

Exact treatment of open finite-dimensional quantum systems: I. Time-independent case

Tomislav P. Živković

Received: 19 November 2007 / Accepted: 4 December 2007 / Published online: 13 February 2008
© Springer Science+Business Media, LLC 2008

Abstract Closed quantum systems that do not interact with the surrounding are described by an eigenvalue equation such as the Schrödinger equation. In particular, one can describe in this way a finite closed quantum system \mathbf{S}_ρ^a that contains ρ eigenvalues and ρ eigenstates. Open quantum systems that interact with surrounding are usually treated within a perturbation expansion method. In a consistent quantum approach this “surrounding” should be treated as another (usually infinite) quantum system \mathbf{S}_∞^b . In formal mathematical terms one has to find a solution of the combined system $\mathbf{S}_\infty \equiv \mathbf{S}_\rho^a \oplus \mathbf{S}_\infty^b$ with emphasize on the properties of the subsystem \mathbf{S}_ρ^a . A new approach for the solution of this problem is presented. One finds that combined system \mathbf{S}_∞ contains embedded eigenstates $|\Psi(\varepsilon, \dots)\rangle$ with continuous eigenvalues ε , and in addition it may contain isolated eigenstates $|\Psi_r\rangle$ with discrete eigenvalues ε_r . Two $\rho \times \rho$ eigenvalue equations, a *generic* eigenvalue equation and a *fractional shift* eigenvalue equation are derived. In almost all cases those two equations produce a complete and exact description of the open quantum system \mathbf{S}_ρ^a . The extremely rare exceptional cases can be also treated accordingly. The suggested method produces correct results, however strong the interaction between quantum systems \mathbf{S}_ρ^a and \mathbf{S}_∞^b . Two examples are presented in order to illustrate various aspects of this method.

Keywords Interaction of quantum systems · Time-independent perturbation · Open quantum systems

T. P. Živković (✉)
Ruđer Bošković Institute, P.O.B. 180, 10002 Zagreb, Croatia
e-mail: zivkovic@irb.hr

1 Introduction

Consider a finite quantum system \mathbf{S}_ρ^a that contains ρ discrete eigenvalues and ρ eigenstates. If this system is closed, it can be described by an eigenvalue equation. However, more interesting is the case when this system is open and when it interacts with its surrounding. In a consistent quantum approach this surrounding should be considered as another (usually infinite) quantum system \mathbf{S}_∞^b . In general, system \mathbf{S}_∞^b can contain several eigenvalue bands and/or several isolated eigenstates. In analogy with standard perturbation expansion approach [1, 2], one can assume that the solution to the system \mathbf{S}_∞^b is known. The problem is to find properties of a system \mathbf{S}_ρ^a that interacts with the known system \mathbf{S}_∞^b . In formal mathematical terms the system \mathbf{S}_ρ^a and its surrounding (system \mathbf{S}_∞^b) form a combined system $\mathbf{S}_\infty \equiv \mathbf{S}_\rho^a \oplus \mathbf{S}_\infty^b$. Thus one has to extract the required information from the solution of this combined system.

There are numerous problems in physics and chemistry of this type. For example, consider the interaction of an isolated molecule with the electromagnetic field [1, 2]. This molecule can be approximated with a system \mathbf{S}_ρ^a containing finite number of eigenvalues E_s and eigenstates $|\Theta_s\rangle$. Those eigenstates interact with one-photon states $|\Theta_\rho, \mathbf{k}\varpi\rangle$ where $|\mathbf{k}\varpi\rangle$ represents a state containing one-photon with momentum \mathbf{k} and polarization ϖ . States $|\Theta_\rho, \mathbf{k}\varpi\rangle$ interact with two-photon states $|\Theta_r, \mathbf{k}'\varpi', \mathbf{k}''\varpi''\rangle$, which in turn interact with three-photon states, etc. [1]. If there is no external electromagnetic field, one can to a very good approximation ignore all states containing multiple photons, and one can associate system \mathbf{S}_∞^b with the set of all one-photon states $|\Theta_\rho, \mathbf{k}\varpi\rangle$ with corresponding eigenvalues. The solution to this system is known since the states $|\mathbf{k}\varpi\rangle$ are essentially plane waves, while $|\Theta_\rho\rangle$ are eigenstates of the isolated molecule. Hence one has formally the interaction of a finite system \mathbf{S}_ρ^a with the known infinite system \mathbf{S}_∞^b . With an appropriate modification, in the similar way can be treated the case when an external electromagnetic field is present. As another example, consider the interaction of the molecule situated on the surface of some solid with this solid. Molecule in isolation can be again approximated with a finite quantum system \mathbf{S}_ρ^a . System \mathbf{S}_∞^b represents a solid with a surface. The solution to this system usually consists of multiple eigenvalue bands $\lambda_\nu(\mathbf{k})$ with the corresponding eigenstates $|\Phi_\nu(\mathbf{k}, \mathbf{l})\rangle$ ($\nu = 1, 2, \dots$) [3]. In addition, system \mathbf{S}_∞^b may contain some discrete eigenvalues λ_i corresponding to the surface states [4]. One is mainly interested in the properties of the molecule (system \mathbf{S}_ρ^a) subject to the interaction with a solid (system \mathbf{S}_∞^b). Again one can assume that the solution to the system \mathbf{S}_∞^b is known. In most cases one knows only an approximate solution of this system [3]. Nevertheless, if this approximate solution is reliable, the problem is to find equally reliable solution of the combined system \mathbf{S}_∞ with emphasize on the properties of the subsystem \mathbf{S}_ρ^a .

Those and similar problems are usually treated either within the formalism of the perturbation expansion method, or using some approximate semi-classical model [1–4]. Both approaches have some drawbacks. If the interaction between the systems \mathbf{S}_ρ^a and \mathbf{S}_∞^b is strong, perturbation expansion may diverge and the entire method fails. Concerning various semi-classical models, those models are only approximate and they can never completely replace exact quantum treatment.

A new method for the solution of such problems will be presented [5–8]. This method produces exact description of a quantum system \mathbf{S}_ρ^a that interacts with a quantum system \mathbf{S}_∞^b , however strong the interaction between those two systems. There is no power series expansion and no divergence problem. This method was initially developed for the case of the interaction of a quantum system \mathbf{S}_1^a that contains only one eigenstate with a quantum system \mathbf{S}_∞^b that contains a single one-parameter eigenvalue band [5]. Next the method was generalized to arbitrary quantum systems \mathbf{S}_∞^b , retaining still the condition that the system \mathbf{S}_1^a contains only one eigenstate [6,7]. Finally the method was generalized to the interaction of an arbitrary finite system \mathbf{S}_ρ^a that interacts with an infinite system \mathbf{S}_∞^b , but with a restriction that \mathbf{S}_∞^b contains a single one-parameter eigenvalue band [8].

In the present paper the most general case of the interaction of an arbitrary finite quantum system \mathbf{S}_ρ^a with an arbitrary infinite quantum system \mathbf{S}_∞^b will be considered. Time-independent version of this method will be presented. Generalization to the time-dependent case is rather straightforward and it can be done along the lines described elsewhere [5–7].

2 Mathematical formulation of a problem

The system \mathbf{S}_ρ^a is an arbitrary ρ -dimensional quantum system. With this system is associated ρ -dimensional space X_ρ^a and it is described by the generalized eigenvalue equation

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

where \mathbf{A} and \mathbf{S}^a are Hermitian operators in X_ρ^a , while \mathbf{S}^a is in addition positive definite in this space. This guaranties reality of the eigenvalues E_s . Eigenstates $|\Theta_s\rangle$ can be orthonormalized according to

$$\langle \Theta_s | \mathbf{S}^a | \Theta_p \rangle = \delta_{s,p}, \tag{1b}$$

Since $|\Theta_s\rangle$ form a complete set in X_ρ^a , this implies

$$\sum_s^\rho |\Theta_s\rangle \langle \Theta_s| \mathbf{S}^a = \mathbf{I}^a. \tag{1c}$$

where \mathbf{I}^a is a unit operator in X_ρ^a . Eigenstates $|\Theta_s\rangle$ of a system \mathbf{S}_ρ^a are called *local* states [8].

The system \mathbf{S}_∞^b is an arbitrary infinite-dimensional quantum system. This system describes any possible surrounding of the system \mathbf{S}_ρ^a . With this system is associated an infinite-dimensional space X_∞^b . In general, this system may contain several eigenvalue bands and/or several discrete eigenstates. Each of those eigenvalue bands may be one-parameter eigenvalue band (nondegenerate eigenvalue band) or it may be a many-parameter eigenvalue band (degenerate eigenvalue band).

Let the system \mathbf{S}_∞^b contain κ eigenvalue bands where κ can assume any value from $\kappa = 1$ to including $\kappa = \infty$ (by assumption, the case $\kappa = 0$ is excluded. See Appendix A). Those eigenvalue bands are described by the eigenvalue equation

$$\mathbf{B} |\Phi_{v,m}(k, l)\rangle = \lambda_v(k) |\Phi_{v,m}(k, l)\rangle, \quad k \in [k_{av}, k_{bv}], \quad v = 1, 2, \dots, \kappa, \quad (2a)$$

where \mathbf{B} is a Hermitian operator, where index v labels various eigenvalue bands, and where each $\lambda_v(k)$ is a monotonic function of a parameter k in the interval $[k_{av}, k_{bv}]$ ($v = 1, \dots, \kappa$). Parameters l and m are optional. Those parameters label possible degeneracy's inside eigenvalue band v . Parameter l represents one or several continuous parameters and parameter m represents one or several discrete parameters. With this convention eigenstates $|\Phi_{v,m}(k, l)\rangle$ of \mathbf{B} can be orthonormalized according to

$$\langle \Phi_{v,m}(k, l) | \Phi_{v',m'}(k', l') \rangle = \delta_{v,v'} \delta_{m,m'} \delta(k - k') \delta(l - l'). \quad (2b)$$

Without loss of generality one can assume that each function $\lambda_v(k)$ is monotonic increasing. In this case all eigenvalues of the eigenvalue band v are confined to the eigenvalue interval $I_v = [a_v, b_v]$ where $a_v = \lambda_v(k_{av})$ and $b_v = \lambda_v(k_{bv})$ are the smallest and the largest possible eigenvalue, respectively. One may have $b_v = \infty$. However, one may not have $a_v = -\infty$, since eigenvalues of \mathbf{S}_∞^b can not assume arbitrary large negative values.

Since each $\lambda_v(k)$ is monotonic, it has well defined inverse

$$\varepsilon = \lambda_v(k), \quad k = \lambda_v^{-1}(\varepsilon), \quad \varepsilon \in [a_v, b_v]. \quad (2c)$$

Union of all eigenvalue intervals $I_v = [a_v, b_v]$ forms a range D of the continuous eigenvalues of \mathbf{S}_∞^b , $D = \cup_v I_v$. This range may consist of one or several disconnected intervals D_μ , where each D_μ is a union of one or several eigenvalue intervals I_v . It is convenient to define a point set \overline{D} which is a complement of D . Accordingly, $D \cup \overline{D} = R$ is the entire real axis.

In addition to continuous eigenvalues $\lambda_v(k)$ and corresponding eigenstates $|\Phi_{v,m}(k, l)\rangle$, system \mathbf{S}_∞^b may contain τ discrete eigenvalues λ_i and τ corresponding eigenstates $|\Phi_i\rangle$. In general, τ can assume any value from $\tau = 0$ to including $\tau = \infty$. Those discrete eigenvalues and eigenstates are described by the eigenvalue equation

$$\mathbf{B} |\Phi_i\rangle = \lambda_i |\Phi_i\rangle, \quad i = 1, 2, \dots, \tau, \quad (3a)$$

Each discrete eigenvalue λ_i satisfies either $\lambda_i \in \overline{D}$ or $\lambda_i \in D$. Corresponding eigenstates $|\Phi_i\rangle$ can be orthonormalized according to

$$\langle \Phi_i | \Phi_j \rangle = \delta_{i,j}, \quad i, j = 1, \dots, \tau, \quad (3b)$$

All discrete eigenstates $|\Phi_i\rangle$ are also orthogonal to all continuous eigenstates $|\Phi_{v,m}(k, l)\rangle$

$$\langle \Phi_i | \Phi_{v,m}(k, l) \rangle = 0. \quad (3c)$$

Eigenstates $|\Phi_i\rangle$ and $|\Phi_{v,m}(k,l)\rangle$ of \mathbf{S}_∞^b form a complete set in the space X_∞^b . Hence those eigenstates satisfy completeness relation

$$\sum_v \sum_m \int |\Phi_{v,m}(k,l)\rangle \langle \Phi_{v,m}(k,l)| dk dl + \sum_i |\Phi_i\rangle \langle \Phi_i| = \mathbf{I}^b. \tag{4}$$

where \mathbf{I}^b is a unit operator in the space X_∞^b .

Above expressions describe an arbitrary quantum system \mathbf{S}_∞^b . Each surrounding of a system \mathbf{S}_ρ^a , however complicated, can be described as such a system.

Relations (1a), (2a) and (3a) describe closed systems \mathbf{S}_ρ^a and \mathbf{S}_∞^b without mutual interaction. An arbitrary interaction between those two systems can be written in the form $\beta\mathbf{V}$ where $\mathbf{V} \neq 0$ is a Hermitian operator and where $\beta \geq 0$ is a coupling parameter. Without loss of generality one can assume that operator \mathbf{V} has nonvanishing matrix elements only between spaces X_ρ^a and X_∞^b . Combined system $\mathbf{S}_\infty \equiv \mathbf{S}_\rho^a \oplus \mathbf{S}_\infty^b$ that includes this interaction is described by the generalized eigenvalue equation

$$\mathbf{C}|\Psi\rangle = \varepsilon \mathbf{S}|\Psi\rangle, \tag{5a}$$

where

$$\mathbf{C} = \mathbf{A} + \mathbf{B} + \beta\mathbf{V}, \quad \mathbf{S} = \mathbf{S}^a + \mathbf{I}^b. \tag{5b}$$

Since \mathbf{S}^a is positive definite in X_ρ^a , operator \mathbf{S} is positive definite in the combined space $X_\infty \equiv X_\rho^a \oplus X_\infty^b$. Eigenvalues ε of (5a) are hence real.

Mathematically, eigenvalue equation (5a) represents an infinite-dimensional eigenvalue problem. The emphasize in the solution of this problem is on the properties of the open system \mathbf{S}_ρ^a that interacts with the infinite system \mathbf{S}_∞^b , and not on the properties of the system \mathbf{S}_∞^b . Such problems are usually treated within the formalism of the perturbation expansion approach where \mathbf{S}_ρ^a is the unperturbed system [1,2]. I will present here a new approach which is not perturbative and which produces an exact solution to this problem, however strong the interaction between systems \mathbf{S}_ρ^a and \mathbf{S}_∞^b .

In the above formulation the system \mathbf{S}_ρ^a was described with a generalized eigenvalue equation (1a). However, by far the most important is the case when $\mathbf{S}^a \equiv \mathbf{I}^a$ is a unit operator in the space X_ρ^a . In the suggested approach there is no substantial difference between the cases $\mathbf{S}^a \neq \mathbf{I}^a$ and $\mathbf{S}^a \equiv \mathbf{I}^a$. Expressions describing the case $\mathbf{S}^a \neq \mathbf{I}^a$ are only slightly more complicated from the expressions describing the case $\mathbf{S}^a \equiv \mathbf{I}^a$. For the sake of generality, the system \mathbf{S}_ρ^a is therefore described with a generalized eigenvalue equation (1a). Concerning the infinite system \mathbf{S}_∞^b , analogous generalization is not so important. This system may represent an electromagnetic field, electronic or vibrational (phonon) states of a solid state, etc. In almost all models such systems are described by base states that are orthonormalized in a standard way [1–3].

Concerning assumption that the system \mathbf{S}_∞^b contains at least one eigenvalue band ($\kappa \neq 0$), the case $\kappa = 0$ is considered elsewhere [9] (see also Appendix A).

3 Solutions of the combined system \mathbf{S}_∞ and description of the open system \mathbf{S}_ρ^a

A general strategy in the solution of the eigenvalue equation (5a) is to approximate infinite system \mathbf{S}_∞^b with a huge but finite system \mathbf{S}_n^b containing n eigenvalues λ_i and n corresponding eigenstates. Infinite combined system $\mathbf{S}_\infty = \mathbf{S}_\rho^a \oplus \mathbf{S}_\infty^b$ is accordingly approximated with a finite $(n + \rho)$ -dimensional combined system $\mathbf{S}_{n+\rho} = \mathbf{S}_\rho^a \oplus \mathbf{S}_n^b$ that has $(n + \rho)$ eigenvalues ε_k and $(n + \rho)$ corresponding eigenstates. There are two kinds of solutions to this finite combined system. If ε_k differs from all the eigenvalues λ_i of the closed system \mathbf{S}_n^b ($\varepsilon_k \notin \{\lambda_j\}$) the corresponding solution is *cardinal*, otherwise it is *singular* [9]. As shown in Appendix A, there are explicit expressions for cardinal and singular solutions of such finite systems [9]. Given those expressions, one can derive their $n \rightarrow \infty$ limit. Provided the approximation of \mathbf{S}_∞ with finite systems $\mathbf{S}_{n+\rho}$ is done in an appropriate way, this limit is well defined [5–8]. One thus derives the required expressions for the infinite combined system \mathbf{S}_∞ .

