_{+} \\ Z_{-} & z_{+} & Z_{+} \end{pmatrix},$$  

(56)

where

$$[Z_{-}]_{m}^{m'} = \Re [\tilde{Z}_{m}^{m'} + (-1)^m \tilde{Z}_{m'}^{m}].$$  

(57)

$$[Z_{+}]_{m}^{m'} = \Re [\tilde{Z}_{m}^{m'} - (-1)^m \tilde{Z}_{m'}^{m}].$$  

(58)

$$[Z_{-}]_{m}^{m'} = \Im [\tilde{Z}_{m}^{m'} + (-1)^m \tilde{Z}_{m'}^{m}].$$  

(59)

$$[Z_{+}]_{m}^{m'} = \Im [\tilde{Z}_{m}^{m'} - (-1)^m \tilde{Z}_{m'}^{m}].$$  

(60)

$$[z_{0}]_{m}^{m'} = \sqrt{2} \Re [\tilde{Z}_{m}^{m'} + (-1)^m \tilde{Z}_{m'}^{m}].$$  

(61)

$$[z_{+}]_{m}^{m'} = \sqrt{2} \Re [\tilde{Z}_{m}^{m'} - (-1)^m \tilde{Z}_{m'}^{m}].$$  

(62)

$$[z_{0}]_{m}^{m'} = \sqrt{2} \Im [\tilde{Z}_{m}^{m'} + (-1)^m \tilde{Z}_{m'}^{m}].$$  

(63)

$$[z_{+}]_{m}^{m'} = \sqrt{2} \Im [\tilde{Z}_{m}^{m'} - (-1)^m \tilde{Z}_{m'}^{m}].$$  

(64)

$$[z_{0}]_{m}^{m'} = [z^{m'}].$$  

(65)

Equations (57)-(65) can be used to transform the complex Hermitian matrices $\tilde{E}, \tilde{A}$ and $\tilde{T}$ into real symmetric matrices $E, A$ and $T$ to form the generalized eigenvalue problem (17).

### 2.6 Numerical results

We illustrate the validity of the real symmetric approximation by considering coupling along the fundamental spheroidal mode (Rayleigh wave) branch for model 1066A + M84A (Gilbert & Dziewonski 1975; Woodhouse & Dziewonski 1984). The perturbations $\delta \rho, \delta \kappa, \delta \mu$ are related to the prescribed variations in shear velocity $\delta \beta$ by the scaling relations $\delta \rho/\rho = 0.4(\delta \beta/\beta), \delta \kappa/\kappa = 1.7(\delta \beta/\beta)$ and $\delta \mu/\mu = 2.4(\delta \beta/\beta)$. The decay rates $\alpha_0$ are calculated using the spherical attenuation model of Masters, Park & Gilbert (1983). Every target multiplet $\nu S_{10}$ to $\nu S_{55}$ is coupled to its five nearest neighbours on either side along the branch; the adequacy of $\nu S_{10}$ to $\nu S_{55}$ is demonstrated for model 1066A + M84A by Um, Dahlen & Park (1991).

The singlet eigenfrequencies of the $\nu S_{55}$ multiplet are compared in Fig. 1. The exact eigenfrequencies $\sigma$ are calculated by solving the complex symmetric generalized eigenvalue problem $(\Omega^2 + V) \cdot u = \sigma^2 (I + T) \cdot u$, whereas the approximate eigenfrequencies $\omega_0 + \delta \omega$ and $\bar{\omega}_0$ are calculated by solving the real symmetric ordinary eigenvalue problem $D \cdot u = \delta \omega u$. The real parts $\omega_0$ and $\bar{\omega}_0$ and $\Re \sigma$ are in excellent agreement; the root-mean-square (rms) differences is only 0.0005 per cent (0.03 Hz). There is a larger discrepancy of order 0.25 per cent, in the decay rates $\sigma_0$ and $\bar{\sigma}_0$; the exact low-frequency singlets decay slightly more rapidly than the exact high-frequency singlets. Fig. 2 shows how the real and imaginary differences $\Re \sigma - \omega_0$ and $\Im \sigma - \sigma_0$ vary along the fundamental mode branch, $\nu S_{10}$ to $\nu S_{55}$; the rms errors are larger for the higher degree multiplets, as expected. Fig. 3 compares the expansion coefficients $u_k$ for a typical singlet (the 28th, counting from the low-frequency end) of the $\nu S_{55}$ multiplet. The imaginary parts $\Im u_k$ of the complex coefficients found by solving...
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0S55 singlets

![Diagram showing exact and approximate eigenfrequencies](image)

**Figure 1.** Dots show exact complex eigenfrequencies \( \sigma \) found by solving \((\mathbf{A} + \mathbf{V}) \cdot \mathbf{u} = \sigma^2 (1 + \mathbf{T}) \cdot \mathbf{u} \). Pluses show the corresponding eigenfrequencies \( \omega_0 + \delta \omega + i \epsilon \), found by solving \( \mathbf{D} \cdot \mathbf{u} = \delta \omega \mathbf{u} \). Both calculations are for the 0S55 multiplet \((\omega_0 = 6.066 \text{ mHz})\) on model 1066A + M84A. The matrices \( \mathbf{A} + \mathbf{V} \), \( 1 + \mathbf{T} \) and \( \mathbf{D} \) are all truncated at \( \pm 5 \) on either side of the target, so the coupling of \( 0 \mathbf{S}_0 \) through \( 0 \mathbf{S}_0 \) is accounted for. Most of the eigenfrequencies are nearly degenerate doublets, even at the high level of resolution shown here.

\((\mathbf{A} + \mathbf{V}) \cdot \mathbf{u} = \sigma^2 (1 + \mathbf{T}) \cdot \mathbf{u} \) are 10–20 times smaller than the real parts \( \Re \epsilon \mathbf{u} \). The approximate real coefficients \( \Re \mathbf{u} \) found by solving \( \mathbf{D} \cdot \mathbf{u} = \delta \omega \mathbf{u} \) are in excellent agreement with the real parts \( \Re \mathbf{u} \) of the exact coefficients; self-coupling dominates and coupling beyond \( \pm 3 \) is relatively weak.

