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On the interaction of two finite-dimensional quantum systems

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Interaction of quantum system $\mathcal{S}^a$ described by the generalised $\rho \times \rho$ eigenvalue equation $\mathbf{A}|\Theta_s\rangle = E_s\mathbf{S}^a|\Theta_s\rangle$ $(s = 1, \ldots, \rho)$ with quantum system $\mathcal{S}^b$ described by the generalised $n \times n$ eigenvalue equation $\mathbf{B}|\Phi_i\rangle = \lambda_i\mathbf{S}^b|\Phi_i\rangle$ $(i = 1, \ldots, n)$ is considered. With the system $\mathcal{S}^a$ is associated ρ-dimensional space X^a_ρ and with the system $\mathcal{S}^b$ is associated an n-dimensional space X^b_n that is orthogonal to X^a_ρ. Combined system $\mathcal{S}$ is described by the generalised $(\rho + n)\times(\rho + n)$ eigenvalue equation $[\mathbf{A} + \mathbf{B} + \mathbf{V}]|\Psi_k\rangle = \varepsilon_k[\mathbf{S}^a + \mathbf{S}^b + \mathbf{P}]|\Psi_k\rangle$ $(k = 1, \ldots, n + \rho)$ where operators $\mathbf{V}$ and $\mathbf{P}$ represent interaction between those two systems. All operators are Hermitian, while operators $\mathbf{S}^a$, $\mathbf{S}^b$ and $\mathbf{S} = \mathbf{S}^a + \mathbf{S}^b + \mathbf{P}$ are, in addition, positive definite. It is shown that each eigenvalue $\varepsilon_k \notin \{\lambda_i\}$ of the combined system is the eigenvalue of the $\rho \times \rho$ eigenvalue equation $[\mathbf{\Omega}(\varepsilon_k) + \mathbf{A}]|\Psi^a_k\rangle = \varepsilon_k\mathbf{S}^a|\Psi^a_k\rangle$. Operator $\mathbf{\Omega}(\varepsilon)$ in this equation is expressed in terms of the eigenvalues λ_i of the system $\mathcal{S}^b$ and in terms of matrix elements $\langle\chi_s|\mathbf{V}|\Phi_i\rangle$ and $\langle\chi_s|\mathbf{P}|\Phi_i\rangle$ where vectors $|\chi_s\rangle$ form a base in X^a_ρ. Eigenstate $|\Psi^a_k\rangle$ of this equation is the projection of the eigenstate $|\Psi_k\rangle$ of the combined system on the space X^a_ρ. Projection $|\Psi^b_k\rangle$ of $|\Psi_k\rangle$ on the space X^b_n is given by $|\Psi^b_k\rangle = (\varepsilon_k\mathbf{S}^b - \mathbf{B})^{-1}(\mathbf{V} - \varepsilon_k\mathbf{P})|\Psi^a_k\rangle$ where $(\varepsilon_k\mathbf{S}^b - \mathbf{B})^{-1}$ is inverse of $(\varepsilon_k\mathbf{S}^b - \mathbf{B})$ in X^b_n. Hence, if the solution to the system $\mathcal{S}^b$ is known, one can obtain all eigenvalues $\varepsilon_k \notin \{\lambda_i\}$ and all the corresponding eigenstates $|\Psi_k\rangle$ of the combined system as a solution of the above $\rho \times \rho$ eigenvalue equation that refers to the system $\mathcal{S}^a$ alone. Slightly more complicated expressions are obtained for the eigenvalues $\varepsilon_k \in \{\lambda_i\}$ and the corresponding eigenstates, provided such eigenvalues and eigenstates exist.

KEY WORDS: interaction of quantum systems, perturbation, diagonalisation, generalised eigenvalue equation, eigenvalues, eigenstates

1. Introduction

Consider quantum system $\mathcal{S}$ consisting of two subsystems $\mathcal{S}^a$ and $\mathcal{S}^b$ that are in mutual interaction. We assume that the solution to the isolated system $\mathcal{S}^b$ is known, and we would like to find an exact solution of the combined system $\mathcal{S} = \mathcal{S}^a \oplus \mathcal{S}^b$. In particular, we would like to find an efficient description of the system $\mathcal{S}^a$ subject to the interaction with the known system $\mathcal{S}^b$. In a standard approach, this is usually done either with some diagonalization method, or with a perturbation expansion. We would like to obtain this solution in a more efficient way, utilising as much as possible the knowledge of the solution to the subsystem $\mathcal{S}^b$.

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There are numerous problems in physics and chemistry of this type. For example, one may consider the interaction of an atom or a molecule (system $\mathcal{S}^a$) that is placed on a surface of some solid state with this solid state (system $\mathcal{S}^b$). Usually an approximate solution to the system $\mathcal{S}^b$ is known. To the extend this solution is reliable, one has a problem of the interaction of a system $\mathcal{S}^a$ with a known system $\mathcal{S}^b$. As another example, consider the effect of various substitution groups (system $\mathcal{S}^a$) in a given molecule. If the solution to the remaining molecular skeleton (system $\mathcal{S}^b$) is known, one would like to obtain in a relatively simple way the solution of the combined system $\mathcal{S}$. To the same type of problems belongs substitution of an atom in a molecule with a heteroatom, creation and destruction of a chemical bond, etc. One may also consider molecular vibrations in the harmonic approximation [1]. If atomic displacements are expressed in terms of Cartesian coordinates, one arrives at the eigenvalue equation of a type $\mathbf{F}|\Psi_k\rangle = \varepsilon_k \mathbf{M}|\Psi_k\rangle$, where $\mathbf{F}$ is a force field matrix, while $\mathbf{M}$ is a diagonal matrix containing on a diagonal atomic masses. Both matrices are Hermitian, and matrix $\mathbf{M}$ is, in addition, positive definite. One may be interested how frequencies and normal modes of some molecular system $\mathcal{S}^a$ are influenced by the interaction of this system with another system $\mathcal{S}^b$ with known frequencies and normal modes. System $\mathcal{S}^b$ may be another molecule, in which case one is looking for frequencies and normal modes of the combined molecular system $\mathcal{S}$. However, system $\mathcal{S}^b$ may be a solid state, with system $\mathcal{S}^a$ representing a molecule that interacts with the surface of this solid state. In this case one usually wants to know how frequencies and normal modes of a molecule $\mathcal{S}^a$ are influenced by the interaction of this molecule with the solid state $\mathcal{S}^b$.

There is another conceptually different class of problems that can be formulated in terms of the interaction of quantum systems $\mathcal{S}^a$ and $\mathcal{S}^b$, where the solution to the system $\mathcal{S}^b$ is known. Assume one has to solve an eigenvalue equation describing some quantum system and one has obtained an approximate solution in a finite base $|\phi_i\rangle$ $(i = 1, \ldots, n)$. One can increase this base with additional vectors $|\chi_s\rangle$ $(s = 1, \ldots, \rho)$ in order to improve the solution. The eigenvalue equation in the original base $\{|\phi_i\rangle\}$ represents system $\mathcal{S}^b$, eigenvalue equation in the augmented base $\{|\phi_i\rangle, |\chi_s\rangle\}$ represents combined system $\mathcal{S}$, and additional vectors $|\chi_s\rangle$ form a base in a system $\mathcal{S}^a$. For example, base vectors $|\phi_i\rangle$ can be atomic orbitals, while the eigenvalues and the eigenstates of the corresponding eigenvalue equation represent molecular orbitals and their energies. One would like to find out how the inclusion of additional atomic orbitals $|\chi_s\rangle$ influences those molecular orbitals and their energies. As another example, assume that base vectors $|\phi_i\rangle$ are resonance structures in a VB model, and one is looking for the VB ground state. One can increase the base set $\{|\phi_i\rangle\}$ with additional resonance structures $|\chi_s\rangle (s = 1, \ldots, \rho)$ in order to decrease ground state energy as much as possible. Since VB resonance structures are in general not orthogonal to each other, the corresponding eigenvalue equation is a generalised eigenvalue equation of a type $\mathbf{H}|\Psi\rangle = \varepsilon \mathbf{S}|\Psi\rangle$ where $\mathbf{S}$ is positive definite.

2. Formulation of a problem

Let us now formulate in more mathematical terms general type of the problem to be considered. We will restrict our discussion to quantum systems involving finite-dimensional spaces. The case of the infinite dimensional systems that may contain eigenvalue bands will be considered elsewhere [2].

We associate with a system $\mathcal{S}^a$ a ρ-dimensional space X^a_ρ and with a system $\mathcal{S}^b$ an n-dimensional space X^b_n. Those spaces are orthogonal to each other, and with the combined system $\mathcal{S}$ is associated an $(n+\rho)$-dimensional space $X_{n+\rho}$. System $\mathcal{S}^a$ alone is described by the generalised eigenvalue equation

$$\mathbf{A}|\Theta_s\rangle = E_s \mathbf{S}^a |\Theta_s\rangle, \quad s = 1, \ldots, \rho, \tag{1a}$$

where $\mathbf{A}$ and $\mathbf{S}^a$ are Hermitian operators acting in the space X^a_ρ, and where $\mathbf{S}^a$ is, in addition, positive definite. No other assumption about those operators is made. Hermiticity of these operators and positive definiteness of $\mathbf{S}^a$ ensures that the eigenvalues E_s are real. In addition, the corresponding eigenstates can be always orthonormalized according to (see appendix):

$$\left\langle \Theta_s \middle| \mathbf{S}^a \middle| \Theta_p \right\rangle = \delta_{sp}. \tag{1b}$$

In a similar way, system $\mathcal{S}^b$ alone is described by the generalised eigenvalue equation

$$\mathbf{B}|\Phi_i\rangle = \lambda_i \mathbf{S}^b |\Phi_i\rangle, \quad i = 1, \ldots, n, \tag{2a}$$

where $\mathbf{B}$ and $\mathbf{S}^b$ are Hermitian operators acting in the space X^b_n and where operator $\mathbf{S}^b$ is, in addition, positive definite. Eigenvalues λ_i are hence real, and the corresponding eigenstates $|\Phi_i\rangle$ can be orthonormalized according to

$$\left\langle \Phi_i \middle| \mathbf{S}^b \middle| \Phi_j \right\rangle = \delta_{ij}. \tag{2b}$$

Relations (1) and (2) describe systems $\mathcal{S}^a$ and $\mathcal{S}^b$ in isolation, that is without mutual interaction. The interaction is introduced by Hermitian operators $\mathbf{V}$ and $\mathbf{P}$, and the eigenvalue equation describing the combined system $\mathcal{S}$ subject to the interaction $(\mathbf{V}, \mathbf{P})$ is

$$\mathbf{H}|\Psi_k\rangle = \varepsilon_k \mathbf{S}|\Psi_k\rangle, \quad k = 1, \ldots, n+\rho, \tag{3a}$$

where

$$\mathbf{H} = \mathbf{A} + \mathbf{B} + \mathbf{V}, \qquad \mathbf{S} = \mathbf{S}^a + \mathbf{S}^b + \mathbf{P}. \tag{3b}$$

Operators $\mathbf{V}$ and $\mathbf{P}$ that describe interaction have nonvanishing matrix elements only between states in the space X^a_ρ and states in the space X^b_n. Hence

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

where $\mathbf{I}^a$ and $\mathbf{I}^b$ are projection operators on spaces X^a_ρ and X^b_n, respectively.

In order to guarantee the reality of the eigenvalues ε_r, operator $\mathbf{S}$ is required to be positive definite in the combined space $X_{n+\rho}$. This requirement imposes some restrictions on the operator $\mathbf{P}$. There is no restriction on the operator $\mathbf{V}$, except that this operator should be Hermitian and that it should connect states in the spaces X^a_ρ and X^b_n.

In analogy to (1b) and (2b), eigenstates $|\Psi_k\rangle$ of the combined system can be orthonormalized according to

$$\langle\Psi_k|\mathbf{S}|\Psi_l\rangle = \delta_{kl}. \tag{3d}$$

The above eigenvalue equations can be formulated as matrix equations in some fixed basis. Let $\{|r\rangle\}$ $(r = 1, \ldots, n)$ be an orthonormalized base in the space X^b_n

$$\langle r|t\rangle = \delta_{rt}, \quad r, t = 1, \ldots, n. \tag{4a}$$

Similarly, let $\{|\chi_s\rangle\}$ $(s = 1, \ldots, \rho)$ be a base in the space X^a_ρ. We make no *a priori* assumption about this base. Given this base, one can define operator $\mathbf{K}^a$ according to

$$\left\langle \chi_s \middle| \mathbf{K}^a \middle| \chi_p \right\rangle = \delta_{sp}. \tag{4b}$$

Since vectors $|\chi_s\rangle$ are by definition linearly independent and complete in X^a_ρ, operator $\mathbf{K}^a$ exists, it is unique, and it is nonsingular in X^a_ρ.

Once chosen, bases $\{|r\rangle\}$ and $\{|\chi_s\rangle\}$ are fixed. For the sake of simplicity, we will use the same notation for various operators and vectors, and their representations in those basis. With this convention $\mathbf{B}$ and $\mathbf{S}^b$ are $n \times n$ matrices with matrix elements $B_{rt} = \langle r|\mathbf{B}|t\rangle$ and $S^b_{rt} = \langle r|\mathbf{S}^b|t\rangle$, respectively, while $|\Phi_i\rangle$ is an n-component column vector with components $\Phi_{ir} = \langle r|\Phi_i\rangle$. Similarly, $\mathbf{A}$ and $\mathbf{S}^a$ are $\rho \times \rho$ matrices with matrix elements $A_{sp} = \langle\chi_s|\mathbf{A}|\chi_p\rangle$ and $S^a_{sp} = \langle\chi_s|\mathbf{S}^a|\chi_p\rangle$, respectively.

In the base $\{|r\rangle, |\chi_s\rangle\}$ of the combined space $X_{n+\rho}$ operators $\mathbf{H} = \mathbf{A} + \mathbf{B} + \mathbf{V}$ and $\mathbf{S} = \mathbf{S}^a + \mathbf{S}^b + \mathbf{P}$ are represented by matrices

$$\mathbf{H} = \begin{bmatrix} \mathbf{B} & \mathbf{U} \\ \mathbf{U}^+ & \mathbf{A} \end{bmatrix}, \qquad \mathbf{S} = \begin{bmatrix} \mathbf{S}^b & \mathbf{X} \\ \mathbf{X}^+ & \mathbf{S}^a \end{bmatrix}, \tag{5}$$

where $\mathbf{U} = \mathbf{I}^b\mathbf{V}\mathbf{I}^a$ and $\mathbf{X} = \mathbf{I}^b\mathbf{P}\mathbf{I}^a$, while $\mathbf{U}^+$ and $\mathbf{X}^+$ denote Hermitian conjugate to $\mathbf{U}$ and $\mathbf{X}$, respectively. According to this representation, combined eigenvalue equation (3a) is an augmented eigenvalue equation, where the eigenvalue equation (2a) containing matrices of order n is augmented by ρ additional rows and ρ additional columns.

Combined system $\mathcal{S}$ is shown schematically in figure 1. Generalised eigenvalue equations (1a)–(3a) allow for a most general treatment of quantum systems $\mathcal{S}^a, \mathcal{S}^b$ and $\mathcal{S}$. Most important is the case $\mathbf{S}^a = \mathbf{I}^a, \mathbf{S}^b = \mathbf{I}^b$ and $\mathbf{P} = 0$ when those equations reduce to normal eigenvalue equations. We will treat those eigenvalue equations in the above most general form. Our aim is to solve the combined eigenvalue equation (3a) given the solution (eigenvalues λ_i and eigenstates $|\Phi_i\rangle$) of the eigenvalue equation (2a). Accordingly, we will consider system $\mathcal{S}^b$ as the original unperturbed system. From this point of view, relation (3a) is a perturbed eigenvalue equation where the "perturbation" is represented by the interaction $(\mathbf{V}, \mathbf{P})$ and by the sys-

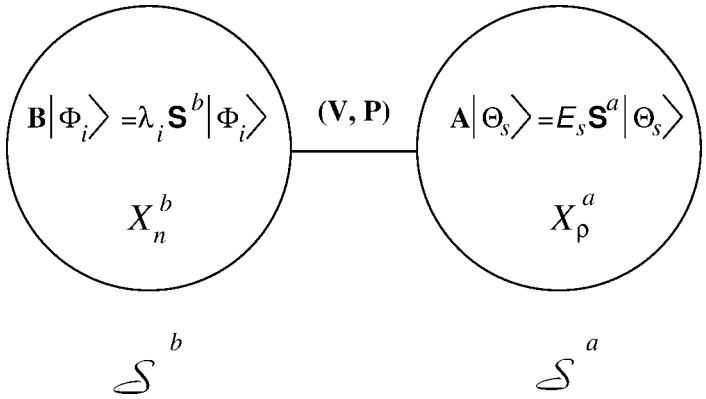

Figure 1. Interaction of the quantum system $\mathcal{S}^a$ described by the generalised eigenvalue equation (1a) with the quantum system $\mathcal{S}^b$ described by the generalised eigenvalue equation (1b). Combined system $\mathcal{S}$ that incorporates generalised interaction $(\mathbf{V}, \mathbf{P})$ is described by the generalised eigenvalue equation (3a).

tem $\mathcal{S}^a$ (operators $\mathbf{A}$ and $\mathbf{S}^a$). Note that in the traditional formulation of the perturbation approach, one usually considers union of systems $\mathcal{S}^a$ and $\mathcal{S}^b$ without mutual interaction as the unperturbed system. We apply here the notion of the unperturbed system to the system $\mathcal{S}^b$ alone. This allows for a more flexible treatment of a combined system $\mathcal{S}$.