As emphasized in a previous section, closed system \mathbf{S}_∞^b may contain discrete eigenvalues $\lambda_i \in \{\lambda_j\}$ as well as continuous eigenvalues $\lambda_\nu(k) \in D$. Combined system \mathbf{S}_∞ may also contain discrete and continuous eigenvalues. By definition, each discrete eigenvalue ε_r of \mathbf{S}_∞ is an *isolated* eigenvalue while each continuous eigenvalue ε of \mathbf{S}_∞ is an *embedded* eigenvalue [8].

Eigenstates $|\Psi_r\rangle$ corresponding to isolated eigenvalues ε_r can be normalized to unity. This normalization is done in accord with the metrics induced by the operator \mathbf{S} . In particular one has [8,9]

$$\langle \Psi_r | \mathbf{S} | \Psi_p \rangle = \delta_{r,p}. \quad (6)$$

One can consider each isolated eigenvalue ε_r of \mathbf{S}_∞ as a continuous function of the coupling parameter β , $\varepsilon_r \equiv \varepsilon_r(\beta)$. From this point of view eigenvalue ε_r may result as perturbed eigenvalue E_s of the local system \mathbf{S}_ρ^a , in which case one has $\varepsilon_r(0) = E_s$. It may also result as a perturbed discrete eigenvalues λ_i of the system \mathbf{S}_∞^b , in which case one has $\varepsilon_r(0) = \lambda_i$. However, if the coupling β is strong enough combined system \mathbf{S}_∞ may contain some additional isolated eigenvalues $\varepsilon_r(\beta)$ that do not result in either of those two ways [5–8].

One can generalize the notion of cardinal and singular solutions defined for finite combined systems $\mathbf{S}_{n+\rho}$ to all isolated as well as to all embedded solutions of the infinite combined system \mathbf{S}_∞ . Each isolated eigenvalue ε_r of \mathbf{S}_∞ is *cardinal* if it differs from all discrete eigenvalues λ_i of the system \mathbf{S}_∞ ($\varepsilon_r \notin \{\lambda_j\}$). Otherwise it is *singular*. This is a natural generalization of the notion of cardinal and singular eigenvalues from the case of finite combined system to isolated eigenvalues of infinite combined system.

Concerning embedded solutions, one finds that each $\varepsilon \in D$ is an embedded eigenvalue of the combined system \mathbf{S}_∞ [5–8]. This eigenvalue is a part of a continuous band of eigenvalues, and the corresponding embedded eigenstates are with respect to this eigenvalue normalized to a δ -function. Those eigenstates are hence of a general type $|\Psi(\varepsilon, \dots)\rangle$ where dots (\dots) denote additional discrete and/or continuous parameters, if any.

A key quantity in the treatment of embedded solutions is a *fractional shift* $x(\varepsilon)$ [5–8]. In general, with each embedded eigenstate $|\Psi(\varepsilon, \dots)\rangle$ is associated a fractional shift $x(\varepsilon)$. Fractional shift has the following interpretation: Imagine infinite system \mathbf{S}_∞^b approximated with a huge but finite system \mathbf{S}_n^b containing n eigenvalues λ_i . The corresponding combined system \mathbf{S}_∞ is accordingly approximated with a huge but finite system $\mathbf{S}_{n+\rho} = \mathbf{S}_\rho^a \oplus \mathbf{S}_n^b$ containing $n + \rho$ eigenvalues ε_k . Consider quantities

$$x(\varepsilon_k) = \frac{\varepsilon_k - \lambda_{k-1}}{\lambda_k - \lambda_{k-1}}, \tag{7}$$

where ε_k are eigenvalues of the combined system $\mathbf{S}_{n+\rho}$ while λ_{k-1} are eigenvalues of the system \mathbf{S}_n^b . In order to have a meaningful $n \rightarrow \infty$ limit of the above expression, all three eigenvalues ε_k , λ_k and λ_{k-1} should be contained in the range D and in addition they should be contained in the same interval $D_\mu \subseteq D$. Each $x(\varepsilon_k)$ is a *fractional shift* of the perturbed eigenvalue ε_k relative to the unperturbed eigenvalue λ_{k-1} [5–8]. Fractional shift is thus defined as the ratio of two infinitesimal quantities: There is an infinitesimal shift $\Delta\varepsilon_k = \varepsilon_k - \lambda_{k-1}$ of the perturbed eigenvalue ε_k relative to the corresponding unperturbed eigenvalue λ_{k-1} . Another infinitesimal quantity is the interval $\Delta\lambda_k = \lambda_k - \lambda_{k-1}$ between two adjacent unperturbed eigenvalues $\lambda_k \in D$. If the infinite system \mathbf{S}_∞ is approximated with finite systems $\mathbf{S}_{n+\rho}$ in an appropriate way [5–8], in a limit $n \rightarrow \infty$ discrete quantities $x(\varepsilon_k)$ converge to one or several functions $x(\varepsilon)$ of a continuous parameter $\varepsilon \in D$ (see Appendix B.2). Each of those functions is well defined everywhere in the range D , with a possible exception of few isolated points. One finds that fractional shift can be confined to the interval $[0, 1)$ (see Sect. 6.2). Fractional shift confined to this interval is a *principal value* of a fractional shift [8]. In this paper it will be assumed that fractional shift is confined to its principal value, i.e. $x(\varepsilon) \in [0, 1)$.

In view of the above picture of the combined system \mathbf{S}_∞ as the $n \rightarrow \infty$ limit of finite combined systems $\mathbf{S}_{n+\rho}$, one can give a following physical interpretation to the notion of a fractional shift: Fractional shift $x(\varepsilon) = 0$ corresponds to the perturbed eigenvalue ε that coincides with some unperturbed eigenvalue λ , while fractional shift $x(\varepsilon) \neq 0$ corresponds to the perturbed eigenvalue ε that does not coincide with any of the unperturbed eigenvalues λ [5–8]. Accordingly, each embedded solution that satisfies $x(\varepsilon) = 0$ is *singular* while each embedded solution that satisfies $x(\varepsilon) \neq 0$ is *cardinal*. This is a natural generalization of the notion of singular and cardinal solutions of the finite combined system $\mathbf{S}_{n+\rho}$ to embedded solutions of the infinite combined system \mathbf{S}_∞ .

In addition to embedded singular solutions which are characterized by fractional shift $x(\varepsilon) = 0$, a special role is also played by embedded cardinal solutions with fractional shift $x(\varepsilon) = 0.5$. This fractional shift corresponds to the perturbed eigenvalue ε that is exactly in a middle between two adjacent infinitesimally close unperturbed eigenvalues λ . Each solution that satisfies $x(\varepsilon) = 0.5$ is called a *resonant* solution and the corresponding point $\varepsilon \in D$ a *resonant point*. This name is due to the resonant shape of the corresponding embedded cardinal eigenstates in the case of the weak coupling (see Sect. 6.2.3.).

3.1 Description of the open system \mathbf{S}_ρ^a

Each isolated as well as each embedded eigenstate of the combined system can be written as a linear combination

$$|\Psi\rangle = |\Psi^a\rangle + |\Psi^b\rangle, \quad (8a)$$

where $|\Psi^a\rangle \in X_\rho^a$ and $|\Psi^b\rangle \in X_\infty^b$ are components of this eigenstate in spaces X_ρ^a and X_∞^b , respectively. Let \mathbf{O} be an observable (linear Hermitian operator) that describes some property of the open system \mathbf{S}_ρ^a and let $|\Psi\rangle$ and $|\Psi'\rangle$ be eigenstates of the combined system \mathbf{S}_∞ . Operator \mathbf{O} can have nonvanishing matrix elements only between the states contained in the space X_ρ^a . This implies

$$\langle\Psi|\mathbf{O}|\Psi'\rangle = \langle\Psi^a|\mathbf{O}|\Psi^{a'}\rangle. \quad (8b)$$

Hence, in order to obtain properties of the open system \mathbf{S}_ρ^a , it is sufficient to know X_ρ^a -components of the (properly normalized) eigenstates of the combined system. The knowledge of X_∞^b -components of those eigenstates is not needed.

In the case of a finite combined system $\mathbf{S}_{n+\rho}$, each cardinal eigenstate has a nonvanishing X_ρ^a -component. Concerning singular eigenstates, one may have two kinds of such eigenstates: strongly singular eigenstates have no X_ρ^a -component, while weakly singular eigenstates have nonvanishing X_ρ^a -component. One finds that a finite combined system $\mathbf{S}_{n+\rho}$ only exceptionally can have some weakly singular eigenstates (see Appendix A). Those properties of cardinal and singular eigenstates in the case of finite combined system $\mathbf{S}_{n+\rho}$ generalize to cardinal and singular eigenstates of the infinite combined system \mathbf{S}_∞ . Consider first embedded eigenstates of the combined system. Each embedded cardinal eigenstate satisfies $|\Psi^a(\varepsilon, \dots)\rangle \neq 0$ while each embedded strongly singular eigenstate satisfies $|\Psi^a(\varepsilon, \dots)\rangle = 0$. Concerning embedded weakly singular eigenstates that have nonvanishing X_ρ^a -component, one may have only a limited number of such eigenstates. However, \mathbf{S}_∞ contains an infinite number of embedded cardinal eigenstates (see Sect. 6). The contribution of embedded weakly singular eigenstates to the properties of the open system \mathbf{S}_ρ^a is hence negligible (see Sect. 6). In conclusion, most important are embedded cardinal eigenstates that have a nonvanishing X_ρ^a component while embedded singular eigenstates are in that respect not important. Similar conclusions apply to isolated eigenstates of the combined system. Here again isolated cardinal eigenstates are most important. However, unlike embedded weakly singular eigenstates, isolated weakly singular eigenstates may in some cases contribute to the properties of the open system \mathbf{S}_ρ^a (this is however quite rare, see Sect. 5).

In conclusion, concerning properties of the open system \mathbf{S}_ρ^a , most important are X_ρ^a -components of embedded cardinal and isolated cardinal eigenstates of the combined system. One finds that those components are described by two key eigenvalue equations. Those are *generic* eigenvalue equation and *fractional shift* eigenvalue equation. Both equations act in the space X_ρ^a and they can be both represented as $\rho \times \rho$ matrix eigenvalue equation. In addition to operators \mathbf{A} and \mathbf{S}^a that according to (1a)

describe closed system \mathbf{S}_ρ^a , those eigenvalue equations involve *characteristic operator* $\mathbf{f}(\varepsilon)$ and *derived operator* $\omega(\varepsilon)$ [8]. Characteristic operator incorporates essential features of the infinite system \mathbf{S}_∞^b and of the interaction of this system with the finite system \mathbf{S}_ρ^a . This operator is basic. Derived operator $\omega(\varepsilon)$ is uniquely determined by the corresponding characteristic operator $\mathbf{f}(\varepsilon)$.

4 Characteristic and derived operators

Key role in the expressions that replace eigenvalue equation (5a) is played by *characteristic operator* $\mathbf{f}(\varepsilon)$. This operator acts in the space X_ρ^a and in this space it is represented by a $\rho \times \rho$ Hermitian matrix. Characteristic operator $\mathbf{f}(\varepsilon)$ is a sum of characteristic operators $\mathbf{f}_\nu(\varepsilon)$ that are associated with eigenvalue bands ν and of the characteristic operator $\mathbf{F}(\varepsilon)$ that is associated with the set $\{\lambda_j\}$ of all discrete eigenvalues λ_i of the system \mathbf{S}_∞^b

$$\mathbf{f}(\varepsilon) = \sum_\nu \mathbf{f}_\nu(\varepsilon) + \mathbf{F}(\varepsilon), \tag{9a}$$

Operator $\mathbf{f}_\nu(\varepsilon)$ associated with the eigenvalue band ν vanishes for each $\varepsilon \notin I_\nu$ and in the interval I_ν it is positive definite with possible exception of few isolated points where it may be zero. In the base $\{|s\rangle\} \in X_\rho^a$ matrix elements $f_{sp}^{(\nu)}(\varepsilon)$ of this operator are (see Appendix B):

$$\begin{aligned} f_{sp}^{(\nu)}(\varepsilon) &\equiv \langle s | \mathbf{f}_\nu(\varepsilon) | p \rangle \\ &= \frac{\sum_m \int \langle s | \mathbf{V} | \Phi_{\nu,m}(k, l) \rangle \langle \Phi_{\nu,m}(k, l) | \mathbf{V} | p \rangle dl}{d\lambda_\nu(k)/dk} \Bigg|_{k=\lambda_\nu^{-1}(\varepsilon)} \cdot \begin{cases} 1 & \text{if } \varepsilon \in I_\nu \\ 0 & \text{if } \varepsilon \notin I_\nu \end{cases} \\ \nu &= 1, \dots, \kappa, \quad s, p = 1, \dots, \rho. \end{aligned} \tag{9b}$$

Without loss of generality one can assume that the states $|s\rangle \in X_\rho^a$ are orthonormalized in a standard way: $\langle s | p \rangle = \delta_{s,p}$.

Each matrix element $f_{sp}^{(\nu)}(\varepsilon)$ is usually an analytic function of ε inside the interval I_ν . However, it is not analytic for each ε , since outside this interval $f_{sp}^{(\nu)}(\varepsilon)$ is identically zero. Since $\mathbf{f}^{(\nu)}(\varepsilon)$ is positive definite almost everywhere inside the interval I_ν and zero outside this interval, each eigenvalue $\xi_i(\varepsilon)$ ($i = 1, \dots, \rho$) of this operator is nonnegative inside I_ν and zero outside I_ν . In particular, if ν is one-parameter eigenvalue band, operator $\mathbf{f}^{(\nu)}(\varepsilon)$ has rank [10] one for each $\varepsilon \in I_\nu$ with a possible exception of few isolated points where this rank vanishes [8]. In this case each eigenvalue $\xi_i(\varepsilon)$ is identically zero ($\xi_i(\varepsilon) = 0$ for each ε) except for only one eigenvalue (say $\xi_1(\varepsilon)$) which is positive for each $\varepsilon \in I_\nu$, except for few isolated points $\varepsilon = \varepsilon_c \in I_\nu$ (if any) where it is zero [8].

Operator $\mathbf{F}(\varepsilon)$ associated with the set $\{\lambda_j\}$ vanishes for each $\varepsilon \notin \{\lambda_j\}$ and it is a δ -type operator in the points $\varepsilon \in \{\lambda_j\}$. This operator is also positive definite, and in the base $\{|s\rangle\}$ matrix elements $F_{sp}(\varepsilon)$ of this operator are

$$F_{sp}(\varepsilon) \equiv \langle s | \mathbf{F}(\varepsilon) | p \rangle = \sum_i \langle s | \mathbf{V} | \Phi_i \rangle \langle \Phi_i | \mathbf{V} | p \rangle \delta(\varepsilon - \lambda_i), \quad s, p = 1, \dots, \rho. \quad (9c)$$

Matrix elements (9b) and (9c) determine characteristic operators $\mathbf{f}_v(\varepsilon)$ and $\mathbf{F}(\varepsilon)$, respectively. According to those expressions, in order to derive those operators one has to know the solution of the unperturbed system \mathbf{S}_∞^b . The knowledge of the solution to this system is a standard assumption in a perturbation expansion approach [1, 2]. Once this solution is known, construction of operators $\mathbf{f}_v(\varepsilon)$ and $\mathbf{F}(\varepsilon)$ is straightforward and computationally simple.

Characteristic operators $\mathbf{f}_v(\varepsilon)$ and $\mathbf{F}(\varepsilon)$ determine derived operators $\omega_v(\varepsilon)$ and $\Omega(\varepsilon)$, respectively. Unlike operator $\mathbf{f}_v(\varepsilon)$ that vanishes outside the interval I_v , the corresponding derived operator $\omega_v(\varepsilon)$ is nonzero in all points outside I_v and in almost all points inside I_v . This operator is expressed in terms of the characteristic operator $\mathbf{f}_v(\varepsilon)$ according to

$$\omega_v(\varepsilon) = P \int \frac{\mathbf{f}_v(\lambda)}{\varepsilon - \lambda} d\lambda, \quad (10a)$$

where P denotes principal Cauchy integral value [11]. In particular

$$\omega_{sp}^{(v)}(\varepsilon) \equiv \langle s | \omega_v(\varepsilon) | p \rangle = P \int \frac{f_{sp}^{(v)}(\lambda)}{\varepsilon - \lambda} d\lambda, \quad s, p = 1, \dots, \rho. \quad (10b)$$

If $\varepsilon \notin I_v$ above expressions are standard integrals. However, if $\varepsilon \in I_v$ sub-integral function on the right-hand side of those expressions may diverge in a point $\lambda = \varepsilon$. In this case one has to take a principal Cauchy integral value of those expressions. If $f_{sp}^{(v)}(\varepsilon)$ is polynomial in the interval I_v , there is a closed expression for the corresponding matrix element $\omega_{sp}^{(v)}(\varepsilon)$ of the derived matrix $\omega_v(\varepsilon)$ [7]. More generally, if $f_{sp}^{(v)}(\varepsilon)$ is an analytic function in this interval, matrix element $\omega_{sp}^{(v)}(\varepsilon)$ can be usually expressed in a closed form as an infinite sum. As shown in the Appendix D, if $q(\lambda)$ is analytic and if a and b are finite ($a \neq -\infty$ and $b \neq \infty$) one has

$$P \int_a^b \frac{q(\lambda)}{\varepsilon - \lambda} d\lambda = q(\varepsilon) \ln \left| \frac{a - \varepsilon}{b - \varepsilon} \right| - g(\varepsilon), \quad (11a)$$

where the function $g(\varepsilon)$ equals

$$g(\varepsilon) = \sum_{i=1}^{\infty} \frac{q^{(i)}(\varepsilon)}{i!} \left[(b - \varepsilon)^i - (a - \varepsilon)^i \right]. \quad (11b)$$

and where ε can assume any real value. In the above expression $q^{(i)}(\varepsilon)$ is i th derivative of the function $q(\varepsilon)$. If $q(\varepsilon)$ is polynomial, $g(\varepsilon)$ is also polynomial. More generally, if $q(\varepsilon)$ is an analytic function with the only singularity in infinity, infinite sum in (11b) is guaranteed to converge for each finite ε . Function $g(\varepsilon)$ defined with this sum is hence also an analytic function with the only singularity in infinity.