Neither the singlet eigenfrequencies \( \sigma \) nor the singlet eigenfunctions \( \mathbf{u} \) are observable; what is important from a practical perspective is how faithfully the real symmetric approximation reproduces synthetic accelerograms. Fig. 4 compares the synthetic vertical acceleration spectra of the 0S55 multiplet at IDA station BDF following the 1978 Oaxaca earthquake; the corresponding time-domain accelerograms are Hann-tapered 20 hr records sampled every 40 s. The exact accelerograms, calculated using equation (40), are of the form

\[
\Re a_{\text{exact}}(t) = \Re \left[ \sum_k A_k^{\text{exact}} \exp (i\omega_k t) \right] H(t),
\]

whereas the approximate accelerograms, calculated using equation (49), are of the form

\[
\Re a_{\text{approx}}(t) = \Re \left[ \sum_k A_k^{\text{approx}} \cos (\omega_k t) \right] \exp (-\alpha t) H(t).
\]

The exact and approximate excitation amplitudes \( A_k^{\text{exact}} \) and \( A_k^{\text{approx}} \) are compared in the stick graphs below the spectra. The approximate amplitudes \( A_k^{\text{approx}} \) agree very well with the real parts \( \Re A_k^{\text{exact}} \) of the exact amplitudes; the imaginary parts \( \Im A_k^{\text{exact}} \) are typically 5–10 times smaller. Once the lines are broadened by dissipation and tapering, the resulting phase and amplitude spectra are virtually indistinguishable. This example illustrates a single multiplet observed at a single station after a single earthquake but it is fairly typical. In general, the contributions from \( \Im A_k^{\text{exact}} \) interfere destructively and contribute little to synthetic accelerograms, whereas the contributions from \( \Re A_k^{\text{exact}} \) are well modelled by the real symmetric approximation. The results of comparing a suite of 300 vertical accelerograms are shown in Fig. 5. The 15 earthquakes and 20 IDA stations employed are listed in tables 1 and 2 of Um, Dahlen & Park (1991); the moment tensors \( M \) are taken from...
real eigenfrequency

imaginary eigenfrequency (decay rate)

Figure 2. Variation of the error in the approximate complex eigenfrequencies \( \omega_0 + \delta \omega + i \alpha_0 \) along the fundamental spheroidal mode dispersion branch, \( \phi S_{10} \) to \( \phi S_{05} \). The quantities plotted are the root-mean-square differences \( \alpha_0 \left[ \sum_\alpha (\Re \alpha_\alpha - \omega_0 - \delta \omega_\alpha) \right]^{1/2} \times 100\% \) (upper graph) and \( \alpha_0 \left[ \sum_\alpha (\Im \alpha_\alpha - \omega_0 - \delta \omega_\alpha) \right]^{1/2} \times 100\% \) (lower graph). Both calculations are for model 1066A + M84A, with the matrices truncated at \( \pm 5 \).

Giardini, Woodhouse & Dziewonski (1985). The quantity plotted is the rms time-domain difference

\[
\sigma_{\text{rms}} = \left[ \frac{1}{T} \int_0^T [a_{\text{exact}}(t) - a_{\text{approx}}(t)]^2 dt \right]^{1/2} \times 100\%. \tag{68}
\]

Both \( a_{\text{exact}}(t) \) and \( a_{\text{approx}}(t) \) are calculated by summing the responses of the \( \phi S_{10} \sim \phi S_{05} \) multiplets; the length \( T \) of each record is
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expansion coefficients of 28th hybrid singlet of $\nu_{55}$ multiplet

approximate

$\nu_{50}$ $\nu_{51}$ $\nu_{52}$ $\nu_{53}$ $\nu_{54}$ $\nu_{55}$ $\nu_{56}$ $\nu_{57}$ $\nu_{58}$ $\nu_{59}$ $\nu_{60}$

exact

real

$\nu_{50}$ $\nu_{51}$ $\nu_{52}$ $\nu_{53}$ $\nu_{54}$ $\nu_{55}$ $\nu_{56}$ $\nu_{57}$ $\nu_{58}$ $\nu_{59}$ $\nu_{60}$

exact

imaginary x 10

$\nu_{50}$ $\nu_{51}$ $\nu_{52}$ $\nu_{53}$ $\nu_{54}$ $\nu_{55}$ $\nu_{56}$ $\nu_{57}$ $\nu_{58}$ $\nu_{59}$ $\nu_{60}$

Figure 3. Exact versus approximate expansion coefficients of the 28th singlet $\nu = \sum \nu_{\nu_{55}} e_{\nu_{55}}$ of the $\nu_{55}$ multiplet. Top shows real coefficients $u_{\nu_{55}}^{\text{approx}}$ calculated by solving $D \cdot u = \delta \omega u$; bottom shows complex coefficients $u_{\nu_{55}}^{\text{exact}}$ calculated by solving $(\Omega^2 + \nu^2) \cdot u = \omega^2 \nu (I + T) \cdot u$. Both calculations are for model 1066A + M84A, with the matrices truncated at $\pm 5 (\nu_{50}$ to $\nu_{55})$. Within each multiplet the basis vectors $e_{\nu_{55}}$ are arranged from left to right in order $(\sqrt{2} X(\theta) \cos \phi, \ldots, X(\theta), \ldots, \sqrt{2} Y(\theta) \sin \phi)$. Height of each line is proportional to $u_{\nu_{55}}^{\text{approx}}$ (top), $Re u_{\nu_{55}}^{\text{exact}}$ (middle), $Im u_{\nu_{55}}^{\text{exact}} \times 10$ (bottom).

