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Augmentation of the generalised $n \times n$ eigenvalue equation to a generalised $(n+1) \times (n+1)$ eigenvalue equation *

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Generalised $n \times n$ eigenvalue equation $\mathbf{B}|\Phi_i\rangle = \lambda_i \mathbf{S}^b|\Phi_i\rangle$ $(i = 1, \ldots, n)$ where $\mathbf{B}$ and $\mathbf{S}^b$ are $n \times n$ Hermitian matrices while $\mathbf{S}^b$ is in addition positive definite is considered. This equation is augmented to a generalised $(n+1)(n+1)$ eigenvalue equation $\mathbf{H}|\Psi_k\rangle = \varepsilon_k \mathbf{S}|\Psi_k\rangle$ $(k = 1, \ldots, n+1)$ where Hermitian matrices $\mathbf{H}$ and $\mathbf{S}$ represent matrices $\mathbf{B}$ and $\mathbf{S}^b$, respectively, augmented by one additional row and one additional column. It is shown how the eigenvalues ε_k and the eigenvectors $|\Psi_k\rangle$ of the augmented eigenvalue equation can be expressed in terms of the eigenvalues λ_i and the eigenvectors $|\Phi_i\rangle$ of the original eigenvalue equation. Operation count to obtain by this method all augmented eigenvalues and eigenvectors is of the order $O(n^2)$. Unless matrices involved are of some special kind such as sparse matrices or alike, this operation count is one order of magnitude smaller than operation count required by other presently known methods. In many practical cases operation count to obtain a single selected eigenvalue and/or eigenvector by this method is of the order $O(n)$. In the case of the generalised eigenvalue equation, all other methods usually require again $O(n^3)$ operations, even if only a single eigenvalue and/or eigenvector is required. Thus in many cases of interest operation count to obtain a selected eigenvalue and/or eigenvector by this method is two orders of magnitude smaller than operation count required by other methods.

KEY WORDS: matrix augmentation, generalised eigenvalue equation, eigenvalue problem, perturbation

1. Introduction

Consider the following problem: The solution of an eigenvalue equation in some base $\{|\phi_i\rangle\}$ $(i = 1, \ldots, n)$ is known. One would like to increase this base with one additional vector $|\Theta\rangle \equiv |\phi_{n+1}\rangle$ in order to improve accuracy of this solution. In general, there may be many candidates for this additional vector, and one would like to find the best one in a most efficient way. For example, base vectors $|\phi_i\rangle$ can be atomic orbitals, while the eigenvectors and eigenvalues of the eigenvalue equation represent molecular orbitals and their energies. One would like to find out how the inclusion of an additional atomic orbital $|\Theta\rangle$ influences those molecular orbitals and their energies. As another

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example, assume that base vectors $|\phi_i\rangle$ are resonance structures in the VB approach and we are looking for the VB ground state. We would like to increase the base set with an additional resonance structure in such a way as to decreases ground state energy as much as possible. Here again there is usually a large number of candidate resonance structures. In addition, VB resonance structures are in general not orthogonal to each other, and the corresponding eigenvalue equation is a generalised eigenvalue equation of a type $\mathbf{H}|\Psi\rangle = \lambda\mathbf{S}|\Psi\rangle$ where $\mathbf{S}$ is positive definite matrix.

In this and similar situations one can use standard approach to diagonalize the augmented eigenvalue equation separately with each candidate base vector $|\Theta\rangle$. Standard diagonalization methods such as Householder, Jacobi or Givens require $O(n^3)$ operations in order to find all n eigenvalues. Additional operation count to find the corresponding eigenvectors is also $O(n^3)$ [1,2]. Those methods do not apply directly to the generalised eigenvalue equation. In order to solve such an equation one usually has to transform it into a normal eigenvalue equation. The obtained eigenvalue equation is then solved in a standard way. If $\mathbf{S}$ is symmetric positive definite matrix, this transformation can be most efficiently done by Cholesky decomposition [1]. However this decomposition alone requires $n^3/6$ operations. In addition, there is yet another operation count needed for the construction of the final eigenvalue equation that is again of the order $O(n^3)$.

In many cases one has to find only one or only a few selected eigenvalues and/or eigenvectors. Direct diagonalization methods are not particularly suitable for such problems. In the case when only a single solution is required, some other method, such as the power method, the Davidson algorithm, the Lanczos method, or the perturbation expansion is usually more efficient. In the power method, one repeatedly calculates the action of a given matrix to previously obtained vectors. Each iteration requires $O(n^2)$ operations. The number of iterations needed to obtain a required accuracy increases with n. The total operation count is hence higher than $O(n^2)$ but lower than $O(n^3)$. However, the power method can be directly applied only for the calculation of extreme eigenvalues. In order to find an arbitrary eigenvalue by this method, one has to calculate matrix inverse, which is again of the order $O(n^3)$ [1,2]. The Lanczos method is more efficient than the power method. Each iterative step of this method requires $O(n^2)$ operations, and intermediate results usually converge to extreme eigenvalues already after a few iterations [1]. Lanczos algorithm is hence faster than $O(n^3)$ if only a few extreme eigenvalues are required. However, this method is again $O(n^3)$ if an arbitrary eigenvalue and/or eigenvector is needed. Davidson's algorithm [3] is usually a method of choice in the large scale CI calculations [4]. Operation count of this algorithm is also less then $O(n^3)$ if only a few eigenvalues and eigenvectors are required [4]. However, this method highly relies on the sparsity of the Hamiltonian. Finally, the perturbation expansion is in general also at least $O(n^3)$. It is less than $O(n^3)$ only if the perturbation is so small that higher expansion terms can be neglected, or if the matrices involved are of some special kind, such as sparse matrices or alike. Thus all those methods are of the order higher than $O(n^2)$, even if only one eigenvalue and/or eigenvector is required. In addition, those methods apply only to a standard eigenvalue equation. In the case of the generalised eigenvalue equation, the problem is much more complex. Additional

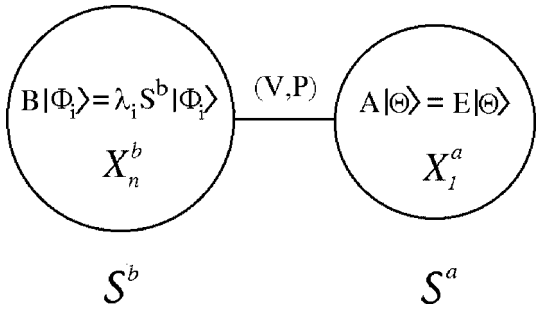

Figure 1. Interaction of a one-dimensional system $\mathcal{S}^a$ with the n-dimensional system $\mathcal{S}^b$. System $\mathcal{S}^a$ is described by a single eigevector $|\Theta\rangle$ with the eigenvalue E. System $\mathcal{S}^b$ is described by a generalised eigenvalue equation (1a). Generalised interaction is (**V**, **P**), and the combined system is described by the generalised eigenvalue equation (4).

operation count that is required is usually of the order $O(n^3)$, even if only a single eigenvalue and/or eigenvector is required. For large matrices this is very time consuming. It is therefore desirable to have some more efficient method to treat this and similar problems.

The problem of the augmentation of the generalised eigenvalue equation can be formulated in terms of the interaction of a one-dimensional quantum system $\mathcal{S}^a$ with the n-dimensional quantum system $\mathcal{S}^b$ (see figure 1). With a system $\mathcal{S}^a$ is associated a one-dimensional space X_1^a and with a system $\mathcal{S}^b$ is associated an n-dimensional space X_n^b. Spaces X_1^a and X_n^b are orthogonal to each other, and with a combined system $\mathcal{S} \equiv \mathcal{S}^a \oplus \mathcal{S}^b$ is associated an $(n+1)$-dimensional space X_{n+1}. System $\mathcal{S}^b$ alone is described by the generalised eigenvalue equation

$$\mathbf{B}|\Phi_i\rangle = \lambda_i \mathbf{S}^b|\Phi_i\rangle, \quad i = 1, \ldots, n. \tag{1a}$$

Operators **B** and $\mathbf{S}^b$ are Hermitian operators acting in the space X_n^b. In addition, we assume that $\mathbf{S}^b$ is positive definite. No other assumption about those operators is made. Hermiticity of those operators and positive definiteness of $\mathbf{S}^b$ guarantees reality of the eigenvalues λ_i and completeness of the corresponding eigenvectors $|\Phi_i\rangle$. In addition, eigenvectors $|\Phi_i\rangle$ can be orthonormalized according to (see appendix):

$$\left\langle \Phi_i \middle| \mathbf{S}^b \middle| \Phi_j \right\rangle = \delta_{ij}, \quad i = 1, \ldots, n. \tag{1b}$$

Let $\{|r\rangle\}_b$ $(r = 1, \ldots, n)$ be an orthonormalized basis in $X_n^b (\langle r|s\rangle = \delta_{rs})$. In this basis operators **B** and $\mathbf{S}^b$ have $n \times n$ matrices with matrix elements $B_{rs} = \langle r|\mathbf{B}|s\rangle$ and $S_{rs}^b = \langle r|\mathbf{S}^b|s\rangle$, respectively, while ket vector $|\Phi_i\rangle$ is in this basis represented as n-component column vector with components $\Phi_{is} = \langle s|\Phi_i\rangle$. For the sake of simplicity we will use the same notation for various operators and vectors, and their matrices in this basis. In particular, eigenvalue equation (1a) can be interpreted as a matrix eigenvalue equation.

System $\mathcal{S}^a$ that interacts with the system $\mathcal{S}^b$ is described by a single normalised eigenvector $|\Theta\rangle$ with the corresponding real eigenvalue E. Formally, one has

$$\mathbf{A}|\Theta\rangle = E|\Theta\rangle \tag{2a}$$

where

$$\mathbf{A} = E|\Theta\rangle\langle\Theta| \tag{2b}$$

is a Hermitian operator in the one-dimensional space X_1^a and where $|\Theta\rangle\langle\Theta| = \mathbf{I}^a$ is a projection operator on this space. One can augment the base $\{|r\rangle\}_b$ of the space X_n^b with the vector $|n+1\rangle \equiv |\Theta\rangle$ to obtain the set $\{|r\rangle\}$ $(r = 1, \ldots, n+1)$ that forms an orthonormalized basis in the combined space X_{n+1}.

Relations (1) and (2) describe systems $\mathcal{S}^b$ and $\mathcal{S}^a$ in isolation, that is without mutual interaction. The interaction is introduced by the Hermitian operators **V** and **P**. Those operators have nonvanishing matrix elements only between vectors in the space X_n^b and vector $|\Theta\rangle \in X_1^a$. Hence

$$\mathbf{V} = \mathbf{I}^b\mathbf{V}\mathbf{I}^a + \mathbf{I}^a\mathbf{V}\mathbf{I}^b, \qquad \mathbf{P} = \mathbf{I}^b\mathbf{P}\mathbf{I}^a + \mathbf{I}^a\mathbf{P}\mathbf{I}^b, \tag{3a}$$

where $\mathbf{I}^b$ and $\mathbf{I}^a$ are projection operators on spaces X_n^b and X_1^a, respectively. Operators **V** and **P** can be also written as

$$\mathbf{V} = |\mathbf{u}\rangle\langle\Theta| + |\Theta\rangle\langle\mathbf{u}|, \qquad \mathbf{P} = |\mathbf{x}\rangle\langle\Theta| + |\Theta\rangle\langle\mathbf{x}|, \tag{3b}$$

where

$$|\mathbf{u}\rangle = \sum_r^n u_r|r\rangle \in X_n^b, \qquad |\mathbf{x}\rangle = \sum_r^n x_r|r\rangle \in X_n^b. \tag{3c}$$

Since vectors $|\mathbf{u}\rangle$ and $|\mathbf{x}\rangle$ are contained in the space X_n^b, relation (3b) implies

$$|\mathbf{u}\rangle = \mathbf{V}|\Theta\rangle, \qquad |\mathbf{x}\rangle = \mathbf{P}|\Theta\rangle. \tag{3d}$$

The eigenvalue equation describing the combined system $\mathcal{S}$ subject to the generalised interaction $(\mathbf{V}, \mathbf{P})$ is

$$\mathbf{H}|\Psi_k\rangle = \varepsilon_k\mathbf{S}|\Psi_k\rangle, \quad k = 1, \ldots, n+1 \tag{4a}$$

where

$$\mathbf{H} = \mathbf{A} + \mathbf{B} + \mathbf{V}, \qquad \mathbf{S} = \mathbf{I}^a + \mathbf{S}^b + \mathbf{P}. \tag{4b}$$

In order to guarantee the reality of the augmented eigenvalues ε_k and completeness of the corresponding eigenvectors $|\Psi_k\rangle$, operator **S** is required to be positive definite in the combined space X_{n+1}. This requirement imposes a restriction on the admissible operators **P** according to the condition given in lemma 1. Concerning operator **V**, there is no restriction on this operator, except that it must be Hermitian and that it should connect vectors in the space X_n^b with the vector $|\Theta\rangle \in X_1^a$.