We will solve eigenvalue equation (3a) following general method of the low rank perturbation (LRP) approach [3]. In this approach it is convenient to distinguish two types of the solution to the perturbed equation. If the eigenvalue ε_k of the combined system $\mathcal{S}$ differs from all the eigenvalues λ_i of the unperturbed system $\mathcal{S}^b$, that is if $\varepsilon_k \notin \{\lambda_i\}$, this eigenvalue and the corresponding eigenstate or eigenstates $|\Psi_k\rangle$ is "cardinal". Otherwise, this eigenvalue and the corresponding eigenstate or eigenstates is "singular" [3]. Most numerous and most important are cardinal eigenvalues and eigenstates. Singular eigenvalues usually arise as a consequence of some symmetry, or as a consequence of some other special condition.

We also distinguish *active* and *passive* unperturbed eigenvalues. This notion is defined relative to the perturbation $(\mathbf{V}, \mathbf{P})$ [3]. Let the unperturbed eigenvalue λ_j be η-degenerate, and let $|\Phi_{j\nu}\rangle$, $(\nu = 1, \ldots, \eta)$ be the corresponding unperturbed eigenstates. By definition, this eigenvalue is passive if all matrix elements $\langle\chi_s|\mathbf{V} - \lambda_j\mathbf{P}|\Phi_{j\nu}\rangle$ $(s = 1, \ldots, \rho; \nu = 1, \ldots, \eta)$ vanish, otherwise it is active. In other words, λ_j is passive if the subspace associated with this eigenvalue is contained in a null subspace of the operator $\mathbf{V} - \lambda_j\mathbf{P}$:

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

3. Solution of the combined eigenvalue equation

In the appendix we derive two theorems that provide a general solution to the combined eigenvalue equation (3a). This solution is expressed in terms of the known solution

to the unperturbed system $\mathcal{S}^b$. In this respect, suggested method resembles the perturbation expansion method, which also requires the knowledge of the solution to the unperturbed system. However, unlike perturbation expansion, the obtained relations provide a solution to the combined system in a closed form. There is no expansion in a power series, and numerical efficiency of the method does not depend on the magnitude of the perturbation. In particular, there is no convergence problem in a limit $n \to \infty$ [2]. If the interaction is strong enough, standard perturbation method usually fails in this limit.

First theorem refers to the cardinal eigenvalues and eigenstates of the combined system:

Theorem 1 (Cardinal eigenvalues and eigenstates). Consider ρ-dimensional system $\mathcal{S}^a$ (equation (1a)), n-dimensional system $\mathcal{S}^b$ (equation (2a)) and combined $(\rho + n)$-dimensional system $\mathcal{S}$ (equation (3a)). Let the eigenstates $|\Phi_i\rangle$ of $\mathcal{S}^b$ be orthonormalized according to (2b). Let further $|\chi_s\rangle \in X^a_\rho$ form a base in X^a_ρ. Then

(a) $\varepsilon_k \notin \{\lambda_i\}$ is an eigenvalue of the combined eigenvalue equation (3a) if and only if it is a root of the function $h(\varepsilon)$

$$h(\varepsilon) \equiv \left|\mathbf{\Omega}(\varepsilon) + \mathbf{A} - \varepsilon \mathbf{S}^a\right| = 0, \quad \varepsilon \notin \{\lambda_i\}, \tag{7}$$

where $\mathbf{\Omega}(\varepsilon)$ is a $\rho \times \rho$ Hermitian matrix with matrix elements

$$\Omega_{sp}(\varepsilon) = \sum_i^n \frac{\langle \chi_s|\mathbf{V} - \varepsilon\mathbf{P}|\Phi_i\rangle\langle\Phi_i|\mathbf{V} - \varepsilon\mathbf{P}|\chi_p\rangle}{\varepsilon - \lambda_i}, \quad \varepsilon \notin \{\lambda_i\}, \tag{8a}$$

while $\mathbf{A}$ and $\mathbf{S}^a$ are $\rho \times \rho$ Hermitian matrices with matrix elements

$$A_{sp} = \langle \chi_s|\mathbf{A}|\chi_p\rangle, \qquad S^a_{sp} = \left\langle \chi_s\middle|\mathbf{S}^a\middle|\chi_p\right\rangle. \tag{9}$$

(b) Let $\varepsilon_k \notin \{\lambda_i\}$ be an eigenvalue of the combined eigenvalue equation (3a). Each eigenstate corresponding to this eigenvalue is of the form

$$|\Psi_k\rangle = \sum_i^n \frac{\sum_s^\rho \langle\Phi_i|\mathbf{V} - \varepsilon_k\mathbf{P}|\chi_s\rangle C^{(k)}_s}{\varepsilon_k - \lambda_i}|\Phi_i\rangle + \sum_s^\rho C^{(k)}_s|\chi_s\rangle, \tag{10}$$

where $C^{(k)}_s$ are components of a column vector $\mathbf{C}^{(k)}$, a nontrivial solution of the matrix equation

$$\left\lfloor \mathbf{\Omega}(\varepsilon_k) + \mathbf{A} - \varepsilon_k\mathbf{S}^a \right\rfloor \mathbf{C}^{(k)} = 0. \tag{11}$$

Inversely, each state (10) where $\mathbf{C}^{(k)}$ is a nontrivial solution of (11) is an eigenstate of (3a) that corresponds to the eigenvalue ε_k. In addition, components $C^{(k)}_s$ of $\mathbf{C}^{(k)}$ satisfy

$$C^{(k)}_s = \left\langle \chi_s\middle|\mathbf{K}^a\middle|\Psi_k\right\rangle, \quad s = 1, \ldots, \rho. \tag{12}$$

According to the above theorem, each nontrivial solution $\mathbf{C}^{(k)}$ of (11) produces an eigenstate of the combined eigenvalue equation. All such eigenstates correspond to the

same eigenvalue ε_k. One can show (see appendix) that linearly independent solutions $\mathbf{C}^{(k)}$ produce linearly independent eigenstates. Hence:

Lemma 1. Degeneracy of the eigenvalue $\varepsilon_k \notin \{\lambda_i\}$ of the combined system equals the nullity of the operator $\mathbf{\Omega}(\varepsilon_k) + \mathbf{A} - \varepsilon_k \mathbf{S}^a$.

Since $\mathbf{\Omega}(\varepsilon_k) + \mathbf{A} - \varepsilon_k \mathbf{S}^a$ is a $\rho \times \rho$ matrix, each cardinal eigenvalue $\varepsilon_k \notin \{\lambda_i\}$ is at most ρ-degenerate.

Second theorem refers to singular eigenvalues and eigenstates of the combined system:

Theorem 2 (Singular eigenvalues and eigenstates). Assume the same conditions as in theorem 1. Let further λ_j be a η-degenerate eigenvalue of the unperturbed eigenvalue equation (2a), and let $|\Phi_{j\nu}\rangle (\nu = 1, \ldots, \eta)$ be the corresponding eigenstates orthonormalized according to (2b). Then

(a) $\varepsilon_k = \lambda_j$ is an eigenvalue of the combined eigenvalue equation (3a) if and only if it satisfies

$$\begin{vmatrix} \mathbf{\Omega}(\varepsilon_k) + \mathbf{A} - \varepsilon_k \mathbf{S}^a & \mathbf{W}^{(k)} \\ \mathbf{W}^{(k)+} & \mathbf{0} \end{vmatrix} = 0, \tag{13}$$

where $\mathbf{A}$ and $\mathbf{S}^a$ are $\rho \times \rho$ Hermitian matrices with matrix elements (9), $\mathbf{\Omega}(\varepsilon_k)$ is a $\rho \times \rho$ Hermitian matrix with matrix elements

$$\Omega_{sp}(\varepsilon_k) = \sum_{i(\lambda_i \neq \varepsilon_k)}^{n} \frac{\langle \chi_s | \mathbf{V} - \varepsilon_k \mathbf{P} | \Phi_i \rangle \langle \Phi_i | \mathbf{V} - \varepsilon_k \mathbf{P} | \chi_p \rangle}{\varepsilon_k - \lambda_i}, \quad \varepsilon_k \in \{\lambda_i\}. \tag{8b}$$

$\mathbf{W}^{(k)}$ is a $\rho \times \eta$ matrix with matrix elements

$$W^{(k)}_{s\nu} = \langle \chi_s | \mathbf{V} - \varepsilon_k \mathbf{P} | \Phi_{j\nu} \rangle, \quad s = 1, \ldots, \rho, \ \nu = 1, \ldots, \eta, \tag{14}$$

while $\mathbf{0}$ is a $\eta \times \eta$ null matrix.

(b) Let $\varepsilon_k = \lambda_j$ be an eigenvalue of the combined eigenvalue equation (3a). Each eigenstate corresponding to this eigenvalue is of the form

$$|\Psi_k\rangle = \sum_{i(\lambda_i \neq \varepsilon_k)}^{n} \frac{\sum_s^{\rho} \langle \Phi_i | \mathbf{V} - \varepsilon_k \mathbf{P} | \chi_s \rangle C^{(k)}_s}{\varepsilon_k - \lambda_i} |\Phi_i\rangle + \sum_s^{\rho} C^{(k)}_s |\chi_s\rangle + \sum_{\nu}^{\eta} D^{(k)}_{\nu} |\Phi_{j\nu}\rangle, \tag{15}$$

where $C^{(k)}_s$ and $D^{(k)}_{\nu}$ are components of a column vector $(\mathbf{C}^{(k)}, \mathbf{D}^{(k)})$, a nontrivial solution of the matrix equation

$$\begin{bmatrix} \mathbf{\Omega}(\varepsilon_k) + \mathbf{A} - \varepsilon_k \mathbf{S}^a & \mathbf{W}^{(k)} \\ \mathbf{W}^{(k)+} & \mathbf{0} \end{bmatrix} \begin{pmatrix} \mathbf{C}^{(k)} \\ \mathbf{D}^{(k)} \end{pmatrix} = 0. \tag{16}$$

Inversely, each state (15) where $(\mathbf{C}^{(k)}, \mathbf{D}^{(k)})$ is a nontrivial solution to (16) is an eigenstate of (3a) corresponding to the eigenvalue $\varepsilon_k = \lambda_j$. In addition, coefficients $C_s^{(k)}$ and $D_\nu^{(k)}$ satisfy

$$C_s^{(k)} = \langle \chi_s | \mathbf{K}^a | \Psi_k \rangle, \quad D_\nu^{(k)} = \langle \Phi_{j\nu} | \mathbf{S}^b | \Psi_k \rangle, \qquad s = 1, \ldots, \rho, \ \nu = 1, \ldots, \eta. \quad (17)$$

Relation (8b) completes the definition of matrix elements $\Omega_{sp}(\varepsilon)$. If $\varepsilon \notin \{\lambda_i\}$ those matrix elements are defined according to (8a), while if $\varepsilon \in \{\lambda_i\}$ they are defined according to (8b). Usually the expression (8a) has singularity in the point $\varepsilon = \lambda_j$ and in this case matrix elements $\Omega_{sp}(\varepsilon)$ of the operator $\mathbf{\Omega}(\varepsilon)$ are not continuous in this point. However, if λ_j is passive, expression (8a) has well-defined limit $\lim_{\varepsilon \to \lambda_j} \Omega_{sp}(\varepsilon) = \Omega_{sp}(\lambda_j)$. In this case each matrix element $\Omega_{sp}(\varepsilon)$ is continuous and analytic in the point $\varepsilon = \lambda_j$. The function $h(\varepsilon)$ is hence also continuous and analytic in this point.

Concerning degeneracy of singular eigenvalues, one finds in analogy to lemma 1.

Lemma 2. Let $\varepsilon_k = \lambda_j$ be a singular eigenvalue of the combined eigenvalue equation. The degeneracy of this eigenvalue equals the number of linearly independent solutions $(\mathbf{C}^{(k)}, \mathbf{D}^{(k)})$ of the matrix equation (16).

Since matrix equation (16) involves a $(\rho + \eta) \times (\rho + \eta)$ matrix, eigenvalue $\varepsilon_k = \lambda_j$ of the combined system can be at most $(\rho + \eta)$-degenerate. One also finds that if $\eta > \rho$ this eigenvalue is at least $(\eta - \rho)$-degenerate. It follows that generalised interaction $(\mathbf{V}, \mathbf{P})$ can alter (decrease or increase) degeneracy of the unperturbed eigenvalue λ_j by at most ρ. This applies also to cardinal eigenvalues, since each cardinal eigenvalue $\varepsilon_k \notin \{\lambda_i\}$ is at most ρ-degenerate.

Theorem 2 supplements theorem 1, and it provides the solution for the remaining singular eigenvalues and eigenstates of the combined eigenvalue equation. Let us analyse in more details those solutions. Condition (13) expresses the requirement that matrix equation (16) should have a nontrivial solution. The solution to this equation is particularly simple if the unperturbed eigenvalue λ_j is passive. In this case $\mathbf{W}^{(k)} = 0$ and (16) implies condition (11) on the vector $\mathbf{C}^{(k)}$. There is no condition on the vector $\mathbf{D}^{(k)}$, and (16) has always a solution $(\mathbf{0}, \mathbf{D}^{(k)})$ where $\mathbf{C}^{(k)} = 0$ while vector $\mathbf{D}^{(k)}$ can assume any value. Each unperturbed eigenstate $|\Phi_{j\nu}\rangle$ is hence an eigenstate of the combined system. In addition, each vector $\mathbf{C}^{(k)}$ that satisfies (11) with $\varepsilon_k = \lambda_j$ generates a solution $(\mathbf{C}^{(k)}, \mathbf{0})$ of (16). According to (15), the corresponding eigenstate is

$$|\Psi_k\rangle = \sum_{i(\lambda_i \neq \varepsilon_k)}^{n} \frac{\sum_s^\rho \langle \Phi_i | \mathbf{V} - \varepsilon_k \mathbf{P} | \chi_s \rangle C_s^{(k)}}{\varepsilon_k - \lambda_i} |\Phi_i\rangle + \sum_s^\rho C_s^{(k)} |\chi_s\rangle. \quad (10')$$

In conclusion, if λ_j is passive, $\varepsilon_k = \lambda_j$ is an eigenvalue of the combined system. Each unperturbed eigenstate $|\Phi_{j\nu}\rangle (\nu = 1, \ldots, \eta)$ is the corresponding eigenstate of the combined system. If, in addition, λ_j satisfies $h(\lambda_j) = 0$, there are additional eigenstates (10′), where $\mathbf{C}^{(k)}$ are nontrivial solutions to (11). Eigenstates (10′) are formally

identical to the eigenstates (10), except that the summation in (10′) excludes all terms that satisfy $\lambda_i = \varepsilon_k$. Each such term is indefinite of a type $0/0$. Note that if λ_j is passive, function $h(\varepsilon)$ is continuous in this point.

If λ_j is active, the problem is slightly more complicated. In this case $\mathbf{W}^{(k)} \neq 0$ and (16) implies a nontrivial condition on a vector $\mathbf{C}^{(k)}$:

$$\mathbf{W}^{(k)+}\mathbf{C}^{(k)} = 0. \tag{16′}$$

General solution to (16) can be now analysed in terms of the solutions to (16′) and in terms of the solutions to the auxiliary equation

$$\mathbf{W}^{(k)}\mathbf{D}^{(k)} = 0. \tag{18}$$

Each nontrivial solution $\mathbf{D}^{(k)}$ to this equation generates a solution $(\mathbf{0}, \mathbf{D}^{(k)})$ to (16). The corresponding eigenstate (15) of the combined system is

$$|\Psi_k\rangle = \sum_{\nu}^{\eta} D_{\nu}^{(k)} |\Phi_{j\nu}\rangle. \tag{15′}$$

If relation (16′) has no nontrivial solution, one has $\mathbf{C}^{(k)} = 0$. In this case eigenstates (15′) where $\mathbf{D}^{(k)}$ is a solution to (18) are the only eigenstates of the combined system corresponding to the eigenvalue $\varepsilon_k = \lambda_j$. In particular, if neither (16′) nor (18) has a nontrivial solution, $\varepsilon = \lambda_j$ is not an eigenvalue of the combined system.