20 hr. The abscissa in each case is the amplitude divided by the scalar moment:

$$A_{\text{scaled}} = \left[ \frac{1}{T} \int_{0}^{T} |u_{\text{exact}}(t)|^2 dt \right]^{1/2}$$

The scaling allows the data from different earthquakes $\nu_{\nu_{55}}$ to be accommodated in a single plot; the moments $[1/2M : M]$ vary from $1.6 \times 10^{19}$ to $1.7 \times 10^{21}$ Nm. Accelerograms with a low scaled amplitude are situated near a node of the Rayleigh wave radiation pattern whereas those with a high scaled amplitude are situated near an antinode. The largest errors are for nearly nodal accelerograms, which, in practice, would probably not be employed in a large-scale inversion. In most cases the error is less than 0.5 per cent. The overall conclusion is that the real symmetric approximation is an excellent one, for Rayleigh waves.
in the period range 150–600 s for model 1066A + M84A. The approximation fails to account for the imaginary parts of the singlet eigenfunctions \( \mathbf{u} \), but their effect on synthetic seismograms is slight.

### 3 SUBSPACE PROJECTION

The subspace projection method is a method of eliminating the small divisor problem which arises in using classical degenerate perturbation theory to calculate the singlet eigenfrequencies \( \sigma \) and eigenvectors \( \mathbf{u} \). Park (1987, 1990), Dahlen (1987) and Um, Dahlen & Park (1991) describe and illustrate the method, starting with the Hermitian analogue to the real symmetric ordinary eigenvalue problem \( \mathbf{D} \cdot \mathbf{u} = \sigma \mathbf{u} \). Here we extend the method to deal with the complex symmetric generalized eigenvalue problem \( (\mathbf{Q}^2 + \mathbf{V}) \cdot \mathbf{u} = \sigma^2(1+\mathbf{T}) \cdot \mathbf{u} \). The test of the subspace projection method conducted by Um, Dahlen & Park (1991) considered only first-order corrections to the eigenfunctions and second-order corrections to the eigenfrequencies; here we extend the analysis to second order in the eigenfunctions and third order in the eigenfrequencies.
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Figure 5. Root-mean-square time-domain differences $\sigma_{rms}$ for a suite of 300 accelerograms, plotted as a function of the scaled root-mean-square amplitudes $A_{scaled}$. The median error associated with the replacement of $(\Omega^2 + V) \cdot u = \sigma^2(I + T) \cdot u$ by $D \cdot u = \delta \omega u$ is 0.28 per cent. Both $\sigma_{approx}(t)$ and $\sigma_{exact}(t)$ are calculated by summing the responses of $\omega S_{10}$ to $\omega S_{35}$, using $\pm 5$ truncation, on model 1066A + M84A.

3.1 Theory

We begin by rewriting $(\Omega^2 + V) \cdot U = (I + T) \cdot U \cdot \Sigma^2$ in the form

$$C \cdot W = W \cdot \Sigma^2,$$

(70)

where

$$W = (I + T)^{1/2} \cdot U,$$

(71)

$$C = (I + T)^{-1/2} \cdot (\Omega^2 + V) \cdot (I + T)^{-1/2}.$$

(72)

Equation (70) is an ordinary eigenvalue problem for the complex symmetric matrix $C = C^T$. If there are no accidental degeneracies, then $W$ is complex orthogonal: $W^T \cdot W = I$. The eigenvector matrix $U$ is given in terms of $W$ by

$$U = (I + T)^{-1/2} \cdot W.$$

(73)

We use a square-root decomposition $I + T = (I + T)^{1/2} \cdot (I + T)^{1/2}$ rather than a Cholesky decomposition $I + T = L \cdot L^T$ as in (31) because it is analytically more convenient.

To implement the subspace projection method, we write $W$ in the form

$$W = P \cdot Q,$$

(74)

where $P$ and $Q$ are both complex orthogonal:

$$P^T \cdot P = I, \quad Q^T \cdot Q = I.$$

(75)

We then use analytical methods to seek a transformation $P$ that renders both

$$B = P^T \cdot C \cdot P$$

(76)
and \( Q \) block diagonal, of the form

\[
\mathbf{B} = \begin{pmatrix}
\mathbf{B}_{00} & \mathbf{B}_{10} & \mathbf{0} \\
\mathbf{0} & \mathbf{B}_{11} & \mathbf{0} \\
& & \ddots
\end{pmatrix}, \quad \mathbf{Q} = \begin{pmatrix}
\mathbf{Q}_{00} & \mathbf{0} \\
\mathbf{0} & \mathbf{Q}_{11} \\
& & \ddots
\end{pmatrix}.
\] (77)

Such a transformation reduces (70) to a number of uncoupled smaller eigenvalue problems of the form \( \mathbf{B}_{kk} \cdot \mathbf{Q}_{kk} = \mathbf{Q}_{kk} \cdot \mathbf{\Sigma}_{k}^2 \), where \( \mathbf{\Sigma}_{k} \) is the diagonal matrix of complex eigenfrequencies \( \sigma \) associated with the \( k \)th multiplet. To find the eigenfrequencies and eigenfunctions associated with the target \( (k = 0) \) multiplet, we only have to solve the target problem

\[
\mathbf{B}_{00} \cdot \mathbf{Q}_{00} = \mathbf{Q}_{00} \cdot \mathbf{\Sigma}_{0}^2.
\] (78)

This reduces the numerical labour substantially, because the dimension of the complex symmetric matrix \( \mathbf{B}_{00} \) is only \((2L + 1) \times (2L + 1)\). The \((2L + 1) \times (2L + 1)\) eigenvector matrix \( \mathbf{Q}_{00} \) is complex orthogonal: \( \mathbf{Q}_{00}^T \cdot \mathbf{Q}_{00} = \mathbf{I}_{00} \).