If operator **S** is positive definite, augmented eigenvectors $|\Psi_k\rangle$ can be orthonormalized according to

$$\langle\Psi_k|\mathbf{S}|\Psi_l\rangle = \delta_{kl}. \tag{4c}$$

This relation is analogous to the relation (1b) that applies to the eigenvectors $|\Phi_i\rangle$ of the eigenvalue equation (1a).

In the augmented basis $\{|r\rangle\}$ operators $\mathbf{V}$, $\mathbf{P}$, $\mathbf{H}$ and $\mathbf{S}$ can be represented as $(n+1) \times (n+1)$ matrices

$$\mathbf{V} = \begin{bmatrix} \mathbf{0} & \mathbf{u} \\ \mathbf{u}^+ & 0 \end{bmatrix}, \qquad \mathbf{P} = \begin{bmatrix} \mathbf{0} & \mathbf{x} \\ \mathbf{x}^+ & 0 \end{bmatrix}, \tag{5a}$$

$$\mathbf{H} = \begin{bmatrix} \mathbf{B} & \mathbf{u} \\ \mathbf{u}^+ & E \end{bmatrix}, \qquad \mathbf{S} = \begin{bmatrix} \mathbf{S}^b & \mathbf{x} \\ \mathbf{x}^+ & 1 \end{bmatrix}, \tag{5b}$$

where $\mathbf{0}$ denotes an $n \times n$ null matrix. In this matrix form $\mathbf{u}$ and $\mathbf{x}$ are n-component column vectors with components $u_r = \langle r|\mathbf{u}\rangle = \langle r|\mathbf{V}|\Theta\rangle$ and $x_r = \langle r|\mathbf{x}\rangle = \langle r|\mathbf{P}|\Theta\rangle$, respectively, while $\mathbf{u}^+$ and $\mathbf{x}^+$ are row vectors, complex conjugated to column vectors $\mathbf{u}$ and $\mathbf{x}$, respectively.

According to the representation (5b), eigenvalue equation (4a) is eigenvalue equation (1a) augmented by one row and one column. Matrix $\mathbf{B}$ in the original eigenvalue equation (1a) is augmented by the new $(n+1)$th row and column. This new row and column is represented by the perturbation vector $\mathbf{u}$ and eigenvalue E of the vector $|\Theta\rangle$. Similarly, matrix $\mathbf{S}^b$ is augmented by a new $(n+1)$th row and column, and this additional row and column is represented by the perturbation vector $\mathbf{x}$.

We will treat system $\mathcal{S}^b$ as the original unperturbed system. From this point of view, "perturbation" is represented by the system $\mathcal{S}^a$ and the interaction $(\mathbf{V}, \mathbf{P})$. Accordingly, we will assume that the solution to the system $\mathcal{S}^b$ (eigenvalues λ_i and eigenvectors $|\Phi_i\rangle$) is known, and using this solution, we will solve the augmented eigenvalue equation (4a) that describes augmented system $\mathcal{S}$. In the same spirit and depending on the context, we will sometimes refer to augmented eigenvalues and eigenvectors as perturbed eigenvalues and eigenvectors, respectively.

2. Solution to the augmentation problem

Augmented eigenvalue equation can be solved following general ideas of the Low Rank Perturbation (LRP) method [5]. In this method, one has to distinguish two types of the perturbed eigenvalues and eigenvectors. If the eigenvalue ε_k of the perturbed system differs from all the eigenvalues λ_i of the unperturbed system, that is if $\varepsilon_k \notin \{\lambda_i\}$, the eigenvalue ε_k and the corresponding eigenvector $|\Psi_k\rangle$ are "cardinal". Otherwise, the eigenvalue ε_k and the corresponding eigenvector or eigenvectors are "singular" [5].

Concerning the unperturbed eigenvalues λ_i, it is convenient to distinguish *active* and *passive* eigenvalues [5]. This notation is defined relative to the interaction $(\mathbf{V}, \mathbf{P})$.

Let the unperturbed eigenvalue λ_j be η-degenerate, and let $|\Phi_{j\nu}\rangle$, $\nu = 1, \ldots, \eta$, be the corresponding unperturbed eigenvectors. The eigenvalue λ_j is *active* if at least one quantity $\langle\Theta|\mathbf{V} - \lambda_j\mathbf{P}|\Phi_{j\nu}\rangle$ $(\nu = 1, \ldots, \eta)$ is nonzero, otherwise it is *passive*. In other words, the eigenvalue λ_j is passive if the space spanned by the unperturbed eigenvectors $|\Phi_{j\nu}\rangle$ $(\nu = 1, \ldots, \eta)$ is contained in a null-space of the operator $(\mathbf{V} - \lambda_j\mathbf{P})$:

$$(\mathbf{V} - \lambda_j\mathbf{P})|\Phi_{j\nu}\rangle = 0, \quad \nu = 1, \ldots, \eta. \tag{6}$$

In the appendix we prove the following two theorems.

Theorem I (Cardinal eigenvalues and eigenvectors). Let $\mathbf{B}$ and $\mathbf{S}^b$ be $n \times n$ Hermitian matrices, let $\mathbf{H} = \mathbf{A} + \mathbf{B} + \mathbf{V}$ and $\mathbf{S} = \mathbf{I}^a + \mathbf{S}^b + \mathbf{P}$ be $(n+1) \times (n+1)$ augmented Hermitian matrices, and let $\mathbf{S}^b$ and $\mathbf{S}$ be positive definite. Let further λ_i $(i = 1, \ldots, n)$ be the eigenvalues of the unperturbed eigenvalue equation (1a), and let $|\Phi_i\rangle$be the corresponding eigenvectors orthonormalized according to (1b). Then

(a) $\varepsilon_k \notin \{\lambda_i\}$ is an eigenvalue of the augmented eigenvalue equation (4a) if and only if it is a root of the function $h(\varepsilon)$

$$h(\varepsilon) \equiv \Omega(\varepsilon) + (\beta - 1)\varepsilon + \alpha + E = 0, \tag{7}$$

where

$$\Omega(\varepsilon) = \sum_i^n \frac{c_i}{\varepsilon - \lambda_i}, \quad c_i = \langle\Theta|\mathbf{V} - \lambda_i\mathbf{P}|\Phi_i\rangle\langle\Phi_i|\mathbf{V} - \lambda_i\mathbf{P}|\Theta\rangle, \tag{8}$$

and where

$$\begin{aligned} \alpha &= \sum_i^n \big[\lambda_i\langle\Theta|\mathbf{P}|\Phi_i\rangle\langle\Phi_i|\mathbf{P}|\Theta\rangle - \langle\Theta|\mathbf{P}|\Phi_i\rangle\langle\Phi_i|\mathbf{V}|\Theta\rangle - \langle\Theta|\mathbf{V}|\Phi_i\rangle\langle\Phi_i|\mathbf{P}|\Theta\rangle\big], \\ \beta &= \sum_i^n \langle\Theta|\mathbf{P}|\Phi_i\rangle\langle\Phi_i|\mathbf{P}|\Theta\rangle. \end{aligned} \tag{9a}$$

(b) Let $\varepsilon_k \notin \{\lambda_i\}$ be an eigenvalue of the augmented eigenvalue equation (4a). This eigenvalue is nondegenerate, and the corresponding eigenvector is

$$|\Psi_k\rangle = \sum_i^n \frac{\langle\Phi_i|\mathbf{V} - \varepsilon_k\mathbf{P}|\Theta\rangle}{\varepsilon_k - \lambda_i}|\Phi_i\rangle + |\Theta\rangle. \tag{10a}$$

In addition, $|\Psi_k\rangle$ satisfies

$$\langle\Theta|\mathbf{V} - \varepsilon_k\mathbf{P}|\Psi_k\rangle = \varepsilon_k - E. \tag{11}$$

The above theorem produces all cardinal ($\varepsilon_k \notin \{\lambda_i\}$) eigenvalues and eigenvectors of the augmented eigenvalue equation (4a). The crucial function $h(\varepsilon)$ is expressed in terms of n unperturbed eigenvalues λ_i, n coefficients c_i, quantities α and β, and the eigenvalue E. According to (8) and (9a) coefficients c_i are nonnegative real numbers, the quantity β is also a nonnegative real number, while α can assume an arbitrary real value. In order for the matrix $\mathbf{S}$ to be positive definite, quantity β must also satisfy the condition $\beta < 1$ (see lemma 1). Coefficients c_i and quantities α and β are ultimately expressed in terms of the unperturbed eigenvalues λ_i and in terms of the matrix elements $\langle\Theta|\mathbf{V}|\Phi_i\rangle$ and $\langle\Theta|\mathbf{P}|\Phi_i\rangle$. Equivalently, those matrix elements can be considered as scalar products $\langle\mathbf{u}|\Phi_i\rangle = \langle\Theta|\mathbf{V}|\Phi_i\rangle$ and $\langle\mathbf{x}|\Phi_i\rangle = \langle\Theta|\mathbf{P}|\Phi_i\rangle$.

Using relations (A2) and (A3) in the appendix quantities α and β can be written in a compact form:

$$\begin{aligned}\alpha &= \langle\Theta|\mathbf{P}(\mathbf{S}^b)^{-1}\mathbf{B}(\mathbf{S}^b)^{-1}\mathbf{P} - \mathbf{V}(\mathbf{S}^b)^{-1}\mathbf{P} - \mathbf{P}(\mathbf{S}^b)^{-1}\mathbf{V}|\Theta\rangle,\\ \beta &= \langle\Theta|\mathbf{P}(\mathbf{S}^b)^{-1}\mathbf{P}|\Theta\rangle\end{aligned} \tag{9b}$$

where $(\mathbf{S}^b)^{-1}$ is the inverse of $\mathbf{S}^b$ in the space X_n^b. Since $\mathbf{S}^b$ is positive definite this inverse exists, and from (A2) one finds $(\mathbf{S}^b)^{-1} = \sum_i |\Phi_i\rangle\langle\Phi_i|$.

Formulas (9b) express quantities α and β in the way that is explicitly independent on the unperturbed eigenvectors $|\Phi_i\rangle$. This is advantageous for some theoretical considerations. Representation (9a) is more convenient for numerical applications.

The case of singular eigenvalues and corresponding eigenvectors is treated in the following theorem.