If (16′) has a nontrivial solution, additional eigenstates are possible. For example, if (16′) and (11) have in common the same nontrivial solution $\mathbf{C}^{(k)}$, relation (16) has a solution $(\mathbf{C}^{(k)}, \mathbf{0})$, which produces an eigenstate of a type (10′). In addition, relation (16) may have solutions of a more general type $(\mathbf{C}^{(k)}, \mathbf{D}^{(k)})$ where $\mathbf{C}^{(k)} \neq 0$ and $\mathbf{D}^{(k)} \neq 0$. Such solutions, if they exist, produce eigenstates of the general type (15).

The above two theorems exhaust all possibilities. All cardinal eigenvalues $\varepsilon_k \notin \{\lambda_i\}$ of the combined eigenvalue equation are roots of the function $h(\varepsilon)$. Once a particular root ε_k of $h(\varepsilon)$ is found, the corresponding eigenstate (eigenstates) is given by equation (10) where vector (vectors) $\mathbf{C}^{(k)}$ is a solution of (11). Concerning remaining singular eigenvalues $\varepsilon_k \in \{\lambda_i\}$, each such eigenvalue coincides with some unperturbed eigenvalue λ_j, and all one has to do is to verify condition (13). This verification can be simplified using relation (16′) and auxiliary relation (18). In particular, each nontrivial solution $\mathbf{D}^{(k)}$ of (18) generates singular eigenstate (15′).

In the computer implementation of the above method, in order to find each particular root ε_k of $h(\varepsilon)$, one has to recalculate in an iterative way this function for many different values of ε. In the case $\mathbf{P} \neq 0$, one can substantially speed up this iteration if the above relations are slightly modified [2]. After some algebra one finds that matrix $\boldsymbol{\Omega}(\varepsilon)$ can be written as

$$\boldsymbol{\Omega}(\varepsilon) = \boldsymbol{\Omega}^0(\varepsilon) + \boldsymbol{\alpha} + \varepsilon\boldsymbol{\beta}, \tag{19}$$

where $\mathbf{\Omega}^0(\varepsilon)$, $\boldsymbol{\alpha}$ and $\boldsymbol{\beta}$ are $\rho \times \rho$ matrices with matrix elements $\Omega^0_{sp}(\varepsilon)$, α_{sp} and β_{sp}, respectively

$$\Omega^0_{sp}(\varepsilon) = \sum_i^n \frac{c^{(i)}_{sp}}{\varepsilon - \lambda_i}, \qquad c^{(i)}_{sp} = \langle \chi_s | \mathbf{V} - \lambda_i \mathbf{P} | \Phi_i \rangle \langle \Phi_i | \mathbf{V} - \lambda_i \mathbf{P} | \chi_p \rangle, \tag{20a}$$

$$\alpha_{sp} = \sum_i^n \big[\lambda_i \langle \chi_s | \mathbf{P} | \Phi_i \rangle \langle \Phi_i | \mathbf{P} | \chi_p \rangle - \langle \chi_s | \mathbf{P} | \Phi_i \rangle \langle \Phi_i | \mathbf{V} | \chi_p \rangle - \langle \chi_s | \mathbf{V} | \Phi_i \rangle \langle \Phi_i | \mathbf{P} | \chi_p \rangle \big], \tag{20b}$$

$$\beta_{sp} = \sum_i^n \langle \chi_s | \mathbf{P} | \Phi_i \rangle \langle \Phi_i | \mathbf{P} | \chi_p \rangle.$$

Relations (7) and (11) accordingly transform into

$$h(\varepsilon) \equiv \big| \mathbf{\Omega}^0(\varepsilon) + \boldsymbol{\alpha} + \mathbf{A} + \varepsilon \big(\boldsymbol{\beta} - \mathbf{S}^a \big) \big| = 0, \tag{7′}$$

$$\big[\mathbf{\Omega}^0(\varepsilon_k) + \boldsymbol{\alpha} + \mathbf{A} + \varepsilon_k \big(\boldsymbol{\beta} - \mathbf{S}^a \big) \big] \mathbf{C} = 0. \tag{11′}$$

The main difference between matrix elements $\Omega_{sp}(\varepsilon)$ of the operator $\mathbf{\Omega}(\varepsilon)$ and matrix elements $\Omega^0_{sp}(\varepsilon)$ of the operator $\mathbf{\Omega}^0(\varepsilon)$ is that those latter matrix elements contain the unknown ε only in the denominator of the sum (20a). This property is useful in order to speed up the iterative recalculation of the function $h(\varepsilon)$ and thus to improve the calculation of each particular root ε_k of $h(\varepsilon)$ [2].

In addition to the explicit expressions for the eigenvalues and eigenstates of the combined system, approximate distribution of the eigenvalues ε_k is also of interest. Due to the interaction, eigenvalues ε_k of the combined system shift relative to the unperturbed eigenvalues λ_i. Maximum possible shift of those eigenvalues is not arbitrary, and it is mainly determined by the dimension ρ of the space X^a_ρ. In the appendix we derive the following.

Interlacing rule. Arrange unperturbed eigenvalues $\lambda_i (i = 1, \ldots, n)$ and perturbed eigenvalues $\varepsilon_k (k = 1, \ldots, n + \rho)$ in a nondecreasing order. Then these eigenvalues are interlaced according to

$$\varepsilon_i \leqslant \lambda_i \leqslant \varepsilon_{i+\rho}, \quad i = 1, \ldots, n. \tag{21}$$

In particular, condition $\lambda_1 \leqslant \varepsilon_{1+\rho}$ implies that at most ρ perturbed eigenvalues $\varepsilon_1, \ldots, \varepsilon_\rho$ can be smaller than the first unperturbed eigenvalue λ_1. Similarly, condition $\varepsilon_n \leqslant \lambda_n$ implies that at most ρ perturbed eigenvalues $\varepsilon_{n+1}, \ldots, \varepsilon_{n+\rho}$ can be larger than the last unperturbed eigenvalue λ_n. Hence at least $n - \rho$ eigenvalues ε_k must be confined to the interval $[\lambda_1, \lambda_n]$.

In the above theorems, no assumption about the base $\{|\chi_s\rangle\}$ in the space X^a_ρ was made. Flexibility in the choice of this base can be utilised in order to cast obtained relations in a more appropriate form for a given problem. Two such choices are particularly important. For some problems, it may be convenient to choose base $\{|\chi_s\rangle\}$ ortho-

normalized according to $\langle\chi_s|\chi_p\rangle = \delta_{sp}$. In this case operator $\mathbf{K}^a$ is a unit operator in $X^a_\rho(\mathbf{K}^a = \mathbf{I}^a)$. Another possible choice is $\{|\chi_s\rangle\} \equiv \{|\Theta_s\rangle\}$. In this case one has $\mathbf{K}^a = \mathbf{S}^a$. Other possible choices are less important.

Above theorems apply to generalised eigenvalue equations (1a)–(3a). All the corresponding relations substantially simplify if these equations are not completely generalised. The most important special case is $\mathbf{P} = 0$. This allows for the unperturbed eigenvalue equations (1a) and (2a) to be still of the most general type. Only the perturbed equation (3a) is slightly restricted with this requirement. This eigenvalue equation 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)–(3a) one has standard eigenvalue equations $\mathbf{A}|\Theta_s\rangle = E_s|\Theta_s\rangle$, $\mathbf{B}|\Phi_i\rangle = \lambda_i|\Phi_i\rangle$ and $\mathbf{H}|\Psi_k\rangle = \varepsilon_k|\Psi_k\rangle$, respectively. Another slightly more general case is the problem of molecular vibrations in harmonic approximation. This problem leads to the eigenvalue equation of the type (3a) where $\mathbf{S} = \mathbf{M}$ is a diagonal matrix, and hence again $\mathbf{P} = 0$.

4. Orthonormalization of eigenstates $|\Psi_k\rangle$

Eigenstates (10) and (15) of the combined system are not orthonormalized. Those eigenstates can be easily orthonormalized according to (3d). This can be done using orthonormality relation (2b) and properties $\mathbf{V}|\chi_s\rangle, \mathbf{P}|\chi_s\rangle \in X^b_n$ and $\mathbf{V}|\Phi_i\rangle, \mathbf{P}|\Phi_i\rangle \in X^a_\rho$.

Concerning normalization, each eigenstate $|\Psi_k\rangle$ of the combined system can be normalized according to

$$\frac{1}{W_k^{1/2}}|\Psi_k\rangle, \tag{22}$$

where $W_k = \langle\Psi_k|\mathbf{S}|\Psi_k\rangle$. If $|\Psi_k\rangle$ is cardinal, it is given by relation (10) while W_k equals (see appendix):

$$W_k = \sum_{sp}^{\rho} C_s^{(k)*} C_p^{(k)} \left[\sum_i^n \frac{\langle\chi_s|\mathbf{V} - \lambda_i\mathbf{P}|\Phi_i\rangle\langle\Phi_i|\mathbf{V} - \lambda_i\mathbf{P}|\chi_p\rangle}{(\varepsilon_k - \lambda_i)^2} - \beta_{sp} + S^a_{sp} \right], \quad \varepsilon_k \notin \{\lambda_i\}. \tag{23a}$$

If $|\Psi_k\rangle$ is singular, it is given by relation (15) and quantity W_k equals

$$W_k = \sum_{sp}^{\rho} C_s^{(k)*} C_p^{(k)} \left[\sum_{i(\lambda_i \neq \varepsilon_k)}^n \frac{\langle\chi_s|\mathbf{V} - \lambda_i\mathbf{P}|\Phi_i\rangle\langle\Phi_i|\mathbf{V} - \lambda_i\mathbf{P}|\chi_p\rangle}{(\varepsilon_k - \lambda_i)^2} - \sum_{i(\lambda_i \neq \varepsilon_k)} \langle\chi_s|\mathbf{P}|\Phi_i\rangle\langle\Phi_i|\mathbf{P}|\chi_p\rangle + S^a_{sp} \right] + \sum_\nu^\eta D_\nu^{(k)*} D_\nu^{(k)}$$
$$+ \sum_{s\nu} \left[C_s^{(k)*} D_\nu^{(k)} \langle\chi_s|\mathbf{P}|\Phi_{j\nu}\rangle + C_s^{(k)} D_\nu^{(k)*} \langle\Phi_{j\nu}|\mathbf{P}|\chi_s\rangle \right], \quad \varepsilon_k = \lambda_j \in \{\lambda_i\}. \tag{23b}$$

In particular, singular eigenstates (15′) are normalized according to

$$|\Psi_k\rangle = \frac{1}{[\sum_\nu^\rho D_\nu^{(k)*} D_\nu^{(k)}]^{1/2}} \sum_\nu^\eta D_\nu^{(k)} |\Phi_{j\nu}\rangle. \tag{15″}$$

Consider now scalar products $\langle\Psi_k|\mathbf{S}|\Psi_l\rangle$ between normalized eigenstates $|\Psi_k\rangle$ and $|\Psi_l\rangle$. If those eigenstates are cardinal, one finds

$$\langle\Psi_k|\mathbf{S}|\Psi_l\rangle = (W_k W_l)^{-1/2} \sum_{sp}^{\rho} C_s^{(k)*} C_p^{(l)} \left[\sum_i^n \frac{\langle\chi_s|\mathbf{V}-\lambda_i\mathbf{P}|\Phi_i\rangle\langle\Phi_i|\mathbf{V}-\lambda_i\mathbf{P}|\chi_p\rangle}{(\varepsilon_k-\lambda_i)(\varepsilon_l-\lambda_i)} - \beta_{sp} + S_{sp}^a \right], \tag{24}$$

where W_k and W_l are given by (23a). Slightly more complicated expressions are obtained in the case of scalar products $\langle\Psi_k|\mathbf{S}|\Psi_l\rangle$ involving singular eigenstates.

In general, if the eigenstates $|\Psi_k\rangle$ and $|\Psi_l\rangle$ correspond to distinct eigenvalues ($\varepsilon_k \neq \varepsilon_l$), they are orthogonal to each other, i.e., $\langle\Psi_k|\mathbf{S}|\Psi_l\rangle = 0$. This orthogonality follows from the hermiticity of operators **A** and **S** and from the fact that **S** is positive definite. In particular, if $|\Psi_k\rangle$ and $|\Psi_l\rangle$ are cardinal eigenstates corresponding to distinct eigenvalues, expression (24) should equal zero. Since suggested method does not enforce orthogonality of calculated eigenstates in any explicit way, this opens the possibility to use this expression as a practical test for the numerical accuracy of those eigenstates [2]. In each numerical calculation due to the finite precision arithmetic, there is always some error accumulation. Therefore, calculated eigenstates $|\Psi_k''\rangle$ slightly differ from exact eigenstates $|\Psi_k\rangle$. If $|\Psi_k''\rangle$ and $|\Psi_l''\rangle$ are calculated eigenstates that correspond to different eigenvalues ($\varepsilon_k \neq \varepsilon_l$), they will be only approximately orthogonal to each other, i.e., numerically one obtains $\langle\Psi_k''|\mathbf{S}|\Psi_l''\rangle \approx 0$. One can use quantities $\langle\Psi_k''|\mathbf{S}|\Psi_l''\rangle$ as an objective measure of the numerical accuracy of those eigenstates. Since cardinal eigenstates are by far most numerous, relation (24) that refers to cardinal eigenstates is sufficient to obtain relatively reliable estimates of the numerical accuracy of calculated eigenstates [2].

If the perturbed eigenvalue ε_k is nondegenerate, one has only to normalize the corresponding eigenstate $|\Psi_k\rangle$ according to the relation (22) or (23), since such an eigenstate is automatically orthogonal to all other eigenstates. However, if the eigenvalue ε_k is degenerate, one has to make an explicit orthonormalization of all the corresponding degenerate eigenstates. In the case of cardinal eigenvalues, this can be done using expression (24) for scalar products $\langle\Psi_k|\mathbf{S}|\Psi_l\rangle$ between degenerate eigenstates ($\varepsilon_k = \varepsilon_l$) and any of the standard orthonormalization procedures, such as Gramm–Schmidt orthonormalization [4,5] or alike. In the case of singular eigenstates, one needs analogous

expression for the scalar products $\langle\Psi_k|\mathbf{S}|\Psi_l\rangle$ between degenerate singular eigenstates. One finds

$$\langle\Psi_k|\mathbf{S}|\Psi_l\rangle = \frac{1}{(W_k W_l)^{1/2}}\Bigg\{\sum_{sp}^{\rho} C_s^{(k)*} C_p^{(l)}\Bigg[\sum_{i(\lambda_i\neq\varepsilon_k)} \frac{\langle\chi_s|\mathbf{V}-\lambda_i\mathbf{P}|\Phi_i\rangle\langle\Phi_i|\mathbf{V}-\lambda_i\mathbf{P}|\chi_p\rangle}{(\varepsilon_k-\lambda_i)^2} - \sum_{i(\lambda_i\neq\varepsilon_k)} \langle\chi_s|\mathbf{P}|\Phi_i\rangle\langle\Phi_i|\mathbf{P}|\chi_p\rangle + S_{sp}^a\Bigg] + \sum_{s\nu}\Big[C_s^{(k)*} D_\nu^{(l)}\langle\chi_s|\mathbf{P}|\Phi_{j\nu}\rangle + C_s^{(l)} D_\nu^{(k)*}\langle\Phi_{j\nu}|\mathbf{P}|\chi_s\rangle\Big] + \sum_{\nu} D_\nu^{(k)*} D_\nu^{(l)}\Bigg\}. \tag{25}$$

In the above expression $|\Psi_k\rangle$ and $|\Psi_l\rangle$ are normalized singular eigenstates corresponding to the same eigenvalue $\varepsilon_k = \varepsilon_l = \lambda_j$.

Orthonormalization of degenerate eigenstates using relations (24) and (25) should be numerically easy to perform, since the dimension of the corresponding degenerate subspace is almost always much smaller then the dimension of the combined space $X_{n+\rho}$.