In analogy to (10a), derived operator $\mathbf{\Omega}(\varepsilon)$ is expressed in terms of the characteristic operator $\mathbf{F}(\varepsilon)$ according to

$$\mathbf{\Omega}(\varepsilon) = P \int \frac{\mathbf{F}(\lambda)}{\varepsilon - \lambda} d\lambda, \tag{12a}$$

Hence and from (9c)

$$\Omega_{sp}(\varepsilon) \equiv \langle s | \mathbf{\Omega}(\varepsilon) | p \rangle = \sum_{i(\lambda_i \neq \varepsilon)} \frac{\langle s | \mathbf{V} | \Phi_i \rangle \langle \Phi_i | \mathbf{V} | p \rangle}{\varepsilon - \lambda_i}, \quad s, p = 1, \dots, \rho. \tag{12b}$$

Note that matrix element $\Omega_{sp}(\varepsilon)$ is finite for each real ε . However, in a point $\varepsilon = \lambda_i \in \{\lambda_j\}$ this matrix element is usually not continuous and (unless $\langle s | \mathbf{V} | \Phi_i \rangle \langle \Phi_i | \mathbf{V} | p \rangle = 0$) one has $\lim_{\varepsilon \rightarrow \lambda_i} \Omega_{sp}(\varepsilon) = \pm \infty$.

In analogy to (9a), derived operators $\omega_v(\varepsilon)$ and $\mathbf{\Omega}(\varepsilon)$ combine to a global derived operator $\omega(\varepsilon)$ according to

$$\omega(\varepsilon) = \sum_v \omega_v(\varepsilon) + \mathbf{\Omega}(\varepsilon), \tag{13a}$$

Matrix elements $\omega_{sp}(\varepsilon)$ of $\omega(\varepsilon)$ are hence

$$\omega_{sp}(\varepsilon) \equiv \langle s | \omega(\varepsilon) | p \rangle = P \int \frac{f_{sp}(\lambda)}{\varepsilon - \lambda} d\lambda, \quad s, p = 1, \dots, \rho. \tag{13b}$$

If the range D and the set $\{\lambda_j\}$ are bounded, above expression implies that each state $|\Theta\rangle \in X_\rho^a$ satisfies

$$\langle \Theta | \omega(\pm\infty) | \Theta \rangle = 0, \tag{14a}$$

One finds that this is true also if the range D and/or the set $\{\lambda_j\}$ is not bounded, provided in the limit $\lambda \rightarrow \infty$ matrix elements $f_{sp}(\lambda)$ satisfy some mild conditions. Further, since $\mathbf{f}(\lambda)$ is nonnegative, for each $\varepsilon \notin D$ and $\varepsilon \notin \{\lambda_j\}$ an arbitrary state $|\Theta\rangle \in X_\rho^a$ satisfies $\langle \Theta | d\omega/d\varepsilon | \Theta \rangle \leq 0$. This holds also if $\varepsilon = \varepsilon_0 \in D$, provided the state $|\Theta\rangle$ satisfies $\mathbf{f}(\varepsilon_0)|\Theta\rangle = 0$. Since $\mathbf{f}(\varepsilon)|\Theta\rangle = 0$ whenever $\varepsilon \notin D$, this can be concisely written as

$$\langle \Theta | d\omega/d\varepsilon | \Theta \rangle \leq 0, \quad \text{if } \mathbf{f}(\varepsilon)|\Theta\rangle = 0 \quad \text{and } \varepsilon \notin \{\lambda_j\}. \tag{14b}$$

Note that if $\varepsilon \in D$ and $\mathbf{f}(\varepsilon)|\Theta\rangle \neq 0$, one may have $\langle \Theta | d\omega/d\varepsilon | \Theta \rangle \leq 0$ as well as $\langle \Theta | d\omega/d\varepsilon | \Theta \rangle > 0$. The condition $\mathbf{f}(\varepsilon)|\Theta\rangle = 0$ is hence essential. Concerning the condition $\varepsilon \notin \{\lambda_j\}$, in the point $\varepsilon \in \{\lambda_j\}$ the derivative $d\omega/d\varepsilon$ is not well defined.

According to the expression (1a), operators \mathbf{A} and \mathbf{S}^a contain all information necessary for the description of the closed system \mathbf{S}_ρ^a . Characteristic operator $\mathbf{f}(\varepsilon)$ contains all additional information necessary for the description of the open system \mathbf{S}_ρ^a .

In order to construct this operator, it is not necessary to specify all the details of the infinite system \mathbf{S}_∞^b and all the details of the interaction of this system with the finite system \mathbf{S}_ρ^a . All what is needed is the knowledge of $\rho \cdot (\rho + 1)/2$ functions (or more precisely distributions [1]) $f_{sp}(\varepsilon)$ ($s \leq p$). There are many different systems \mathbf{S}_∞^b that may produce the same functions $f_{sp}(\varepsilon)$. If the details of the system \mathbf{S}_∞^b and of the interaction of this system with the system \mathbf{S}_ρ^a are not known, one can model those functions in such a way as to satisfy some required properties and/or some known data of the combined system.

5 Isolated solutions of the combined system \mathbf{S}_∞

As emphasized in Sect. 3, isolated eigenvalues of the combined system may be cardinal as well as singular. By definition, isolated eigenvalue ε_r of the combined system is cardinal if it differs from all discrete eigenvalues of the closed system \mathbf{S}_∞^b , $\varepsilon_r \notin \{\lambda_j\}$. Otherwise it is singular. Isolated cardinal eigenvalues and the corresponding eigenstates of the combined system can be obtained as a solution of the generic eigenvalue equation

$$\left[\beta^2 \boldsymbol{\omega}(\varepsilon_r) + \mathbf{A} \right] |\theta_r\rangle = \varepsilon_r \mathbf{S}^a |\theta_r\rangle, \quad \varepsilon_r \notin \{\lambda_j\}, \quad (15a)$$

If there is no interaction ($\beta = 0$) this equation reduces to the eigenvalue equation (1a) that describes closed system \mathbf{S}_ρ^a .

For simplicity and unless required in order to avoid possible ambiguity, in the above and in the following expressions explicit dependence on the parameter β will not be written. Since eigenvalue ε_r and eigenstate $|\theta_r\rangle$ depend on this parameter, in an explicit full notation one should write $\varepsilon_r \equiv \varepsilon_r(\beta)$ and $|\theta_r\rangle \equiv |\theta_r(\beta)\rangle$.

Expression (15a) is a nonlinear eigenvalue equation. It may have eigenvalues $\varepsilon_r \in \overline{D}$ as well as eigenvalues $\varepsilon_r \in D$. As shown in the Appendix B.1, each eigenvalue $\varepsilon_r \in \overline{D}$ of this equation is an isolated eigenvalue of the combined system. Corresponding eigenstate $|\theta_r\rangle \in X_\rho^a$ determines X_ρ^a -component $|\Psi_r^a\rangle$ of the isolated eigenstate $|\Psi_r\rangle$ according to

$$|\Psi_r^a\rangle = \frac{1}{\sqrt{Q_r}} |\theta_r\rangle, \quad (15b)$$

where

$$Q_r = \langle \theta_r | \mathbf{S}^a | \theta_r \rangle - \beta^2 \langle \theta_r | d\boldsymbol{\omega}/d\varepsilon_r | \theta_r \rangle. \quad (15c)$$

Concerning eigenvalues $\varepsilon_r \in D$ of (15a), those eigenvalues are *resonant points* [8] and they are related to the embedded solutions of the combined system [8] (see Sect. 6.2.3.). In a special case when in a point $\varepsilon = \varepsilon_r$ there is an eigenstate $|\theta_r\rangle$ of (15a) that in addition to (15a) satisfies

$$\mathbf{f}(\varepsilon_r) |\theta_r\rangle = 0, \quad (16)$$

this point is an *anomal point*. One finds that in each anomal point combined system has an isolated solution. Eigenvalue of this isolated solution is eigenvalue ε_r of the generic eigenvalue equation (15a). In addition, component $|\Psi_r^a\rangle$ of the corresponding isolated eigenstate $|\Psi_r\rangle$ is again given by expressions (15b,c) where $|\theta_r\rangle$ satisfies (15a) and (16).

In conclusion, eigenvalues and eigenstates of the generic eigenvalue equation determine all cardinal isolated eigenvalues $\varepsilon_r \notin \{\lambda_j\}$ of the combined system and all X_ρ^a -components of the corresponding eigenstates $|\Psi_r\rangle$. If $\varepsilon_r \in \overline{D}$ this solution is determined by the generic eigenvalue equation (15a). However, if $\varepsilon_r \in D$ the corresponding eigenstate $|\theta_r\rangle$ should satisfy additional condition (16).

Consider now eigenvalue ε_r of the generic eigenvalue equation as a function of a coupling parameter β . As shown in the Appendix E, the rate of change of the eigenvalue $\varepsilon_r \equiv \varepsilon_r(\beta)$ as β increases is

$$\frac{\partial \varepsilon_r}{\partial \beta} = \frac{2\beta \langle \theta_r | \boldsymbol{\omega}(\varepsilon_r) | \theta_r \rangle}{\langle \theta_r | \mathbf{S}^a | \theta_r \rangle - \beta^2 \langle \theta_r | d\boldsymbol{\omega}/d\varepsilon_r | \theta_r \rangle}, \quad \varepsilon_r \notin \{\lambda_j\}. \tag{17}$$

If $\varepsilon_r \in \overline{D}$ expression (14b) implies $\langle \theta_r | d\boldsymbol{\omega}/d\varepsilon_r | \theta_r \rangle \leq 0$. Since $\langle \theta_r | \mathbf{S}^a | \theta_r \rangle > 0$, the sign of the derivative $(\partial \varepsilon_r / \partial \beta)$ equals the sign of the matrix element $\langle \theta_r | \boldsymbol{\omega}(\varepsilon_r) | \theta_r \rangle$. Hence for each $\varepsilon_r \in \overline{D}$ and $\varepsilon_r \notin \{\lambda_j\}$ eigenvalue $\varepsilon_r = \varepsilon_r(\beta)$, considered as a function of a parameter β , increases (decreases) if matrix element $\langle \theta_r | \boldsymbol{\omega}(\varepsilon_r) | \theta_r \rangle$ is positive (negative). Let $\lambda_1 \in \{\lambda_j\}$ be the smallest isolated eigenvalue of \mathbf{S}_∞^b and let $a_1 = \lambda_1(k_{a1})$ be the smallest left edge of all intervals $I_\nu \subseteq D$. Consider extreme left subinterval $\overline{I}_{left} = (-\infty, \min(\lambda_1, a_1))$ of \overline{D} . Due to (14) one has $\langle \theta_r | \boldsymbol{\omega}(\varepsilon_r) | \theta_r \rangle \leq 0$ if $\varepsilon_r \in \overline{I}_{left}$. In a similar way one finds $\langle \theta_r | \boldsymbol{\omega}(\varepsilon_r) | \theta_r \rangle \geq 0$ if $\varepsilon_r \in \overline{I}_{right}$ where \overline{I}_{right} is analogous extreme right subinterval of \overline{D} (provided this right subinterval exist, i.e. provided D as well as $\{\lambda_j\}$ is bounded from above). Accordingly, in the subinterval \overline{I}_{left} of \overline{D} eigenvalue $\varepsilon_r(\beta)$ is a decreasing function of β , while in the subinterval \overline{I}_{right} of \overline{D} it is an increasing function of β . Thus the effect of the coupling β is to repeal each isolated eigenvalue $\varepsilon_r(\beta)$ (that is sufficiently far from the range D) away from this range.

Expressions (15) and (16) describe isolated cardinal solutions of the combined system (with eigenvalues $\varepsilon_r \notin \{\lambda_j\}$). One can derive similar expressions for isolated singular solutions that satisfy $\varepsilon_r \in \{\lambda_j\}$. Those expressions can be derived from expressions (A8) in the same way as expression (15a) is derived from the expression (A5a). However, isolated singular solutions are usually not important. First, there are many systems \mathbf{S}_∞^b that have no discrete eigenvalue λ_i . If this is the case, the corresponding combined system \mathbf{S}_∞ has no isolated singular solution (though it may have and usually has isolated cardinal solutions). For example, a free electromagnetic field is such a system which has no discrete eigenvalue. Second, unless some special conditions are met, combined system \mathbf{S}_∞ can have isolated singular eigenvalue $\varepsilon_r = \lambda_i$ only if the degeneracy of discrete unperturbed eigenvalue $\lambda_i \in \{\lambda_j\}$ exceeds dimension ρ of the space X_ρ^a . Further, since singular eigenvalue ε_r equals some unperturbed eigenvalue λ_i . It is much easier to find singular eigenvalues (and corresponding eigenstates) than to find cardinal eigenvalues which can assume any value $\varepsilon_r \notin \{\lambda_i\}$. Finally, even

when the system \mathbf{S}_∞ contains some isolated singular eigenvalue $\varepsilon_r \in \{\lambda_i\}$, the corresponding eigenstate $|\Psi_r\rangle$ is usually strongly singular with no X_ρ^a -component. Such eigenstates do not contribute to the properties of the open system \mathbf{S}_ρ^a . Nonvanishing X_ρ^a -components have only isolated weakly singular eigenstates which are usually quite rare (see Appendix A and B.1).

5.1 Probabilities associated with isolated eigenstates

Once $|\Psi_r^a\rangle \in X_\rho^a$ is known, one can find all related properties of the open system \mathbf{S}_ρ^a . For example, probability amplitude to find isolated eigenstate $|\Psi_r\rangle$ in the local state $|\Theta_s\rangle$ equals $\langle\Theta_s|\mathbf{S}|\Psi_r\rangle$ [8]. Hence and according to (15b,c), probability $w_{r,s}$ to find isolated eigenstate $|\Psi_r\rangle$ in the local state $|\Theta_s\rangle$ equals

$$w_{r,s} \equiv |\langle\Theta_s|\mathbf{S}|\Psi_r\rangle|^2 = \frac{\langle\theta_r|\mathbf{S}^a|\Theta_s\rangle\langle\Theta_s|\mathbf{S}_a|\theta_r\rangle}{\langle\theta_r|\mathbf{S}^a|\theta_r\rangle - \beta^2\langle\theta_r|d\boldsymbol{\omega}/d\varepsilon_r|\theta_r\rangle}. \quad (18a)$$

Since $\{|\Theta_s\rangle\}$ is a complete orthonormalized set in X_ρ^a , probability w_r to find isolated eigenstate $|\Psi_r\rangle$ in a local system \mathbf{S}_ρ^a equals a sum $\sum_s w_{r,s}$. Hence and due to (1c)

$$w_r \equiv \sum_s w_{r,s} = \frac{\langle\theta_r|\mathbf{S}^a|\theta_r\rangle}{\langle\theta_r|\mathbf{S}^a|\theta_r\rangle - \beta^2\langle\theta_r|d\boldsymbol{\omega}/d\varepsilon_r|\theta_r\rangle}. \quad (18b)$$

According to (15b,c), this probability equals norm of the X_ρ^a -component of the isolated eigenstate $|\Psi_r\rangle$

$$w_r = \langle\Psi_r^a|\mathbf{S}^a|\Psi_r^a\rangle. \quad (18c)$$

Obviously $w_r \leq 1$. Probability to find isolated eigenstate $|\Psi_r\rangle$ in a system \mathbf{S}_ρ^a can never exceed one.

6 Embedded solutions of the combined system \mathbf{S}_∞

Embedded solutions of the combined system depend on a continuous parameter ε and they exist for each $\varepsilon \in D$, while for $\varepsilon \notin D$ those solutions do not exist. With each embedded solution is associated a fractional shift $x(\varepsilon)$ [5–8] which is defined as the $n \rightarrow \infty$ limit of quantities (7) (see Appendix B.2). As emphasized in Sect. 3, there are two kinds of embedded solutions: singular solutions that satisfy $x(\varepsilon) = 0$ and cardinal solutions that satisfy $x(\varepsilon) \neq 0$.