Theorem II (Singular eigenvalues and eigenvectors). Assume the same conditions as in theorem I. Let λ_j be η-degenerate unperturbed eigenvalue, and let $|\Phi_{j\nu}\rangle$ $(\nu = 1, \ldots, \eta)$ be the corresponding eigenvectors. Then

(a) If the unperturbed eigenvalue λ_j is active and degenerate $(\eta > 1)$, then $\varepsilon_k = \lambda_j$ is a $(\eta - 1)$-degenerate eigenvalue of the augmented system. The corresponding $(\eta - 1)$ eigenvectors are linear combinations of the unperturbed eigenvectors $|\Phi_{j\nu}\rangle$:

$$|\Psi\rangle = \sum_{\nu}^{\eta} D_\nu |\Phi_{j\nu}\rangle \tag{12a}$$

where the coefficients D_ν satisfy

$$\sum_{\nu}^{\eta} \langle\Theta|\mathbf{V} - \varepsilon_k\mathbf{P}|\Phi_{j\nu}\rangle D_\nu = 0. \tag{12b}$$

If the unperturbed eigenvalue λ_j is not degenerate $(\eta = 1)$, the value $\varepsilon_k = \lambda_j$ is not an eigenvalue of the augmented system.

(b) If the unperturbed eigenvalue λ_j is passive, then $\varepsilon_k = \lambda_j$ is an eigenvalue of the augmented system with the following two possibilities:

(b1) If $h(\varepsilon_k) \neq 0$, this eigenvalue is η-degenerate, and the corresponding η eigenvectors can be chosen to coincide with η-unperturbed eigenvectors $|\Phi_{j\nu}\rangle$.

$$|\Psi\rangle = |\Phi_{j\nu}\rangle, \quad \nu = 1, \ldots, \eta; \tag{13}$$

(b2) If $h(\varepsilon_k) = 0$, this eigenvalue is $(\eta+1)$-degenerate. First η eigenvectors corresponding to this eigenvalue are given by (13), while an additional eigenvector is

$$|\Psi_k\rangle = \sum_{i(\lambda_i \neq \varepsilon_k)}^{n} \frac{\langle\Phi_i|\mathbf{V} - \varepsilon_k\mathbf{P}|\Theta\rangle}{\varepsilon_k - \lambda_i}|\Phi_i\rangle + |\Theta\rangle \tag{10b}$$

where i $(\lambda_i \neq \varepsilon_k)$ denotes the summation over all i such that $\lambda_i \neq \varepsilon_k$. This eigenvector satisfies relation (11) with $\varepsilon_k = \lambda_j$.

In the expression (10b) of the above theorem summation excludes all terms with $\lambda_i = \varepsilon_k$. Since $\varepsilon_k = \lambda_j$ is passive, all such terms are formally of the type $0/0$. If we make the convention to neglect those terms, then relation (10b) becomes a special case of the relation (10a). In addition, condition $h(\varepsilon_k) = 0$ is relation (7) with $\varepsilon = \lambda_j$. This shows that each root of the function $h(\varepsilon)$ is an eigenvalue of the augmented eigenvalue equation, either cardinal or singular. If the unperturbed eigenvalue λ_j is active, the function $h(\varepsilon)$ has singularity in the point $\varepsilon = \lambda_j$, and hence it can have no root in this point. However, if the unperturbed eigenvalue λ_j is passive, this function is finite and analytic in the point $\varepsilon = \lambda_j$. In this case, it is possible for $h(\varepsilon)$ to have a root $\varepsilon_k = \lambda_j \in \{\lambda_i\}$. This root is also an eigenvalue of the augmented eigenvalue equation. In conclusion, the set of all roots to the function $h(\varepsilon)$ contains all cardinal eigenvalues of the augmented eigenvalue equation. In addition, it may also contain some singular eigenvalues of this equation.

The above two theorems provide complete solution to the matrix augmentation problem. In order to find eigenvalues and eigenvectors of the augmented eigenvalue equation, one has first to find roots of $h(\varepsilon)$. Once a particular root $\varepsilon = \varepsilon_k$ is obtained, this root is an augmented eigenvalue, and the corresponding eigenvector is given by relation (10a). This produces all cardinal and possibly some singular eigenvalues and eigenvectors. The remaining singular eigenvalues and eigenvectors are trivial to find. Each η-degenerate $(\eta > 1)$ unperturbed eigenvalue λ_j that is active generates an $(\eta - 1)$-degenerate perturbed eigenvalue $\varepsilon_k = \lambda_j$. The corresponding eigenvectors are given by relation (12a), where the coefficients D_v satisfy (12b). Each η-degenerate unperturbed eigenvalue λ_j that is passive generates either η- or $(\eta + 1)$-degenerate perturbed eigenvalue $\varepsilon_k = \lambda_j$. First η eigenvectors coincide with the η unperturbed eigenvectors (equation (13)). The one extra eigenvector, which exists only if $h(\lambda_j) = 0$, is already obtained during the search for the roots of $h(\varepsilon)$ and the corresponding eigenvectors. This completes derivation of augmented eigenvalues and eigenvectors by the LRP method. In addition it shows that the augmentation of the original eigenvalue equation by a single row and a single column can change (decrease or increase) the degeneracy of each particular unperturbed eigenvalue λ_j at most by one.

Above theorems apply to generalised eigenvalue equations (1a) and (4a) where $\mathbf{S}^b$ is an arbitrary positive definite Hermitian operator acting in the space X_n^b, while $\mathbf{V}$ is an arbitrary Hermitian operator connecting spaces X_n^b and X_1^a. Similarly, $\mathbf{P}$ is an arbitrary Hermitian operator connecting those two spaces that satisfies the condition of lemma 1. All the obtained relations simplify if the corresponding equations are not completely general. The most important special case is $\mathbf{P} = 0$. In this case $\alpha = \beta = 0$ and hence $h(\varepsilon) \equiv \Omega(\varepsilon) + E - \varepsilon$. Condition $\mathbf{P} = 0$ is relatively mild and it allows for the unperturbed eigenvalue equation (1a) to be still of a most general type. There are no restrictions on the interaction $\mathbf{V}$ that connects spaces X_n^b and X_1^a, and the eigenvalue equation describing the combined system is still a generalised eigenvalue equation, though not of a most general type. One has $\mathbf{P} = 0$ in a special but highly important case when instead

of generalised eigenvalue equations (1a) and (4a) one has standard eigenvalue equations $\mathbf{B}|\Phi_i\rangle = \lambda_i|\Phi_i\rangle$ and $\mathbf{H}|\Psi_k\rangle = \varepsilon_k|\Psi_k\rangle$, respectively.

3. Orthonormalization of perturbed eigenvectors

Perturbed eigenvectors (10) and (12) are not orthonormalized. All perturbed eigenvectors can be orthonormalized according to (4c). This can be done using relation (1b) and the property $\mathbf{P}|\Theta\rangle \in X_n^b$.

Concerning normalisation, one finds that each cardinal eigenvector should be normalised according to

$$\frac{1}{\sqrt{W_k}}|\Psi_k\rangle \tag{14a}$$

where $|\Psi_k\rangle$ is given by (10a) and where (see appendix)

$$W_k = \sum_i^n \frac{|\langle\Phi_i|\mathbf{V} - \lambda_i\mathbf{P}|\Theta\rangle|^2}{(\varepsilon_k - \lambda_i)^2} + 1 - \beta. \tag{14b}$$

In a similar way are normalised singular eigenvectors (10b). Singular eigenvectors (12a) are normalised according to

$$|\Psi\rangle = \frac{1}{\sqrt{\sum_\nu D_\nu^* D_\nu}} \sum_\nu^\eta D_\nu|\Phi_{j\nu}\rangle. \tag{14c}$$

In particular, each singular eigenvector of type (13) is already properly normalised.

Concerning mutual orthogonality of perturbed eigenvectors, eigenvectors $|\Psi_k\rangle$ and $|\Psi_l\rangle$ that correspond to distinct eigenvalues ($\varepsilon_k \neq \varepsilon_l$) are already orthogonal to each other. This is a consequence of the hermiticity of operators $\mathbf{H}$ and $\mathbf{S}$, and the fact that $\mathbf{S}$ is positive definite. Since each cardinal eigenvector is nondegenerate, it is orthogonal to all other eigenvectors. In particular, if $|\Psi_k\rangle$ and $|\Psi_l\rangle$ are distinct cardinal eigenvectors, they satisfy $\langle\Psi_k|\mathbf{S}|\Psi_l\rangle = 0$. If those eigenvectors are normalised one finds

$$\langle\Psi_k|\mathbf{S}|\Psi_l\rangle \equiv \frac{1}{\sqrt{W_k W_l}}\left[\sum_i^n \frac{|\langle\Theta|\mathbf{V} - \lambda_i\mathbf{P}|\Phi_i\rangle|^2}{(\varepsilon_k - \lambda_i)(\varepsilon_l - \lambda_i)} + 1 - \beta\right] = 0 \tag{15a}$$

where W_k and W_l are given by (14b).

Similar relation is obtained if $|\Psi_k\rangle$ is a normalised cardinal eigenvector and if $|\Psi_l\rangle$ is a normalised singular eigenvector of type (10b), or if both eigenvectors are normalised singular eigenvectors of type (10b). Another possible combination is that $|\Psi_k\rangle$ is a normalised cardinal eigenvector while $|\Psi_l\rangle$ is a normalised singular eigenvector (14c). In this case one obtains

$$\langle\Psi_l|\mathbf{S}|\Psi_k\rangle = \frac{1}{\sqrt{W_k \sum_\nu D_\nu^* D_\nu}} \frac{\sum_\nu^\eta D_\nu^* \langle\Phi_{j\nu}|\mathbf{V} - \varepsilon_l\mathbf{P}|\Theta\rangle}{\varepsilon_k - \varepsilon_l} = 0. \tag{15b}$$

This relation is equivalent to the condition (12b) imposed on the coefficients D_v that determine singular eigenvector $|\Psi_l\rangle$.

One can write right hand sides of relations (15) in a simpler form, without normalisation constants. However, written in the above form those relations can be directly used as a test for the numerical accuracy of the suggested method [6]. In any numerical calculation due to the finite precision arithmetic there is always some error accumulation. Therefore, calculated eigenvectors $|\Psi_k''\rangle$ slightly differ from exact eigenvectors $|\Psi_k\rangle$. If $|\Psi_k''\rangle$ and $|\Psi_l''\rangle$ are calculated eigenvectors that correspond to different eigenvalues, they will be only approximately orthogonal to each other. Numerically one obtains $\langle\Psi_k''|\mathbf{S}|\Psi_l''\rangle \approx 0$. In order for quantities $\langle\Psi_k''|\mathbf{S}|\Psi_l''\rangle$ to be an objective measure of the numerical error, vectors $|\Psi_k''\rangle$ and $|\Psi_l''\rangle$ should be normalised.

Since eigenvectors that correspond to distinct eigenvalues are automatically orthogonal to each other, relations (14) are sufficient to orthonormalize all cardinal eigenvectors and, in addition, all nondegenerate singular eigenvectors. If there is any degenerate singular eigenvalue $\varepsilon_k = \lambda_j$, corresponding eigenvectors can be orthonormalized using some standard orthonormalization procedures such as Gramm–Schmidt orthonormalization [1,2] and relations (1b) and (12). This extra orthonormalization should be numerically simple and easy to perform, since the dimension of the corresponding degenerate subspace is in most cases much smaller than the dimension of the combined space X_{n+1}.