5. Numerical considerations

An important practical aspect of the above approach is numerical efficiency. Since cardinal solutions are by far the most numerous, main numerical load in solving perturbed eigenvalue equation involves the search for the root or roots of the function $h(\varepsilon)$. After a particular root ε_k of $h(\varepsilon)$ is found, operation count to find the corresponding eigenstate or eigenstates (10) is relatively small. We will now estimate those operation counts. Most interesting is the case when the known system $\mathcal{S}^b$ is much larger than the system $\mathcal{S}^a$, i.e., when $n \gg \rho$. To be more specific, we will assume $\rho < n^{1/2}$. For the sake of simplicity, eigenvalue equation (3a) with real matrices will be considered. In the case of more general complex matrices various operation counts are slightly enhanced, but qualitative order of magnitude estimates are the same as in the case of real matrices.

Operation count 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 [4]. 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 order to initiate calculation of the roots of $h(\varepsilon)$, one has first to find ρn matrix elements $\langle\chi_s|\mathbf{V}|\Phi_i\rangle = \sum_r^n \langle\chi_s|\mathbf{V}|r\rangle\langle r|\Phi_i\rangle$ and ρn matrix elements $\langle\chi_s|\mathbf{P}|\Phi_i\rangle = \sum_r^n \langle\chi_s|\mathbf{P}|r\rangle\langle r|\Phi_i\rangle$. In a most general case involving real matrices this requires $2\rho n^2$ multiplications, n multiplications per matrix element. However, in some cases this operation count can be considerably smaller. For example, in the case $\mathbf{P} = 0$ one has $\langle\chi_s|\mathbf{P}|\Phi_i\rangle = 0$, and this decreases operation count by factor two. Further, if the sys-

tem $\mathcal{S}^b$ is very large, system $\mathcal{S}^a$ usually interacts in a direct way with only relatively small fraction of $\mathcal{S}^b$. In such cases, only relatively few base vectors $|r\rangle \in X_n^b$ of the system $\mathcal{S}^b$ are involved in the interaction with the system $\mathcal{S}^a$. The number of operations required to calculate matrix elements $\langle\chi_s|\mathbf{V}|\Phi_i\rangle$ and $\langle\chi_s|\mathbf{P}|\Phi_i\rangle$ accordingly reduces, and it is usually of the order $O(\rho n)$. Finally, matrix elements $\langle\chi_s|\mathbf{V}|\Phi_i\rangle$ and $\langle\chi_s|\mathbf{P}|\Phi_i\rangle$ can be given in an explicit analytic form. This may eliminate the need for the calculation of those matrix elements. Thus, depending on a problem, this preparatory phase may require anything from zero to $2\rho n^2$ operations.

Once matrix elements $\langle\chi_s|\mathbf{V}|\Phi_i\rangle$ and $\langle\chi_s|\mathbf{P}|\Phi_i\rangle$ are known, one has to find root or roots ε_k of the function $h(\varepsilon)$. This function is usually discontinuous in each point $\varepsilon \in \{\lambda_i\}$, while in each interval $I_r \equiv (\lambda_r, \lambda_{r+1})$ it is continuous and analytic. Assume that a root or roots of $h(\varepsilon)$ in the particular interval I_r is required. Most root finding methods start with some initial approximate root $\varepsilon_k^{(0)} \in I_r$, which is then iteratively improved. This iteration requires multiple recalculation of the function $h(\varepsilon)$. At this point one may use either expression (7) or expression (7′). Consider, for example, expression (7). Each recalculation of $h(\varepsilon)$ using this expression involves calculation of $\rho(\rho+1)/2$ functions $\Omega_{sp}(\varepsilon)$ followed by calculation of the determinant (7). Calculation of each function $\Omega_{sp}(\varepsilon)$ requires n multiplications and n divisions, while calculation of the $\rho \times \rho$ determinant requires $\rho^3/3$ operations [4,5]. One finds that in order to calculate function $h(\varepsilon)$ for a particular value of ε one needs approximately $\rho(\rho+2)n + \rho^3/3 \approx \rho(\rho+2)n$ operations. If the number of iterative recalculations of a function $h(\varepsilon)$ is It_k, this amounts to $N_k \approx It_k\rho(\rho+2)n$ operations required to obtain root ε_k of $h(\varepsilon)$. The number of iterations It_k depends on many factors, in particular on the choice of the initial approximate root $\varepsilon_k^{(0)}$. However, this number is on average essentially independent on the dimensions n and ρ [3,6]. Operation count to obtain a single root of $h(\varepsilon)$ is hence of the order $\approx O(\rho^2 n)$. The same order of magnitude estimate is obtained if instead of the expression (7) one uses expression (7′). There are however some differences. In the case of the relation (7′), in addition to the calculation of matrix elements $\langle\chi_s|\mathbf{V}|\Phi_i\rangle$ and $\langle\chi_s|\mathbf{P}|\Phi_i\rangle$, initial preparatory phase requires also calculation of coefficients $c_{sp}^{(i)}$ and of matrix elements α_{sp} and β_{sp}. Calculation of those quantities can be done with approximately $\rho n(2\rho+3) \approx 2\rho^2 n$ additional operations. This slightly increases operation count for the initial preparatory phase. Further, in each iterative recalculation of $h(\varepsilon)$, instead of $\rho(\rho+1)/2$ functions $\Omega_{sp}(\varepsilon)$ one has to calculate $\rho(\rho+1)/2$ functions $\Omega_{sp}^0(\varepsilon)$. Calculation of each function $\Omega_{sp}^0(\varepsilon)$ requires only n operations, since coefficients $c_{sp}^{(i)}$ do not depend on ε. This decreases operation count for the calculation of each particular root of $h(\varepsilon)$ approximately by factor two. In addition, using relation (7′) substantial further decrease in the operation count can be obtained [2]. Nevertheless, the total operation count to produce a single root of $h(\varepsilon)$ is still of the order $\approx O(\rho^2 n)$.

Once a root ε_k of $h(\varepsilon)$ is obtained, calculation of the corresponding eigenstate requires approximately $\rho^3/3$ operations to solve (11) followed by $O(\rho n)$ operations to construct the corresponding eigenstate (10). If normalization is required, calculation of the quantity W_k according to (23a) requires additional $O(\rho n)$ operations. For $\rho < n^{1/2}$ this adds to approximately $O(\rho n)$ operations per normalized eigenstate.

In conclusion, in order to find the root or roots of $h(\varepsilon)$ there is initial preparatory phase which requires, depending on the problem, anything from zero to $O(\rho n^2)$ operations. After this is done, calculation of each particular root ε_k of $h(\varepsilon)$ requires approximately $O(\rho^2 n)$ operations. Once ε_k is known, calculation of the corresponding normalised eigenstate requires $O(\rho n)$ operations. If all eigenvalues and eigenstates are needed, total operation count is of the order $O(\rho^2 n^2)$. This is a rough order of magnitude estimate. More precise estimate depends on many details, such as selection of the relation (7) or (7′) to calculate function $h(\varepsilon)$, average number of iterations required to obtain a single root of this function, details of the particular algorithm implementation, etc. Nevertheless, it shows that if $\rho \approx n^{1/2}$ the operation count to obtain all eigenvalues and/or eigenstates of the combined eigenvalue equation is of the order $O(n^3)$. In comparison, standard diagonalization methods such as Householder, Givens or Jacoby require also $O(n^3)$ operations in order to calculate all eigenvalues and/or eigenstates of a normal eigenvalue equation [4,5]. In the case of generalised eigenvalue equation, one has first to transform such an equation into a normal eigenvalue equation in order to solve it by one of the standard diagonalization methods. If **S** is symmetric positive definite, this transformation is most efficiently done by Cholesky decomposition [4]. One of the presently best algorithms for the solution of the generalised eigenvalue equation involving real Hermitian matrices combines Cholesky decomposition with the symmetric QR algorithm [4]. Total operation count of this algorithm is $7n^3$ [4].

Above analysis shows that, as far as numerical efficiency of the suggested method is concerned, the break-even point with standard diagonalization methods is approximately at $\rho \approx Cn^{1/2}$, where constant C depends on the details of algorithm implementation. If $\rho \ll n^{1/2}$, and if all the eigenvalues and/or eigenstates are required, suggested method should be numerically more efficient than standard diagonalization methods.

In some cases only a single eigenvalue and/or eigenstate is required. Standard diagonalization methods are not particularly suitable for such problems. Some other method, such as power method, the Lanczos method, the Davidson algorithm, or the perturbation expansion is usually more efficient. Operation count for the power method and Lanczos method is higher then $O(n^2)$ but less than $O(n^3)$ [4,5]. Lanczos method is substantially more efficient than power method. However, both methods are suitable only for few extreme eigenvalues, and those methods are again of the order $O(n^3)$ if an arbitrary eigenvalue and/or eigenstate is required. Davidson's algorithm has also an operation count less than $O(n^3)$ if only a few solutions are required [7]. This algorithm is usually a method of choice in a large scale CI calculations [7]. However, this method highly relies on the scarcity of the Hamiltonian. Finally, operation count for the perturbation expansion 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 $O(n^2)$. In addition, those methods apply only to a normal eigenvalue equation. In a case of a generalised eigenvalue equation, there is an additional operation count of the order $O(n^3)$ associated with the construction of the corresponding normal eigenvalue equa-

tion. Hence, in this case one has again $O(n^3)$ operations, even if a single eigenvalue and/or eigenstate is required.

Suggested method is more efficient. Most unfavourable is the case when one has to calculate matrix elements $\langle\chi_s|\mathbf{V}|\Phi_i\rangle$ and $\langle\chi_s|\mathbf{P}|\Phi_i\rangle$ and when in addition most of the matrix elements $\langle\chi_s|\mathbf{V}|r\rangle$ and $\langle\chi_s|\mathbf{P}|r\rangle$ are nonzero. In this case, operation count to find a single eigenvalue and/or eigenstate is dominated by the calculation of those matrix elements, which is of the order $O(\rho n^2)$. This is less than $O(n^3)$ especially if ρ is small, but still at least $O(n^2)$. However, if the formation of the above matrix elements does not require as many as $O(\rho n^2)$ operations, this operation count can be significantly smaller. For example, if matrix elements $\langle\chi_s|\mathbf{V}|r\rangle$ and $\langle\chi_s|\mathbf{P}|r\rangle$ are sparse, or if matrix elements $\langle\chi_s|\mathbf{V}|\Phi_i\rangle$ and $\langle\chi_s|\mathbf{P}|\Phi_i\rangle$ are a priori known, initial operation count required to construct matrix elements $\langle\chi_s|\mathbf{V}|\Phi_i\rangle$ and $\langle\chi_s|\mathbf{P}|\Phi_i\rangle$ can be as low as $O(\rho n)$ or even smaller. In this case, operation count to obtain a particular eigenvalue and/or eigenstate is dominated by the calculation of the corresponding root of $h(\varepsilon)$ which is of the order $O(\rho^2 n)$. Hence if $\rho \ll n^{1/2}$ operation count to obtain a single eigenvalue and/or eigenstate by this method can be substantially smaller than $O(n^2)$.

For the special case $\rho = 1$ suggested method and the above estimates were successfully verified by the computer program written by the author [6]. In this program, random matrices of the order $n = 100$ up to including $n = 5 \cdot 10^6$ were considered [6].

6. System $\mathcal{S}^a$ in the interaction with a known system $\mathcal{S}^b$ as a nonlinear eigenvalue problem

Relations obtained in theorems 1 and 2 can be cast into a more familiar form. Each eigenstate $|\Psi_k\rangle$ of the combined system is a linear combination

$$|\Psi_k\rangle = \left|\Psi_k^a\right\rangle + \left|\Psi_k^b\right\rangle, \tag{26}$$

where $|\Psi_k^a\rangle \in X_\rho^a$ and $|\Psi_k^b\rangle \in X_n^b$ are projections of this eigenstate on subspaces X_ρ^a and X_n^b, respectively. If $|\Psi_k\rangle$ is a normalized cardinal eigenstate of the combined system, one has

$$\left|\Psi_k^a\right\rangle = W_k^{-1/2} \sum_s^\rho C_s^{(k)} |\chi_s\rangle, \tag{27a}$$

$$\left|\Psi_k^b\right\rangle = \sum_i^n \frac{\langle\Phi_i|\mathbf{V} - \varepsilon_k\mathbf{P}|\Psi_k^a\rangle}{\varepsilon_k - \lambda_i} |\Phi_i\rangle, \quad \varepsilon_k \notin \{\lambda_i\}, \tag{27b}$$

where $\mathbf{C}^{(k)}$ is a nontrivial solution to (11), while W_k is given by (23a).

All properties of the system $\mathcal{S}^a$ alone, such as expectation values of various observables that refer to this system, can be deduced from the state $|\Psi_k^a\rangle$. Similarly, all properties of the system $\mathcal{S}^b$ can be deduced from the state $|\Psi_k^b\rangle$. Only those properties that refer to both systems require the knowledge of the complete eigenstate $|\Psi_k\rangle$. Accordingly, the state $|\Psi_k^a\rangle$ contains a full description of the system $\mathcal{S}^a$, while the state

$|\Psi_k^b\rangle$ contains a full description of the system $\mathcal{S}^b$. Note that neither $|\Psi_k^a\rangle$ nor $|\Psi_k^b\rangle$ is normalized. Only a combined eigenstate $|\Psi_k\rangle$ is normalized.

Further and according to (27b), the state $|\Psi_k^b\rangle \in X_n^b$ is fully determined by the state $|\Psi_k^a\rangle \in X_\rho^a$ and by the corresponding eigenvalue ε_k. Thus, the state $|\Psi_k^a\rangle$ that describes system $\mathcal{S}^a$ and the corresponding eigenvalue ε_k completely determines the eigenstate $|\Psi_k\rangle$ of the combined system $\mathcal{S}$.

Using (2a) and (2b) one can express the inverse of $(\varepsilon\mathbf{S}^b - \mathbf{B})$ in the space X_n^b as

$$\big(\varepsilon\mathbf{S}^b - \mathbf{B}\big)^{-1} = \sum_i^n \frac{|\Phi_i\rangle\langle\Phi_i|}{\varepsilon - \lambda_i}, \quad \varepsilon \notin \{\lambda_i\}. \tag{28}$$

Expression (27b) can be hence written in a compact form

$$\big|\Psi_k^b\big\rangle = \big(\varepsilon_k\mathbf{S}^b - \mathbf{B}\big)^{-1}(\mathbf{V} - \varepsilon_k\mathbf{P})\big|\Psi_k^a\big\rangle. \tag{27b$'$}$$

Consider now relations (7) and (11). Those relations combine into a single equation

$$[\mathbf{\Omega}(\varepsilon_k) + \mathbf{A}]\big|\Psi_k^a\big\rangle = \varepsilon_k\mathbf{S}^a\big|\Psi_k^a\big\rangle, \tag{29}$$

where $\mathbf{\Omega}(\varepsilon)$, $\mathbf{A}$ and $\mathbf{S}^a$ are operators that act in the space X_ρ^a and that in the base $\{|\chi_s\rangle\}$ have matrix elements (8) and (9), respectively. Using (28) operator $\mathbf{\Omega}(\varepsilon)$ can be expressed in a compact form

$$\mathbf{\Omega}(\varepsilon) = (\mathbf{V} - \varepsilon\mathbf{P})\big(\varepsilon\mathbf{S}^b - \mathbf{B}\big)^{-1}(\mathbf{V} - \varepsilon\mathbf{P}). \tag{8a$'$}$$

In a similar way relations (7$'$) and (11$'$) combine into

$$\big[\mathbf{\Omega}^0(\varepsilon_k) + \boldsymbol{\alpha} + \mathbf{A}\big]\big|\Psi_k^a\big\rangle = \varepsilon_k\big(\mathbf{S}^a - \boldsymbol{\beta}\big)\big|\Psi_k^a\big\rangle. \tag{29$'$}$$

Operators $\mathbf{\Omega}^0(\varepsilon)$, $\boldsymbol{\alpha}$ and $\boldsymbol{\beta}$ can be also written in a compact form

$$\mathbf{\Omega}^0(\varepsilon) = \big(\mathbf{V} - \mathbf{P}\mathbf{S}^{-b}\mathbf{B}\big)\big(\varepsilon\mathbf{S}^b - \mathbf{B}\big)^{-1}\big(\mathbf{V} - \mathbf{B}\mathbf{S}^{-b}\mathbf{P}\big), \tag{20a$'$}$$

$$\boldsymbol{\alpha} = \mathbf{P}\mathbf{S}^{-b}\mathbf{B}\mathbf{S}^{-b}\mathbf{P} - \mathbf{V}\mathbf{S}^{-b}\mathbf{P} - \mathbf{P}\mathbf{S}^{-b}\mathbf{V}, \qquad \boldsymbol{\beta} = \mathbf{P}\mathbf{S}^{-b}\mathbf{P}, \tag{20b$'$}$$

where $\mathbf{S}^{-b} \equiv (\mathbf{S}^b)^{-1} = \sum_i |\Phi_i\rangle\langle\Phi_i|$ is inverse of $\mathbf{S}^b$ in the space X_n^b, i.e., $\mathbf{S}^{-b}\mathbf{S}^b = \mathbf{S}^b\mathbf{S}^{-b} = \mathbf{I}^b$.