To find \( \mathbf{P} \) we insert the binomial expansion

\[
(1 + \mathbf{T})^{-1/2} = 1 - \frac{1}{2} \mathbf{T} + \frac{3}{8} \mathbf{T}^2 + \cdots
\] (79)

in (72) and expand the matrix \( \mathbf{C} \) in powers of \( \mathbf{T} \) and \( \mathbf{V} \). The result can be written in the form

\[
\mathbf{C} = \mathbf{\Omega}^2 + \mathbf{C}^{(1)} + \mathbf{C}^{(2)} + \mathbf{C}^{(3)} + \cdots,
\] (80)

where the superscripts denote the order. The \( \infty \times \infty \) matrices \( \mathbf{C}^{(1)}, \mathbf{C}^{(2)} \) and \( \mathbf{C}^{(3)} \) are composed of submatrices \( \mathbf{C}^{(1)}_{kk}, \mathbf{C}^{(2)}_{kk} \) and \( \mathbf{C}^{(3)}_{kk} \), given by

\[
\mathbf{C}^{(1)}_{kk} = \mathbf{V}_{kk} - \frac{1}{2}(\omega_k^2 + \omega_k^2)\mathbf{T}_{kk},
\]
(81)

\[
\mathbf{C}^{(2)}_{kk} = -\frac{3}{8} \sum_{k'} \sum_{k''} \left[ \mathbf{T}_{kk'} \cdot \mathbf{V}_{k''k'} + \mathbf{V}_{kk'} \cdot \mathbf{T}_{k''k'} \right] + \sum_{k''} \sum_{k'''} \left( 3\omega_k^2 + 2\omega_k^2 + 3\omega_k^2 \right) \mathbf{T}_{kk} \cdot \mathbf{T}_{k''k''}.
\]
(82)

\[
\mathbf{C}^{(3)}_{kk} = -\frac{1}{16} \left( \sum_{k''} \sum_{k'''} \left( 5\omega_k^4 + 3\omega_k^2 + 3\omega_k^2 + 5\omega_k^4 \right) \mathbf{T}_{kk} \cdot \mathbf{T}_{k''k''} \right) + \mathbf{C}^{(2)}_{kk} - \mathbf{T}_{kk} \cdot \mathbf{T}_{k''k''}.
\] (83)

The orthonormality condition \( \mathbf{P}^T \cdot \mathbf{P} = \mathbf{I} \) can be written in terms of the submatrices \( \mathbf{P}_{kk} \) and \( \mathbf{P}_{kk'}^T \) in the form

\[
\sum_{k''} \mathbf{P}_{kk} \cdot \mathbf{P}_{k''k''} = \mathbf{I}_{kk''}
\] (84)

Here \( \mathbf{I}_{kk} \) is the \((2L + 2k + 1) \times (2L + 2k + 1)\) identity, and \( \mathbf{I}_{kk'k'} = 0 \) if \( k \neq k' \). Note that \( \mathbf{P}_{kk}^T \) denotes the \( kk' \) submatrix of \( \mathbf{P}^T \), not the transpose of \( \mathbf{P}_{kk} \). Following Dahlen (1987) we expand \( \mathbf{P}_{kk} \) and \( \mathbf{P}_{kk'}^T \) in the form

\[
\mathbf{P}_{kk} = \mathbf{I}_{kk} + \mathbf{P}_{(1)}^{(1)} + \mathbf{P}_{(2)}^{(2)} + \mathbf{P}_{(3)}^{(3)} + \cdots,
\]
(85)

\[
\mathbf{P}_{kk'}^T = \mathbf{I}_{kk'} - \mathbf{P}_{(1)}^{(1)} - \mathbf{P}_{(2)}^{(2)} + \mathbf{P}_{(3)}^{(3)} + \cdots.
\] (86)

It is easily verified that (85) and (86) satisfy (84) correct to third order. Written out in terms of submatrices, the condition that \( \mathbf{B} \) be block diagonal is

\[
\mathbf{B}_{kk} = \sum_{k''} \mathbf{P}_{kk''}^T \cdot \mathbf{C}_{kk''} \cdot \mathbf{P}_{k''k''} = \mathbf{0}, \quad \text{for } k \neq k'.
\] (87)

Inserting (85) and (86) into (87) and equating terms of like order leads to a systematic determination, successively, of \( \mathbf{P}_{(1)}^{(1)}, \mathbf{P}_{(2)}^{(2)}, \mathbf{P}_{(3)}^{(3)}, \ldots \) for \( k \neq k' \). The square matrices \( \mathbf{P}_{(1)}^{(1)}, \mathbf{P}_{(2)}^{(2)}, \mathbf{P}_{(3)}^{(3)}, \ldots \) are indeterminate, but it can be verified that the target response \( a_0(t) \) is independent of these matrices. This indeterminacy at every order reflects the non-uniqueness of the block-diagonalizing transformation \( \mathbf{P} \); a convenient choice, which determines \( \mathbf{P} \) uniquely, is to require that \( \mathbf{P} \) reduces to the identity in the limit of a vanishingly small perturbation:

\[
\mathbf{P}_{(1)}^{(1)} = \mathbf{P}_{(2)}^{(2)} = \mathbf{P}_{(3)}^{(3)} = \cdots = \mathbf{0}.
\] (88)

From (87) we find, to first and second order, respectively,

\[
\mathbf{P}_{(1)}^{(1)} = (\omega_k^2 - \omega_k^2)^{-1} \mathbf{C}_{kk}^{(1)}, \quad k \neq k'.
\] (89)
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Inserting (80) and (88)–(90) into (76) we find that $B_{kk'}$ is given correct to third order by

$$B_{kk'} = \omega_0^2 B_{kk'} + C_{kk'}^{(1)} + C_{kk'}^{(2)} + \sum_{k \neq k'} (\omega_0^2 - \omega_k^2)^{-1} [C_{kk'}^{(1)} \cdot C_{kk'}^{(1)} + C_{kk'}^{(1)} \cdot C_{kk'}^{(2)} + C_{kk'}^{(2)} \cdot C_{kk'}^{(2)}]$$

$$- \frac{1}{2} \sum_{k \neq k'} (\omega_0^2 - \omega_k^2)^{-2} [C_{kk'}^{(1)} \cdot C_{kk'}^{(1)} + C_{kk'}^{(1)} \cdot C_{kk'}^{(2)} + C_{kk'}^{(2)} \cdot C_{kk'}^{(2)}] + \sum_{k \neq k', k' \neq 0} (\omega_0^2 - \omega_k^2)^{-1} (\omega^2 - \omega_k^2)^{-1} C_{kk'}^{(1)} \cdot C_{kk'}^{(1)} + C_{kk'}^{(1)} \cdot C_{kk'}^{(2)} + C_{kk'}^{(2)} \cdot C_{kk'}^{(3)} .$$