4. Global distribution of perturbed eigenvalues

All cardinal eigenvalues of the augmented eigenvalue equation are roots of the function $h(\varepsilon)$. In order to find efficiently those roots, one has to investigate in more details a global behaviour of this function. According to the expression (7), each cardinal eigenvalue lies on the intersection of the function $\Omega(\varepsilon)$ and a line $g(\varepsilon) = (1-\beta)\varepsilon - \alpha - E$. Conversely, each intersection of $\Omega(\varepsilon)$ and $g(\varepsilon)$ is an eigenvalue of the augmented eigenvalue equation, either cardinal or singular. Further, the function $\Omega(\varepsilon)$ is continuous and analytic everywhere, except in the points $\varepsilon = \lambda_j$ where the unperturbed eigenvalue λ_j is active. If namely this eigenvalue is active, there is at least one unperturbed eigenvector $|\Phi_{jv}\rangle$ such that $\langle\Theta|\mathbf{V} - \lambda_j\mathbf{P}|\Phi_{jv}\rangle \neq 0$**.** Hence $c_j \neq 0$, and the function $\Omega(\varepsilon)$ has a singularity in the point $\varepsilon = \lambda_j$. Since each coefficient c_i is nonnegative, it follows that if the unperturbed eigenvalue λ_j is active, functions $\Omega(\varepsilon)$ and $h(\varepsilon)$ satisfy

$$\lim_{\varepsilon\to\lambda_j^+} h(\varepsilon) = \lim_{\varepsilon\to\lambda_j^+} \Omega(\varepsilon) = \infty, \qquad \lim_{\varepsilon\to\lambda_j^-} h(\varepsilon) = \lim_{\varepsilon\to\lambda_j^-} \Omega(\varepsilon) = -\infty \tag{16a}$$

where $\varepsilon \to \lambda_j^+$ and $\varepsilon \to \lambda_j^-$ denotes right and left limits, respectively. If the unperturbed eigenvalue λ_j is passive, functions $\Omega(\varepsilon)$ and $h(\varepsilon)$ are finite and analytic in the point $\varepsilon = \lambda_j$.

One also finds

$$\lim_{\varepsilon\to\pm\infty} \Omega(\varepsilon) = 0. \tag{16b}$$

Since $c_i \geqslant 0$ the derivative of a function $\Omega(\varepsilon)$ is negative, i.e., $\mathrm{d}\Omega(\varepsilon)/\mathrm{d}\varepsilon < 0$. In addition, one finds (see appendix):

Lemma 1. Matrix $\mathbf{S} = \mathbf{I}^a + \mathbf{S}^b + \mathbf{P}$ is positive definite if and only if $\beta = \langle\Theta|\mathbf{P}(\mathbf{S}^b)^{-1}\mathbf{P}|\Theta\rangle$ satisfies $\beta < 1$, i.e.,

$$\beta \equiv \sum_i^n \langle\Theta|\mathbf{P}|\Phi_i\rangle\langle\Phi_i|\mathbf{P}|\Theta\rangle < 1. \tag{17}$$

According to this lemma, the slope $1 - \beta$ of a line $g(\varepsilon)$ must be positive. Since the derivative of the function $\Omega(\varepsilon)$ is negative, relations (16) and (17) imply

Lemma 2. (a) The function $h(\varepsilon)$ has negative derivative

$$\frac{\mathrm{d}h(\varepsilon)}{\mathrm{d}\varepsilon} < 0 \tag{18a}$$

on the entire real axis, except in those points $\varepsilon = \lambda_j$ where the unperturbed eigenvalue λ_j is active.

(b) In the limit $\varepsilon \to \pm\infty$ one has

$$\lim_{\varepsilon\to\pm\infty} \frac{\mathrm{d}h(\varepsilon)}{\mathrm{d}\varepsilon} = \beta - 1 < 0. \tag{18b}$$

The function $h(\varepsilon)$ is thus monotonically decreasing function on the entire real axis, except in those points $\varepsilon = \lambda_j$ where the unperturbed eigenvalue λ_j is active. In such points the function $h(\varepsilon)$ diverges. Hence and from (7) it follows that if the adjacent unperturbed eigenvalues λ_s and λ_{s+1} are active, and if these eigenvalues differ from each other, then there is exactly one root ε_k of $h(\varepsilon)$ in the open interval $(\lambda_s, \lambda_{s+1})$. This root is a cardinal eigenvalue of the augmented eigenvalue equation, and there is no other eigenvalue of this equation in the interval $(\lambda_s, \lambda_{s+1})$. According to (18b), the same applies to the intervals $(-\infty, \lambda_1)$ and (λ_n, ∞), provided the extreme unperturbed eigenvalues λ_1 and λ_n are active.

More generally, if λ_s and λ_p $(\lambda_s < \lambda_p)$ are active eigenvalues of the unperturbed system which are not necessarily adjacent, and if all the intervening eigenvalues $\lambda_j \in (\lambda_s, \lambda_p)$ are passive, then there is exactly one root $\varepsilon = \varepsilon_k$ of $h(\varepsilon)$ in the open interval (λ_s, λ_p). This root is an eigenvalue of the augmented eigenvalue equation (4a), and this eigenvalue can be either cardinal or singular. It is singular if it coincides with some passive unperturbed eigenvalue $\lambda_j \in (\lambda_s, \lambda_p)$, otherwise it is cardinal.

This implies that if all the unperturbed eigenvalues λ_i $(i = 1, \ldots, n)$ are nondegenerate and active, they are interlaced with the perturbed eigenvalues ε_k according to

$$\varepsilon_1 < \lambda_1 < \varepsilon_2 < \lambda_2 < \cdots < \varepsilon_n < \lambda_n < \varepsilon_{n+1}. \tag{19}$$

Relation (19) describes global distribution of the perturbed eigenvalues in the special but important case when all eigenvalues λ_i of the unperturbed system are nondegen-

erate and active. Those conditions can be relaxed. If the eigenvalue equation (1a) has some degenerate and/or passive eigenvalues λ_i, there is always an infinitesimal variation of the matrix elements of a matrix **B** such that the resulting eigenvalue equation has all eigenvalues nondegenerate and active. Eigenvalues of this slightly perturbed eigenvalue equation and the eigenvalues of the corresponding augmented eigenvalue equation satisfy interlacing condition (19). However, each eigenvalue of the eigenvalue equation (1a) is a continuous function of the matrix elements of the matrix **B**. Each eigenvalue of the augmented eigenvalue equation (4a) is also a continuous function of the matrix elements of the matrix **B**. Hence we have the following

Interlacing rule. Let the initial eigenvalues λ_i and the augmented eigenvalues ε_k be arranged in the nondecreasing order. Then:

(a) Eigenvalues ε_k of the augmented system are interlaced with the eigenvalues λ_i of the initial system according to

$$\varepsilon_1 \leqslant \lambda_1 \leqslant \varepsilon_2 \leqslant \lambda_2 \leqslant \cdots \leqslant \varepsilon_n \leqslant \lambda_n \leqslant \varepsilon_{n+1}. \tag{20a}$$

(b) If the adjacent unperturbed eigenvalues λ_i and λ_{i+1} are distinct and active, then in the relation (20a) a strict inequality applies

$$\lambda_i < \varepsilon_{i+1} < \lambda_{i+1}. \tag{20b}$$

Concerning point (b) of the above rule, there are additional possibilities that either one or both of the adjacent unperturbed eigenvalues λ_i and λ_{i+1} ($\lambda_i \neq \lambda_{i+1}$) is passive. If this is the case, perturbed eigenvalue ε_{i+1} may coincide with the passive unperturbed eigenvalue. In order to investigate this case in more details, one has to calculate the function $h(\varepsilon)$ in the point of the passive unperturbed eigenvalue or eigenvalues. For example, if λ_i and λ_{i+1} are adjacent and distinct unperturbed eigenvalues, and if λ_i is passive while λ_{i+1} is active, one has to calculate $h(\lambda_i)$. If $h(\lambda_i) > 0$, and since $h(\varepsilon)$ is monotonically decreasing in the interval $[\lambda_i, \lambda_{i+1})$, there is a root of $h(\varepsilon)$ in this interval, and hence $\lambda_i < \varepsilon_{i+1} < \lambda_{i+1}$. Augmented eigenvalue ε_{i+1} is thus cardinal. If however $h(\lambda_i) < 0$, there is no cardinal eigenvalue in this interval. Hence and due to (20a) one has $\lambda_i = \varepsilon_{i+1} < \lambda_{i+1}$ and ε_{i+1} is singular. In a similar way one can analyse other possibilities.

In many cases extreme eigenvalues ε_1 and ε_{n+1} are of special interest. Consider for example the smallest perturbed eigenvalue ε_1. According to the above analyse one has $\varepsilon_1 < \lambda_1$, unless the unperturbed eigenvalue λ_1 is passive and unless in addition $h(\lambda_1) \geqslant 0$. Thus the augmented eigenvalue equation will decrease the lowest eigenvalue λ_1 whenever this eigenvalue is active. If however this eigenvalue is passive, it will be decreased by the perturbation if and only if $h(\lambda_1) < 0$.

Note finally that interlacing rule depends on the condition (17) that guarantees matrix **S** to be positive definite. If this condition is not satisfied, matrix **S** is not positive definite, and some of the perturbed eigenvalues may be complex. There is even the possibility for the perturbed system to have less then $(n + 1)$ eigenvalues, in which case this system is defective.

5. Numerical considerations

Numerically the above suggested method has two important features, relatively small storage requirement, and relatively small operation count.

Consider first storage requirement. In a standard approach in order to solve generalised eigenvalue equation (4a) one has to store in a computer memory matrix elements H_{ij} and S_{ij} of matrices $\mathbf{H}$ and $\mathbf{S}$. If those matrices are real symmetric, and if the symmetry $H_{ij} = H_{ji}$ and $S_{ij} = S_{ji}$ is fully exploited, this requires the storage of approximately n^2 matrix elements. If those matrices are Hermitian but not real, storage doubles and equals approximately $2n^2$. Additional storage is needed in order to perform diagonalization and to keep various intermediate results. In all those cases standard storage requirement is of the order $O(n^2)$. In the LRP approach in order to find the eigenvalues of the augmented eigenvalue equation (4a) one has to find roots of the function $h(\varepsilon)$. This function is fully defined by n unperturbed eigenvalues λ_i, n real coefficients c_i, and three additional quantities α, β and E. Minimum additional storage is needed in order to obtain roots of $h(\varepsilon)$. The entire storage requirement is hence approximately $2n$ which is of the order $O(n)$. This storage is an order of magnitude smaller than the storage required in a standard approach.

If besides the eigenvalues the corresponding eigenvectors are also needed, the LRP storage is slightly enhanced, but it is still of the order $O(n)$. In conclusion, whether only eigenvalues or also eigenvectors are required, in both cases LRP storage requirement is of the order $O(n)$. This is substantial saving in storage, especially for large n. Consequently, with the LRP approach one can easily treat matrix augmentation problem for matrices of the order of few millions on a standard PC computer.

Consider now operation count. This quantity is usually expressed in terms of the number of flops needed to perform a particular algorithm. A flop roughly constitutes the effort of doing a floating point add, a floating point multiply, and a little subscribing [1]. Thus, the number of flops approximately equals the number of multiplicative operations $(\times, \div)$. Therefore, one can estimate operation count by estimating the number of multiplicative operations.

In the LRP approach all cardinal eigenvalues, and in addition some singular eigenvalues of the perturbed eigenvalue equation are roots of the function $h(\varepsilon)$. Hence, the main numerical load involves the search of those roots. For the sake of simplicity, we will consider real matrix augmentation problem where matrices involved are real symmetric. Generalisation to arbitrary Hermitian matrices is straightforward.