Relations (29) and (29$'$) are nonlinear eigenvalue equations in the space X_ρ^a. Consider, for example, relation (29). Solutions of this equation are all eigenvalues $\varepsilon_k \notin \{\lambda_i\}$ of a combined system $\mathcal{S}$ and the corresponding eigenstates $|\Psi_k^a\rangle$ that describe system $\mathcal{S}^a$. According to (27b), those eigenvalues and eigenstates determine projections $|\Psi_k^b\rangle$ and hence corresponding eigenstates $|\Psi_k\rangle$ of the combined system. Thus equation (29) is an equation that explicitly describes system $\mathcal{S}^a$ subject to the interaction with the system $\mathcal{S}^b$, but implicitly it describes the entire interacting system $\mathcal{S}$. All operators in this equation act in the ρ-dimensional space X_ρ^a. Operators $\mathbf{A}$ and $\mathbf{S}^a$ alone describe the system $\mathcal{S}^a$ in the absence of the interaction with the system $\mathcal{S}^b$. The entire interaction with

this system and influence of this system on the system $\mathcal{S}^a$ is succinctly expressed by the operator $\mathbf{\Omega}(\varepsilon)$.

Eigenvalue equation (29) is a $\rho \times \rho$ eigenvalue equation. In this respect, it is similar to the eigenvalue equation (1a) that describes the system $\mathcal{S}^a$ alone and that is also a $\rho \times \rho$ eigenvalue equation. Formally, eigenvalue equation (29) is a perturbed eigenvalue equation (1a), where the role of the perturbation is assumed by the operator $\mathbf{\Omega}(\varepsilon)$. However, though this eigenvalue equation refers only to the ρ-dimensional space X^a_ρ, it has as a solution all cardinal eigenvalues and eigenstates of the combined system. Hence, this equation can have as many as $(\rho + n)$ distinct eigenvalues and eigenstates. This is possible since (29) is not a linear eigenvalue equation. The eigenvalue ε_k of this equation appears on the right-hand side of (29), but it also appears as an argument of the operator $\mathbf{\Omega}(\varepsilon)$ on the left-hand side of this equation. This equation is hence nonlinear, and it can have much more solutions than the dimension ρ of the space X^a_ρ. Therefore, eigenstates $|\Psi^a_k\rangle$ of (29) are usually not orthogonal to each other. If this equation has more solutions than the dimension ρ of the space X^a_ρ, which is almost always the case, corresponding eigenstates are linearly dependent. Orthonormalized and linearly independent are only complete eigenstates $|\Psi_k\rangle$ that describe the combined system $\mathcal{S}$. Note, however, that if $\varepsilon_k \notin \{\lambda_i\}$ is a degenerate eigenvalue of the combined system, and if $|\Psi_{kv}\rangle$ are the corresponding (linearly independent) eigenstates, then $|\Psi^a_{kv}\rangle$ are also linearly independent (see appendix).

Consider the effect of the slow inclusion of the interaction between systems $\mathcal{S}^a$ and $\mathcal{S}^b$. In the absence of the interaction, there is a sharp separation between those two systems. There exist a complete set $\{|\Psi_k\rangle\}$ of the eigenstates of the combined system such that each eigenstate $|\Psi_k\rangle$ refers either entirely to the subsystem $\mathcal{S}^a$ or entirely to the subsystem $\mathcal{S}^b$. One arrives at the same conclusion formally from the eigenvalue equation (29). Namely, if $\mathbf{V} = \mathbf{P} = 0$ one has $\mathbf{\Omega}(\varepsilon) = 0$ and this equation reduces to the eigenvalue equation (1a). One thus obtains ρ linearly independent eigenstates $|\Psi^a_k\rangle \equiv |\Theta_s\rangle \in X^a_\rho$. Since $\mathbf{V} = \mathbf{P} = 0$, (27) implies $|\Psi^b_k\rangle = 0$. Hence $|\Psi_k\rangle = |\Psi^a_k\rangle$ are ρ eigenstates of the combined system. Remaining n eigenstates of this system coincide with unperturbed eigenstates $|\Phi_i\rangle \in X^b_n$. By definition, those eigenstates are singular ($\varepsilon_i = \lambda_i$), and therefore they are not obtained as a solution of the equation (29) that produces all cardinal and may produce only some singular eigenstates.

If the interaction is nonzero, one has $\mathbf{\Omega}(\varepsilon) \neq 0$ and there is no more clear separation between systems $\mathcal{S}^a$ and $\mathcal{S}^b$. Almost every eigenstate $|\Psi_k\rangle$ of the combined system has in this case a nonvanishing component $|\Psi^a_k\rangle \in X^a_\rho$ as well as a nonvanishing component $|\Psi^b_k\rangle \in X^b_\rho$. In addition, interaction usually shifts almost every unperturbed eigenvalue, and therefore large majority of the perturbed eigenvalues ε_k is cardinal ($\varepsilon_k \notin \{\lambda_i\}$). If a particular unperturbed eigenvalue is not effected by the interaction, this is due either to some symmetry, or to some other special condition. Since all cardinal eigenvalues are solutions of the equation (29), with the inclusion of the interaction, however small, this equation suddenly acquires a huge number of solutions. However, if the interaction is small, either the component $|\Psi^a_k\rangle \in X^a_\rho$, or the component $|\Psi^b_k\rangle \in X^b_\rho$ of the eigenstate $|\Psi_k\rangle$ will be usually dominant. If the component $|\Psi^a_k\rangle$ is dominant, it is proper to inter-

pret the state $|\Psi_k\rangle$ as the state describing system $\mathcal{S}^a$ subject to the perturbation by the system $\mathcal{S}^b$. However, if the component $|\Psi_k^b\rangle$ is dominant, it is proper to interpret the state $|\Psi_k\rangle$ as the state describing system $\mathcal{S}^b$ perturbed by the interaction with the system $\mathcal{S}^a$. Thus in most cases one can still associate each eigenstate $|\Psi_k\rangle$ of the combined system either with the system $\mathcal{S}^a$, or with the system $\mathcal{S}^b$. With the increase of the interaction, this association becomes more blurred and it is more difficult to associate the state $|\Psi_k\rangle$ either with $\mathcal{S}^a$ or with $\mathcal{S}^b$.

Above relations apply to the general case $\mathbf{P} \neq 0$. If $\mathbf{P} = 0$ those relations simplify. In particular, relations (27) reduce to

$$\left|\Psi_k^a\right\rangle = W_k^{-1/2} \sum_s^{\rho} C_s^{(k)} |\chi_s\rangle, \tag{30a}$$

$$\left|\Psi_k^b\right\rangle = \sum_i^n \frac{\langle\Phi_i|\mathbf{V}|\Psi_k^a\rangle}{\varepsilon_k - \lambda_i} |\Phi_i\rangle, \tag{30b}$$

while relation (23a) simplifies to

$$W_k = \sum_{sp}^{\rho} C_s^{(k)*} C_p^{(k)} \left[\sum_i^n \frac{\langle\chi_s|\mathbf{V}|\Phi_i\rangle\langle\Phi_i|\mathbf{V}|\chi_p\rangle}{(\varepsilon_k - \lambda_i)^2} + S_{sp}^a \right], \quad \varepsilon_k \notin \{\lambda_i\}. \tag{31a}$$

For completeness, note that if $\mathbf{P} = 0$ relation (23b) that refers to singular eigenstates simplifies to

$$W_k = \sum_{sp}^{\rho} C_s^{(k)*} C_p^{(k)} \left[\sum_{i\,(\lambda_i \neq \varepsilon_k)}^n \frac{\langle\chi_s|\mathbf{V}|\Phi_i\rangle\langle\Phi_i|\mathbf{V}|\chi_p\rangle}{(\varepsilon_k - \lambda_i)^2} + S_{sp}^a \right] + \sum_{\nu}^{\eta} D_{\nu}^{(k)*} D_{\nu}^{(k)},$$

$$\varepsilon_k = \lambda_j \in \{\lambda_i\}. \tag{31b}$$

In addition, one obtains $\boldsymbol{\alpha} = 0$, $\boldsymbol{\beta} = 0$ and $\boldsymbol{\Omega}(\varepsilon) \equiv \boldsymbol{\Omega}^0(\varepsilon)$. In particular,

$$\Omega_{sp}(\varepsilon) \equiv \Omega_{sp}^0(\varepsilon) = \sum_i^n \frac{\langle\chi_s|\mathbf{V}|\Phi_i\rangle\langle\Phi_i|\mathbf{V}|\chi_p\rangle}{\varepsilon - \lambda_i}, \quad \varepsilon \notin \{\lambda_i\}. \tag{8a$'$}$$

Relation (29′) hence reduces to the relation (29).

In a metrics induced by the positive definite operator $\mathbf{S}$ one can define the probability w_k^a to find the eigenstate $|\Psi_k\rangle$ in the system $\mathcal{S}^a$

$$w_k^a = \left\langle\Psi_k^a\middle|\mathbf{S}\middle|\Psi_k^a\right\rangle = \frac{1}{W_k} \sum_{sp}^{\rho} C_s^{(k)*} C_p^{(k)} \left\langle\chi_s\middle|\mathbf{S}^a\middle|\chi_p\right\rangle \tag{32a}$$

as well as the probability w_k^b to find this eigenstate in the system $\mathcal{S}^b$:

$$w_k^b = \left\langle\Psi_k^b\middle|\mathbf{S}\middle|\Psi_k^b\right\rangle = \sum_i^n \frac{|\langle\Phi_i|\mathbf{V}|\Psi_k^a\rangle|^2}{(\varepsilon_k - \lambda_i)^2}. \tag{32b}$$

If the base vectors $|\chi_s\rangle$ in X^a_ρ are chosen to coincide with the eigenstates $|\Theta_s\rangle$, expression (32a) simplifies to

$$w^a_k = \frac{1}{W_k}\sum_s^\rho C^{(k)*}_s C^{(k)}_s. \tag{32a$'$}$$

From (32) one finds

$$w^a_k + w^b_k = 1. \tag{33}$$

This relation must be satisfied in order for quantities w^a_k and w^b_k to be interpreted as probabilities. In the general case $\mathbf{P} \neq 0$ relation (33) can be satisfied only with an artificial definitions of probabilities w^a_k and w^b_k. Namely, one has $\langle\Psi^a_k|\mathbf{S}|\Psi^b_k\rangle = \langle\Psi^a_k|\mathbf{P}|\Psi^b_k\rangle$ and if $\mathbf{P} \neq 0$ components $|\Psi^a_k\rangle$ and $|\Psi^b_k\rangle$ of $|\Psi_k\rangle$ are in general not orthogonal to each other in the metrics defined by the operator $\mathbf{S}$. As a consequence, $w^a_k + w^b_k \neq 1$ and quantities w^a_k and w^b_k cannot be interpreted as probabilities. One can avoid this drawback by using the metrics induced by the operator $\mathbf{S}' = \mathbf{S}^a + \mathbf{S}^b$ instead of the metrics induced by the operator $\mathbf{S}$. In this metrics, one can define quantities $w^{a\prime}_k$ and $w^{b\prime}_k$ that satisfy $w^{a\prime}_k + w^{b\prime}_k = 1$. However, there is a drawback to this definition as well. Namely, in this metrics eigenstates $|\Psi_k\rangle$ and $|\Psi_l\rangle$ that correspond to mutually distinct eigenvalues satisfy $\langle\Psi_k|\mathbf{S}'|\Psi_l\rangle = -\langle\Psi_k|\mathbf{P}|\Psi_l\rangle$. Hence, in this metrics those eigenstates are usually not orthogonal to each other. The same applies to the metrics induced by the unit operator $\mathbf{I}$. All those problems are avoided if $\mathbf{P} = 0$.

Until now, we have considered cardinal solutions to the combined system. Those solutions are most numerous and most important. In the case of singular solutions slightly more complicated relations are obtained. Component $|\Psi^a_k\rangle \in X^a_\rho$ of a normalized eigenstate $|\Psi_k\rangle$ is still given by the relation (27a) where the quantity W_k is now given by (23b). However, component $|\Psi^b_k\rangle \in X^b_n$ of this eigenstate is

$$\big|\Psi^b_k\big\rangle = \sum_{i\,(\lambda_i\neq\varepsilon_k)}^{n} \frac{\sum_s^\rho \langle\Phi_i|\mathbf{V}-\varepsilon_k\mathbf{P}|\Psi^a_k\rangle}{\varepsilon_k-\lambda_i}|\Phi_i\rangle + \big|\Psi^{jb}_k\big\rangle, \quad \varepsilon_k = \lambda_j, \tag{34}$$

where $|\Psi^{jb}_k\rangle = W_k^{-1/2}\sum_\nu D^{(k)}_\nu|\Phi_{j\nu}\rangle$. In addition, relations (13) and (16) combine into

$$\big[\mathbf{\Omega}(\varepsilon_k)+\mathbf{A}\big]\big|\Psi^a_k\big\rangle + [\mathbf{V}-\varepsilon_k\mathbf{P}]\big|\Psi^{jb}_k\big\rangle = \varepsilon_k\mathbf{S}^a\big|\Psi^a_k\big\rangle, \tag{35a}$$

$$\langle\Phi_{j\nu}|\mathbf{V}-\varepsilon_k\mathbf{P}\big|\Psi^a_k\big\rangle = 0, \quad \varepsilon_k = \lambda_j. \tag{35b}$$

Unlike relation (29) that involves only the state $|\Psi^a_k\rangle \in X^a_\rho$ which refers to the system $\mathcal{S}^a$ alone, relations (35) contain also the state $|\Psi^{jb}_k\rangle \in X^b_n$ that refers to the system $\mathcal{S}^b$. Those relations thus partially mix spaces X^a_ρ and X^b_n. This is less appealing than elegant relations (29) and (29$'$) that involve only the space X^a_ρ. However, this drawback is highly compensated by the fact that there are usually very few singular solutions.

7. Generalisation to the time dependent eigenvalue equation

Relation (3a) is time-independent. The above method can be easily generalised to the time-dependent eigenvalue equation

$$i\hbar\frac{\partial}{\partial t}\mathbf{S}\big|\Psi(t)\big\rangle = \mathbf{H}\big|\Psi(t)\big\rangle. \tag{36}$$

An arbitrary solution $|\Psi(t)\rangle$ to this equation is a linear combination

$$\big|\Psi(t)\big\rangle = \sum_{k}^{n+\rho} c_k|\Psi_k\rangle \mathrm{e}^{-\mathrm{i}\varepsilon_k t/\hbar}, \tag{37}$$

where $|\Psi_k\rangle$ are orthonormalized eigenstates of the time independent eigenvalue equation (3a), ε_k are the corresponding eigenvalues and c_k are unknown coefficients to be determined from the initial conditions. In analogy to (26) one has

$$\big|\Psi(t)\big\rangle = \big|\Psi^a(t)\big\rangle + \big|\Psi^b(t)\big\rangle, \tag{38}$$

where $|\Psi^a(t)\rangle \in X^a_\rho$ and $|\Psi^b(t)\rangle \in X^b_n$ are projections of $|\Psi_k(t)\rangle$ on subspaces X^a_ρ and X^b_n, respectively. Hence

$$\big|\Psi^a(t)\big\rangle = \sum_{k}^{n+\rho} c_k\big|\Psi^a_k\big\rangle \mathrm{e}^{-\mathrm{i}\varepsilon_k t/\hbar}, \qquad \big|\Psi^b(t)\big\rangle = \sum_{k}^{n+\rho} c_k\big|\Psi^b_k\big\rangle \mathrm{e}^{-\mathrm{i}\varepsilon_k t/\hbar}. \tag{39}$$

Eigenvalues ε_k and eigenstates $|\Psi^a_k\rangle$ can be obtained as solutions of relations (29) and (35). Once ε_k and $|\Psi^a_k\rangle$ are known, projection $|\Psi^b_k\rangle$ of the eigenstate $|\Psi_k\rangle$ on the space X^b_n can be easily derived. Above relations hence provide a general method for the solution of the time dependent eigenvalue equation (36). In general, summations in expressions (37) and (39) involve cardinal as well as singular eigenstates $|\Psi_k\rangle$. However, the number of cardinal eigenstates is usually much larger than the number of singular eigenstates. Hence, for large n one can in most cases neglect the contribution of singular eigenstates.