It is unnecessary to calculate $B_{kk'}^2$, since only $B_{kk'}^2 = 0$ contributes to (91). A more convenient form for $B_{kk'}$ can be formed by inserting (81)–(83) into (91) and collecting terms. The algebra is heavy; we found it helpful to use Mathematica (Wolfram 1988). For notational convenience we define the matrices

$$H_{kk'} = V_{kk'} - \omega_0^2 T_{kk'} .$$

The final result depends only on the matrices $T_{0k}$, $T_{k0}$ and $H_{kk'}$:

$$B_{kk'} = \omega_0^2 B_{kk'} + B_{kk'}^{(1)} + B_{kk'}^{(2)} + B_{kk'}^{(3)} ,$$

where

$B_{kk'}^{(1)} = \text{H}_{kk'} \cdot \omega_0^2 T_{kk'}$.

$B_{kk'}^{(2)} = \omega_0^2 T_{kk'} \cdot T_{0k} + \frac{1}{2} (H_{kk'} \cdot H_{k0} + H_{k0} \cdot H_{kk'}) + \sum_{k \neq 0} (\omega_0^2 - \omega_k^2)^{-1} H_{kk} \cdot H_{k0} .

B_{kk'}^{(3)} = \frac{1}{2} (H_{kk'} \cdot H_{k0} + H_{k0} \cdot H_{kk'}) + \text{H}_{kk'} \cdot H_{k0}

- \frac{1}{2} \sum_{k \neq k'} (\omega_0^2 - \omega_k^2)^{-1} [2 (T_{0k} \cdot H_{kk} + H_{kk} \cdot T_{0k}) + H_{kk} \cdot H_{k0} + H_{k0} \cdot H_{kk'} + H_{k0} \cdot H_{k0} + T_{kk'} \cdot H_{k0} + H_{kk'} \cdot H_{k0}] .

- \frac{1}{2} \sum_{k \neq k', k' \neq 0} (\omega_0^2 - \omega_k^2)^{-1} [H_{kk'} \cdot H_{kk'} + H_{kk'} \cdot H_{k0} + H_{k0} \cdot H_{k0} + H_{k0} \cdot H_{k0} + H_{k0} \cdot H_{k0}] .

To calculate the target eigenvectors $u$ and the transformed source and receiver vectors $r'$ and $s'$, we need to find $U_{kk'}$ and $T_{kk'}$, $k \neq 0$. These are obtained by inserting (79) and (88)–(90) into $U^T = Q^T \cdot P^T \cdot (1 + T)^{-1/2}$. Correct to second order this gives the result

$$U_{kk'} = Q_{kk'} \cdot \left[ k_{kk'} - \frac{1}{4} T_{kk'} + \frac{1}{4} T_{kk'} \cdot T_{kk'} + \frac{5}{4} \sum_{k' \neq 0} T_{kk'} \cdot T_{kk'} \cdot T_{kk'} \right]

- \frac{1}{2} \sum_{k \neq k'} (\omega_0^2 - \omega_k^2)^{-1} C_{kk'}^{(1)} \cdot T_{kk'} + \frac{1}{2} \sum_{k \neq k'} (\omega_0^2 - \omega_k^2)^{-2} C_{kk'}^{(1)} \cdot C_{kk'}^{(1)} .

U_{kk'} = K_{kk'} \cdot \left[ -\frac{1}{4} T_{kk'} + (\omega_0^2 - \omega_k^2)^{-1} C_{kk'}^{(1)} + \frac{1}{4} T_{kk'} \cdot T_{kk'} + \frac{5}{4} \sum_{k' \neq k} T_{kk'} \cdot T_{kk'} + (\omega_0^2 - \omega_k^2)^{-1} C_{kk'}^{(1)}

- (\omega_0^2 - \omega_k^2)^{-2} C_{kk'}^{(1)} \cdot C_{kk'}^{(1)} - \frac{1}{2} \sum_{k' \neq 0} (\omega_0^2 - \omega_k^2)^{-1} C_{kk'}^{(1)} \cdot C_{kk'}^{(1)} \right],

k \neq 0 .

Inserting (81) and (82) and combining terms using Mathematica, we obtain the final result

$$U_{kk'} = Q_{kk'} \cdot \left[ K_{kk'} + K_{kk'}^{(2)} \right],

U_{kk'} = Q_{kk'} \cdot \left[ K_{kk'}^{(1)} + K_{kk'}^{(2)} \right],

k \neq 0 ,

where

$$K_{kk'}^{(1)} = -\frac{1}{4} T_{kk'},

K_{kk'}^{(2)} = \frac{3}{4} T_{kk'} \cdot T_{kk'} + \frac{1}{4} \sum_{k' \neq 0} (\omega_0^2 - \omega_k^2)^{-1} T_{kk'} \cdot H_{k0} - \frac{3}{4} \sum_{k \neq 0} (\omega_0^2 - \omega_k^2)^{-1} H_{k0} \cdot T_{kk'} + \frac{1}{2} \sum_{k \neq 0} (\omega_0^2 - \omega_k^2)^{-2} H_{k0} \cdot H_{k0} .

K_{kk'}^{(1)} = (\omega_0^2 - \omega_k^2)^{-1} H_{k0},

K_{kk'}^{(2)} = -(\omega_0^2 - \omega_k^2)^{-1} H_{k0} \cdot T_{k0} - \frac{1}{2} (\omega_0^2 - \omega_k^2)^{-1} T_{k0} \cdot H_{k0} .