6.1 Embedded singular solutions

Let $X^{b\varepsilon}$ be the subspace of the space X_∞^b that contains all band eigenstates of \mathbf{S}_∞^b with the eigenvalue $\varepsilon \in D$. In other words, this subspace contains all eigenstates $|\Phi_{v,m}(k,l)\rangle$ that satisfy $k = \lambda_v^{-1}(\varepsilon)$ and where v , m and l can assume any admissible

value. Since $\varepsilon \in D$, the space $X^{b\varepsilon}$ is nonempty and it contains at least one eigenstate $|\Phi_{\nu,m}(k, l)\rangle$. This space may contain a finite as well as an infinite number of such eigenstates. As shown in the Appendix B.2, X^a_ρ -component and the corresponding $X^{b\varepsilon}$ -component of embedded singular eigenstates with the eigenvalue ε are solutions of the equations

$$\mathbf{h}(\varepsilon) |\varphi(\varepsilon, \dots)\rangle = -\beta \mathbf{VP}^\varepsilon |\phi(\varepsilon, \dots)\rangle, \tag{19a}$$

$$\mathbf{f}(\varepsilon) |\varphi(\varepsilon, \dots)\rangle = 0, \tag{19b}$$

where

$$\mathbf{h}(\varepsilon) = \beta^2 \boldsymbol{\omega}(\varepsilon) + \mathbf{A} - \varepsilon \mathbf{S}^a. \tag{19c}$$

and where \mathbf{P}^ε is a projection operator on the subspace $X^{b\varepsilon}$. Since operator $\mathbf{h}(\varepsilon)$ acts in the space X^a_ρ while \mathbf{P}^ε is a projection on $X^{b\varepsilon}$, one has $|\varphi(\varepsilon, \dots)\rangle \in X^a_\rho$ and $|\phi(\varepsilon, \dots)\rangle \in X^{b\varepsilon}$. Above expressions generalize expressions (A8) which produce all singular solutions of a finite combined system $\mathbf{S}_{n+\rho}$ to the singular embedded solutions of infinite combined system \mathbf{S}_∞ .

In analogy to a finite system $\mathbf{S}_{n+\rho}$, infinite system \mathbf{S}_∞ may contain embedded strongly singular eigenstates which have no X^a_ρ -component as well as embedded weakly singular eigenstates which have a nonvanishing X^a_ρ -component. In the case of embedded strongly singular eigenstates one has $|\varphi(\varepsilon, \dots)\rangle = 0$ and expressions (19) reduce to

$$\mathbf{VP}^\varepsilon |\phi(\varepsilon, \dots)\rangle = 0, \tag{20a}$$

If $|\phi(\varepsilon, \dots)\rangle$ is a solution of (20a) the corresponding strongly singular eigenstate of the combined system is

$$|\Psi(\varepsilon, \dots)\rangle \equiv \left| \Psi^b(\varepsilon, \dots) \right\rangle = \frac{1}{\sqrt{\langle \phi(\varepsilon, \dots) | \phi(\varepsilon, \dots) \rangle}} |\phi(\varepsilon, \dots)\rangle. \tag{20b}$$

Embedded strongly singular eigenstates are due to the degeneracy of the unperturbed eigenvalues $\lambda_\nu(k)$. For example, if the system \mathbf{S}_∞^b is described by the eigenvalue equation

$$\mathbf{B} |\Phi_m(k)\rangle = \lambda(k) |\Phi_m(k)\rangle, \quad k \in [k_a, k_b], \quad m = 1, 2, \dots, \eta, \tag{21a}$$

where m is discrete parameter which can assume η values, each eigenvalue $\lambda(k)$ is η -degenerate. In this case $X^{b\varepsilon}$ is a η -dimensional space spanned by η unperturbed eigenstates $|\Phi_m(k)\rangle$ where $k = \lambda^{-1}(\varepsilon)$. Projection on this space is

$$\mathbf{P}^\varepsilon = \sum_m^\eta |\Phi_m(k)\rangle \langle \Phi_m(k)|, \quad k = \lambda^{-1}(\varepsilon), \tag{21b}$$

and each state $|\phi(\varepsilon, \dots)\rangle \in X^{b\varepsilon}$ is a linear combination

$$|\phi(\varepsilon, \dots)\rangle = \sum_m^\eta c_m |\Phi_m(k)\rangle, \quad k = \lambda^{-1}(\varepsilon), \quad (21c)$$

where c_m are unknown coefficients. In a matrix form expression (20a) reads

$$\sum_m^\eta c_m \langle s | \mathbf{V} | \Phi_m(k)\rangle = 0, \quad s = 1, \dots, \rho, \quad k = \lambda^{-1}(\varepsilon). \quad (21d)$$

This is a set of ρ homogenous linear equations in η unknowns c_m . If $\eta > \rho$, for each $\varepsilon \in [a, b] \equiv [\lambda(k_a), \lambda(k_b)]$ combined system has at least $\eta - \rho$ linearly independent strongly singular eigenstates with the eigenvalue ε . Each such eigenstate is a linear combination (21c) where coefficients c_m satisfy (21d). If η is large, the number of strongly singular eigenstates can be substantial. For example, if instead of the discrete parameter m one has a continuous parameter l (see expressions (B11) in the Appendix B.2), then for each $\varepsilon \in [a, b]$ combined system has a c -infinite number of linearly independent strongly singular eigenstates with this eigenvalue.

The set of all embedded strongly singular eigenstates with the eigenvalue $\varepsilon \in D$ spans *passive* subspace $X^{b\varepsilon-}$ of the space $X^{b\varepsilon}$. According to (20a) this subspace is a nullspace [10] of the operator \mathbf{VP}^ε . It is the largest linear space, subspace of $X^{b\varepsilon}$, such that no vector in this space interacts with the space X_ρ^a . Orthogonal complement of $X^{b\varepsilon-}$ in the space $X^{b\varepsilon}$ is *active* subspace $X^{b\varepsilon+}$ of $X^{b\varepsilon}$. Each vector in this space interacts with the space X_ρ^a . Dimension of active subspace $X^{b\varepsilon+}$ is at most ρ , while passive subspace $X^{b\varepsilon-}$ can have any dimension from zero to including ∞ .

In addition to active and passive spaces $X^{b\varepsilon+}$ and $X^{b\varepsilon-}$ associated with the particular eigenvalue $\varepsilon = \lambda(k) \in D$, one can consider global active space X_∞^{b+} which is orthogonal sum of all active spaces $X^{b\varepsilon+}$ as well as global passive space X^{b-} which is orthogonal sum of all passive spaces $X^{b\varepsilon-}$. In analogy to (A12b) those spaces satisfy $X_\infty^{b+} \oplus X^{b-} = X_\infty^b$.

Consider now embedded weakly singular eigenstates. Those eigenstates satisfy $|\varphi(\varepsilon, \dots)\rangle \neq 0$ and conditions (19a) and (19b) are nontrivial. One finds that those eigenstates may exist only for some isolated eigenvalues $\varepsilon = \varepsilon_0 \in D$. In addition, for each $\varepsilon_0 \in D$ one may have at most ρ such eigenstates (see Appendix A and B.2). Hence the combined system may contain at most a finite number of such eigenstates (or in some extreme cases a denumerable (\aleph_0) number of such eigenstates). Since each such eigenstate is orthogonal to all embedded strongly singular eigenstates, those eigenstates satisfy $|\phi(\varepsilon, \dots)\rangle \in X^{b\varepsilon_0+}$.

One can have two kinds of embedded weakly singular eigenstates depending on whether $\mathbf{h}(\varepsilon_0)|\varphi(\varepsilon_0, \dots)\rangle \neq 0$ or $\mathbf{h}(\varepsilon_0)|\varphi(\varepsilon_0, \dots)\rangle = 0$. One finds that embedded weakly singular eigenstates which satisfy $\mathbf{h}(\varepsilon_0)|\varphi(\varepsilon_0, \dots)\rangle \neq 0$ do not contribute to the properties of the open system \mathbf{S}_ρ^a . This follows from the fact that such eigenstates may exist only in some isolated points $\varepsilon_0 \in D$. The set of all such points is of measure zero (at most \aleph_0) and hence all relevant integrals over those eigenstates vanish.

Another possibility is $\mathbf{f}(\varepsilon_a)|\varphi(\varepsilon_a, \dots)\rangle = 0$ and $\mathbf{h}(\varepsilon_a)|\varphi(\varepsilon_a, \dots)\rangle = 0$ for some $\varepsilon = \varepsilon_a$. Those expressions are recognized as relations (15a) and (16) which describe isolated eigenstates of the combined system (see Sect. 6.2.4). Each point $\varepsilon = \varepsilon_a$ where there is a nontrivial state $|\varphi\rangle$ such that $\mathbf{h}(\varepsilon_a)|\varphi\rangle = 0$ as well as $\mathbf{f}(\varepsilon_a)|\varphi\rangle = 0$ is an *anomalous* point [8]. One finds that the general method described in the Appendix B.2 breaks down in anomalous points, and in such a point the combined system may have one or several isolated eigenstates [5–8].

To summarize, in the case of embedded singular eigenstates most numerous are usually embedded strongly singular eigenstates which are given by expressions (20). Those eigenstates are due to the degeneracy of the corresponding unperturbed eigenvalue and for each $\varepsilon \in D$ they span the nullspace of \mathbf{VP}^ε . However, those eigenstates have no component in the space X_ρ^a and hence they do not contribute to the properties of the open system \mathbf{S}_ρ^a . On the other hand, embedded weakly singular eigenstates which do have nonvanishing X_ρ^a -component may exist only for some isolated eigenvalues $\varepsilon = \varepsilon_0 \in D$. There is hence a limited number of such eigenstates. One finds that to the properties of the open system \mathbf{S}_ρ^a may contribute only those weakly singular eigenstates which are anomalous. However, those eigenstates are isolated and they are taken care by corresponding expressions which produce isolated eigenvalues and eigenstates. In conclusion, embedded singular eigenstates do not contribute to the properties of the open system \mathbf{S}_ρ^a .

6.2 Embedded cardinal solutions

Embedded cardinal eigenstates of the combined system have nonvanishing fractional shift ($x(\varepsilon) \neq 0$) and nonvanishing X_ρ^a component. Those eigenstates contribute to the properties of the open system \mathbf{S}_ρ^a and they can be obtained as a solution of the fractional shift eigenvalue equation [8] (see Appendix B.2).

$$\mathbf{h}(\varepsilon)|\varphi_d(\varepsilon)\rangle = X_d(\varepsilon)\mathbf{f}(\varepsilon)|\varphi_d(\varepsilon)\rangle, \tag{22a}$$

where $\mathbf{h}(\varepsilon)$ is given by (19c) and where

$$X_d(\varepsilon) = -\pi\beta^2 \cot(\pi x_d(\varepsilon)), \quad \varepsilon \in D, \quad d = 1, 2, \dots, r(\varepsilon), \quad r(\varepsilon) \leq \rho. \tag{22b}$$

For simplicity, in the above expressions is omitted dependence on the parameter β . On this parameter depend quantities $\mathbf{h}(\varepsilon)$, $|\varphi_d(\varepsilon)\rangle$, $X_d(\varepsilon)$ and $x_d(\varepsilon)$, but not $\mathbf{f}(\varepsilon)$. Hence in an explicit full notation one should write $\mathbf{h}(\varepsilon) \equiv \mathbf{h}(\varepsilon, \beta)$, $|\varphi_d(\varepsilon)\rangle \equiv |\varphi_d(\varepsilon, \beta)\rangle$, $X_d(\varepsilon) \equiv X_d(\varepsilon, \beta)$ and $x_d(\varepsilon) \equiv x_d(\varepsilon, \beta)$.

Eigenvalue equation (22) produces X_ρ^a -components of cardinal eigenstates $|\Psi_d(\varepsilon)\rangle$ as well as the corresponding fractional shifts $x_d(\varepsilon)$. Index d is used to label multiple fractional shifts associated with degenerate cardinal eigenstates. Fractional shift $x_d(\varepsilon)$ is determined by the eigenvalue $X_d(\varepsilon)$ of the fractional shift eigenvalue equation according to (22b) and it is confined to the interval $[1 - \rho, 1]$ [8].

$$1 - \rho \leq x_d(\varepsilon) \leq 1. \tag{23}$$

Since for each integer m one has $\cot(\pi(x_d(\varepsilon) + m)) = \cot(\pi x_d(\varepsilon))$, expression (22b) determines fractional shift up to an additive integer constant. No other quantity to be derived in this paper is sensitive to this constant. Hence one can confine fractional shift $x_d(\varepsilon)$ to the interval $[0, 1)$. This is a *principal value* of a fractional shift. As emphasized in Sect. 3, in this paper it will be assumed that the fractional shift is confined to its principal value.

Fractional shift $x_d(\varepsilon)$ in conjuncture with the corresponding eigenstate $|\varphi_d(\varepsilon)\rangle$ of the fractional shift eigenvalue equation determines X_ρ^a -component $|\Psi_d^a(\varepsilon)\rangle$ of the embedded eigenstate $|\Psi_d(\varepsilon)\rangle$ according to [8]

$$|\Psi_d^a(\varepsilon)\rangle = \frac{\sin(\pi x_d(\varepsilon))}{\pi\beta\sqrt{\langle\varphi_d(\varepsilon)|\mathbf{f}(\varepsilon)|\varphi_d(\varepsilon)\rangle}} |\varphi_d(\varepsilon)\rangle, \quad (24a)$$

Using (22b) one can express $\sin(\pi x_d(\varepsilon))$ in terms of the eigenvalue $X_d(\varepsilon)$ of the fractional shift equation. Thus one finds

$$|\Psi_d^a(\varepsilon)\rangle = \frac{\beta}{\sqrt{\pi^2\beta^4 + (X_d(\varepsilon))^2\langle\varphi_d(\varepsilon)|\mathbf{f}(\varepsilon)|\varphi_d(\varepsilon)\rangle}} |\varphi_d(\varepsilon)\rangle. \quad (24b)$$

Fractional shift eigenvalue equation reduces to the generic eigenvalue equation if $X_d(\varepsilon) = 0$, i.e. if fractional shift equals $x_d(\varepsilon) = 0.5$. In particular, if $\varepsilon_r \equiv \varepsilon_r(\beta)$ is an eigenvalue of the generic eigenvalue equation (15a) and if $|\theta_r\rangle \equiv |\theta_r(\beta)\rangle$ is the corresponding eigenstate, then there is an eigenstate $|\varphi_r(\varepsilon)\rangle \equiv |\varphi_r(\varepsilon, \beta)\rangle$ of the fractional shift eigenvalue equation (22a) such that $X_r(\varepsilon_r(\beta), \beta) = 0$ and (up to the norm and phase) $|\theta_r(\beta)\rangle \equiv |\varphi_r(\varepsilon_r(\beta), \beta)\rangle$. Each solution to (15a) can be hence considered as a special case of solutions to (22a). Accordingly, one could obtain both, isolated as well as embedded solutions, using only fractional shift eigenvalue equation. However, it is more convenient to use both equations in order to have a clear separation between isolated eigenstates which are solutions of the generic eigenvalue equation (15a) and embedded eigenstates which are solutions of the fractional shift eigenvalue equation (22a).

As shown in a previous section, embedded singular eigenstates do not contribute to the properties of the open system \mathbf{S}_ρ^a . In addition to this difference between embedded cardinal and embedded singular eigenstates, there is another important difference between those two types of eigenstates. For each $\varepsilon \in D$ one may have at most ρ linearly independent embedded cardinal eigenstates (see next section). Hence those eigenstates can be labeled with discrete label d as $|\Psi_d(\varepsilon)\rangle$ (as this is done in the expression (22a)). On the other hand, strongly singular eigenstates may depend on additional discrete and/or continuous parameters induced by the system \mathbf{S}_∞^b . Each embedded strongly singular eigenstate is hence of a general type $|\Psi(\varepsilon, \dots)\rangle$ where dots (\dots) represents those additional parameters, if any. In particular, for each eigenvalue $\varepsilon \in D$ the set of all strongly singular eigenstates spans the nullspace of $\mathbf{V}\mathbf{P}^\varepsilon$ and one may have an infinite number of such eigenstates (see Sect. 6.1.). It is fortunate that those eigenstates are not required for the description of the open system \mathbf{S}_ρ^a and that

(as far as properties of this open system are considered) embedded cardinal eigenstates are sufficient.

6.2.1 Basic properties of the solutions to the fractional shift eigenvalue equation

In a base $\{|s\rangle\} \in X_\rho^a$ fractional shift equation is a $\rho \times \rho$ matrix eigenvalue equation. Standard $\rho \times \rho$ eigenvalue equation involving Hermitian matrix has ρ eigenvalues and ρ orthonormalized eigenstates. However, fractional shift equation is a generalized eigenvalue equation with Hermitian operator $\mathbf{f}(\varepsilon)$ on the right hand side of this equation. Hence for each ε the number $r(\varepsilon)$ of linearly independent eigenstates $|\varphi_d(\varepsilon)\rangle$ of this equation may be anything from $r(\varepsilon) = 0$ to $r(\varepsilon) = \rho$. If $\mathbf{h}(\varepsilon)$ is regular (which is usually the case) this number equals rank of the operator $\mathbf{f}(\varepsilon)$, i.e. $r(\varepsilon) = \text{rank}(\mathbf{f}(\varepsilon))$.