One is usually interested in the time evolution of a state $|\Psi(t)\rangle$ that is at $t = 0$ prepared in a well-defined state $|\Psi(0)\rangle$. In particular, if $|\Psi(0)\rangle \equiv |\Theta_s\rangle \in X^a_\rho$, at some latter time t this state will evolve in the state $|\Theta_s(t)\rangle \notin X^a_\rho$. Similarly, if $|\Psi(0)\rangle \equiv |\Phi_i\rangle \in X^b_n$, at some later time t this state will evolve in the state $|\Phi_i(t)\rangle \notin X^b_n$.

We will now consider in more details time evolution of the states $|\Theta_s(t)\rangle$ and $|\Phi_i(t)\rangle$. For the sake of simplicity, we will restrict our consideration to the case $\mathbf{P} = 0$. Generalisation to the case $\mathbf{P} \neq 0$ is straightforward, and can be obtained along the same lines.

If $\mathbf{P} = 0$ then (see appendix)

$$\big|\Theta_s(t)\big\rangle = \sum_{k}^{n+\rho}\frac{1}{W_k^{1/2}}\left[\sum_{p}^{\rho} C_p^{(k)*}\big\langle\chi_p\big|\mathbf{S}^a\big|\Theta_s\big\rangle\right]|\Psi_k\rangle \mathrm{e}^{-\mathrm{i}\varepsilon_k t/\hbar}. \tag{40}$$

It is convenient to choose base vectors $|\chi_p\rangle$ to coincide with the eigenstates $|\Theta_p\rangle$. With such a choice (40) simplifies to

$$\big|\Theta_s(t)\big\rangle = \sum_k^{n+\rho} \frac{C_s^{(k)*}}{W_k^{1/2}} |\Psi_k\rangle \mathrm{e}^{-\mathrm{i}\varepsilon_k t/\hbar}. \tag{41a}$$

Hence

$$\big|\Theta_s^a(t)\big\rangle = \sum_k^{n+\rho} \frac{C_s^{(k)*}}{W_k^{1/2}} \big|\Psi_k^a\big\rangle \mathrm{e}^{-\mathrm{i}\varepsilon_k t/\hbar}, \qquad \big|\Theta_s^b(t)\big\rangle = \sum_k^{n+\rho} \frac{C_s^{(k)*}}{W_k^{1/2}} \big|\Psi_k^b\big\rangle \mathrm{e}^{-\mathrm{i}\varepsilon_k t/\hbar}. \tag{41b}$$

We emphasise that relations (41) contain implicit assumption that all relevant quantities are expressed in the base $\{|\Theta_s\rangle\}$. In particular, if $|\Psi_k\rangle$ is cardinal, the vector $\mathbf{C}^{(k)}$ is a solution of (11) where matrices $\mathbf{\Omega}(\varepsilon_k)$, $\mathbf{A}$ and $\mathbf{S}^a$ are expressed in the base $\{|\Theta_s\rangle\}$. In this base operators $\mathbf{A}$ and $\mathbf{S}^a$ are diagonal, and one has $A_{sp} = E_s\delta_{sp}$ and $S^a_{sp} = \delta_{sp}$.

Since the states $|\Theta_s\rangle \equiv |\Theta_s(0)\rangle$ form a base in X^a_ρ, relations (40) and (41) determine time evolution of each state $|\Psi(t)\rangle$ that is at $t = 0$ prepared in the system $\mathcal{S}^a$.

In a similar way one finds time evolution of states $|\Phi_i(t)\rangle$:

$$\big|\Phi_i(t)\big\rangle = \sum_k \frac{1}{W_k^{1/2}} \frac{\sum_s^\rho \langle\chi_s|\mathbf{V}|\Phi_i\rangle C_s^{(k)*}}{\varepsilon_k - \lambda_i} |\Psi_k\rangle \mathrm{e}^{-\mathrm{i}\varepsilon_k t/\hbar}, \quad \lambda_i \notin \{\varepsilon_k\}, \tag{42a}$$

$$\big|\Phi_{jv}(t)\big\rangle = \sum_{k(\varepsilon_k\neq\lambda_j)} \frac{1}{W_k^{1/2}} \frac{\sum_s^\rho \langle\chi_s|\mathbf{V}|\Phi_{jv}\rangle C_s^{(k)*}}{\varepsilon_k - \lambda_j} |\Psi_k\rangle \mathrm{e}^{-\mathrm{i}\varepsilon_k t/\hbar} + \left[\sum_{k(\varepsilon_k=\lambda_j)} \frac{D_v^{(k)*}}{W_k^{1/2}} |\Psi_k\rangle\right] \mathrm{e}^{-\mathrm{i}\lambda_j t/\hbar},$$
$$\lambda_j \in \{\varepsilon_k\}. \tag{42b}$$

Relation (42a) applies to the case when unperturbed eigenvalue λ_i is not a singular eigenvalue if the combined system, while (42b) applies to the case when λ_j is a singular eigenvalue of the combined system. In this latter case one has an extra contribution to the states $|\Phi_{jv}(t)\rangle$ that involves singular eigenstates $|\Psi_k\rangle$ with $\varepsilon_k = \lambda_j$. As discussed above, the contribution of such eigenstates is usually negligible, especially for large n.

Since the states $|\Phi_i\rangle \equiv |\Phi_i(0)\rangle$ form a base in X^b_ρ, relations (42) determine time evolution of each state $|\Psi(t)\rangle$ that is at $t = 0$ prepared in the system $\mathcal{S}^b$. Relations (41) and (42) hence determine time evolution of an arbitrary state $|\Psi(t)\rangle \in X_{n+\rho}$.

From the above relations one easily obtains all necessary probability amplitudes. For example, if in X^a_ρ the base $\{|\chi_s\rangle\} \equiv \{|\Theta_s\rangle\}$ is used, probability amplitudes $\langle\Theta_p|\mathbf{S}|\Theta_s(t)\rangle \equiv \langle\Theta_p|\mathbf{S}|\Theta^a_s(t)\rangle (p = 1, \ldots, \rho)$ and $\langle\Phi_i|\mathbf{S}|\Theta_s(t)\rangle \equiv \langle\Phi_i|\mathbf{S}|\Theta^b_s(t)\rangle$ $(i = 1, \ldots, n)$ are found to be

$$\langle\Theta_p|\mathbf{S}\big|\Theta_s(t)\big\rangle = \sum_k^{\rho+n} \frac{1}{W_k} C_s^{(k)*} C_p^{(k)} \mathrm{e}^{-\mathrm{i}\varepsilon_k t/\hbar}, \tag{43}$$

$$\langle \Phi_i|\mathbf{S}\big|\Theta_s(t)\big\rangle = \sum_k \frac{C_s^{(k)*}}{W_k} \frac{\sum_p^{\rho} \langle \Phi_i|\mathbf{V}|\Theta_p\rangle C_p^{(k)}}{\varepsilon_k - \lambda_i} \mathrm{e}^{-\mathrm{i}\varepsilon_k t/\hbar}, \quad \lambda_i \notin \{\varepsilon_k\}, \tag{44a}$$

$$\langle \Phi_{j\nu}|\mathbf{S}\big|\Theta_s(t)\big\rangle = \sum_{k(\varepsilon_k \neq \lambda_j)} \frac{C_s^{(k)*}}{W_k} \frac{\sum_p^{\rho} \langle \Phi_{j\nu}|\mathbf{V}|\Theta_p\rangle C_p^{(k)}}{\varepsilon_k - \lambda_j} \mathrm{e}^{-\mathrm{i}\varepsilon_k t/\hbar} + \left[\sum_{k(\varepsilon_k = \lambda_j)} \frac{C_s^{(k)*} D_\nu^{(k)}}{W_k} \right] \mathrm{e}^{-\mathrm{i}\lambda_j t/\hbar}, \quad \lambda_j \in \{\varepsilon_k\}. \tag{44b}$$

Probability amplitudes $\langle \Theta_p|\mathbf{S}|\Theta_s(t)\rangle$ refer to the space X_ρ^a and they determine time evolution of a system $\mathcal{S}^a$. On the other hand, probability amplitudes $\langle \Phi_i|\mathbf{S}|\Theta_s(t)\rangle$ refer to the space X_n^b and they determine transition probabilities for a state that is at time $t = 0$ prepared in a system $\mathcal{S}^a$ to be found at time t in some state $|\Phi_i\rangle$ of a system $\mathcal{S}^b$.

For $t = 0$ above relations in conjunction with orthonormality relation (1b) and orthogonality condition $\langle \Phi_i|\mathbf{S}|\Theta_s\rangle \equiv \langle \Phi_i|\mathbf{S}|\Theta_s(0)\rangle = 0$ imply

$$\langle \Theta_p|\mathbf{S}|\Theta_s\rangle = \sum_k^{\rho+n} \frac{1}{W_k} C_s^{(k)*} C_p^{(k)} = \delta_{sp}, \tag{45}$$

$$\langle \Phi_i|\mathbf{S}|\Theta_s\rangle = \sum_k \frac{C_s^{(k)*}}{W_k} \frac{\sum_p^{\rho} \langle \Phi_i|\mathbf{V}|\Theta_p\rangle C_p^{(k)}}{\varepsilon_k - \lambda_i} = 0, \quad \lambda_i \notin \{\varepsilon_k\}, \tag{46a}$$

$$\langle \Phi_{j\nu}|\mathbf{S}|\Theta_s\rangle = \sum_{k(\varepsilon_k \neq \lambda_j)} \frac{C_s^{(k)*}}{W_k} \frac{\sum_p^{\rho} \langle \Phi_{j\nu}|\mathbf{V}|\Theta_p\rangle C_p^{(k)}}{\varepsilon_k - \lambda_j} + \left[\sum_{k(\varepsilon_k = \lambda_j)} \frac{C_s^{(k)*} D_\nu^{(k)}}{W_k} \right] = 0, \quad \lambda_j \in \{\varepsilon_k\}. \tag{46b}$$

Probability amplitudes $\langle \Theta_s|\mathbf{S}|\Phi_i(t)\rangle$ and $\langle \Phi_j|\mathbf{S}|\Phi_i(t)\rangle$ can be derived in a similar way.

8. Example of the interaction of two quantum systems

In order to illustrate the above method, consider the interaction of a two-dimensional system $\mathcal{S}_2^a$ with a known three-dimensional system $\mathcal{S}_3^b$.

Let the system $\mathcal{S}_2^a$ be described by the generalised eigenvalue equation (1a) where in a base $\{|\chi_s\rangle\}$ one has

$$\mathbf{A} = \begin{bmatrix} 1 & -0.5 \\ -0.5 & 0 \end{bmatrix}, \qquad \mathbf{S}^a = \begin{bmatrix} 1 & 0.3 \\ 0.3 & 1 \end{bmatrix}. \tag{47}$$

Let the system $\mathcal{S}_3^b$ be described by the generalised eigenvalue equation (2a) where in a base $\{|r\rangle\}$

$$\mathbf{B} = \begin{bmatrix} 1 & 2 & 3 \\ 2 & 2 & 1 \\ 3 & 1 & 5 \end{bmatrix}, \qquad \mathbf{S}^b = \begin{bmatrix} 1 & 0.5 & 0.2 \\ 0.5 & 1.2 & 0.5 \\ 0.2 & 0.5 & 1.3 \end{bmatrix}. \tag{48}$$

Let further the combined system $\mathcal{S}_5$ that includes the interaction between systems $\mathcal{S}_2^a$ and $\mathcal{S}_3^b$ be described by the generalised eigenvalue equation (3a) where in a base $\{|r\rangle, |\chi_s\rangle\}$

$$\mathbf{H} = \begin{bmatrix} \mathbf{B} & \mathbf{I}^b\mathbf{V}\mathbf{I}^a \\ \mathbf{I}^a\mathbf{V}\mathbf{I}^b & \mathbf{A} \end{bmatrix}, \qquad \mathbf{S} = \begin{bmatrix} \mathbf{S}^b & \mathbf{I}^b\mathbf{P}\mathbf{I}^a \\ \mathbf{I}^a\mathbf{P}\mathbf{I}^b & \mathbf{S}^a \end{bmatrix} \tag{49a}$$

and where generalised interaction $(\mathbf{V}, \mathbf{P})$ is given by

$$\mathbf{I}^a\mathbf{V}\mathbf{I}^b = \begin{bmatrix} 1 & 2 & -1 \\ 1 & 2 & 3 \end{bmatrix}, \qquad \mathbf{I}^a\mathbf{P}\mathbf{I}^b = \begin{bmatrix} 0.3 & -0.5 & 0.2 \\ 0.3 & 0.1 & -0.4 \end{bmatrix}. \tag{49b}$$

One finds that this combined system has eigenvalues

$$\begin{aligned} &\varepsilon_1 = -2.32918, \qquad \varepsilon_2 = -1.50057, \qquad \varepsilon_3 = 0.06038, \\ &\varepsilon_4 = 4.35986, \qquad \varepsilon_5 = 60.42988. \end{aligned} \tag{50a}$$

The corresponding eigenstates are

$$\begin{aligned} |\Psi_1\rangle &= \begin{pmatrix} 1.11912 \\ -0.49548 \\ -0.39826 \\ -0.51397 \\ 0.05630 \end{pmatrix}, \qquad |\Psi_2\rangle = \begin{pmatrix} 0.35630 \\ 0.29638 \\ -0.02665 \\ -0.37694 \\ -0.73890 \end{pmatrix}, \qquad |\Psi_3\rangle = \begin{pmatrix} 0.53374 \\ -0.49000 \\ 0.20859 \\ 0.40996 \\ -0.57247 \end{pmatrix}, \\ |\Psi_4\rangle &= \begin{pmatrix} 0.07052 \\ 0.63770 \\ 0.27950 \\ 0.44679 \\ 0.34263 \end{pmatrix}, \qquad |\Psi_5\rangle = \begin{pmatrix} 1.17903 \\ -2.38652 \\ 1.73945 \\ -2.44302 \\ 1.36072 \end{pmatrix}. \end{aligned} \tag{50b}$$

This can be verified by inserting those eigenvalues and eigenstates in the eigenvalue equation (3a) with matrices **H** and **S** as given by (49). One can also verify that eigenstates (50b) are orthonormalized according to (3d).

We will now solve the same eigenvalue equation by the above suggested method. In this method, in order to solve combined eigenvalue equation, one has to know the solution of the eigenvalue equation (2a) describing the system $\mathcal{S}_3^b$. This system has three eigenvalues and three corresponding eigenstates orthonormalized according to (2b). One finds

$$\lambda_1 = -1.66138, \qquad \lambda_2 = 1.89610, \qquad \lambda_3 = 5.20405, \tag{51a}$$

$$|\Phi_1\rangle = \begin{pmatrix} 0.99832 \\ -0.56029 \\ -0.32137 \end{pmatrix}, \quad |\Phi_2\rangle = \begin{pmatrix} 0.23961 \\ 0.86544 \\ -0.26545 \end{pmatrix}, \quad |\Phi_3\rangle = \begin{pmatrix} 0.45738 \\ -0.39004 \\ 0.86160 \end{pmatrix}. \quad (51b)$$

We first notice that unperturbed eigenvalues λ_i and perturbed eigenvalues ε_k satisfy interlacing rule. For example, $\varepsilon_1 = -2.32918 < \lambda_1 = -1.66138 < \varepsilon_3 = 0.06038$ in accord with (21), etc.

From (49b) and (51b) one derives matrix elements $\langle\chi_s|\mathbf{V}|\Phi_i\rangle \equiv \langle\mathbf{u}_s|\Phi_i\rangle$ and $\langle\chi_s|\mathbf{P}|\Phi_i\rangle \equiv \langle\mathbf{x}_s|\Phi_i\rangle$:

$$\begin{aligned} &\langle\mathbf{u}_1|\Phi_1\rangle = 0.19912, && \langle\mathbf{u}_2|\Phi_1\rangle = -1.08638, \\ &\langle\mathbf{u}_1|\Phi_2\rangle = 2.23594, && \langle\mathbf{u}_2|\Phi_2\rangle = 1.17415, \\ &\langle\mathbf{u}_1|\Phi_3\rangle = -1.18430, && \langle\mathbf{u}_2|\Phi_3\rangle = 2.26211, \\ &\langle\mathbf{x}_1|\Phi_1\rangle = 0.51537, && \langle\mathbf{x}_2|\Phi_1\rangle = 0.37202, \\ &\langle\mathbf{x}_1|\Phi_2\rangle = -0.41393, && \langle\mathbf{x}_2|\Phi_2\rangle = 0.26461, \\ &\langle\mathbf{x}_1|\Phi_3\rangle = 0.50456, && \langle\mathbf{x}_2|\Phi_3\rangle = -0.24643. \end{aligned} \quad (52)$$

One can now proceed using relation (11) that has a nontrivial solution if the determinant $h(\varepsilon)$ given by (7) is zero. Equivalently, one can use relation (11′) that has a nontrivial solution if determinant $h(\varepsilon)$ as expressed by relation (7′) is zero. For the sake of illustration we will apply this latter approach.