- (\omega_0^2 - \omega_k^2)^{-2} H_{k0} \cdot H_{k0} + (\omega_0^2 - \omega_k^2)^{-1} \sum_{k' \neq 0} (\omega_0^2 - \omega_k^2)^{-1} H_{k0} \cdot H_{k0} .

k \neq 0 .
The acceleration response of the target multiplet in this approximation is
\[ a_0(t) = \mathcal{B} [r_0^T \cdot \exp(i\mathbf{z}_0) \cdot s_0^T]H(t), \]
where
\[ r_0 = Q_{00}^T \cdot [I_{00} + K^{(1)}_{00} + K^{(2)}_{00}] \cdot r_0 + Q_{00}^T \cdot \sum_{k=0} K_{0k}^{(1)} + K_{0k}^{(2)} \cdot r_k, \]
\[ s_0 = Q_{00}^T \cdot [I_{00} + K^{(1)}_{00} + K^{(2)}_{00}] \cdot s_0 + Q_{00}^T \cdot \sum_{k=0} K_{0k}^{(1)} + K_{0k}^{(2)} \cdot s_k. \]

The above results retain all terms of third order in the eigenfrequencies and second order in the eigenfunctions. To find the target eigenfrequencies to second order and the target eigenfunctions to first order, we ignore \( B_{0k}^{(3)}, K_{0k}^{(3)} \) and \( K_{0k}^{(3)} \). For brevity we refer to the two cases as the second-order and first-order subspace projections approximations, respectively.

The algebraic structure of the multiplet coupling problem is summarized in Fig. 6. A portion of a perturbation matrix \( Z \) (either \( E \), \( A \) or \( T \)) is shown; the numbers and degree of shading depict the order at which the various terms affect the response of the target (centre) multiplet. Every \( \times \times \times \) matrix \( Z \) is block diagonal, with zeros in the lower left and upper right corners, if the model of the lateral heterogeneity is bandlimited. The number of non-zero submatrices \( Z_{kk} \) on either side of the target is the maximum spherical harmonic degree \( K \) of the earth model. To zeroth order in the eigenfunctions and first order in the eigenfrequencies, only \( Z_{00} \) contributes; this is the isolated multiplet (self-coupling) approximation:
\[ H_{00} \cdot Q_{00} = Q_{00} \cdot Z^0. \]

To first order in the eigenfunctions and second order in the eigenfrequencies, only the coupling between the target and each of its neighbours, as specified by the matrices \( Z_{0k} \) and \( Z_{00} \), is accounted for. To second order in the eigenfunctions and third order in the eigenfrequencies, both \( Z_{kk} \) self-coupling of neighbouring multiplets \( -K \leq k \leq K \) and \( Z_{kk} \) coupling between neighbours \( -K \leq k, k' \leq K \) affect the target multiplet. Contributions from \( Z_{kk} \) with \( k, k' < K \) and \( k, k' > K \) do not arise until the next order; the coupling propagates order by order up and down the diagonals of the \( \times \times \times \) matrices \( Z \) due to the successive incorporation of terms of the form \( Z_{0k} \cdot Z_{kk} \cdot Z_{kk}^* \cdot Z_{kk}^{**} \cdot Z_{kk}^{***} \cdot Z_{kk}^{****} \), etc. Truncation at \( \pm K \) should almost
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always be justified because the coupling strength $\epsilon_k$ is proportional to $(\omega_0^2 - \omega_k^2)^{-1}$ and the ignored terms are of third order and higher in $\epsilon_k$. The eigenfrequencies are always calculated to one higher order of accuracy than the eigenfunctions.

3.2 Real symmetric approximation

Subspace projection can also be applied to the real symmetric eigenvalue problem $D \cdot u = \delta u u$. In this case it is convenient to define the real auxiliary matrices

$$F_{kk'} = \mathbf{E}_{kk'} - \omega_0^2 \mathbf{T}_{kk'}.$$  

We find the real perturbations $\delta \omega$ to the target eigenfrequency $\omega_0$ correct to third order by solving the $(2l + 1) \times (2l + 1)$ real symmetric eigenvalue problem

$$[D^{(1)}_{00} + D^{(2)}_{00} + D^{(3)}_{00}] \cdot \mathbf{Q}_{00} = \mathbf{Q}_{00} \cdot \Delta_0.$$  

The matrices $D^{(1)}_{00}$, $D^{(2)}_{00}$ and $D^{(3)}_{00}$ are given by

$$2\omega_0 D^{(1)}_{00} = \mathbf{E}_{00} = \mathbf{E}_{00} - \omega_0^2 \mathbf{T}_{00},$$

$$2\omega_0 D^{(2)}_{00} = \sum_{k \neq \omega} \left(\omega_0^2 - \omega_k^2\right)^{-1} \mathbf{F}_{0k} \cdot \mathbf{F}_{k0},$$

$$2\omega_0 D^{(3)}_{00} = -\frac{1}{2} \sum_{k \neq \omega} \left(\omega_0^2 - \omega_k^2\right)^{-2} \left[\mathbf{F}_{0k} \cdot \mathbf{F}_{k0} + \mathbf{F}_{0k} \cdot \mathbf{F}_{k0} + \mathbf{F}_{0k} \cdot \mathbf{F}_{k0} \right] + \sum_{k \neq \omega} \sum_{k' \neq \omega} \left(\omega_0^2 - \omega_k^2\right)^{-1} \left(\omega_0^2 - \omega_{k'}^2\right)^{-1} \mathbf{F}_{0k} \cdot \mathbf{F}_{k'k} \cdot \mathbf{F}_{k'0}. $$