In order to initiate calculation of the roots of $h(\varepsilon)$, one has first to calculate $2n$ matrix elements $\langle\Theta|\mathbf{V}|\Phi_i\rangle$ and $\langle\Theta|\mathbf{P}|\Phi_i\rangle$. In the base $\{|r\rangle\}$ one has $\langle\Theta|\mathbf{V}|\Phi_i\rangle = \sum_r \langle\Theta|\mathbf{V}|r\rangle\langle r|\Phi_i\rangle$ and $\langle\Theta|\mathbf{P}|\Phi_i\rangle = \sum_r \langle\Theta|\mathbf{P}|r\rangle\langle r|\Phi_i\rangle$. In a most general case involving real matrices, calculation of these matrix elements requires $2n^2$ multiplications. However, in many cases this operation count is much smaller. For example, most of the matrix elements $\langle\Theta|\mathbf{V}|r\rangle$ and $\langle\Theta|\mathbf{P}|r\rangle$ may be zero. If n is large this is usually the case, since in the majority of standard problems vector $|\Theta\rangle$ that describes system $\mathcal{S}^a$ usually interacts only with relatively few base vectors $|r\rangle$ of the system $\mathcal{S}^b$. As n increases one usually

finds that the number of nonzero matrix elements $\langle\Theta|\mathbf{V}|r\rangle$ and $\langle\Theta|\mathbf{P}|r\rangle$ is of the order substantially lower than $O(n)$, in many cases of the order $O(1)$. This reduces above operation count to $O(n)$. In some other cases matrix elements $\langle\Theta|\mathbf{V}|\Phi_i\rangle$ and $\langle\Theta|\mathbf{P}|\Phi_i\rangle$ may be given in a closed analytical form, which eliminates the corresponding operation count. Once these matrix elements are known, next step is to construct the function $h(\varepsilon)$. This requires calculation of n coefficients c_i and calculation of the quantities α and β. Calculation of coefficients c_i requires $2n$ multiplications, while calculation of quantities α and β requires approximately $3n$ multiplications. Hence the construction of the function $h(\varepsilon)$ requires approximately $5n$ multiplications, which is of the order $O(n)$. In conclusion, this preparatory phase, which is needed in order to obtain the function $h(\varepsilon)$, requires at most $O(n^2)$ operations ($2n^2 + 5n$ multiplications), but it can be as low as $O(n)$ operations ($5n$ multiplications). This estimate applies to a most general matrix augmentation problem involving real symmetric matrices. In the important special case $\mathbf{P} = 0$ one has $\langle\Theta|\mathbf{P}|\Phi_i\rangle = 0$ and $\alpha = \beta = 0$. Operation count accordingly decreases to at most $(n^2 + n)$ multiplications, or to as few as only n multiplications. Operation count equals $(n^2 + n)$ if one has to calculate matrix elements $\langle\Theta|\mathbf{V}|\Phi_i\rangle$ and if in addition almost all matrix elements $\langle\Theta|\mathbf{V}|r\rangle$ are nonzero. Operation count equals n if matrix elements $\langle\Theta|\mathbf{V}|\Phi_i\rangle$ are *a priori* known, and it is of the order $O(n)$ (but higher than n) if the number of nonzero matrix elements $\langle\Theta|\mathbf{V}|r\rangle$ is of the order $O(1)$.

Once the function $h(\varepsilon)$ is constructed, next step is to find root or roots ε_k of this function. Most root finding methods start with some initial approximate root $\varepsilon_k^{(0)}$, which is then iteratively improved. This iteration requires on average It recalculations of the function $h(\varepsilon)$ and (depending on the method) its derivative for various values of ε. Each recalculation of the function $h(\varepsilon)$ requires approximately n divisions. If the derivative of $h(\varepsilon)$ is also needed, one has to perform an additional n multiplications. Hence this last step requires, depending on the method, either $It \cdot n$ or $2 \cdot It \cdot n$ multiplicative operations per root. This is $O(n)$ operations per root, or $O(n^2)$ operations if all roots of $h(\varepsilon)$ are required. Once a particular root is obtained, the corresponding eigenvector (10a) can be easily derived with essentially n divisions. Concerning normalisation, the quantity W_k given by (14b) can be calculated with n additional multiplicative operations. Total operation count to find all eigenvalues and all normalized eigenvectors is hence of the order $O(n^2)$. This compares very favourable with the operation count of various direct matrix diagonalization methods, such as Jacobi, Givens and Householder, which require $O(n^3)$ operations in order to obtain all eigenvalues and/or eigenvectors [1,2]. In addition, if a single eigenvalue and/or eigenvector is required, and if matrix elements $\langle\Theta|\mathbf{V}|\Phi_i\rangle$ and $\langle\Theta|\mathbf{P}|\Phi_i\rangle$ are known, or if the number of nonzero matrix elements $\langle\Theta|\mathbf{V}|r\rangle$ and $\langle\Theta|\mathbf{P}|r\rangle$ is of the order $O(1)$, this can be done with as few as $O(n)$ operations.

6. Numerical results

In order to verify the LRP matrix augmentation method and to estimate its performance, a computer program was written by the author. The program was written in C++, and the calculation was done on a 1.5 GHz Pentium 4 PC computer. In a calcu-

lation double precision floating point numbers that require eight bytes per number and that are accurate to approximately 15 significant digits were used. Instead of arbitrary Hermitian matrices, real Hermitian matrices were considered. Those matrices are symmetric. There are essentially no new features if instead of real Hermitian more general complex Hermitian matrices are treated. The restriction to real matrices is of no consequence as far as the numerical verification of the suggested method is concerned.

Concerning verification of the LRP method, LRP results were directly compared with the results obtained by the standard diagonalization method. This was done only for relatively small matrices ($n \leqslant 1000$). Due to the excessive storage requirement, it was not possible to perform a standard diagonalization on a PC computer in the case of large matrices. Actual calculation was simulated with random matrices. Matrix $\mathbf{B}$ was constructed as real symmetric matrix with matrix elements chosen as uniform random numbers in some predefined interval. In a similar way was constructed matrix $\mathbf{S}^b$. In order for this matrix to be positive definite, diagonal elements of $\mathbf{S}^b$ were chosen as relatively large random positive numbers, while off-diagonal elements were chosen as relatively small random numbers. With such a choice resulting matrix is diagonally dominant, and if the intervals for random diagonal and of-diagonal matrix elements are selected in an appropriate way, it is positive definite. After matrices $\mathbf{B}$ and $\mathbf{S}^b$ were constructed, generalised eigenvalue equation (1) was solved in a standard way using the combination of the Cholesky decomposition and the symmetric QR algorithm [1]. This was done in two steps. In the first step matrix $\mathbf{S}^b$ was decomposed by Cholesky decomposition according to $\mathbf{S}^b = \mathbf{G} \cdot \mathbf{G}^T$ where $\mathbf{G}$ is a lower triangular matrix and where $\mathbf{G}^T$ is transpose of $\mathbf{G}$ [1]. In this way, generalised eigenvalue equation (1a) was transformed into a simple eigenvalue equation $\mathbf{C}|\phi_i\rangle = \lambda_i|\phi_i\rangle$ where $\mathbf{C} = \mathbf{G}^{-1}\mathbf{B}(\mathbf{G}^T)^{-1}$ and where $|\phi_i\rangle = \mathbf{G}^T|\Phi_i\rangle$. In the second step, the obtained eigenvalue equation was solved using symmetric QR algorithm. This algorithm involves initial Householder tridiagonalization followed by the QR algorithm proper [1]. This standard approach that combines Cholesky decomposition with the symmetric QR algorithm is one of the best methods to solve generalised symmetric eigenvalue equation. It requires about $7n^3$ flops [1]. Once the unperturbed eigenvectors $|\Phi_i\rangle$ are obtained, they were orthonormalized according to the relation (1b). Concerning augmented eigenvalue equation, matrix elements $\langle\Theta|\mathbf{V}|r\rangle$ and $\langle\Theta|\mathbf{P}|r\rangle$ were also constructed as uniform random numbers in some predefined interval. In order for the matrix $\mathbf{S}$ to be positive definite, matrix elements $\langle\Theta|\mathbf{P}|\Phi_i\rangle$ should satisfy the condition (17) of lemma 1. In the base $\{|r\rangle\}$ this condition reads $\sum_{rp}\langle\Theta|\mathbf{P}|r\rangle\langle r|(\mathbf{S}^b)^{-1}|p\rangle\langle p|\mathbf{P}|\Theta\rangle < 1$. Accordingly, random matrix elements $\langle\Theta|\mathbf{P}|r\rangle$ were rescaled in order to satisfy this condition. Eigenvalue E was also treated as random quantity. Once the augmented eigenvalue equation was constructed in this way, it was solved by the LRP approach and by a standard diagonalization method. In this way, one could verify LRP eigenvalues and eigenvectors by a direct comparison with eigenvalues and eigenvectors obtained in a standard way. This comparison did show that the LRP matrix augmentation method is numerically accurate and reliable.

In order to estimate the performance of the LRP approach, the unperturbed system was simulated in the way that is more appropriate for this method. Unperturbed

eigenvalues λ_i were chosen as random numbers in some predefined interval. In a similar way was chosen eigenvalue E. Matrix elements $\langle\Theta|\mathbf{V}|\Phi_i\rangle$ and $\langle\Theta|\mathbf{P}|\Phi_i\rangle$ were also simulated as random numbers, and those later matrix elements were subject to the condition (17) of lemma 1. Next a LRP calculation was performed. This calculation was repeated for various matrices of the order $n = 10^2$ up to including $n = 5 \cdot 10^6$. In order to cover this entire range, five different sets of such calculations were done. In the first set matrices of order $n = 10^2(10^2)9 \cdot 10^2$ were considered, in the second set matrices of order $n = 10^3(10^3)9 \cdot 10^3$ were considered, in the third set matrices of order $n = 10^4(10^4)9 \cdot 10^4$ were considered, in the forth set matrices of the order $n = 10^5(10^5)9 \cdot 10^5$ were considered, while in the fifth set huge matrices of the order $n = 10^6(10^6)5 \cdot 10^6$ were considered. The entire calculation was repeated few times with various choices for predefined intervals for random quantities λ_i, $\langle\Theta|\mathbf{V}|\Phi_i\rangle$ and $\langle\Theta|\mathbf{P}|\Phi_i\rangle$. In this way, one could simulate the case of the weak as well as strong and very strong interactions. This was done covering few orders of magnitude, starting with the weak interaction (relatively small quantities $\langle\Theta|\mathbf{V}|\Phi_i\rangle$) to very strong interaction (relatively large quantities $\langle\Theta|\mathbf{V}|\Phi_i\rangle$).

According to the above discussion, LRP operation count per eigenvalue and per eigenvector should be proportional to the dimension n of the generalised eigenvalue equation. However, the corresponding times are only approximately proportional to the operation count. Depending on the matrix dimension and internal computer architecture, some operations are done faster using computer cache, while some require access to the computer RAM that is slower. Hence average time needed to perform a single flop depends on the relative speed of cache and RAM memory access, on the amount of memory that can be stored in the computer cache, on the cache status, and on the dimension n of matrices involved. In addition, in the case of cardinal eigenvalues, operation count depends on the number of iterations that are required to obtain the corresponding root of the function $h(\varepsilon)$. This number varies from eigenvalue to eigenvalue, and for each particular eigenvalue ε_k it strongly depends on the choice of the initial approximate eigenvalue $\varepsilon_k^{(0)}$. According to the interlacing rule each cardinal eigenvalue ε_k $(2 \leqslant k \leqslant n)$ satisfies $\lambda_{k-1} < \varepsilon_k < \lambda_k$. In the present computer program, this initial approximation was chosen as $\varepsilon_k^{(0)} = (\lambda_{k-1} + \lambda_k)/2$. This is a very crude approximation, and much better choices, based on some approximate estimation of the perturbed eigenvalue are possible. Nevertheless, this choice is relatively unbiased, and it is good enough for the assessment of the LRP performance. In view of all above factors obtained times per eigenvalue and per eigenvector can be only approximately proportional to the matrix dimension n.

Typical results of the LRP method are shown in tables 1 and 2. In table 1 are given times required to calculate a single eigenvalue ε_k, while in table 2 are given times required to calculate a single normalised eigenvector $|\Psi_k\rangle$, once the corresponding eigenvalue ε_k is known. In the case of large matrices, calculation of all eigenvalues and/or eigenvectors was quite time consuming, and therefore in this case only a relatively small number of randomly selected eigenvalues and eigenvectors were calculated. This is indicated with an asterisk (*) in those tables.