Using relations (20) and (52) one obtains matrix elements of matrices $\mathbf{\Omega}^0(\varepsilon)$, $\boldsymbol{\alpha}$ and $\boldsymbol{\beta}$

$$\begin{aligned} \Omega^0_{11}(\varepsilon) &= \frac{1.11373}{\varepsilon-\lambda_1} + \frac{9.12516}{\varepsilon-\lambda_2} + \frac{14.51632}{\varepsilon-\lambda_3}, \\ \Omega^0_{22}(\varepsilon) &= \frac{0.21932}{\varepsilon-\lambda_1} + \frac{0.45215}{\varepsilon-\lambda_2} + \frac{12.56382}{\varepsilon-\lambda_3}, \\ \Omega^0_{12}(\varepsilon) \equiv \Omega^0_{21}(\varepsilon) &= \frac{-0.49423}{\varepsilon-\lambda_1} + \frac{2.03125}{\varepsilon-\lambda_2} - \frac{13.50483}{\varepsilon-\lambda_3}, \end{aligned} \quad (53a)$$

$$\begin{aligned} &\alpha_{11} = 4.04931, && \alpha_{22} = 1.52069, && \alpha_{12} = \alpha_{21} = -2.22630, \\ &\beta_{11} = 0.69151, && \beta_{22} = 0.26914, && \beta_{12} = \beta_{21} = -0.04214. \end{aligned} \quad (53b)$$

Inserting (47) and (53) into (7′) one obtains

$$h(\varepsilon) \equiv \begin{vmatrix} \Omega^0_{11}(\varepsilon) + 5.04931 - 0.30849\varepsilon & \Omega^0_{12}(\varepsilon) - 2.72630 - 0.34214\varepsilon \\ \Omega^0_{21}(\varepsilon) - 2.72630 - 0.34214\varepsilon & \Omega^0_{22}(\varepsilon) + 1.52069 - 0.73086\varepsilon \end{vmatrix} = 0. \quad (54)$$

Roots of this equation are cardinal eigenvalues of the combined system. One easily verifies that eigenvalues (50a) satisfy (54). In addition, one finds that there are no other

solutions to (54). This shows that relation (7′) produces correct eigenvalues of the combined system. Moreover, in this particular case the function $h(\varepsilon)$ has exactly five roots. Since the combined system is five-dimensional, those are all eigenvalues of this system, and there are no singular solutions.

Once the particular eigenvalue ε_k is found as a root of $h(\varepsilon)$, the corresponding cardinal eigenstate (10) is determined by the column vector $\mathbf{C}^{(k)}$, nontrivial solution to the matrix equation (11′):

$$\begin{bmatrix} \Omega^0_{11}(\varepsilon_k) + 5.04931 & \Omega^0_{12}(\varepsilon_k) - 2.72630 \\ \Omega^0_{21}(\varepsilon_k) - 2.72630 & \Omega^0_{22}(\varepsilon_k) + 1.52069 \end{bmatrix} \begin{pmatrix} C_1 \\ C_2 \end{pmatrix} = \varepsilon_k \begin{bmatrix} 0.30849 & 0.34214 \\ 0.34214 & 0.73086 \end{bmatrix} \begin{pmatrix} C_1 \\ C_2 \end{pmatrix}. \tag{55}$$

Using obtained eigenvalues ε_k one finds:

$$\begin{aligned} &\mathbf{C}^{(1)} = \begin{pmatrix} 1 \\ -0.10954 \end{pmatrix}, \qquad \mathbf{C}^{(2)} = \begin{pmatrix} 1 \\ 1.96028 \end{pmatrix}, \qquad \mathbf{C}^{(3)} = \begin{pmatrix} 1 \\ -1.39639 \end{pmatrix}, \\ &\mathbf{C}^{(4)} = \begin{pmatrix} 1 \\ 0.76687 \end{pmatrix}, \qquad \mathbf{C}^{(5)} = \begin{pmatrix} 1 \\ -0.55698 \end{pmatrix}. \end{aligned} \tag{56}$$

Inserting above vectors into (10) and using (50a), (51a) and (52) one obtains, up to the normalisation constant, eigenstates (50b) of the combined system. One can also calculate quantities W_k according to (23a) and normalize those eigenstates. One thus obtains eigenstates (50b) up to the sign. This shows that suggested method produces correct cardinal eigenstates of the combined system.

From a numerical point of view above example is not very interesting. It can be solved more efficiently by many other methods. However, it illustrates main features of the suggested method, its advantageous and possible drawbacks.

Eigenvalue equation (55) that describes the system $\mathcal{S}^a_2$ subject to the interaction (49b) with the known system $\mathcal{S}^b_3$ is a 2×2 eigenvalue equation. In this example, system $\mathcal{S}^b_3$ was relatively small three-dimensional system. However, dimension n of this system can be arbitrary large. All cardinal solutions of the combined system will be still the solution of the 2×2 eigenvalue equation that is similar to the eigenvalue equation (55). If singular eigenvalues exist, dimension of the corresponding eigenvalue equation will be slightly larger than 2×2, but still much smaller than the dimension of the combined space X_{n+2}. Thus if the dimension of the system $\mathcal{S}^b$ is large enough, this method will be numerically much more efficient than other known methods.

9. Conclusion

Quantum system $\mathcal{S}$ consisting of subsystems $\mathcal{S}^a$ and $\mathcal{S}^b$ is considered. With a system $\mathcal{S}^a$ is associated a ρ-dimensional space X^a_ρ and with a system $\mathcal{S}^b$ is associated an

n-dimensional space X_n^b that is orthogonal to the space X_ρ^a. System $\mathcal{S}^a$ alone is described by the generalised $\rho \times \rho$ eigenvalue equation $\mathbf{A}|\Theta_s\rangle = E_s\mathbf{S}^a|\Theta_s\rangle (s = 1, \ldots, \rho)$, where $\mathbf{A}$ and $\mathbf{S}^a$ are Hermitian operators, while $\mathbf{S}^a$ is, in addition, positive definite. Similarly, system $\mathcal{S}^b$ alone is described by the 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 Hermitian operators, while $\mathbf{S}^b$ is, in addition, positive definite. It is assumed that the solution to this system (eigenvalues λ_i and the corresponding eigenstates $|\Phi_i\rangle$) is known. The combined quantum system $\mathcal{S} = \mathcal{S}^a \oplus \mathcal{S}^b$ is described by a generalised eigenvalue equation $[\mathbf{A} + \mathbf{B} + \mathbf{V}]|\Psi_k\rangle = \varepsilon_k[\mathbf{S}^a + \mathbf{S}^b + \mathbf{P}]|\Psi_k\rangle$, where operators $\mathbf{V}$ and $\mathbf{P}$ describe generalised interaction between subsystems $\mathcal{S}^a$ and $\mathcal{S}^b$. Formulation in terms of generalised eigenvalue equations allows for a most general treatment of the combined system $\mathcal{S}$ and its subsystems $\mathcal{S}^a$ and $\mathcal{S}^b$.

New method for the solution of the combined system is derived. In this method one distinguishes cardinal ($\varepsilon_k \notin \{\lambda_i\}$) and singular ($\varepsilon_k \in \{\lambda_i\}$) eigenvalues and the corresponding eigenstates of the combined system. Efficiency of this method does not depend on the magnitude of the interaction. Most important feature of this method is replacement of the huge $(\rho + n)(\rho + n)$ eigenvalue equation that describes the combined system with much smaller eigenvalue equation that refers essentially to the system $\mathcal{S}^a$. In particular, all cardinal solutions can be derived from the $\rho \times \rho$ eigenvalue equation $[\mathbf{\Omega}(\varepsilon_k) + \mathbf{A}]|\Psi_k^a\rangle = \varepsilon_k\mathbf{S}^a|\Psi_k^a\rangle$ that refers to the system $\mathcal{S}^a$ alone. Formally, this equation is eigenvalue equation $\mathbf{A}|\Theta_s\rangle = E_s\mathbf{S}^a|\Theta_s\rangle$ that described isolated system $\mathcal{S}^a$ subject to the perturbation $\mathbf{\Omega}(\varepsilon)$. This perturbation is a Hermitian operator acting in the space X_ρ^a. It is expressed in terms of the eigenvalues λ_i of the system $\mathcal{S}^b$ and in terms of matrix elements $\langle\chi_s|\mathbf{V}|\Phi_i\rangle$ and $\langle\chi_s|\mathbf{P}|\Phi_i\rangle$, where vectors $|\chi_s\rangle$ form a base in X_ρ^a. Those quantities incorporate essential features of the system $\mathcal{S}^b$ and of the interaction $(\mathbf{V}, \mathbf{P})$ between the two systems. Eigenstate $|\Psi_k^a\rangle$ of this equation is the projection of the eigenstate $|\Psi_k\rangle$ on the space X_ρ^a. This eigenstate describes all properties of the system $\mathcal{S}^a$. Once $|\Psi_k^a\rangle$ is known, the projection $|\Psi_k^b\rangle$ of $|\Psi_k\rangle$ on the space X_n^b can be easily obtained. Thus, if the solution to the system $\mathcal{S}^b$ is known, one can obtain all cardinal solutions of the combined system as a solution to the above eigenvalue equation that refers to a system $\mathcal{S}^a$ alone. Slightly more complicated expression is obtained for singular eigenvalues $\varepsilon_k \in \{\lambda_i\}$ and the corresponding eigenstates, provided such eigenvalues and eigenstates exist.

The method can be easily generalised to the time-dependent eigenvalue equation $i\hbar\mathbf{S}\partial/\partial t|\Psi(t)\rangle = \mathbf{H}|\Psi(t)\rangle$. In conclusion, the system $\mathcal{S}^a$ that interacts with potentially very huge known system $\mathcal{S}^b$ can be described in an exact way with an eigenvalue equation that refers essentially to the system $\mathcal{S}^a$. In this eigenvalue equation the role of the "perturbation" is assumed by the operator $\mathbf{\Omega}(\varepsilon)$ that incorporates basic features of the system $\mathcal{S}^b$ and of the interaction between the two systems. In general, one has to know the solution to the system $\mathcal{S}^b$ in order to construct this operator. However, in practical applications one can use a different approach. Even if the solution to the system $\mathcal{S}^b$ is not known, one can model this operator in such a way as to reproduce some known properties of the system $\mathcal{S}^a$. This modelling should be assisted with the knowledge of the general structure of the operator $\mathbf{\Omega}(\varepsilon)$ and with possible partial knowledge of the system $\mathcal{S}^b$ and the nature of the interaction between the two systems. Such an approach

may provide a reasonably good description of a system $\mathcal{S}^a$ that interacts with a relatively large and not completely known system $\mathcal{S}^b$.

In the case $\rho = 1$ the suggested method and its performance was successfully verified by the computer program using random matrices as large as $n = 5 \cdot 10^6$ [6].

Appendix

A.1. Basic relations

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

$$\mathbf{A}_0|\phi_s\rangle = E_s|\phi_s\rangle, \tag{A.1}$$

where

$$\mathbf{A}_0 = \big(\mathbf{S}^a\big)^{-1/2}\mathbf{A}\big(\mathbf{S}^a\big)^{-1/2}, \qquad |\phi_s\rangle = \big(\mathbf{S}^a\big)^{1/2}|\Theta_s\rangle. \tag{A.1′}$$

Hermiticity of $\mathbf{A}$ and $\mathbf{S}^a$ implies hermiticity of $\mathbf{A}_0$, and the eigenvalues E_s of the eigenvalue equation (1a) are hence real. Further, eigenstates $|\phi_s\rangle$ of $\mathbf{A}_0$ can be orthonormalized according to $\langle\phi_s|\phi_p\rangle = \delta_{sp}$, which implies (1b). The set $\{|\Theta_s\rangle\}$ is hence complete. In a similar way one shows that eigenstates $|\Phi_i\rangle$ of (2a) and eigenstates $|\Psi_k\rangle$ of (3a) can be orthonormalized according to (2b) and (3d), respectively.

Define operators $\mathbf{I}^a$, $\mathbf{I}^b$ and $\mathbf{I}$:

$$\mathbf{I}^a = \sum_s^\rho |\chi_s\rangle\langle\chi_s|\mathbf{K}^a, \qquad \mathbf{I}^b = \sum_i^n |\Phi_i\rangle\langle\Phi_i|\mathbf{S}^b, \qquad \mathbf{I} = \sum_k^{n+\rho} |\Psi_k\rangle\langle\Psi_k|\mathbf{S}. \tag{A.2}$$

Using (4b) one finds $\mathbf{I}^a|\chi_p\rangle = |\chi_p\rangle$ for each vector $|\chi_p\rangle \in X^a_\rho$. Since these vectors form a base in X^a_ρ, operator $\mathbf{I}^a$ is a projection operator on this space. In a similar way one finds that $\mathbf{I}^b$ is a projection operator on the space X^b_n, while $\mathbf{I}$ is a projection operator on the combined space $X_{n+\rho}$, i.e., it is a unit operator. One also has $\mathbf{I} = \mathbf{I}^a + \mathbf{I}^b$.

Multiplying perturbed eigenvalue equation (3a) from left with $\langle\Phi_i|$ and using (2) and relations $\langle\Phi_i|\mathbf{A} = \langle\Phi_i|\mathbf{S}^a = 0$ one obtains

$$(\varepsilon_k - \lambda_i)\big\langle\Phi_i\big|\mathbf{S}^b\big|\Psi_k\big\rangle = \langle\Phi_i|\mathbf{V} - \varepsilon_k\mathbf{P}|\Psi_k\rangle.$$

Since $|\Phi_i\rangle \in X^b_n$ one has $\langle\Phi_i|(\mathbf{V} - \varepsilon\mathbf{P}) \in X^a_\rho$. Hence $\langle\Phi_i|(\mathbf{V} - \varepsilon\mathbf{P}) = \langle\Phi_i|(\mathbf{V} - \varepsilon\mathbf{P})\mathbf{I}^a$. Using (A.2) one finds

$$(\varepsilon_k - \lambda_i)\big\langle\Phi_i\big|\mathbf{S}^b\big|\Psi_k\big\rangle = \sum_s^\rho \langle\Phi_i|\mathbf{V} - \varepsilon_k\mathbf{P}|\chi_s\rangle\big\langle\chi_s\big|\mathbf{K}^a\big|\Psi_k\big\rangle, \quad i = 1, \ldots, n. \tag{A.3}$$

Multiplying perturbed eigenvalue equation (3a) from left with $\langle\chi_s|$ and using $\langle\chi_s|\mathbf{B} = \langle\chi_s|\mathbf{S}^b = 0$ one finds

$$\langle\chi_s|\mathbf{V} - \varepsilon_k\mathbf{P}|\Psi_k\rangle + \big\langle\chi_s\big|\mathbf{A} - \varepsilon_k\mathbf{S}^a\big|\Psi_k\big\rangle = 0.$$

Further $\mathbf{A} - \varepsilon\mathbf{S}^a = (\mathbf{A} - \varepsilon\mathbf{S}^a)\mathbf{I}^a$, and hence

$$\langle\chi_s|\mathbf{V} - \varepsilon_k\mathbf{P}|\Psi_k\rangle + \sum_p^{\rho}\langle\chi_s|\mathbf{A} - \varepsilon_k\mathbf{S}^a|\chi_p\rangle\langle\chi_p|\mathbf{K}^a|\Psi_k\rangle = 0, \quad s = 1, \ldots, \rho. \tag{A.4}$$

In particular, for $\{|\chi_s\rangle\} \equiv \{|\Theta_s\rangle\}$ this relation simplifies to

$$\langle\Theta_s|\mathbf{V} - \varepsilon_k\mathbf{P}|\Psi_k\rangle + (E_s - \varepsilon_k)\langle\Theta_s|\mathbf{S}^a|\Psi_k\rangle = 0, \quad s = 1, \ldots, \rho. \tag{A.4$'$}$$

Relations (A.3) and (A.4) are starting relations for the derivation of theorems 1 and 2.