Equation (113) corrects a sign error in equation (83) of Dahlen (1987). The eigenvectors $\mathbf{U}_{0k}$ and $\mathbf{U}_{0k}$, $k \neq 0$, are given correct to second order by

$$\mathbf{U}_{00} = \mathbf{Q}_{00} \cdot [\mathbf{I}_{00} + \mathbf{K}_{00} + \mathbf{K}_{00}^{(2)}],$$

$$\mathbf{U}_{0k} = \mathbf{Q}_{0k} \cdot [\mathbf{K}_{0k}^{(1)} + \mathbf{K}_{0k}^{(2)}], \quad k \neq 0,$$

where

$$\mathbf{K}_{00}^{(1)} = 0,$$

$$\mathbf{K}_{0k}^{(1)} = -\frac{1}{2} \sum_{\omega \neq \omega} \left(\omega_0^2 - \omega_\omega\right)^{-1} \mathbf{F}_{0k} \cdot \mathbf{F}_{k0},$$

$$\mathbf{K}_{0k}^{(2)} = (\omega_0^2 - \omega_k^2)^{-2} \mathbf{F}_{0k} \cdot \mathbf{F}_{k0},$$

$$\mathbf{K}_{0k}^{(1)} = (\omega_0^2 - \omega_k^2)^{-1} \mathbf{F}_{0k} \cdot \mathbf{F}_{k0}, \quad k \neq 0,$$

$$\mathbf{K}_{0k}^{(1)} = -(\omega_0^2 - \omega_k^2)^{-2} \mathbf{F}_{0k} \cdot \mathbf{F}_{k0} + (\omega_0^2 - \omega_k^2)^{-1} \sum_{k' \neq \omega} \left(\omega_0^2 - \omega_{k'}^2\right)^{-1} \mathbf{F}_{0k} \cdot \mathbf{F}_{k'k}. \quad k \neq 0.$$

The target acceleration response in this approximation is

$$a_{\omega} (t) = \left[ r_{\omega} \right] \cdot \cos (\omega_0 t + \Delta_\omega) \cdot s_\omega \exp (-\alpha t)H(t),$$

where $r_0$ and $s_\omega$ are again given by (106) and (107).

3.3 Numerical results

In this section we compare both the second-order and first-order subspace projection approximations with the exact variational method; as before, we consider $\pm 5$ coupling along the fundamental spheroidal mode branch, $\nu S_{10}$ to $\nu S_{55}$, on model 1066A + M84A. The singlet eigenfrequencies $\sigma$ of the $\nu S_{55}$ multiplet are compared in Fig. 7. Both the real and imaginary eigenfrequencies are slightly better predicted by the second-order theory than by the first-order theory; this is more evident in Fig. 8, which shows how the real and imaginary differences $Re \sigma_{\text{exact}} - Re \sigma_{\text{approx}}$ and $Im \sigma_{\text{exact}} - Im \sigma_{\text{approx}}$ vary along the fundamental mode branch, $\nu S_{10}$ to $\nu S_{55}$. The factor-of-four improvement for $\nu S_{55}$, from 0.0012 to 0.0003 per cent for the real eigenfrequencies and from 0.04 to 0.01 per cent for the imaginary eigenfrequencies, is consistent with the magnitude of the cumulative coupling strength, $\epsilon_{\text{rms}} = 0.25$ (Um, Dahlen & Park 1991). Figs 9 and 10 compare the first-order and second-order eigenfunction expansion coefficients $u_k$ for the 28th singlet of the $\nu S_{55}$ multiplet. Both coefficients $Re u_k^{\text{approx}}$ and $Im u_k^{\text{approx}}$ are indiscernible from the exact coefficients $Re u_k^{\text{exact}}$ and $Im u_k^{\text{exact}}$ at the resolution shown.

Figs 11 and 12 compare the vertical acceleration spectra at IDA station BDF following the 1978 Oaxaca earthquake. As before, the spectra are calculated using Hann-tapered 20 hr records with a 40 s sample interval. There are slight inaccuracies in the excitation amplitudes $A_k^{\text{approx}}$ calculated using first-order eigenfunctions which conspire to give rise to a 1–2 $\mu$Hz shift in the position of the broadened spectral peak to lower frequencies. The corresponding amplitudes $A_k^{\text{approx}}$ calculated using second-order eigenfunctions, on the other hand, are extremely accurate; both the amplitude and phase of the broadened spectral peak are faithfully reproduced. The rms time-domain differences $\sigma_{\text{rms}}$ for the same suite of 300 vertical accelerograms...
Figure 7. Dots show exact complex eigenfrequencies $\alpha_{\text{exact}}$ found by solving $(\Omega^2 + V) \cdot \mathbf{u} = \alpha^2(t + T) \cdot \mathbf{u}$. Pluses show approximate complex eigenfrequencies $\alpha_{\text{approx}}$ found using first-order (top) and second-order (bottom) subspace projection. Both calculations are for the $a_{S_{55}}$ multiplet on model 1066A + M84A, with the matrices truncated at ±5.

Figure 8. Variation of the root-mean-square differences $\alpha_{\text{approx}} \cdot |\Sigma \beta' \alpha^{\text{exact}} - \beta' \alpha^{\text{approx}}|^{1/2} \times 100\%$ (top) and $\alpha_{\text{approx}} \cdot |\Sigma \beta' \alpha^{\text{exact}} - \beta' \alpha^{\text{approx}}|^{1/2} \times 100\%$ (bottom) along the fundamental spheroidal mode dispersion branch, $\phi_{910}$ to $\phi_{S_{55}}$. Pluses and dots show first-order and second-order subspace projection results, respectively. All calculations are for model 1066A + M84A, with the matrices truncated at ±5.
Figure 9. Exact versus approximate expansion coefficients of the 28th singlet $u = \sum u_k e_k$ of the $S_{28}$ multiplet. The approximate coefficients are calculated using first-order subspace projection. All calculations are for model $1066A + M84A$, with the matrices truncated at $\pm 5$ ($u_{\text{S}&u}$ to $u_{\text{S}0}$). Within each multiplet the basis vectors $e_k$ are arranged from left to right in order $(\sqrt{V}/\chi(\theta) \cos \phi, \ldots, \chi(\theta), \ldots, \sqrt{V}/\chi(\theta) \sin \phi)$. Height of each line is proportional to $\Re u_k^{\text{approx}}$ (top), $\Re u_k^{\text{exact}}$ (second from top), $\Im u_k^{\text{exact}} \times 10$ (third from top) and $\Im u_k^{\text{approx}} \times 10$ (bottom). The differences $\Re u_k^{\text{exact}} - \Re u_k^{\text{approx}}$ and $\Im u_k^{\text{exact}} - \Im u_k^{\text{approx}}$ are too small to be discerned at the resolution shown.