In general, eigenstates $|\varphi_d(\varepsilon)\rangle$ of the fractional shift eigenvalue equation are not orthogonal to each other. Hence usually $\langle \Psi_d^a(\varepsilon) | \mathbf{S}^a | \Psi_{d'}^a(\varepsilon) \rangle \neq 0$ ($d \neq d'$). Orthogonal to each other are complete embedded eigenstates $|\Psi_d(\varepsilon)\rangle$, but not necessarily their X_ρ^a -components. However, those components satisfy

$$\langle \Psi_d^a(\varepsilon) | \mathbf{f}(\varepsilon) | \Psi_{d'}^a(\varepsilon) \rangle = 0, \quad d \neq d'. \tag{25}$$

This can be easily derived from (22a). Note further that all $r(\varepsilon)$ embedded eigenstates $|\Psi_d(\varepsilon)\rangle$ ($d = 1, \dots, r(\varepsilon)$) have the same eigenvalue ε and hence each linear combination of those eigenstates is again an embedded eigenstate of the combined system with this eigenvalue. However, corresponding linear combination of the eigenstates $|\varphi_d(\varepsilon)\rangle$ of the fractional shift equation is usually not an eigenstate of this equation. Each eigenstate $|\varphi_d(\varepsilon)\rangle$ of (22a) has well defined fractional shift $x_d(\varepsilon)$. Hence, unless $x_d(\varepsilon) = x_{d'}(\varepsilon)$, linear combination $a|\varphi_d(\varepsilon)\rangle + b|\varphi_{d'}(\varepsilon)\rangle$ is not an eigenstate of (22a) and it has not well defined fractional shift.

In the analysis of the solutions to the fractional shift eigenvalue equation important are some *characteristic points* $\varepsilon \in D$. Those are *singular*, *critical* and *resonant* points [8].

Singular points $\varepsilon_0 \in D$ correspond to embedded singular solutions of the combined system. Each such solution satisfies $x(\varepsilon_0) = 0$ and it describes perturbed eigenvalue that in the limit $n \rightarrow \infty$ coincides with some unperturbed eigenvalue (see Appendix B.2). As shown in Sect. 6.1., singular solutions are treated by the Eq. 19. According to (22b), fractional shift $x_d(\varepsilon_0) = 0$ corresponds to the eigenvalue $X_d(\varepsilon_0) = \pm\infty$ of the fractional shift equation. Infinite value of $X_d(\varepsilon_0)$ is not a proper eigenvalue of this equation. This is consistent with the fact that fractional shift equation produces all embedded cardinal solutions and no singular solution. However, one can consider some singular solutions as a limit case of cardinal solutions. If $\lim_{\varepsilon \rightarrow \varepsilon_0} X_d(\varepsilon) \mathbf{f}(\varepsilon) |\varphi_d(\varepsilon)\rangle$ is well defined and finite and if $\lim_{\varepsilon \rightarrow \varepsilon_0} X_d(\varepsilon) = \pm\infty$, one must have $\lim_{\varepsilon \rightarrow \varepsilon_0} \mathbf{f}(\varepsilon) |\varphi_d(\varepsilon)\rangle = 0$. In this case in a point $\varepsilon = \varepsilon_0$ one has a singular solution. Accordingly, in addition to embedded cardinal solutions fractional shift equation can (as a limit case) produce some embedded singular solutions. Those solutions may exist only in some isolated points $x_0 \in D$.

Second type of characteristic points are critical points. If the system \mathbf{S}_∞^b contains a single one-parameter eigenvalue band, operator $\mathbf{f}(\varepsilon)$ has rank one for each interior point $\varepsilon \in D$, except possibly for some isolated points $\varepsilon_c \in D$ where this rank vanishes. Such points were named *critical* points [8]. One can generalize the notion of critical point to arbitrary system \mathbf{S}_∞^b where characteristic operator $\mathbf{f}(\varepsilon)$ may have any rank $\leq \rho$. In general, global characteristic operator $\mathbf{f}(\varepsilon)$ can contain several characteristic operators $\mathbf{f}_\nu(\varepsilon)$ which correspond to various eigenvalue bands. Rank $r_\nu(\varepsilon) = \text{rank}(\mathbf{f}_\nu(\varepsilon))$ associated with the eigenvalue band ν is constant for each $\varepsilon \in I_\nu$ which is an interior point in I_ν , except possibly for some isolated points $\varepsilon_c \in I_\nu$. By definition, those isolated points are *critical* points. This is a natural generalization of the notion of a critical point from the case of a single one-parameter eigenvalue band to a general case of several multiparameter eigenvalue bands.

Third type of characteristic points are *resonant* points. In a resonant point $\varepsilon_r \in D$ operator $\mathbf{h}(\varepsilon_r)$ is singular. Hence there is at least one eigenstate $|\varphi_d(\varepsilon)\rangle \in X_\rho^a$ of fractional shift eigenvalue equation such that $\mathbf{h}(\varepsilon_r)|\varphi_d(\varepsilon_r)\rangle = 0$. This expression is the same as the generic eigenvalue equation (15a) where $\varepsilon_r \in D$. There are two possibilities: either $\mathbf{f}(\varepsilon_r)|\varphi_d(\varepsilon_r)\rangle \neq 0$ or $\mathbf{f}(\varepsilon_r)|\varphi_d(\varepsilon_r)\rangle = 0$. If $\mathbf{f}(\varepsilon_r)|\varphi_d(\varepsilon_r)\rangle \neq 0$ and if the coupling β is sufficiently small, in some neighborhood of this resonant point density $\rho_d(\varepsilon) = \langle \Psi_d^a(\varepsilon) | \mathbf{S}^a | \Psi_d^a(\varepsilon) \rangle$ of the X_ρ^a -component of the embedded eigenstate $|\Psi_d(\varepsilon)\rangle$ exhibits a strong resonance feature. This is a rationale for the name *resonant point* [8]. Another possibility is $\mathbf{f}(\varepsilon_r)|\varphi_d(\varepsilon_r)\rangle = 0$. If this is the case, the point $\varepsilon = \varepsilon_r$ is an *anomalous* point. In such a point combined system may have one or several isolated eigenstates [8]. In Sects. 6.2.3. and 6.2.4. those two possibilities are discussed in more details.

6.2.2 Probabilities associated with embedded cardinal eigenstates

Component $|\Psi_d^a(\varepsilon)\rangle$ of the embedded cardinal eigenstate $|\Psi_d(\varepsilon)\rangle$ determines all related properties of the open system \mathbf{S}_ρ^a . In particular, probability amplitude to find local state $|\Theta_s\rangle$ in this eigenstate equals $\langle \Theta_s | \mathbf{S} | \Psi_d(\varepsilon) \rangle$ [8]. Hence and due to (24b) probability density $\rho_{d,s}(\varepsilon)$ to find this state in the embedded eigenstate $|\Psi_d(\varepsilon)\rangle$ equals

$$\rho_{d,s}(\varepsilon) \equiv |\langle \Theta_s | \mathbf{S} | \Psi_d(\varepsilon) \rangle|^2 = \frac{\beta^2 \langle \varphi_d(\varepsilon) | \mathbf{S}^a | \Theta_s \rangle \langle \Theta_s | \mathbf{S}^a | \varphi_d(\varepsilon) \rangle}{[\pi^2 \beta^4 + (X_d(\varepsilon))^2] \langle \varphi_d(\varepsilon) | \mathbf{f}(\varepsilon) | \varphi_d(\varepsilon) \rangle}, \quad (26a)$$

One can also consider total probability $C_{d,s}$ to find local state $|\Theta_s\rangle$ in any of the embedded eigenstates $|\Psi_d(\varepsilon)\rangle$ corresponding to index d . By definition, this probability equals

$$C_{d,s} = \int \rho_{d,s}(\varepsilon) d\varepsilon. \quad (26b)$$

Of more practical interest is probability density $\sigma_s(\varepsilon)$ to find local state $|\Theta_s\rangle$ in any of the embedded eigenstates $|\Psi_d(\varepsilon)\rangle$ with the eigenvalue ε . In other words, $\sigma_s(\varepsilon)$ is a probability density to find local state $|\Theta_s\rangle$ with the eigenvalue $\varepsilon \in D$:

$$\sigma_s(\varepsilon) = \sum_d \rho_{d,s}(\varepsilon) = \sum_d |\langle \Theta_s | \mathbf{S} | \Psi_d(\varepsilon) \rangle|^2, \tag{27a}$$

Corresponding total probability S_s to find local state $|\Theta_s\rangle$ in any of the embedded eigenstates of the combined system equals

$$S_s \equiv \sum_d C_{d,s} = \int \sigma_s(\varepsilon) d\varepsilon. \tag{27b}$$

In conjuncture with isolated eigenvalues ε_r and corresponding probabilities $w_{r,s}$, probability density $\sigma_s(\varepsilon)$ determines eigenvalue distribution (or spectral distribution) of the local state $|\Theta_s\rangle$. In other words, if \mathbf{S}_ρ^a is an open system and if one measures eigenvalue of the local state $|\Theta_s\rangle$, one should find each isolated eigenvalue ε_r with the probability $w_{r,s}$ and each embedded eigenvalue $\varepsilon \in D$ with probability density $\sigma_s(\varepsilon)$.

In analogy to (18b) one can also consider probability density $\rho_d(\varepsilon)$ to find embedded eigenstate $|\Psi_d(\varepsilon)\rangle$ in a local system \mathbf{S}_ρ^a , i.e. to find this eigenstate in any of the local states $|\Theta_s\rangle$. Due to (1c) one has

$$\rho_d(\varepsilon) \equiv \sum_s \rho_{d,s}(\varepsilon) = \frac{\beta^2 \langle \varphi_d(\varepsilon) | \mathbf{S}^a | \varphi_d(\varepsilon) \rangle}{[\pi^2 \beta^4 + X_d(\varepsilon)^2] \langle \varphi_d(\varepsilon) | \mathbf{f}(\varepsilon) | \varphi_d(\varepsilon) \rangle}, \tag{28a}$$

This equals norm of the X_d^a -component of the embedded cardinal eigenstate $|\Psi_d(\varepsilon)\rangle$:

$$\rho_d(\varepsilon) = \langle \Psi_d^a(\varepsilon) | \mathbf{S}^a | \Psi_d^a(\varepsilon) \rangle. \tag{28b}$$

Above expression is formally identical to the expression (18c).

Densities $\sigma_s(\varepsilon)$ have a direct physical interpretation. However, densities $\rho_d(\varepsilon)$ are more convenient mathematically since those densities are given by simple expressions (28). For each $\varepsilon \in D$ those two densities satisfy

$$\sum_s \sigma_s(\varepsilon) = \sum_d \rho_d(\varepsilon) \tag{29a}$$

Hence

$$\sum_s S_s = \sum_d C_d \tag{29b}$$

where

$$C_d \equiv \sum_s C_{d,s} = \int \rho_d(\varepsilon) d\varepsilon. \tag{29c}$$

6.2.3 Emergence of resonance in the case of the weak coupling

As shown in the Appendix E, if $\mathbf{f}(\varepsilon)$ is smooth in a point $\varepsilon \in D$ and if $X_d(\varepsilon) \equiv X_d(\varepsilon, \beta)$ is nondegenerate, one has

$$\frac{\partial X_d(\varepsilon, \beta)}{\partial \varepsilon} = \frac{\langle \varphi_d(\varepsilon, \beta) | \beta^2 d\boldsymbol{\omega}(\varepsilon)/d\varepsilon - \mathbf{S}^a - X_d(\varepsilon, \beta) d\mathbf{f}(\varepsilon)/d\varepsilon | \varphi_d(\varepsilon, \beta) \rangle}{\langle \varphi_d(\varepsilon, \beta) | \mathbf{f}(\varepsilon) | \varphi_d(\varepsilon, \beta) \rangle}, \quad (30)$$

where $|\varphi_d(\varepsilon, \beta)\rangle$ is eigenstate of the fractional shift eigenvalue equation corresponding to the eigenvalue $X_d(\varepsilon, \beta)$. For clarity, in the above and in the following expressions dependence on β is explicitly written.

Above expression is the rate of change of the eigenvalue $X_d(\varepsilon, \beta)$ of the fractional shift equation with respect to parameter ε . Let the eigenvalue E_s of \mathbf{S}_ρ^a satisfy $E_s \in D$ and let this eigenvalue be nondegenerate. If $\mathbf{f}(E_s)|\Theta_s\rangle \neq 0$ and if β is sufficiently small, components $|\Psi_d^a(\varepsilon, \beta)\rangle \in X_\rho^a$ of embedded eigenstates $|\Psi_d(\varepsilon, \beta)\rangle$ can be in the vicinity of the resonant point $\varepsilon = \varepsilon_s(\beta)$ approximated as (see Appendix E)

$$\begin{aligned} |\Psi_d^a(\varepsilon, \beta)\rangle &\approx \\ |\Psi_d^a(\varepsilon, \beta)\rangle^\circ &= \frac{\beta}{\sqrt{\pi^2 \beta^4 + a_s(\beta)^2 (\varepsilon - \varepsilon_s(\beta))^2} \sqrt{\langle \theta_s(\beta) | \mathbf{f}(\varepsilon_s) | \theta_s(\beta) \rangle}} |\theta_s(\beta)\rangle \delta_{s,d}, \end{aligned} \quad (31a)$$

where

$$a_s(\beta) \equiv -\frac{\partial X_s(\varepsilon_s(\beta), \beta)}{\partial \varepsilon_s} = \frac{\langle \theta_s(\beta) | \mathbf{S}^a - \beta^2 d\boldsymbol{\omega}(\varepsilon_s)/d\varepsilon_s | \theta_s(\beta) \rangle}{\langle \theta_s(\beta) | \mathbf{f}(\varepsilon_s(\beta)) | \theta_s(\beta) \rangle}, \quad \varepsilon \in \Delta(\varepsilon_s), \quad (31b)$$

and where $|\theta_s(\beta)\rangle$ is the eigenstate and $\varepsilon_s(\beta)$ the corresponding eigenvalue of the generic eigenvalue equation (15a) that satisfy $|\theta_s(0)\rangle = |\Theta_s\rangle$ and $\varepsilon_s(0) = E_s$. Since E_s is nondegenerate, generic eigenvalue equation has exactly one solution that satisfy those conditions. Approximation (31) is valid in some (small) neighborhood $\Delta(\varepsilon_s)$ of the point $\varepsilon = \varepsilon_s(\beta)$. In particular, if $\varepsilon \in \Delta(\varepsilon_s)$ and if $d \neq s$ one has $|\Psi_d^a(\varepsilon, \beta)\rangle \approx 0$. According to (31a) probability density $\rho_d(\varepsilon, \beta) = \langle \Psi_d^a(\varepsilon, \beta) | \mathbf{S} | \Psi_d^a(\varepsilon, \beta) \rangle$ can be approximated as

$$\rho_d(\varepsilon, \beta) \approx \rho_d^0(\varepsilon, \beta) = \rho_s^0(\varepsilon, \beta) \delta_{d,s}, \quad \varepsilon \in \Delta(\varepsilon_s), \quad (32a)$$

where

$$\rho_s^0(\varepsilon, \beta) = \frac{\beta^2 K_s(\beta)}{\pi^2 \beta^4 + a_s(\beta)^2 (\varepsilon - \varepsilon_s(\beta))^2}, \quad K_s(\beta) = \frac{\langle \theta_s(\beta) | \mathbf{S}^a | \theta_s(\beta) \rangle}{\langle \theta_s(\beta) | \mathbf{f}(\varepsilon_s) | \theta_s(\beta) \rangle}, \quad (32b)$$

and where $a_s(\beta)$ is given by (31b). Density $\rho_s^0(\varepsilon, \beta)$ represents a universal resonance curve [12] centered at the point $\varepsilon = \varepsilon_s(\beta)$ and with the width $\Delta\varepsilon_s(\beta)$

$$\Delta\varepsilon_s(\beta) = \frac{\pi\beta^2}{a_s(\beta)} = \frac{\pi\beta^2 \langle \theta_s(\beta) | \mathbf{f}(\varepsilon_s) | \theta_s(\beta) \rangle}{\langle \theta_s(\beta) | \mathbf{S}^a - \beta^2 d\boldsymbol{\omega}(\varepsilon_s)/d\varepsilon_s | \theta_s(\beta) \rangle} \tag{33a}$$

Height of this curve equals $\rho_s^0(\varepsilon_s, \beta)$ and it has the area $w_s^0(\beta) = \int \rho_s^0(\varepsilon, \beta) d\varepsilon$

$$\rho_s^0(\varepsilon_s(\beta), \beta) = \frac{\langle \theta_s(\beta) | \mathbf{S}^a | \theta_s(\beta) \rangle}{\pi^2 \beta^2 \langle \theta_s(\beta) | \mathbf{f}(\varepsilon_s) | \theta_s(\beta) \rangle}, \tag{33b}$$

$$w_s^0(\beta) = \frac{\langle \theta_s(\beta) | \mathbf{S}^a | \theta_s(\beta) \rangle}{\langle \theta_s(\beta) | \mathbf{S}^a | \theta_s(\beta) \rangle - \beta^2 \langle \theta_s(\beta) | d\boldsymbol{\omega}(\varepsilon_s)/d\varepsilon_s | \theta_s(\beta) \rangle} \equiv \frac{K_s(\beta)}{a_s(\beta)}. \tag{33c}$$

The area $w_s^0(\beta)$ is an approximation of a total probability to find any of the states $|\Theta_s\rangle$ with the eigenvalue ε anywhere in the interval $\Delta(\varepsilon_s)$. Note that expression (33c) is formally identical to the expression (18b) for the probability to find isolated eigenstate $|\Psi_r\rangle$ in a local system \mathbf{S}_ρ^a .