Table 1
Times (in seconds) needed to calculate a single augmented eigenvalue by the LRP method.

n	10^2	10^3	10^4	10^5	10^6
$1 \cdot n$	0.000035	0.00036	0.0036	0.035*	0.33*
$2 \cdot n$	0.000072	0.00075	0.0072	0.070*	0.62*
$3 \cdot n$	0.00011	0.0011	0.010	0.10*	0.95*
$4 \cdot n$	0.00015	0.0014	0.014	0.13*	1.32*
$5 \cdot n$	0.00018	0.0018	0.018*	0.17*	1.68*
$6 \cdot n$	0.00022	0.0022	0.021*	0.21*	
$7 \cdot n$	0.00026	0.0026	0.025*	0.24*	
$8 \cdot n$	0.00030	0.0029	0.028*	0.28*	
$9 \cdot n$	0.00033	0.0032	0.031*	0.31*	

* Times based on the calculation of randomly selected eigenvalues.

Table 2
Times (in seconds) needed to calculate a single augmented eigenvector by the LRP method.

n	10^2	10^3	10^4	10^5	10^6
$1 \cdot n$	0.0000062	0.000064	0.00067	0.0070*	0.071*
$2 \cdot n$	0.000013	0.00013	0.0014	0.014*	0.14*
$3 \cdot n$	0.000019	0.00019	0.0021	0.021*	0.21*
$4 \cdot n$	0.000025	0.00026	0.0028	0.029*	0.29*
$5 \cdot n$	0.000032	0.00033	0.0035*	0.035*	0.36*
$6 \cdot n$	0.000039	0.00040	0.0042*	0.043*	
$7 \cdot n$	0.000044	0.00046	0.0049*	0.050*	
$8 \cdot n$	0.000051	0.00053	0.0056*	0.057*	
$9 \cdot n$	0.000057	0.00060	0.0063*	0.065*	

* Times based on the calculation of randomly selected eigenvectors.

Times reported in table 1 are obtained under the assumption that quantities $\langle\Theta|\mathbf{V}|\Phi_i\rangle$ and $\langle\Theta|\mathbf{P}|\Phi_i\rangle$ are known. This assumption is in the spirit with the LRP approach, and it is justified in many cases, especially if n is large. If those quantities are not known, and if in addition almost all matrix elements $\langle\Theta|\mathbf{V}|r\rangle$ and $\langle\Theta|\mathbf{P}|r\rangle$ are nonzero, there is an overall overhead of approximately $2n^2$ multiplications required to calculate these quantities. This is an extreme case, and all intermediate cases are possible. Usually vector $|\Theta\rangle$ interacts only with $O(1)$ base vectors $|r\rangle$ of the system $\mathcal{S}^b$, and this overhead reduces to $O(n)$. In the extreme case of the $O(n^2)$ overhead, times in table 1 should be interpreted as approximate times per eigenvalue, rather than individual times required to obtain selected eigenvalue. If all eigenvalues are calculated, main numerical load is due to multiple iterative recalculations of the function $h(\varepsilon)$, and the per eigenvalue overhead due to the calculation of quantities $\langle\Theta|\mathbf{V}|\Phi_i\rangle$ and $\langle\Theta|\mathbf{P}|\Phi_i\rangle$ is relatively small.

Furthermore, times reported in tables 1 and 2 are average times taken over many choices of random matrices. For all previous reasons, those times are subject to relatively large fluctuations. Those fluctuations are particularly large in the case of the eigenvalues (table 1) since for each n the average number of iterations per eigenvalue and hence the operation count depends on the selected random matrix. However, in the case of the corresponding eigenvectors (table 2) operation count depends only on the matrix dimension n, and not on the particular choice of this matrix. Fluctuations are hence smaller and they are mainly due to variations in the use of computer cache.

Times required to calculate a particular eigenvalue are in general slightly better than linear (table 1). This indicates that on average large matrices require slightly smaller number of iterations per eigenvalue. This result of course depends on the particular choice of the initial approximation $\varepsilon_k^{(0)}$ and it may vary with this choice. Nevertheless, the deviation from linearity in table 1 is very mild over many orders of magnitude, and this strongly suggests that the average operation count per eigenvalue is indeed proportional to n. In addition, one can devise an algorithm that significantly improves convergence and stability of the iterative calculation of the eigenvalues [6]. Thus, times reported in table 1 can be substantially reduced. Simultaneously fluctuations of the operation counts per eigenvalue are also reduced. The details of this improved algorithm for the calculation of the augmented eigenvalues will be given elsewhere [6].

Once the particular eigenvalue ε_k is known, operation count to obtain the corresponding eigenvector is to the very good approximation proportional to n. As shown in table 2, average time per eigenvector is slightly worst than linear. This result can be attributed to the relatively better use of computer cache in the case of small matrices. If the matrix is sufficiently small, it is possible for all input data to fit into computer cache, while if the matrix is large this is not possible. Hence, on average, time required to perform a single flop is smaller in the case of a small matrix, and it should slowly increase with the increase of n. The deviation from linearity in table 2 is however very mild over many orders of magnitude, and hence one can conclude that the LRP operation count per eigenvector is to a very good approximation proportional to n.

As an example, consider the case $n = 1000$. In this case, LRP algorithm requires about 0.42 seconds in order to obtain all eigenvalues and eigenvectors of the augmented eigenvalue equation. Standard method that combines the Cholesky decomposition with the symmetric QR algorithm [1] requires about 120 seconds in order to solve the same problem. The case $n = 1000$ was the largest case to be solved by this standard method. If all solutions are required, relative advantage of the LRP approach increases linearly with the increase of n. Thus already in the case $n = 10^4$ LRP approach requires about 43 seconds in order to find all augmented solutions, while the above standard algorithm would require, provided it could be done on a PC computer, more than 33 hours. Relative advantage of the LRP approach is even more pronounced if only a single eigenvalue and/or eigenvector is required. If matrix elements $\langle\Theta|\mathbf{V}|\Phi_i\rangle$ and $\langle\Theta|\mathbf{P}|\Phi_i\rangle$ that define augmented interaction are given by the conditions of the matrix augmentation problem, and if $n = 10^4$, one needs only about 0.0043 seconds in order to obtain any particular augmented eigenvalue and the corresponding eigenvector. If matrices are as large

as $n = 10^6$, this time increases to only about 0.4 seconds. Even when matrix elements $\langle\Theta|\mathbf{V}|\Phi_i\rangle$ and $\langle\Theta|\mathbf{P}|\Phi_i\rangle$ are not known, operation count to obtain any particular eigenvalue and/or eigenvector is still very small and of the order $O(n)$, provided vector $|\Theta\rangle$ interacts only with relatively few base vectors $|r\rangle$ of the system $\mathcal{S}^b$.

7. Conclusions

Augmentation of the generalised $n \times n$ eigenvalue equation $\mathbf{B}|\Phi_i\rangle = \lambda_i \mathbf{S}^b|\Phi_i\rangle$ $(i = 1, \ldots, n)$ by a single row and a single column to the generalised $(n+1)(n+1)$ eigenvalue equation $\mathbf{H}|\Psi_k\rangle = \varepsilon_k \mathbf{S}|\Psi_k\rangle$ $(k = 1, \ldots, n+1)$ is considered. Following ideas of the LRP approach [5], the solution of the augmented eigenvalue equation is expressed in a closed form in terms of the eigenvalues λ_i and orthonormalized eigenvectors $|\Phi_i\rangle$ of the original eigenvalue equation.

It is found that the operation count to obtain all augmented eigenvalues and all augmented eigenvectors by this method is of the order $O(n^2)$. Other presently known methods usually require $O(n^3)$ operations in order to obtain all augmented eigenvalues and eigenvectors. Even in the case when only a single eigenvalue and/or eigenvector is required, operation count of those other methods is still higher than $O(n^2)$. Unless matrices involved are of some special kind, such as sparse matrices, or unless the perturbation is small, operation count to find an arbitrary eigenvalue and/or eigenvector is again of the order $O(n^3)$. The problem is substantially more complex in the case of the generalised eigenvalue equation. However, LRP method in many cases requires only $O(n)$ operations in order to find any particular eigenvalue and/or eigenvector of the generalised eigenvalue equation. This operation count is as low as $O(n)$ if matrix elements $\langle\Theta|\mathbf{V}|\Phi_i\rangle$ and $\langle\Theta|\mathbf{P}|\Phi_i\rangle$ are known, or if the number of nonzero matrix elements $\langle\Theta|\mathbf{V}|r\rangle$ and $\langle\Theta|\mathbf{P}|r\rangle$ is of the order $O(1)$. First assumption applies to some problems involving huge matrices, when matrix elements $\langle\Theta|\mathbf{V}|\Phi_i\rangle$ and $\langle\Theta|\mathbf{P}|\Phi_i\rangle$ are given in an analytic closed form. Second assumption applies to the case when system $\mathcal{S}^a$ described by the vector $|\Theta\rangle$ interacts only with relatively few base vectors $|r\rangle$ of the system $\mathcal{S}^b$. This is usually the case in most practical problems. In conclusion, if all eigenvalues and/or eigenvectors are required, LRP solution to the matrix augmentation problem is usually one order of magnitude faster than other presently known methods. If only a single eigenvalue and/or eigenvector is required, in many cases of interest, LRP approach is two orders of magnitude faster than other methods.

The storage requirement of the LRP approach is also favourable. Direct diagonalization methods usually require the storage of matrix elements of all matrices involved. This is of the order $O(n^2)$. However, the storage requirement of the LRP approach is of the order $O(n)$. Hence, one can treat by these method very large matrices. In the present manuscript, matrices as large as $5 \cdot 10^6 \times 5 \cdot 10^6$ were considered on a standard PC computer.

Matrix augmentation problem naturally arises whenever one knows a solution to an eigenvalue equation and one wants to improve this solution by the extension of the initial vector space with some additional vectors. Many practical problems are of this

kind. For example, one may know the solution of some MO calculation in a selected base set of atomic orbitals. This solution can be always improved with the inclusion of additional atomic orbitals in the original basic set. Relative importance of candidate orbitals and their influence on the resulting eigenvalues and eigenvectors can be very efficiently analysed by the suggested LRP method.

Appendix

A.1. Proof of theorems I and II

If $\mathbf{S}^b$ is Hermitian and positive definite in X_n^b, $(\mathbf{S}^b)^{-1/2}$ is also Hermitian and positive definite. Eigenvalue equation (1a) is hence equivalent to

$$\mathbf{B}_0|\phi_i\rangle = \lambda_i|\phi_i\rangle \tag{A1}$$

where

$$\mathbf{B}_0 = \left(\mathbf{S}^b\right)^{-1/2}\mathbf{B}\left(\mathbf{S}^b\right)^{-1/2}, \qquad |\phi_i\rangle = \left(\mathbf{S}^b\right)^{1/2}|\Phi_i\rangle. \tag{A1$'$}$$

Hermiticity of $\mathbf{B}$ and $\mathbf{S}^b$ implies hermiticity of $\mathbf{B}_0$, and the eigenvalues λ_i of the unperturbed equation (1a) are hence real. Further, eigenvectors $|\phi_i\rangle$ of $\mathbf{B}_0$ can be orthonormalized according to $\langle\phi_i|\phi_j\rangle = \delta_{ij}$, which implies (1b). The set $\{|\Phi_i\rangle\}$ is hence complete. Similar conclusion applies to the perturbed eigenvalue equation (4a).