Figure 10. Same as Fig. 9, with $\Re u_k^{\text{approx}}$ and $\Im u_k^{\text{approx}}$ calculated using second-order rather than first-order subspace projection.
Figure 11. Amplitude and phase of the $\delta_{55}$ multiplet observed on a vertical accelerometer at IDA station BDF following the 1978 Oaxaca, Mexico earthquake. Solid lines show the exact spectrum; dotted lines show the corresponding spectrum calculated using the first-order subspace projection approximation. Line spectra below compare the exact and approximate singlet excitation amplitudes $\Re A_{\text{approx}}$ (top), $\Im A_{\text{approx}}$ (second from top), $\Re A_{\text{exact}}$ (third from top) and $\Im A_{\text{exact}}$ (bottom). The exact amplitudes are plotted at $\delta_{01}^e$, and the approximate amplitudes are plotted at $\Re \delta_{02}^e$.

considered above are shown in Fig. 13. Going to second order typically leads to an improvement of more than a factor of five; in most cases, the error of the second-order approximation is less than 1 per cent. The largest errors, as before, are for stations situated near a node of the Rayleigh wave radiation pattern.

4 COMPUTATION TIMES

All the eigenvalue computations are performed using standard EISPACK routines. For maximum accuracy, we use the path CBAL–CORTH–COMQR2–CBAK2 to solve both the large-scale complex symmetric eigenvalue problem $C \cdot W = W \cdot \Sigma^2$ and the reduced complex symmetric eigenvalue problem $B_{\nu\nu} \cdot Q_{\nu\nu} = Q_{\nu\nu} \cdot \Sigma^2$ that arises in the subspace projection method. A Gram–Schmidt procedure is applied to each nearly degenerate doublet to force the biorthogonality relations $W^\top \cdot W = I$ and $Q_{\nu\nu}^\top \cdot Q_{\nu\nu} = I$. All the eigenvalues and eigenvectors of $C$ are obtained; however, only those associated with the target multiplet are retained and the rest are discarded. The Cholesky decomposition of the kinetic energy matrix $I + T = L \cdot L^\top$ is performed using the routine REDUC, and the real and imaginary parts of the eigenvectors $W$ are separately back transformed to
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Figure 12. Same as Fig. 11, except that the singlet eigenfrequencies $\omega_{\text{approx}}$ and excitation amplitudes $A_\text{approx}$ are computed using the second-order rather than the first-order subspace projection approximation.

We solve the large-scale real symmetric eigenvalue problem $D \cdot U = U \cdot \Delta$ by first searching for the eigenvalues of a target multiplet using the routines TRED1 and TRIDIB. The corresponding eigenvectors are then obtained by inverse iteration using the routines TINVIT and TRBAK1. All the eigenvalues and eigenvectors of the reduced real symmetric problem $D_{\text{reduced}} \cdot U_{\text{reduced}} = U_{\text{reduced}} \cdot \Delta$, are computed using the routines TRED2 and TQL2.

Table 1 is a comparison of computation times needed to calculate all the singlet eigenfrequencies and eigenfunctions along the fundamental spheroidal mode dispersion branch, $\nu_{\text{approx}} \approx \nu_{55}$. The computations were performed on a Sun SPARC 2 with 64 megabytes of memory, except for the complex symmetric variational calculations, which were executed on a Sun SPARC 2 with 128 megabytes of memory. The actual computation time for the complex symmetric variational method is 11 times that shown (147 hr). We divide by 11 for a fair comparison on the grounds that approximately 10/11 of the eigenvalues and eigenvectors that are calculated are discarded. We attempted to use the path CBAL–COMHES–COMLR–CINVIT–CBABK2 to solve only for the complex target eigenvectors, but were unsuccessful; the tabulated time (13.4 hr) assumes that a more stable complex inverse iteration procedure can be found. We did not attempt to develop such a procedure because the real symmetric approximation (for which inverse iteration works very well) is so accurate. All the computations are for model 1066A + M84A, with the matrices truncated at $\pm 5$. 

$U = L^{-T} \cdot W$ using the routine REBAK.
Figure 13. Root-mean-square time-domain differences $\sigma_{\text{rms}}$ for a suite of 300 synthetic vertical accelerograms, plotted as a function of the scaled root-mean-square amplitudes $A_{\text{scaled}}$. Both $a_{\text{approx}}(t)$ and $a_{\text{exact}}(t)$ are calculated by summing the responses of $a_{S_{10}}$ to $a_{S_{55}}$, using $\pm 5$ truncation, on model 1066A + M84A. The median error of the first-order subspace projection accelerograms is 3.33 per cent and whereas that of the second-order subspace projection accelerograms is 0.45 per cent.

Table 1. Time needed to compute all singlet eigenfrequencies and eigenfunctions for $a_{S_{10}}$ to $a_{S_{55}}$.

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5 CONCLUSION

The results in this paper can be used as the basis for an efficient scheme of calculating accurate synthetic long-period seismograms on a non-rotating, aspherical, anelastic earth model. A complex-to-real spherical earth basis transformation eliminates the need to solve explicitly for the dual singlet eigenfunctions. Subspace projection, carried to second order in the
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Normal mode multiplet coupling, third order in the eigenfrequencies, is a rapid and accurate method of solving either the exact complex symmetric generalized eigenvalue problem \((\Omega^2 + \mathbf{V}) \cdot \mathbf{u} = \alpha^2 (I + \mathbf{T}) \cdot \mathbf{u}\) or the approximate real symmetric ordinary eigenvalue problem \(\mathbf{D} \cdot \mathbf{u} = \delta \omega \mathbf{u}\). Taken together, the procedures described here halve the memory requirements and reduce the computation time by about a factor of 30.

ACKNOWLEDGMENTS

We thank Jeffrey Park for providing his original variational and subspace projection computer codes; this work would not have been possible without his generosity. Financial support for this work was provided by the US National Science Foundation under Grant EAR-9001531. Some computation was performed at the Pittsburgh Supercomputing Center.

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