A.2. Proof of theorem 1

Let $\varepsilon_k \notin \{\lambda_i\}$ be a cardinal eigenvalue of the perturbed equation. Dividing (A.3) by $(\varepsilon_k - \lambda_i)$ $(i = 1, \ldots, n)$, multiplying by $|\Phi_i\rangle$, summing over i, adding to both sides of the obtained relation $\mathbf{I}^a|\Psi_k\rangle \equiv \sum_s |\chi_s\rangle\langle\chi_s|\mathbf{K}^a|\Psi_k\rangle$ and using (A.2), one derives expression (10) where coefficients $C_s^{(k)}$ are given by (12). This relation expresses the perturbed eigenstate $|\Psi_k\rangle$ as a linear combination of unperturbed eigenstates $|\Phi_i\rangle$ that span the space X_n^b and states $|\chi_s\rangle$ that span the space X_ρ^a. Next one has to determine unknown coefficients $C_s^{(k)}$. Multiplying expression (10) from left with $\langle\chi_p|(\mathbf{V} - \varepsilon_k\mathbf{P})$ one obtains

$$\langle\chi_s|\mathbf{V} - \varepsilon_k\mathbf{P}|\Psi_k\rangle = \sum_p^{\rho}\Omega_{sp}(\varepsilon_k)C_p^{(k)}, \tag{A.5}$$

where $\Omega(\varepsilon)$ is given by (8a).

Comparing (A.4) and (A.5) one finds

$$\sum_p^{\rho}\left[\Omega_{sp}(\varepsilon_k) + \langle\chi_s|\mathbf{A} - \varepsilon_k\mathbf{S}^a|\chi_p\rangle\right]C_p^{(k)} = 0. \tag{A.6}$$

This is relation (11). It is a homogenous linear set of ρ linear equations in ρ unknowns $C_p^{(k)}$. In order for the eigenstate (10) to be nontrivial, at least one coefficient $C_p^{(k)}$ must be nonzero. Hence (A.6) should have a nontrivial solution. However, this relation has a nontrivial solution if and only if the determinant of a system vanishes, which gives condition (7).

This proves that the necessary condition for $\varepsilon \equiv \varepsilon_k$ to be an eigenvalue of the perturbed equation (3a) is that it satisfies (7). Further, it shows that if $\varepsilon \equiv \varepsilon_k$ is a perturbed eigenvalue, the corresponding eigenstates are all of the form (10), where the coefficients $C_p^{(k)}$ are components of a column vector $\mathbf{C}^{(k)}$, nontrivial solution of a matrix equation (11).

Following the above derivation backwards one finds that the inverse is also true. Each root $\varepsilon \equiv \varepsilon_k \notin \{\lambda_i\}$ of (7) is an eigenvalue of the perturbed equation (3a), and all the corresponding eigenstates are of a type (10), where coefficients $C_p^{(k)} = \langle\chi_p|\mathbf{K}^a|\Psi_k\rangle$ satisfy (11). This proves theorem 1.

A.3. Proof of theorem 2

Assume the same conditions as in theorem 1. Let $\varepsilon_k = \lambda_j$ be a singular eigenvalue of the perturbed eigenvalue equation (3a). Let further λ_j be a η-degenerate eigenvalue of the unperturbed equation (2a), and let $|\Phi_{j\nu}\rangle$ $(\nu = 1, \ldots, \eta)$ be the corresponding unperturbed eigenstates.

Dividing (A.3) by $(\varepsilon_k - \lambda_i)(\lambda_i \neq \varepsilon_k)$, multiplying by $|\Phi_i\rangle$, summing over i, adding to both sides of the obtained relation $\sum_s |\chi_s\rangle\langle\chi_s|\mathbf{K}^a|\Psi_k\rangle + \sum_\nu \langle\Phi_{j\nu}|\mathbf{S}^b|\Psi_k\rangle|\Phi_{j\nu}\rangle$ and using (A.2), one derives expression (15) where coefficients $C_s^{(k)}$ and $D_\nu^{(k)}$ are given by (17). This relation expresses the perturbed eigenstate $|\Psi_k\rangle$ as a linear combination of unperturbed eigenstates $|\Phi_i\rangle$ that span the space X_n^b and states $|\chi_s\rangle$ that span the space X_ρ^a.

Next one has to determine unknown coefficients $C_s^{(k)}$ and $D_\nu^{(k)}$. Multiplying (15) from left with $\langle\chi_p|(\mathbf{V} - \varepsilon_k\mathbf{P})$ one obtains

$$\langle\chi_s|\mathbf{V} - \varepsilon_k\mathbf{P}|\Psi_k\rangle = \sum_p^\rho \Omega_{sp}(\varepsilon_k)C_p^{(k)} + \sum_\nu^\eta \langle\chi_s|\mathbf{V} - \varepsilon_k\mathbf{P}|\Phi_{j\nu}\rangle D_\nu^{(k)}, \tag{A.7}$$

where $\Omega_{sp}(\varepsilon_k)$ is given by (8b).

Comparing (A.4) with (A.7) one finds

$$\sum_p^\rho \big[\Omega_{sp}(\varepsilon_k) + \big\langle\chi_s\big|\mathbf{A} - \varepsilon_k\mathbf{S}^a\big|\chi_p\big\rangle\big]C_p^{(k)} + \sum_\nu^\eta \langle\chi_s|\mathbf{V} - \varepsilon_k\mathbf{P}|\Phi_{j\nu}\rangle D_\nu^{(k)} = 0,$$
$$s = 1, \ldots, \rho. \tag{A.8}$$

Further, relation (A.3) for $i = j$ implies

$$\sum_p^\rho \langle\Phi_{j\nu}|\mathbf{V} - \varepsilon_k\mathbf{P}|\chi_p\rangle C_p^{(k)} = 0, \quad \nu = 1, \ldots, \eta. \tag{A.9}$$

Relations (A.8) and (A.9) form a homogenous linear set of $\rho + \eta$ linear equations in $\rho + \eta$ unknowns $C_p^{(k)}$ and $D_\nu^{(k)}$. Expressed in a matrix form those relations are equivalent to relation (16). This relation has a (nontrivial) solution if and only if the determinant of a system vanishes, which gives condition (13).

This proves that the necessary condition for $\varepsilon_k = \lambda_j$ to be a singular eigenvalue of the perturbed equation (3a) is that it satisfies (13). Further, it shows that if $\varepsilon_k = \lambda_j$ is a perturbed eigenvalue, the corresponding eigenstates are all of the form (15) where the coefficients $C_p^{(k)}$ and $D_\nu^{(k)}$ are given by (17). Moreover, those coefficients are components of a column vector $(\mathbf{C}^{(k)}, \mathbf{D}^{(k)})$ that is a nontrivial solution of a matrix equation (16).

Following the above derivation backwards one finds that those conditions are also sufficient. If $\varepsilon_k = \lambda_j$ satisfies (13) it is a singular eigenvalue of the perturbed eigenvalue equation (3a). Further, each nontrivial solution $(\mathbf{C}^{(k)}, \mathbf{D}^{(k)})$ of (16) generates according to (15) the corresponding eigenstate. This proves theorem 2.

A.4. Proof of lemmas 1 and 2

By definition, nullity of the operator $\mathbf{\Omega}(\varepsilon_k)+\mathbf{A}-\varepsilon_k\mathbf{S}^a$ is the number of the linearly independent solutions to (11). Let $\mathbf{C}^{(kr)}$ $(r = 1,\ldots,l)$ be those linearly independent solutions. According to (10) each vector $\mathbf{C}^{(kr)}$ generates a perturbed eigenstate $|\Psi_{kr}\rangle$. Assume those perturbed eigenstates to be linearly dependent. Then there exist a nontrivial set of coefficients c_r such that $\sum_r c_r|\Psi_{kr}\rangle = 0$. Since $|\Phi_i\rangle \in X_n^b$ while $|\chi_s\rangle \in X_\rho^a$, this and (10) implies $\sum_s \sum_r C_s^{(kr)} c_r|\chi_s\rangle = 0$. Since base vectors $|\chi_s\rangle$ are linearly independent, one has $\sum_r c_r C_s^{(kr)} = 0$ $(s = 1,\ldots,\rho)$. Thus vectors $\mathbf{C}^{(kr)}$ are linearly dependent, contrary to the assumption. Hence the eigenstates $|\Psi_{kr}\rangle$ must be linearly independent. This shows that the degeneracy of ε_k equals the number of linearly independent solutions $\mathbf{C}^{(k)}$ to (10), which completes the proof.

Note that the above derivation proves not only that eigenvectors $|\Psi_{kr}\rangle$ are linearly independent, but also that the projections $|\Psi_{kr}^a\rangle \equiv \sum_s C_s^{(kr)}|\chi_s\rangle$ of those eigenstates on the space X_ρ^a are linearly independent.

Lemma 2 can be proven in the same way.

A.5. Proof of the interlacing rule

Let the unperturbed eigenvalues λ_i $(i = 1,\ldots,n)$ and the perturbed eigenvalues ε_k $(k = 1,\ldots,n+\rho)$ be arranged in a nondecreasing order. In the special case $\rho = 1$ those eigenvalues are interlaced according to [6]

$$\varepsilon_1 \leqslant \lambda_1 \leqslant \varepsilon_2 \leqslant \lambda_2 \leqslant \cdots \leqslant \lambda_n \leqslant \varepsilon_{n+1}. \tag{A.10}$$

According to a matrix representation (5), transition from the unperturbed equation (2a) to the perturbed equation (3a) represents augmentation of this equation by ρ additional rows and ρ additional columns. One can obtain this augmentation applying ρ times matrix augmentation by a single row and a single column. Thus, a general case $\rho > 1$ can be obtained as a result of ρ successive applications of the $\rho = 1$ case. However, to each $\rho = 1$ case interlacing relation (A.10) applies. By induction, one obtains general interlacing rule (21). For example, let $\rho = 2$. One can obtain this case by two $\rho = 1$ augmentations. Denote perturbed eigenvalues obtained after first augmentation by $\varepsilon_1',\ldots,\varepsilon_{n+1}'$ and denote perturbed eigenvalues obtained after second augmentation by $\varepsilon_1,\ldots,\varepsilon_{n+2}$. According to (A.10) one has

$$\varepsilon_1' \leqslant \lambda_1 \leqslant \varepsilon_2' \leqslant \lambda_2 \leqslant \cdots \leqslant \lambda_n \leqslant \varepsilon_{n+1}'.$$

After first augmentation, eigenvalues $\varepsilon_1',\ldots,\varepsilon_{n+1}'$ assume the role of the unperturbed eigenvalues λ_i, and hence applying (A.10) once more one obtains

$$\varepsilon_1 \leqslant \varepsilon_1' \leqslant \varepsilon_2 \leqslant \varepsilon_2' \leqslant \cdots \leqslant \varepsilon_{n+1}' \leqslant \varepsilon_{n+2}.$$

Combining those two relations one finds $\varepsilon_i \leqslant \lambda_i$ and $\lambda_i \leqslant \varepsilon_{i+2}$. This is relation (21) for the case $\rho = 2$.

A.6. Proof of orthonormality relations (23)–(25)

Using relations (2b) and (3d) one finds that each cardinal eigenstate should be normalized according to $W_k^{-1/2}|\Psi_k\rangle$ where $|\Psi_k\rangle$ is given by (10) and where

$$W_k = \sum_{sp}^{\rho} C_s^{(k)*} C_p^{(k)} \left\{ \sum_i^n \left[\frac{\langle\chi_s|\mathbf{V}-\varepsilon_k\mathbf{P}|\Phi_i\rangle\langle\Phi_i|\mathbf{V}-\varepsilon_k\mathbf{P}|\chi_p\rangle}{(\varepsilon_k-\lambda_i)^2} + \frac{\langle\chi_s|\mathbf{V}-\varepsilon_k\mathbf{P}|\Phi_i\rangle\langle\Phi_i|\mathbf{P}|\chi_p\rangle}{\varepsilon_k-\lambda_i} + \frac{\langle\chi_s|\mathbf{P}|\Phi_i\rangle\langle\Phi_i|\mathbf{V}-\varepsilon_k\mathbf{P}|\chi_p\rangle}{\varepsilon_k-\lambda_i} \right] + S_{sp}^a \right\}.$$

In the case of singular eigenstates (15) one finds

$$W_k = \sum_{sp}^{\rho} C_s^{(k)*} C_p^{(k)} \left\{ \sum_{i(\lambda_i\neq\varepsilon_k)}^n \left[\frac{\langle\chi_s|\mathbf{V}-\varepsilon_k\mathbf{P}|\Phi_i\rangle\langle\Phi_i|\mathbf{V}-\varepsilon_k\mathbf{P}|\chi_p\rangle}{(\varepsilon_k-\lambda_i)^2} + \frac{\langle\chi_s|\mathbf{V}-\varepsilon_k\mathbf{P}|\Phi_i\rangle\langle\Phi_i|\mathbf{P}|\chi_p\rangle}{\varepsilon_k-\lambda_i} + \frac{\langle\chi_s|\mathbf{P}|\Phi_i\rangle\langle\Phi_i|\mathbf{V}-\varepsilon_k\mathbf{P}|\chi_p\rangle}{\varepsilon_k-\lambda_i} \right] + S_{sp}^a \right\} + \sum_{\nu}^{\eta} D_\nu^{(k)*} D_\nu^{(k)}.$$

With some algebra above expressions transform into relations (23).

Consider now scalar products $\langle\Psi_k|\mathbf{S}|\Psi_l\rangle$ between normalized eigenstates $|\Psi_k\rangle$ and $|\Psi_l\rangle$. If both eigenstates are cardinal, one finds:

$$\langle\Psi_k|\mathbf{S}|\Psi_l\rangle = (W_k W_l)^{-1/2} \sum_{sp}^{\rho} C_s^{(k)*} C_p^{(k)} \left\{ \sum_i^n \left[\frac{\langle\chi_s|\mathbf{V}-\varepsilon_k\mathbf{P}|\Phi_i\rangle\langle\Phi_i|\mathbf{V}-\varepsilon_l\mathbf{P}|\chi_p\rangle}{(\varepsilon_k-\lambda_i)(\varepsilon_l-\lambda_i)} + \frac{\langle\chi_s|\mathbf{V}-\varepsilon_k\mathbf{P}|\Phi_i\rangle\langle\Phi_i|\mathbf{P}|\chi_p\rangle}{\varepsilon_k-\lambda_i} + \frac{\langle\chi_s|\mathbf{P}|\Phi_i\rangle\langle\Phi_i|\mathbf{V}-\varepsilon_l\mathbf{P}|\chi_p\rangle}{\varepsilon_l-\lambda_i} \right] + S_{sp}^a \right\}.$$

This relation can be transformed into (24). In the same way relation (25) can be derived.

A.7. Time dependent eigenvalue equation

Relations (A.2) imply

$$|\Theta_s\rangle = \sum_k |\Psi_k\rangle\langle\Psi_k|\mathbf{S}|\Theta_s\rangle, \quad s = 1, \ldots, \rho, \tag{A.11a}$$

$$|\Phi_i\rangle = \sum_k |\Psi_k\rangle\langle\Psi_k|\mathbf{S}|\Phi_i\rangle, \quad i = 1, \ldots, n, \tag{A.11b}$$

where $|\Psi_k\rangle$ are orthonormalized according to (3d).

If $\mathbf{P} = 0$ relations (30) and (34) imply

$$\langle\Theta_s|\mathbf{S}|\Psi_k\rangle \equiv \langle\Theta_s|\mathbf{S}\big|\Psi_k^a\big\rangle = \frac{1}{W_k^{1/2}} \sum_p^{\rho} C_p^{(k)} \big\langle\Theta_s\big|\mathbf{S}^a\big|\chi_p\big\rangle, \tag{A.12}$$

$$\langle\Phi_j|\mathbf{S}|\Psi_k\rangle \equiv \langle\Phi_j|\mathbf{S}\big|\Psi_k^b\big\rangle = \frac{1}{W_k^{1/2}} \frac{\sum_p^{\rho} \langle\Phi_j|\mathbf{V}|\chi_p\rangle C_p^{(k)}}{\varepsilon_k - \lambda_j}, \quad \varepsilon_k \neq \lambda_j, \tag{A.13a}$$

$$\langle\Phi_{j\nu}|\mathbf{S}|\Psi_k\rangle \equiv \langle\Phi_{j\nu}|\mathbf{S}\big|\Psi_k^b\big\rangle = \frac{D_\nu^{(k)}}{W_k^{1/2}}, \quad \varepsilon_k = \lambda_j. \tag{A.13b}$$

The case (A.13b) can happen only if $|\Psi_k\rangle$ is singular and if in addition the corresponding eigenvalue equals $\varepsilon_k = \lambda_j$. Index ν labels possible degeneracy of the unperturbed eigenstates $|\Phi_{j\nu}\rangle$ that have common eigenvalue λ_j.

From (A.11a), (A.12) and (37) one obtains relation (40), while (A.11b) and (A.13) imply relations (42).

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