Define operator

$$\mathbf{I}^b = \sum_i^n |\Phi_i\rangle\langle\Phi_i|\mathbf{S}^b. \tag{A2}$$

Using (1b) one finds $\mathbf{I}^b|\Phi_i\rangle = |\Phi_i\rangle$ for each eigenvector $|\Phi_i\rangle$ of the eigenvalue equation (1a). Since these eigenvectors form a complete set in X_n^b, operator $\mathbf{I}^b$ is a unit operator in this space. Hence

$$\mathbf{I} = \mathbf{I}^b + |\Theta\rangle\langle\Theta| \tag{A2$'$}$$

is a unit operator in the augmented space X_{n+1}. In a similar way, one obtains identity

$$\mathbf{B} = \sum_i^n \mathbf{S}^b|\Phi_i\rangle\lambda_i\langle\Phi_i|\mathbf{S}^b. \tag{A3}$$

We now derive theorems I and II following general ideas of the LRP approach [5].

Relations (4) and (3) imply

$$\left[\mathbf{B} + (\mathbf{V} - \varepsilon_k\mathbf{P})|\Theta\rangle\langle\Theta| + |\Theta\rangle\langle\Theta|(\mathbf{V} - \varepsilon_k\mathbf{P}) + (E - \varepsilon_k)|\Theta\rangle\langle\Theta|\right]|\Psi_k\rangle = \varepsilon_k\mathbf{S}^b|\Psi_k\rangle.$$

Multiplying this expression from left by $\langle\Phi_i|$, and using (1a) and the orthogonality $\langle\Phi_i|\Theta\rangle = 0$, one finds

$$(\varepsilon_k - \lambda_i)\left\langle\Phi_i\middle|\mathbf{S}^b\middle|\Psi_k\right\rangle = \langle\Phi_i|\mathbf{V} - \varepsilon_k\mathbf{P}|\Theta\rangle\langle\Theta|\Psi_k\rangle, \quad i = 1, \ldots, n. \tag{A4}$$

Multiplying the same expression with $\langle\Theta|$ and using properties $\langle\Theta|\mathbf{B} = \langle\Theta|\mathbf{S}^b = 0$ and $\langle\Theta|\mathbf{V}|\Theta\rangle = \langle\Theta|\mathbf{P}|\Theta\rangle = 0$ one obtains

$$\langle\Theta|\mathbf{V} - \varepsilon_k\mathbf{P}|\Psi_k\rangle + (E - \varepsilon_k)\langle\Theta|\Psi_k\rangle = 0. \tag{A5}$$

Relations (A4) and (A5) are our starting relations for the derivation of theorems I and II.

Cardinal eigenvalues ($\varepsilon_k \notin \{\lambda_i\}$)

Let $\varepsilon_k \notin \{\lambda_i\}$ be an eigenvalue of the perturbed eigenvalue equation (4a). Divide (A4) by $(\varepsilon_k - \lambda_i)$ $(i = 1, \ldots, n)$, multiply the obtained relation by $|\Phi_i\rangle$ and sum over i to obtain:

$$\sum_i^n |\Phi_i\rangle\langle\Phi_i|\mathbf{S}^b|\Psi_k\rangle = \langle\Theta|\Psi_k\rangle \sum_i^n \frac{\langle\Phi_i|\mathbf{V} - \varepsilon_k\mathbf{P}|\Theta\rangle}{\varepsilon_k - \lambda_i}|\Phi_i\rangle.$$

Adding to both sides of this relation $|\Theta\rangle\langle\Theta|\Psi_k\rangle$ and using (A2) one finds:

$$|\Psi_k\rangle = \langle\Theta|\Psi_k\rangle \sum_i^n \frac{\langle\Phi_i|\mathbf{V} - \varepsilon_k\mathbf{P}|\Theta\rangle}{\varepsilon_k - \lambda_i}|\Phi_i\rangle + \langle\Theta|\Psi_k\rangle|\Theta\rangle. \tag{A6}$$

Since $|\Psi_k\rangle$ is nontrivial, one must have $\langle\Theta|\Psi_k\rangle \neq 0$. Without loss of generality one can choose $\langle\Theta|\Psi_k\rangle = 1$. With this choice (A6) reduces to (10a) while (A5) reduces to (11).

Next one has to determine the perturbed eigenvalue ε_k. Multiplying (10a) from left by $\langle\Theta|(\mathbf{V} - \varepsilon_k\mathbf{P})$ one obtains

$$\langle\Theta|\mathbf{V} - \varepsilon_k\mathbf{P}|\Psi_k\rangle = \Omega_0(\varepsilon_k), \tag{A7}$$

where

$$\Omega_0(\varepsilon) = \sum_i^n \frac{\langle\Theta|\mathbf{V} - \varepsilon\mathbf{P}|\Phi_i\rangle\langle\Phi_i|\mathbf{V} - \varepsilon\mathbf{P}|\Theta\rangle}{\varepsilon - \lambda_i}, \quad \varepsilon \notin \{\lambda_i\}. \tag{A8}$$

Relation (A5) and condition $\langle\Theta|\Psi\rangle = 1$ imply

$$\Omega_0(\varepsilon_k) = \varepsilon_k - E. \tag{A9}$$

Eigenvalue ε_k is hence a root of (A9). In order to facilitate numerical evaluation of the function $\Omega_0(\varepsilon)$ for multiple values of ε, it is convenient to eliminate dependence on ε from the numerator of a sum in (A8). Using the identity

$$\begin{aligned}(a - \varepsilon b)\big(a^* - \varepsilon b^*\big) = (a - \lambda b)\big(a^* - \lambda b^*\big) + (\lambda - \varepsilon)\big[(a - \lambda b)b^* + \big(a^* - \lambda b^*\big)b\big] \\ + (\lambda - \varepsilon)^2 bb^*\end{aligned}$$

one finds

$$\Omega_0(\varepsilon) = \Omega(\varepsilon) + \alpha + \varepsilon\beta, \tag{A10}$$

where the function $\Omega(\varepsilon)$ is given by (8) while the quantities α and β are given by (9a). Relation (A9) is hence equivalent to

$$\Omega(\varepsilon_k) = (1-\beta)\varepsilon_k - E - \alpha$$

which is condition (7).

This proves that a necessary condition for $\varepsilon_k \notin \{\lambda_i\}$ to be an eigenvalue of the perturbed eigenvalue equation (4a) is that it should satisfy $h(\varepsilon_k) = 0$ and that the corresponding eigenvector is given by (10a). The inverse is also true. If $\varepsilon_k \notin \{\lambda_i\}$ satisfies $h(\varepsilon_k) = 0$, then according to the above derivation it is an eigenvalue of the augmented equation (4a), and (10a) is the corresponding eigenvector. This completes the proof of theorem I.

Singular eigenvalues ($\varepsilon_k \in \{\lambda_i\}$)

Let $\varepsilon_k = \lambda_j$ be a singular eigenvalue of the perturbed eigenvalue equation (4a). Let further λ_j be a η-degenerate eigenvalue of the original unperturbed system, and let $|\Phi_{j\nu}\rangle$ ($\nu = 1, \ldots, \eta$) be the corresponding unperturbed eigenvectors. Inserting $\varepsilon_k = \lambda_j$ in relation (A4) one obtains for $i = j$

$$\langle \Phi_{j\nu}|\mathbf{V} - \varepsilon_k \mathbf{P}|\Theta\rangle\langle\Theta|\Psi_k\rangle = 0, \quad \nu = 1, \ldots, \eta. \tag{A11}$$

Dividing (A4) by $(\varepsilon_k - \lambda_i)$ ($\lambda_i \neq \varepsilon_k$), multiplying the obtained relation by $|\Phi_i\rangle$ and summing over i one finds:

$$\sum_{i(\lambda_i \neq \varepsilon_k)}^{n} |\Phi_i\rangle\langle\Phi_i|\mathbf{S}^b|\Psi_k\rangle = \sum_{i(\lambda_i \neq \varepsilon_k)}^{n} \frac{\langle\Phi_i|\mathbf{V} - \varepsilon_k\mathbf{P}|\Theta\rangle\langle\Theta|\Psi_k\rangle}{\varepsilon_k - \lambda_i}|\Phi_i\rangle.$$

Adding to both sides of this relation $|\Theta\rangle\langle\Theta|\Psi_k\rangle + \sum_\nu |\Phi_{j\nu}\rangle\langle\Phi_{j\nu}|\mathbf{S}^b|\Psi_k\rangle$ and using (A2) one finds

$$|\Psi_k\rangle = \langle\Theta|\Psi_k\rangle \sum_{i(\lambda_i \neq \varepsilon_k)}^{n} \frac{\langle\Phi_i|\mathbf{V} - \varepsilon_k\mathbf{P}|\Theta\rangle}{\varepsilon_k - \lambda_i}|\Phi_i\rangle + \langle\Theta|\Psi_k\rangle|\Theta\rangle + \sum_{\nu}^{\eta} D_\nu|\Phi_{j\nu}\rangle \tag{A12}$$

where

$$D_\nu = \langle\Phi_{j\nu}|\mathbf{S}^b|\Psi_k\rangle, \quad \nu = 1, \ldots, \eta. \tag{A12'}$$

Relation (A12) expresses the perturbed eigenvector $|\Psi_k\rangle$as a linear combination of the unperturbed eigenvectors $|\Phi_i\rangle$ and a vector $|\Theta\rangle$. Next one has to determine unknown coefficients $\langle\Theta|\Psi_k\rangle$ and D_ν.

Multiplying (A12) from left by $\langle\Theta|(\mathbf{V} - \varepsilon_k\mathbf{P})$ one obtains

$$\langle\Theta|\mathbf{V} - \varepsilon_k\mathbf{P}|\Psi_k\rangle = \langle\Theta|\Psi_k\rangle\Omega_0(\varepsilon_k) + \sum_{\nu}^{\eta} D_\nu\langle\Theta|\mathbf{V} - \varepsilon_k\mathbf{P}|\Phi_{j\nu}\rangle \tag{A13}$$

where

$$\Omega_0(\varepsilon_k) = \sum_{i(\lambda_i \neq \varepsilon_k)}^{n} \frac{\langle \Theta | \mathbf{V} - \varepsilon_k \mathbf{P} | \Phi_i \rangle \langle \Phi_i | \mathbf{V} - \varepsilon_k \mathbf{P} | \Theta \rangle}{\varepsilon_k - \lambda_i}. \tag{A8′}$$

Relation (A8′) extends the definition of the function $\Omega_0(\varepsilon)$ to the points $\varepsilon \in \{\lambda_i\}$. If $\varepsilon \notin \{\lambda_i\}$ this function is defined according to (A8), while if $\varepsilon \in \{\lambda_i\}$ it is defined according to (A8′). Note that if λ_j is active expression (A8) has a pole in a point $\varepsilon = \lambda_j$. The function $\Omega_0(\varepsilon)$ is hence not continuous in this point. However, if λ_j is passive, expression (A8) is finite in the point $\varepsilon = \lambda_j$ and one finds that the function $\Omega_0(\varepsilon)$ is continuous and analytic in this point.

We now distinguish two cases. The eigenvalue λ_j can be either active or passive.

Case I: the eigenvalue λ_j is active

If the unperturbed eigenvalue λ_j is active, there is at least one unperturbed eigenvector $|\Phi_{j\nu}\rangle$ such that $\langle \Theta | \mathbf{V} - \lambda_j \mathbf{P} | \Phi_{j\nu} \rangle \neq 0$. Hence (A11) implies $\langle \Theta | \Psi_k \rangle = 0$. Inserting into (A12) one obtains $|\Psi_k\rangle = \sum_\nu D_\nu |\Phi_{j\nu}\rangle$. Further, (A5) implies $\langle \Theta | \mathbf{V} - \lambda_j \mathbf{P} | \Psi_k \rangle = 0$ and (A13) thus reduces to (12b). This proves that if the singular eigenvalue $\lambda_j = \varepsilon_k$ is active, all the corresponding eigenvectors are linear combinations (12a) of the unperturbed eigenvectors $|\Phi_{j\nu}\rangle$ with the coefficients D_ν that satisfy (12b). The inverse is also true. If $|\Psi\rangle$ is a linear combination (12a) of the unperturbed eigenvectors $|\Phi_{j\nu}\rangle$ with the coefficients D_ν that satisfy (12b), it is an augmented eigenvector corresponding to the eigenvalue $\varepsilon_k = \lambda_j$. Thus if λ_j is a η-degenerate unperturbed eigenvalue, $\varepsilon_k = \lambda_j$ is a $(\eta - 1)$-degenerate perturbed eigenvalue. In particular, if the unperturbed eigenvalue λ_j is nondegenerate $(\eta = 1)$, $\varepsilon_k = \lambda_j$ is not the eigenvalue of the perturbed system.