From the expression (31) one finds in a similar way probability densities $\rho_{d,p}(\varepsilon, \beta) = |\langle \Theta_p | \mathbf{S}^a | \Psi_d(\varepsilon, \beta) \rangle|^2$ and $\sigma_p(\varepsilon, \beta) \equiv \sum_d \rho_{d,p}(\varepsilon, \beta)$. Since β is small one has $|\theta_s(\beta)\rangle \approx |\theta_s(0)\rangle = |\Theta_s\rangle$. Hence those densities satisfy

$$\begin{aligned} \sigma_{d,p}(\varepsilon, \beta) &\approx \rho_s^0(\varepsilon, \beta) \delta_{d,p} \delta_{p,s}, \\ \sigma_p(\varepsilon, \beta) &\equiv \sum_d \rho_{d,p}(\varepsilon, \beta) \approx \rho_s^0(\varepsilon, \beta) \delta_{p,s}, \quad \varepsilon \in \Delta(\varepsilon_s). \end{aligned} \tag{33d}$$

In addition, in the case of small β expression (33c) implies $w_s^0(\beta) \approx 1$.

In conclusion, if $E_s \in D$ is nondegenerate and if $\mathbf{f}(E_s) |\Theta_s\rangle \neq 0$, for sufficiently small interaction parameter β there is an embedded eigenstate $|\Psi_s(\varepsilon, \beta)\rangle$ with the property that component $|\Psi_s^a(\varepsilon, \beta)\rangle$ of this eigenstate exhibits a strong resonance feature in the neighborhood $\Delta(\varepsilon_s)$ of the resonant point $\varepsilon = \varepsilon_s(\beta)$, while X_ρ^a -components of all other embedded eigenstates $|\Psi_d(\varepsilon, \beta)\rangle$ ($d \neq s$) are negligible in $\Delta(\varepsilon_s)$ [8]. In particular, probability density $\sigma_s(\varepsilon, \beta)$ to find local state $|\Theta_s\rangle$ with the eigenvalue $\varepsilon \in D$ exhibits a strong resonance feature in $\Delta(\varepsilon_s)$. The same applies to the probability density $\rho_s(\varepsilon, \beta)$ and one has $\rho_s(\varepsilon, \beta) \approx \sigma_s(\varepsilon, \beta)$. This property is rational for the name “resonant point” [8].

Similar results are obtained if $E_s \in D$ is degenerate. However, in this case there are several eigenstates $|\theta_r(\beta)\rangle$ of a generic eigenvalue equation that satisfy $|\theta_r(0)\rangle = |\Theta_s\rangle$ and one may have several closed spaced resonant structures corresponding to the degeneracy of E_s [8].

Emergence of resonance in the case of the weak coupling is usually derived within the formalism of the time-independent perturbation expansion approach [1,2]. If a system of particles interacts weakly with the field (such as e.g. electromagnetic field), there are two main effects of such an interaction. First, due to this interaction each eigenvalue E_s of this system shifts to a new position ε_s . Second, this shifted eigenvalue

is not sharp and it acquires the shape of the universal resonance curve [1]. As shown above, both effects are correctly described within the small β limit of the suggested approach.

6.2.4 Anomal points and isolated solutions

As shown in a previous section, if β is sufficiently small the width $\Delta\varepsilon_s(\beta)$ of the universal resonance curve (32b), as calculated according to (33a), is small. This implies emergence of resonance in the case of small β . However, if $\langle\theta_r(\beta)|\mathbf{f}(\varepsilon_r)|\theta_r(\beta)\rangle$ is sufficiently small one may have small $\Delta\varepsilon_s(\beta)$ even for large β . Accordingly, open system \mathbf{S}_ρ^a may display a strong resonant features even in the case of strong interaction with its surrounding. Such an extreme case is the case of anomal point $\beta = \beta_a$ where $\varepsilon_a = \varepsilon_r(\beta_a)$. In this point there is at least one eigenstate $|\theta_r(\beta)\rangle$ of the generic eigenvalue equation such that $\mathbf{h}(\varepsilon_a)|\theta_r(\beta_a)\rangle = 0$ and $\mathbf{f}(\varepsilon_a)|\theta_r(\beta_a)\rangle = 0$. This implies $\langle\theta_r(\beta_a)|\mathbf{f}(\varepsilon_a)|\theta_r(\beta_a)\rangle = 0$. Corresponding eigenvalue $X_r(\varepsilon_a, \beta_a)$ of a fractional shift eigenvalue equation can assume any value and fractional shift $x_r(\varepsilon_a, \beta_a)$ is hence not well defined [8]. However, this case can be analyzed as a limit $\lim_{\beta \rightarrow \beta_a} \langle\theta_r(\beta)|\mathbf{f}(\varepsilon_r)|\theta_r(\beta)\rangle$. Let $\varepsilon_r(\beta)$ be nondegenerate in the point $\beta = \beta_a$. In the process $\beta \rightarrow \beta_a$ the width $\Delta\varepsilon_r(\beta)$ of resonance curve (32b) decreases, approximate probability (33c) improves, and in a limit $\Delta\varepsilon_r(\beta) \rightarrow 0$ it is exact. In this limit resonant shape at the anomal point $\varepsilon_a = \varepsilon_r(\beta_a)$ becomes infinitely narrow and infinitely high. One obtains qualitatively the same result in the case when $\varepsilon_r(\beta)$ is degenerate in the point $\beta = \beta_a$. In general, such infinitely narrow and infinitely high densities correspond to one or several isolated eigenstates [8]. One finds that components $|\Psi_r^a\rangle \in X_\rho^a$ of those eigenstates are given by expressions (15b,c) (see Appendix E). Thus all cardinal isolated eigenstates, those with eigenvalues $\varepsilon_r \notin D$ as well as those with eigenvalues $\varepsilon_r \in D$, are described by the same expressions (15–16).

7 Completeness relations

As shown in the Appendix C, isolated eigenstates and embedded cardinal eigenstates of the combined system satisfy

$$\sum_r w_{r,s} + S_s = 1, \quad s = 1, \dots, \rho, \quad (34a)$$

where

$$w_{r,s} = |\langle\Theta_s|\mathbf{S}^a|\Psi_r\rangle|^2, \quad S_s = \sum_d \int |\langle\Theta_s|\mathbf{S}^a|\Psi_d(\varepsilon)\rangle|^2 d\varepsilon \quad (34b)$$

Quantity $w_{r,s}$ is a probability to find local state $|\Theta_s\rangle$ in the isolated eigenstate $|\Psi_r\rangle$ of the combined system, while S_s is a probability to find this state in any of the embedded cardinal eigenstate $|\Psi_d(\varepsilon)\rangle$ of the combined system. Relation (34a) thus expresses the fact that one must find each local state $|\Theta_s\rangle \in X_\rho^a$ with certainly either in

some isolated eigenstate $|\Psi_r\rangle$ of the combined system, or in some embedded cardinal eigenstate $|\Psi_d(\varepsilon)\rangle$ of this system.

Note that expression (34a) does not contain any contribution from embedded singular eigenstates. As shown in Sect. 6.1, those eigenstates do not contribute to the properties of the open system \mathbf{S}_ρ^a .

Quantities $w_{r,s}$ and S_s are given by expressions (18a), (26a) and (27). Summing expression (34a) over s one finds

$$\sum_r w_r + \sum_s S_s = \rho, \tag{34c}$$

where probabilities $w_r = \sum_s w_{r,s}$ are given by expression (18b).

Expressions (34) are completeness relations. Those expressions are satisfied for each value of the coupling parameter β , however large. Expressions (34) thus provide an efficient way for the verification of the suggested method [8].

8 Open two-dimensional quantum systems

Above, a general method for the exact treatment of open finite-dimensional quantum system \mathbf{S}_ρ^a was presented. However, of special importance are open two-dimensional systems \mathbf{S}_2^a [13]. In the case of such systems generic eigenvalue equation and fractional shift eigenvalue equation simplify. For clarity, in the following expressions dependence on the coupling parameter β will be explicitly shown.

Isolated eigenvalues and eigenstates of the combined system as well as resonant points are solutions of the generic equation (15a). This equation has a nontrivial solution if and only if the determinant of the system vanishes. In a 2×2 case condition $|\mathbf{h}(\varepsilon_r, \beta)| = 0$ reads

$$|\mathbf{h}(\varepsilon_r, \beta)| \equiv h_{11}(\varepsilon_r, \beta)h_{22}(\varepsilon_r, \beta) - h_{12}(\varepsilon_r, \beta)h_{21}(\varepsilon_r, \beta) = 0, \tag{35a}$$

where

$$h_{sp}(\varepsilon, \beta) \equiv \beta^2 \omega_{sp}(\varepsilon) + A_{sp} - \varepsilon S_{sp}^a, \tag{35b}$$

are matrix elements of the operator $\mathbf{h}(\varepsilon, \beta)$ in the base $\{|s\rangle\}$.

Hence

$$\beta^4 |\boldsymbol{\omega}(\varepsilon_r)| + \beta^2 \Gamma(\varepsilon_r) + |\mathbf{A} - \varepsilon_r \mathbf{S}^a| = 0, \tag{36a}$$

where

$$\begin{aligned} \Gamma(\varepsilon) &= Tr(\boldsymbol{\omega}(\varepsilon)) Tr(\mathbf{A} - \varepsilon \mathbf{S}^a) - Tr(\boldsymbol{\omega}(\varepsilon)(\mathbf{A} - \varepsilon \mathbf{S}^a)) \\ &\equiv \omega_{11}(\varepsilon) (A_{22} - \varepsilon S_{22}^a) + \omega_{22}(\varepsilon) (A_{11} - \varepsilon S_{11}^a) - \omega_{12}(\varepsilon) (A_{21} - \varepsilon S_{21}^a) \\ &\quad - \omega_{21}(\varepsilon) (A_{12} - \varepsilon S_{12}^a). \end{aligned} \tag{36b}$$

and where $\omega_{sp}(\varepsilon)$ are matrix elements of the derived operator $\omega(\varepsilon)$, while $|\omega(\varepsilon)|$ and $|\mathbf{A} - \varepsilon \mathbf{S}^a|$ are determinants of $\omega(\varepsilon)$ and $(\mathbf{A} - \varepsilon \mathbf{S}^a)$, respectively. Each solution $\varepsilon = \varepsilon_r(\beta)$ of (36a) is an eigenvalue of the generic eigenvalue equation. Once this eigenvalue is obtained, the corresponding eigenstate $|\theta_r\rangle \equiv |\theta_r(\beta)\rangle$ is:

$$|\theta_r(\beta)\rangle = h_{12}(\varepsilon_r, \beta) |1\rangle - h_{11}(\varepsilon_r, \beta) |2\rangle. \quad (37)$$

This applies to the usual case when either $h_{12}(\varepsilon_r, \beta) \neq 0$ or $h_{11}(\varepsilon_r, \beta) \neq 0$. However, if for some $\beta = \beta_0$ one has $h_{12}(\varepsilon_r, \beta_0) = 0$ and $h_{11}(\varepsilon_r, \beta_0) = 0$, in this case eigenvalue $\varepsilon_r(\beta_0)$ is degenerate and each linear combination of $|1\rangle$ and $|2\rangle$ is the corresponding eigenstate.

If $\varepsilon_r(\beta) \notin D$, eigenstate (37) determines X_ρ^a -component $|\Psi_r^a\rangle$ of the isolated eigenstate $|\Psi_r\rangle$ according to expressions (15b,c). If however $\varepsilon_r(\beta) \in D$, one has an isolated eigenstate in this point only if the additional condition (16) is satisfied. Provided this is the case, X_ρ^a -component of this eigenstate is again given by expressions (15b,c) and the point $\varepsilon = \varepsilon_r$ is an anomalous point.

Consider now solutions of expression (36a) from another point of view. This expression is quadratic in $x = \beta^2$ and one can solve this expression for β to obtain two solutions of a type $\beta = \beta(\varepsilon)$

$$\beta_{1,2}(\varepsilon) = \left[\frac{-\Gamma(\varepsilon) \pm \sqrt{\Gamma(\varepsilon)^2 - 4|\omega(\varepsilon)||\mathbf{A} - \varepsilon \mathbf{S}^a|}}{2|\omega(\varepsilon)|} \right]^{1/2}. \quad (38a)$$

The quantity

$$\Lambda(\varepsilon) = \Gamma(\varepsilon)^2 - 4|\omega(\varepsilon)||\mathbf{A} - \varepsilon \mathbf{S}^a|, \quad (38b)$$

is discriminant [14] of the quadratic equation (36a). Since β must be real, solutions (38a) exist only if $\Lambda(\varepsilon) \geq 0$. In addition, the expression inside square brackets in (38a) must be nonnegative. If this is the case, one has two solutions $\beta_{1,2}(\varepsilon)$ if $\Lambda(\varepsilon) > 0$, one solution $\beta(\varepsilon)$ if $\Lambda(\varepsilon) = 0$ and no solution if $\Lambda(\varepsilon) < 0$. One has also to consider a special case $|\omega(\varepsilon)| = 0$ when quadratic equation (36a) reduces to a linear equation (in $x = \beta^2$) with a solution

$$\beta(\varepsilon) = \sqrt{-\frac{|\mathbf{A} - \varepsilon \mathbf{S}^a|}{\Gamma(\varepsilon)}}, \quad \text{if } |\omega(\varepsilon)| = 0. \quad (38c)$$

The same expression is obtained as the $|\omega(\varepsilon)| \rightarrow 0$ limit of the expression (38a). Provided $\Gamma(\varepsilon) \neq 0$ and provided the expression under the square root in (38c) is nonnegative, parameter β is real and finite. This is an admissible solution to (36a). However, if the expression under the square root in (38c) is negative, parameter β is complex which is not an admissible solution.

Solutions (38) of a type $\beta = \beta(\varepsilon)$ are convenient mathematically since those solutions are given in a closed form. However, physically are more important inverse solutions of a type $\varepsilon = \varepsilon(\beta)$ since each such solution is an eigenvalue of the generic

eigenvalue equation. In general, one can have several solutions of a type $\varepsilon = \varepsilon(\beta)$ while one can have at most two solutions of a type $\beta = \beta(\varepsilon)$. Note that if $\beta = 0$ eigenvalues of the generic equation coincide with local eigenvalues E_1 and E_2 . Hence, among all such solutions one must have two solutions $\varepsilon = \varepsilon_1(\beta)$ and $\varepsilon = \varepsilon_2(\beta)$ that satisfy $\varepsilon_1(0) = E_1$ and $\varepsilon_2(0) = E_2$, respectively.

Consider next fractional shift eigenvalue equation (22a). This equation has a non-trivial solution if and only if determinant of a system vanishes. In the case of a two-dimensional system \mathbf{S}_2^a this implies

$$X_d(\varepsilon, \beta)^2 |\mathbf{f}(\varepsilon)| - X_d(\varepsilon, \beta) \Xi(\varepsilon, \beta) + |\mathbf{h}(\varepsilon, \beta)| = 0, \quad \varepsilon \in D, \tag{39a}$$

where

$$\begin{aligned} \Xi(\varepsilon, \beta) &= Tr \mathbf{h}(\varepsilon, \beta) Tr \mathbf{f}(\varepsilon) - Tr [\mathbf{h}(\varepsilon, \beta) \mathbf{f}(\varepsilon)] \\ &\equiv h_{11}(\varepsilon, \beta) f_{22}(\varepsilon) + h_{22}(\varepsilon, \beta) f_{11}(\varepsilon) - h_{12}(\varepsilon, \beta) f_{21}(\varepsilon) - h_{21}(\varepsilon, \beta) f_{12}(\varepsilon). \end{aligned} \tag{39b}$$

and where $|\mathbf{f}(\varepsilon)|$ and $|\mathbf{h}(\varepsilon, \beta)|$ are determinants of $\mathbf{f}(\varepsilon)$ and $\mathbf{h}(\varepsilon, \beta)$, respectively.

Solutions of the above equation are eigenvalues $X_d(\varepsilon, \beta)$ of a fractional shift eigenvalue equation. Those eigenvalues must be real.