Case II: the eigenvalue λ_j is passive

If the unperturbed eigenvalue λ_j is passive, all quantities $\langle \Theta | \mathbf{V} - \lambda_j \mathbf{P} | \Phi_{j\nu} \rangle$ vanish and (A11) does not imply $\langle \Theta | \Psi_k \rangle = 0$. There are hence two possibilities, either $\langle \Theta | \Psi_k \rangle = 0$ or $\langle \Theta | \Psi_k \rangle \neq 0$.

If $\langle \Theta | \Psi_k \rangle = 0$, we obtain similar result as in the case when λ_j is active. However, since λ_j is now passive, there is no condition (12b) on the coefficients D_ν. Hence all the unperturbed eigenvectors $|\Phi_{j\nu}\rangle$ are also the perturbed eigenvectors.

If $\langle \Theta | \Psi_k \rangle \neq 0$ one can without loss of generality choose $\langle \Theta | \Psi_k \rangle = 1$. In addition, and since $|\Phi_{j\nu}\rangle$ are already shown to be the perturbed eigenvectors, one can in the relation (A12) choose $D_\nu = 0$ $(\nu = 1, \ldots, \eta)$. With this choice relation (A12) reduces to (10b), while relation (A13) reduces to

$$\Omega_0(\lambda_j) = \langle \Theta | \mathbf{V} - \lambda_j \mathbf{P} | \Psi_k \rangle \tag{A14}$$

which is relation (A7) with $\varepsilon_k = \lambda_j$.

In analogy to (A10) one finds that the quantity $\Omega_0(\lambda_j)$ can be written as

$$\Omega_0(\lambda_j) = \Omega(\lambda_j) + \alpha + \lambda_j \beta$$

where

$$\Omega(\lambda_j) = \sum_{i(\lambda_i \neq \lambda_j)} \frac{\langle\Theta|\mathbf{V} - \lambda_i\mathbf{P}|\Phi_i\rangle\langle\Phi_i|\mathbf{V} - \lambda_i\mathbf{P}|\Theta\rangle}{\lambda_j - \lambda_i}.$$

Since eigenvalue λ_j is passive the function $\Omega(\varepsilon)$ is continuous and analytic in the point $\varepsilon = \lambda_j$. Further, (A5) implies $\langle\Theta|\mathbf{V} - \lambda_j\mathbf{P}|\Psi_k\rangle = \lambda_j - E$ which is equation (11) with $\varepsilon_k = \lambda_j$. Inserting into (A14) one finally obtains

$$\Omega(\lambda_j) = (1 - \beta)\lambda_j - \alpha - E.$$

This proves that in order for the vector (10b) to be an eigenvector of the perturbed system, $\varepsilon_k = \lambda_j$ should satisfy $h(\varepsilon_k) = 0$. One easily shows that the inverse is also true, if $\varepsilon_k = \lambda_j$ satisfies $h(\varepsilon_k) = 0$, then the vector (10b) is an eigenvector corresponding to this eigenvalue. This completes the proof of theorem II.

A.2. Proof of relations (14) and (15)

Using property (1b) one finds that each cardinal eigenvector should be normalised according to $W_k^{-1/2}|\Psi_k\rangle$ where $|\Psi_k\rangle$ is given by (10a) and where

$$W_k = \sum_i^n \frac{|\langle\Phi_i|\mathbf{V} - \varepsilon_k\mathbf{P}|\Theta\rangle|^2}{(\varepsilon_k - \lambda_i)^2} + \sum_i^n \frac{\langle\Phi_i|\mathbf{V} - \varepsilon_k\mathbf{P}|\Theta\rangle\langle\Theta|\mathbf{P}|\Phi_i\rangle + \langle\Phi_i|\mathbf{P}|\Theta\rangle\langle\Theta|\mathbf{V} - \varepsilon_k\mathbf{P}|\Phi_i\rangle}{\varepsilon_k - \lambda_i} + 1.$$

With some algebra this expression can be transformed into (14b). One also finds that normalised cardinal eigenvectors $|\Psi_k\rangle$ and $|\Psi_l\rangle$ should satisfy

$$\langle\Psi_k|\mathbf{S}|\Psi_l\rangle \equiv \frac{1}{\sqrt{W_k W_l}}\left\{\sum_i^n\left[\frac{\langle\Theta|\mathbf{V} - \varepsilon_k\mathbf{P}|\Phi_i\rangle\langle\Phi_i|\mathbf{V} - \varepsilon_l\mathbf{P}|\Theta\rangle}{(\varepsilon_k - \lambda_i)(\varepsilon_l - \lambda_i)} + \frac{\langle\Theta|\mathbf{V} - \varepsilon_k\mathbf{P}|\Phi_i\rangle\langle\Phi_i|\mathbf{P}|\Theta\rangle}{\varepsilon_k - \lambda_i} + \frac{\langle\Theta|\mathbf{P}|\Phi_i\rangle\langle\Phi_i|\mathbf{V} - \varepsilon_l\mathbf{P}|\Theta\rangle}{\varepsilon_l - \lambda_i}\right] + 1\right\} = 0.$$

This expression is equivalent to (15a). In a similar way, if $|\Psi\rangle$ is singular eigenvector (14c) with the eigenvalue $\varepsilon_l = \lambda_j$ and $|\Psi_k\rangle$ is normalised cardinal eigenvector, one finds

$$\langle\Psi|\mathbf{S}|\Psi_k\rangle = \frac{1}{\sqrt{W_k \sum_\nu D_\nu^* D_\nu}}\left[\frac{\sum_\nu D_\nu^*\langle\Phi_{j\nu}|\mathbf{V} - \varepsilon_k\mathbf{P}|\Theta\rangle}{\varepsilon_k - \lambda_j} + \sum_\nu D_\nu^*\langle\Phi_{j\nu}|\mathbf{P}|\Theta\rangle\right]$$

which is equivalent to (15b).

A.3. Proof of lemma 1

If matrix $\mathbf{S} = \mathbf{I}^a + \mathbf{S}^b + \mathbf{P}$ is positive definite then $\langle\Psi|\mathbf{S}|\Psi\rangle > 0$ for each nontrivial vector $|\Psi\rangle \in X_{n+1}$. One can write vector $|\Psi\rangle$ as a sum $|\Psi\rangle = |\Psi^b\rangle + y_{n+1}|\Theta\rangle$ where $|\Psi^b\rangle \in X_n^b$ and where $y_{n+1} = \langle\Theta|\Psi\rangle$ is the $(n+1)$th component of the vector $|\Psi\rangle$. Hence

$$\langle\Psi|\mathbf{S}|\Psi\rangle = \langle\Psi^b|\mathbf{S}^b|\Psi^b\rangle + y_{n+1}^*\langle\Theta|\mathbf{P}|\Psi^b\rangle + y_{n+1}\langle\Psi^b|\mathbf{P}|\Theta\rangle + y_{n+1}^* y_{n+1} > 0. \quad \text{(A15)}$$

There are two possibilities, either $y_{n+1} = 0$ or $y_{n+1} \neq 0$. If $y_{n+1} = 0$ relation (A15) reduces to $\langle\Psi|\mathbf{S}|\Psi\rangle = \langle\Psi^b|\mathbf{S}^b|\Psi^b\rangle > 0$. Since $\mathbf{S}^b$ is by assumption positive definite in X^b, this relation is true for each nontrivial $|\Psi^b\rangle \in X^b$. If $y_{n+1} \neq 0$, one can normalise vector $|\Psi\rangle$ in such a way that $y_{n+1} = 1$. Hence

$$\langle\Psi|\mathbf{S}|\Psi\rangle = \langle\Psi^b|\mathbf{S}^b|\Psi^b\rangle + \langle\Theta|\mathbf{P}|\Psi^b\rangle + \langle\Psi^b|\mathbf{P}|\Theta\rangle + 1 > 0. \quad \text{(A15}'\text{)}$$

This expression is a function of $|\Psi^b\rangle \in X^b$, and it has a minimum for some vector $|\Psi_0^b\rangle$. The variation of the right hand side of (A15′) should vanish for $|\Psi^b\rangle = |\Psi_0^b\rangle$, i.e., $\delta\langle\Psi_0^b|\mathbf{S}^b|\Psi_0^b\rangle + \delta\langle\Theta|\mathbf{P}|\Psi_0^b\rangle + \delta\langle\Psi_0^b|\mathbf{P}|\Theta\rangle = 0$. From this condition one finds $|\Psi_0^b\rangle = -(\mathbf{S}^b)^{-1}\mathbf{P}|\Theta\rangle$ and hence $\langle\Psi_0^b + \Theta|\mathbf{S}|\Psi_0^b + \Theta\rangle = 1 - \langle\Theta|\mathbf{P}(\mathbf{S}^b)^{-1}\mathbf{P}|\Theta\rangle$. Thus if the matrix $\mathbf{S}$ is positive definite, one must have $\langle\Theta|\mathbf{P}(\mathbf{S}^b)^{-1}\mathbf{P}|\Theta\rangle < 1$. The inverse is also true. Assume that $\langle\Theta|\mathbf{P}(\mathbf{S}^b)^{-1}\mathbf{P}|\Theta\rangle < 1$ and let vector $|\Psi\rangle$ satisfy $y_{n+1} = 1$. One can write this vector as a linear combination $|\Psi\rangle = c|\Psi_0^b\rangle + |\delta\Psi\rangle + |\Theta\rangle$ where c is some constant, and where the variation $|\delta\Psi\rangle$ is contained in the space X_n^b and it is orthogonal to the vector $|\Psi_0^b\rangle$ ($\langle\delta\Psi|\mathbf{S}|\Psi_0^b\rangle = 0$, $|\delta\Psi\rangle \in X_n^b$). This implies

$$\langle\Psi|\mathbf{S}|\Psi\rangle = 1 + \left[|c|^2 - \left(c + c^*\right)\right]\langle\Theta|\mathbf{P}\left(\mathbf{S}^b\right)^{-1}\mathbf{P}|\Theta\rangle + \langle\delta\Psi|\mathbf{S}^b|\delta\Psi\rangle.$$

Since $\mathbf{S}^b$ is by assumption positive definite, one has $\langle\delta\Psi|\mathbf{S}^b|\delta\Psi\rangle \geqslant 0$. Further, for each complex c one has $[|c|^2 - (c + c^*)] \geqslant -1$. Hence $\langle\Psi|\mathbf{S}|\Psi\rangle \geqslant 1 - \langle\Theta|\mathbf{P}(\mathbf{S}^b)^{-1}\mathbf{P}|\Theta\rangle$. This proves that if $\langle\Theta|\mathbf{P}(\mathbf{S}^b)^{-1}\mathbf{P}|\Theta\rangle < 1$ one has $\langle\Psi|\mathbf{S}|\Psi\rangle > 0$ for each vector $|\Psi\rangle \in X_{n+1}$ which satisfies $y_{n+1} \neq 0$. If however $y_{n+1} = 0$, then one directly obtains $\langle\Psi|\mathbf{S}|\Psi\rangle = \langle\Psi|\mathbf{S}^b|\Psi\rangle > 0$. Thus for each nontrivial $|\Psi\rangle$ one has $\langle\Psi|\mathbf{S}|\Psi\rangle > 0$, and matrix $\mathbf{S}$ is hence positive definite.

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