If $|\mathbf{f}(\varepsilon)| \neq 0$ expression (39a) has formally two solutions

$$X_{1,2}(\varepsilon, \beta) = \frac{\Xi(\varepsilon, \beta) \pm \sqrt{\Xi(\varepsilon, \beta)^2 - 4 |\mathbf{f}(\varepsilon)| |\mathbf{h}(\varepsilon, \beta)|}}{2 |\mathbf{f}(\varepsilon)|}. \tag{40a}$$

The quantity

$$\Pi(\varepsilon) = \Xi(\varepsilon)^2 - 4 |\mathbf{f}(\varepsilon)| |\mathbf{h}(\varepsilon)|, \tag{40b}$$

is discriminant [14] of the quadratic equation (39a). Using definition (39b) and since $|\mathbf{f}(\varepsilon)| \geq 0$, one finds $\Pi(\varepsilon) \geq 0$. The quantity (40a) is hence guaranteed to be real for each $\varepsilon \in D$. In conclusion, if $|\mathbf{f}(\varepsilon)| \neq 0$ expression (39a) has two real solutions with possible exception of some isolated points $\varepsilon = \varepsilon_0 \in D$ where $\Pi(\varepsilon_0, \beta) = 0$ and where this expression has only one real solution $X(\varepsilon_0, \beta)$.

Another possibility is $|\mathbf{f}(\varepsilon)| = 0$. In this case expression (39a) has only one solution

$$X(\varepsilon, \beta) = \frac{|\mathbf{h}(\varepsilon, \beta)|}{\Xi(\varepsilon, \beta)}, \quad \text{if } |\mathbf{f}(\varepsilon)| = 0. \tag{40c}$$

The same expression is obtained as the $|\mathbf{f}(\varepsilon)| \rightarrow 0$ limit of the expression (40a).

One has $|\mathbf{f}(\varepsilon)| = 0$ for each $\varepsilon \in D$ if the system \mathbf{S}_∞^b that interacts with the two-dimensional system \mathbf{S}_2^a contains a single one-parameter eigenvalue band [8]. In this case for each $\varepsilon \in D$ combined system has at most only one embedded eigenstate.

Once $X_d(\varepsilon, \beta)$ is obtained as a solution of (39a), X_2^a -component $|\Psi_d^a(\varepsilon, \beta)\rangle$ of the embedded eigenstate $|\Psi_d(\varepsilon, \beta)\rangle$ is given by expressions (24) where

$$|\varphi_d(\varepsilon, \beta)\rangle = [h_{12}(\varepsilon, \beta) - X_d(\varepsilon, \beta)f_{12}(\varepsilon)]|1\rangle + [X_d(\varepsilon, \beta)f_{11}(\varepsilon) - h_{11}(\varepsilon, \beta)]|2\rangle. \quad (41)$$

This is nondegenerate case. If however both coefficients in the above expression are zero, eigenvalue $X_d(\varepsilon, \beta)$ is degenerate and in this case each linear combination of $|1\rangle$ and $|2\rangle$ is the corresponding eigenstate.

Note that in a resonant point $\varepsilon = \varepsilon_r$ one has $X_d(\varepsilon_r, \beta) = 0$ either for $d = 1$ or for $d = 2$. If this is the case expression (41) reduces to the expression (37).

9 Examples

Let me illustrate the above method with some examples. In order to cover various aspects of open quantum systems, two different two-dimensional quantum systems in the interaction with two different surroundings will be considered.

9.1 Example E1

As a first example consider the system \mathbf{S}_2^a that is in the base $\{|s\rangle\}$ characterized by matrices

$$\mathbf{A} = \begin{pmatrix} 0.5 & -0.25 \\ -0.25 & 0.6 \end{pmatrix}, \quad \mathbf{S}^a = \begin{pmatrix} 1.1 & 0.1 \\ 0.1 & 1 \end{pmatrix}, \quad (42a)$$

In order to illustrate most general case, this system is described by a generalized eigenvalue equation (1a) where $\mathbf{S}^a \neq \mathbf{I}^a$. Eigenvalues and eigenstates of this system are

$$E_1 = 0.25474, \quad E_2 = 0.85536, \quad (42b)$$

$$|\Theta_1\rangle = \begin{pmatrix} 0.72621 \\ 0.57942 \end{pmatrix}, \quad |\Theta_2\rangle = \begin{pmatrix} 0.62454 \\ -0.82064 \end{pmatrix}, \quad (42c)$$

where $|\Theta_s\rangle$ are orthonormalized according to (1b).

In (42c) and in the following expressions I will freely mix bracket notation with a standard vector notation. Strictly, this is not allowed and one should write, for example, $|\Theta_1\rangle = 0.72621|1\rangle + 0.57942|2\rangle$, etc. Nevertheless, with a due caution one can use slightly inaccurate notation (42c).

Let the surrounding of the system \mathbf{S}_2^a contain a single eigenvalue band in the interval $D \equiv I_1 = [a_1, b_1] = [-1, 1]$ and let this surrounding contain no isolated eigenvalues λ_i . As emphasized in Sect. 4, interaction of this eigenvalue band with the system \mathbf{S}_2^a is described by the characteristic operator $\mathbf{f}_1(\varepsilon)$ which is identically zero outside the interval I_1 and which is nonnegative inside this interval. As an example of such an operator consider

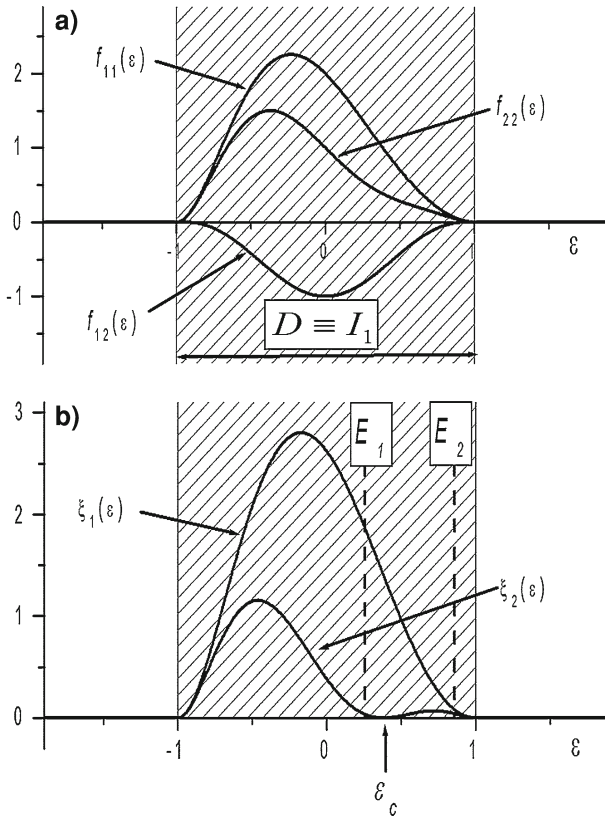


Fig. 1 Example E1. (a) Matrix elements $f_{sp}(\epsilon)$ of the characteristic matrix $\mathbf{f}(\epsilon)$. (b) Eigenvalues $\xi_s(\epsilon)$ of the characteristic matrix. Eigenvalues E_1 and E_2 of the local system \mathbf{S}_2^a are inside the range D

$$\mathbf{f}_1(\epsilon) = \begin{pmatrix} f_{11}^{(1)}(\epsilon) & f_{12}^{(1)}(\epsilon) \\ f_{21}^{(1)}(\epsilon) & f_{22}^{(1)}(\epsilon) \end{pmatrix} \equiv \begin{pmatrix} q_{11}^{(1)}(\epsilon) & q_{12}^{(1)}(\epsilon) \\ q_{21}^{(1)}(\epsilon) & q_{22}^{(1)}(\epsilon) \end{pmatrix} \cdot \begin{cases} 1 & \text{if } \epsilon \in I_1 \\ 0 & \text{otherwise} \end{cases} \quad (43a)$$

where $q_{sp}^{(1)}(\epsilon)$ are polynomials

$$\begin{aligned} q_{11}^{(1)}(\epsilon) &= (\epsilon^2 - 1)^2 (2\epsilon^2 - 2\epsilon + 1), \\ q_{22}^{(1)}(\epsilon) &= (\epsilon^2 - 1)^2 (\epsilon^2 - 2\epsilon + 2), \\ q_{12}^{(1)}(\epsilon) &\equiv q_{21}^{(1)}(\epsilon) = (\epsilon^2 - 1)^3. \end{aligned} \quad (43b)$$

Matrix elements $f_{sp}^{(1)}(\epsilon)$ are identical to polynomials $q_{sp}^{(1)}(\epsilon)$ inside the interval I_1 , and they are identically zero outside this interval. Since \mathbf{S}_∞^b contains only this single eigenvalue band, one has $\mathbf{f}(\epsilon) \equiv \mathbf{f}_1(\epsilon)$ and hence $f_{sp}(\epsilon) \equiv f_{sp}^{(1)}(\epsilon)$. In Fig. 1a are shown those matrix elements, while in Fig. 1b are shown eigenvalues $\xi_1(\epsilon)$ and $\xi_2(\epsilon)$ of the characteristic matrix $\mathbf{f}(\epsilon)$. Since polynomials $q_{sp}^{(1)}(\epsilon)$ are zero on both

end-points of the interval I_1 , those matrix elements and eigenvalues are continuous at those end-points and they vanish outside the range D . As required, eigenvalues $\xi_s(\varepsilon)$ are nonnegative (see Fig. 1b). Diagonal matrix elements $f_{ss}(\varepsilon)$ of $\mathbf{f}(\varepsilon)$ are also nonnegative (see Fig. 1a). Rank of matrix $\mathbf{f}(\varepsilon)$ equals two for each interior point $\varepsilon \in D$ (excluding end-points $a_1 = -1$ and $b_1 = 1$ of this interval), except for the critical point $\varepsilon = \varepsilon_c = 0.38197$ where $\text{rank}(\mathbf{f}(\varepsilon_c)) = 1$ and where eigenvalue $\xi_2(\varepsilon)$ of $\mathbf{f}(\varepsilon)$ vanishes: $\xi_2(\varepsilon_c) = 0$.

$$\text{rank}(\mathbf{f}(\varepsilon)) = \begin{cases} 2 & \text{if } \varepsilon \in D \text{ \& } \varepsilon \neq \varepsilon_c \\ 1 & \text{if } \varepsilon = \varepsilon_c = 0.38197 \\ 0 & \text{if } \varepsilon \in \overline{D} \end{cases} \quad (44)$$

Since for almost each $\varepsilon \in D$ one has $\text{rank}(\mathbf{f}(\varepsilon)) > 1$, this characteristic matrix corresponds to multiparameter eigenvalue band. The case of the interaction of a system \mathbf{S}_ρ^a with a system \mathbf{S}_∞^b that contains a single one-parameter eigenvalue band is considered elsewhere [8].

In Fig. 1b are also shown eigenvalues E_1 and E_1 of the (closed) local system \mathbf{S}_2^a . Both eigenvalues are contained inside the eigenvalue band I_1 of the system \mathbf{S}_∞^b .

Once characteristic matrix $\mathbf{f}_1(\varepsilon)$ is known, corresponding derived matrix $\omega_1(\varepsilon)$ is given by expressions (10). In particular, since matrix elements of $\mathbf{f}_1(\varepsilon)$ are polynomials inside the interval $D \equiv I_1$, one can use expressions (11) to obtain:

$$\begin{aligned} \omega_{11}^{(1)}(\varepsilon) &= q_{11}^{(1)}(\varepsilon) \ln \left| \frac{\varepsilon+1}{\varepsilon-1} \right| - g_{11}^{(1)}(\varepsilon), \\ \omega_{22}^{(1)}(\varepsilon) &= q_{22}^{(1)}(\varepsilon) \ln \left| \frac{\varepsilon+1}{\varepsilon-1} \right| - g_{22}^{(1)}(\varepsilon), \\ \omega_{12}^{(1)}(\varepsilon) &\equiv \omega_{21}^{(1)}(\varepsilon) = q_{12}^{(1)}(\varepsilon) \ln \left| \frac{\varepsilon+1}{\varepsilon-1} \right| - g_{12}^{(1)}(\varepsilon), \end{aligned} \quad (45a)$$

where $q_{sp}^{(1)}(\varepsilon)$ are polynomials (43b), while $g_{sp}^{(1)}(\varepsilon)$ are polynomials:

$$\begin{aligned} g_{11}^{(1)}(\varepsilon) &= 4\varepsilon^5 - 4\varepsilon^4 - \frac{14}{3}\varepsilon^3 + \frac{20}{3}\varepsilon^2 - \frac{6}{5}\varepsilon - \frac{32}{15}, \\ g_{22}^{(1)}(\varepsilon) &= 2\varepsilon^5 - 4\varepsilon^4 + \frac{2}{3}\varepsilon^3 + \frac{20}{3}\varepsilon^2 - \frac{28}{5}\varepsilon - \frac{32}{15}, \\ g_{12}^{(1)}(\varepsilon) &\equiv g_{21}^{(1)}(\varepsilon) = 2\varepsilon^5 - \frac{16}{3}\varepsilon^3 + \frac{22}{5}\varepsilon. \end{aligned} \quad (45b)$$

Since $\mathbf{f}(\varepsilon) \equiv \mathbf{f}_1(\varepsilon)$ one has $\omega(\varepsilon) \equiv \omega_1(\varepsilon)$. In Fig. 2a are shown matrix elements $\omega_{sp}(\varepsilon)$, while in Fig. 2b are shown eigenvalues $\mu_1(\varepsilon)$ and $\mu_2(\varepsilon)$ of the derived matrix $\omega(\varepsilon)$. All those quantities are finite and continuous functions of ε for each real ε , including end-points $a_1 = -1$ and $b_1 = 1$ of the interval I_1 . This follows from the property $\lim_{x \rightarrow 0} (x \ln(x)) = 0$ and from the fact that matrix elements of the operator $\mathbf{f}_1(\varepsilon)$ are polynomials that vanish at those end-points [7]. Note further that in accord with the requirement (14b), both eigenvalues are decreasing functions of ε for each $\varepsilon \notin D = [-1, 1]$. However, if $\varepsilon \in D$ those eigenvalues may be decreasing as well as

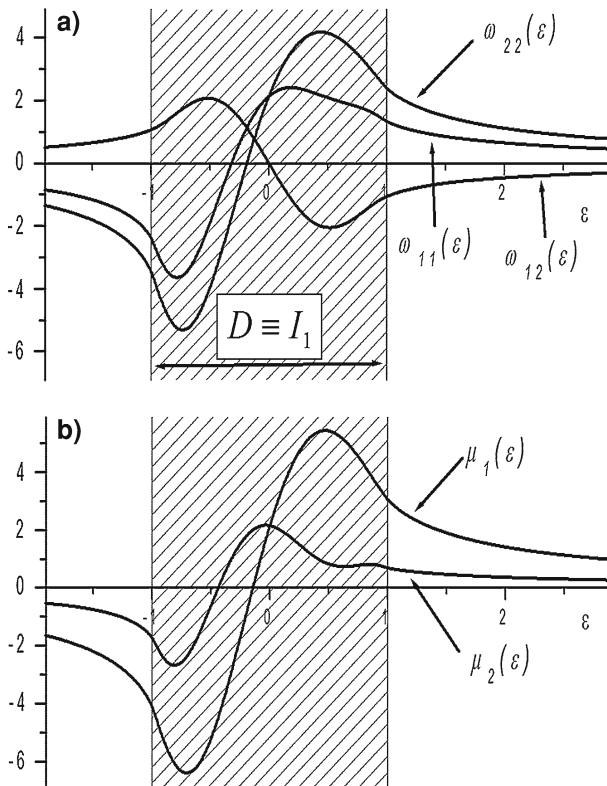


Fig. 2 Example E1. (a) Matrix elements $\omega_{sp}(\varepsilon)$ of the derived matrix $\omega(\varepsilon)$. (b) Eigenvalues $\mu_s(\varepsilon)$ of the derived matrix $\omega(\varepsilon)$

increasing functions of ε (see Fig. 2b). The same applies to diagonal matrix elements $\omega_{ss}(\varepsilon)$ of the derived matrix $\omega(\varepsilon)$ (see Fig. 2a).

Generic eigenvalue equation (15a) produces all cardinal isolated solutions of the combined system and all resonant points. In the case of a two dimensional system \mathbf{S}_2^a , this equation reduces to the Eqs. 36 and 37. Equation 36 produces eigenvalues of the generic eigenvalue equation while Eq. 36 produces all the corresponding eigenstates.

Solutions of the Eq. 36 of a type $\varepsilon = \varepsilon(\beta)$ are shown in Fig. 3. There are six such solutions: $\varepsilon_{R1}(\beta)$, $\varepsilon_{R2}(\beta)$, $\varepsilon_1(\beta)$, $\varepsilon_2(\beta)$, $\varepsilon_{L1}(\beta)$ and $\varepsilon_{L2}(\beta)$. Those solutions are eigenvalues of a generic eigenvalue equation considered as functions of the coupling parameter β . Eigenvalues inside the range D are resonant points, while eigenvalues outside this range are isolated eigenvalues of the combined system.

If there is no interaction ($\beta = 0$) eigenvalues of the generic equation reduce to local eigenvalues. In particular, one has $\varepsilon_{R1}(0) = E_1$ and $\varepsilon_{R2}(0) = E_2$. Both eigenvalues are contained in the range D . As the coupling β increases, those two eigenvalues change as continuous functions $\varepsilon_{R1}(\beta)$ and $\varepsilon_{R2}(\beta)$. For small β one has $\varepsilon_{R1}(\beta), \varepsilon_{R2}(\beta) \in D$ and those eigenvalues are resonant points. However, if the coupling is as strong as $\beta > \beta_{R2}$ one has $\varepsilon_{R2}(\beta) \notin D$ and this eigenvalue becomes right

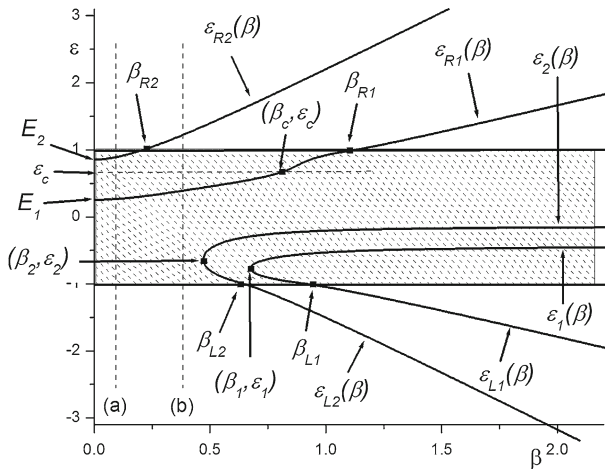


Fig. 3 Eigenvalues $\varepsilon_r(\beta)$ of the generic equation considered as functions of the coupling β . Eigenvalue distributions of local states $|\Theta_s\rangle$ for the coupling β corresponding to lines (a) and (b) are shown in Figs. 5 and 6, respectively. For details see text

isolated eigenvalue of the combined system. Also, if $\beta > \beta_{R1}$ one finds $\varepsilon_{R1}(\beta) \notin D$ and this eigenvalue becomes another right isolated eigenvalue of the combined system. As $\beta > \beta_{R1}$ further increases, isolated eigenvalues $\varepsilon_{R1}(\beta)$ and $\varepsilon_{R2}(\beta)$ continue to increase. This is in accord with expressions (14) and (17) that imply $\partial\varepsilon_R/\partial\beta > 0$ for each right isolated eigenvalue $\varepsilon_R \in \bar{I}_{right}$ where \bar{I}_{right} is extreme right subinterval of \bar{D} (see Sect. 5). In the above example $\bar{I}_{right} = (b_1, \infty)$. Hence for each $\beta > \beta_{R1}$ combined system has two right isolated eigenvalues. This is maximum number of extreme right isolated eigenvalues that combined system with $\rho = 2$ may have.

In the points β_{R1} and β_{R2} one has $\varepsilon = b_1 = 1$. Inserting this value into (36a) and using expressions (45) (which imply $\omega_{11}(1) = 4/3, \omega_{22}(1) = 12/5$ and $\omega_{12}(1) = -16/15$) one finds

$$2.06222 \cdot \beta^4 - 2.72 \cdot \beta^2 + 0.1175 = 0 \tag{46a}$$

This is quadratic equation in the unknown $x = \beta^2$. Since $\beta \geq 0$ there are two solutions, $\beta_{R2} = 0.21146$ and $\beta_{R1} = 1.12883$.

Consider now remaining four eigenvalues $\varepsilon_{L1}(\beta), \varepsilon_{L2}(\beta), \varepsilon_1(\beta)$ and $\varepsilon_2(\beta)$. Note that $\varepsilon_{L1}(\beta)$ and $\varepsilon_1(\beta)$ are two branches of one and the same analytic function $\beta = \beta_1(\varepsilon)$, while $\varepsilon_{L2}(\beta)$ and $\varepsilon_2(\beta)$ are two branches of another analytic function $\beta = \beta_2(\varepsilon)$. It is more convenient to analyze those functions in a form $\beta = \beta_1(\varepsilon)$ and $\beta = \beta_2(\varepsilon)$ using expressions (38). Condition $d\beta_1(\varepsilon)/d\varepsilon = 0$ determines the point $(\beta_1, \varepsilon_1) = (0.67519, -0.76673)$ while condition $d\beta_2(\varepsilon)/d\varepsilon = 0$ determines the point $(\beta_2, \varepsilon_2) = (0.47058, -0.63563)$. Eigenvalues $\varepsilon_{L1}(\beta)$ and $\varepsilon_1(\beta)$ exist only if $\beta \geq \beta_1$ while eigenvalues $\varepsilon_{L2}(\beta)$ and $\varepsilon_2(\varepsilon)$ exist only if $\beta \geq \beta_2$. For each β (where defined) eigenvalues $\varepsilon_1(\beta)$ and $\varepsilon_2(\beta)$ are inside the range D and hence these eigenvalues are resonant points. Concerning eigenvalues $\varepsilon_{L1}(\beta)$ and $\varepsilon_{L2}(\beta)$, as β increases one has at first $\varepsilon_{L1}(\beta), \varepsilon_{L2}(\beta) \in D$ and those eigenvalues are resonant points. However, if the

coupling is as strong as $\beta > \beta_{L2}$ one has $\varepsilon_{L2}(\beta) \notin D$ and this eigenvalue becomes left isolated eigenvalue of the combined system. Also, if $\beta > \beta_{L1}$ one finds $\varepsilon_{L1}(\beta) \notin D$ and this eigenvalue becomes another left isolated eigenvalue of the combined system. As $\beta > \beta_{L1}$ further increases, isolated eigenvalues $\varepsilon_{L1}(\beta)$ and $\varepsilon_{L2}(\beta)$ continue to decrease. This is in accord with expressions (14) and (17) that imply $\partial\varepsilon_L/\partial\beta < 0$ for each left isolated eigenvalue $\varepsilon_L \in \bar{I}_{left}$ where \bar{I}_{left} is extreme left subinterval of \bar{D} . In the above example $\bar{I}_{left} = (-\infty, a_1)$. Hence for each $\beta > \beta_{L1}$ combined system has two left isolated eigenvalues. This is maximum number of extreme left isolated eigenvalues that combined system with $\rho = 2$ may have.

In the points β_{L1} and β_{L2} one has $\varepsilon = a_1 = -1$. In analogy to (46a) one finds

$$7.18222 \cdot \beta^4 - 9.06667 \cdot \beta^2 + 2.5375 = 0. \tag{46b}$$

which implies $\beta_{L2} = 0.64717$ and $\beta_{L1} = 0.91845$.

Figure 3 provides detailed interaction landscape of the open system \mathbf{S}_2^a that interacts with its surrounding (system \mathbf{S}_∞^b). Note that left isolated eigenvalues $\varepsilon_{L1}(\beta)$ and $\varepsilon_{L2}(\beta)$ cannot be derived by any standard perturbation expansion method. Those eigenvalues do not exist in the point $\beta = 0$ and hence no perturbation expansion in this point can reproduce those eigenvalues.

Once eigenvalues $\varepsilon_{R1}(\beta)$, $\varepsilon_{R2}(\beta)$, $\varepsilon_{L1}(\beta)$ and $\varepsilon_{L2}(\beta)$ are obtained as a solution of (36a), one can derive corresponding isolated eigenstates according to (37) and (15b,c). Those eigenstates determine all related properties of the combined system. In particular, probabilities $w_{r,s}$ and $w_r = w_{r,1} + w_{r,2}$ are given by expressions (18). Those probabilities are shown in Fig. 4. In Fig. 4a are shown probabilities $w_{R1,s} \equiv |\langle \Theta_s | \mathbf{S}^a | \Psi_{R1} \rangle|^2$ to find right isolated eigenstate $|\Psi_{R1}\rangle$ in a local state $|\Theta_s\rangle$, as well as global probability $w_{R1} = w_{R1,1} + w_{R1,2}$ to find this eigenstate in a local system \mathbf{S}_2^a . Since right isolated eigenvalue $\varepsilon_{R1}(\beta)$ exists only if $\beta > \beta_{R1} = 1.12883$, those probabilities are zero if $\beta < \beta_{R1}$. As β continuously increases from $\beta = 0$, in a point $\beta = \beta_{R1}$ those probabilities discontinuously jump to $w_{R1}(\beta_{R1}+) = 0.44324$, $w_{R1,1}(\beta_{R1}+) = 0.43952$ and $w_{R1,2}(\beta_{R1}+) = 0.00372$, respectively (see Fig. 4a). Similarly, right isolated eigenvalue $\varepsilon_{R2}(\beta)$ exists only if $\beta > \beta_{R2} = 0.21146$. As β continuously increases, in this point corresponding probabilities discontinuously jump from zero to $w_{R2}(\beta_{R2}+) = 0.81727$, $w_{R2,1}(\beta_{R2}+) = 0.00026$ and $w_{R2,2}(\beta_{R2}+) = 0.81701$, respectively (see Fig. 4b). In Fig. 4c and d are shown corresponding probabilities for left isolated eigenstates $|\Psi_{L1}\rangle$ and $|\Psi_{L2}\rangle$, respectively. Probabilities w_{L1} and $w_{L1,s}$, considered as functions of coupling parameter β , are zero if $\beta \leq \beta_{L1} = 0.91845$ and in this point those probabilities discontinuously jump to values $w_{L1}(\beta_{L1}+) = 0.17524$, $w_{L1,1}(\beta_{L1}+) = 0.17171$ and $w_{L1,2}(\beta_{L1}+) = 0.00353$, respectively (see Fig. 4c). Similarly, probabilities w_{L2} and $w_{L2,s}$, considered as functions of coupling parameter β , are zero if $\beta \leq \beta_{L2} = 0.64717$ and in this point those probabilities discontinuously jumps to the values $w_{L2}(\beta_{L2}+) = 0.18305$, $w_{L2,1}(\beta_{L2}+) = 0.00787$ and $w_{L2,2}(\beta_{L2}+) = 0.17518$, respectively (see Fig. 4d).

It remains to determine whether the combined system contains any anomalous point where this system could also have an isolated eigenstate. Each anomalous point $\varepsilon = \varepsilon_c$ is an interior point of a range D and in this point one must have a nontrivial state $|\theta_c\rangle$

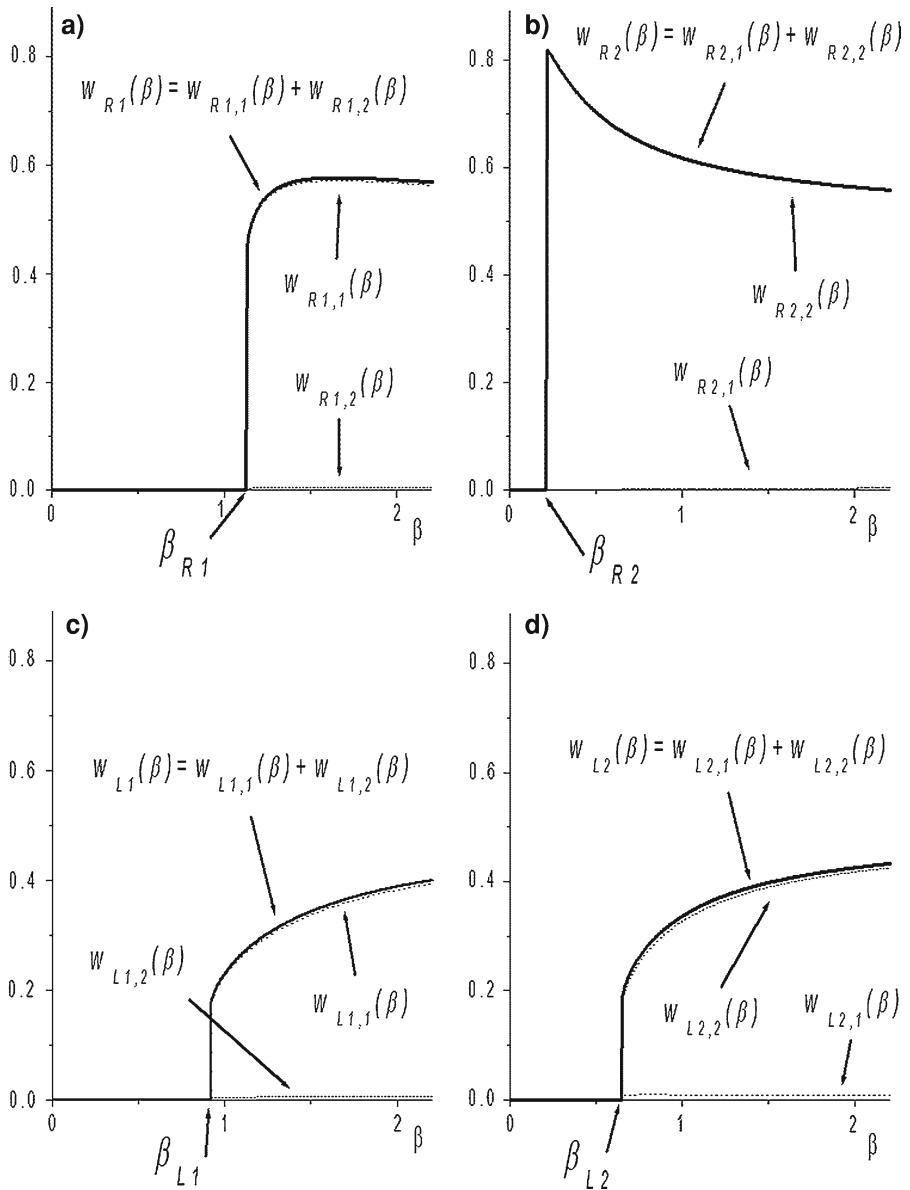


Fig. 4 Probabilities $w_{r,s}(\beta) \equiv |\langle \Theta_s | \mathbf{S} | \Psi_r(\beta) \rangle|^2$ to find isolated eigenstate $|\Psi_r(\beta)\rangle$ in a local state $|\Theta_s\rangle$ and probabilities $w_r = w_{r,1} + w_{r,2}$ to find this eigenstate in the system \mathbf{S}_2^r . **(a)** Probabilities corresponding to the eigenstate $|\Psi_{R1}\rangle$. **(b)** Probabilities corresponding to the eigenstate $|\Psi_{R2}\rangle$. **(c)** Probabilities corresponding to the eigenstate $|\Psi_{L1}\rangle$. **(d)** Probabilities corresponding to the eigenstate $|\Psi_{L2}\rangle$

that satisfies $\mathbf{f}(\varepsilon_c) |\theta_c\rangle = 0$ as well as $\mathbf{h}(\varepsilon_c) |\theta_c\rangle = 0$. First condition implies that in this point rank of a characteristic matrix $\mathbf{f}(\varepsilon)$ must be smaller than the dimension ρ of the space X_ρ^a . According to (44), only a point $\varepsilon = \varepsilon_c = 0.38197$ has such a property. Second condition implies that an anomalous point must be a resonant point that satisfies (36a). The solution $\beta = \beta(\varepsilon)$ of (36a) is given by (38a). Inserting $\varepsilon = \varepsilon_c$ into this

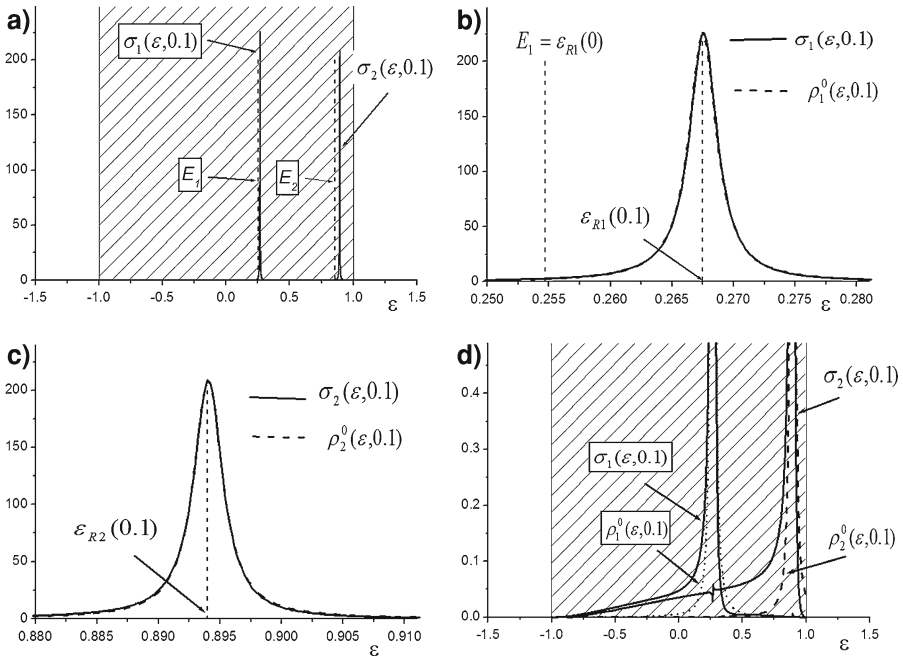


Fig. 5 Eigenvalue distributions of local states $|\Theta_1\rangle$ and $|\Theta_2\rangle$ in the case $\beta = 0.1$. Those distributions correspond to the line (a) in Fig. 3. **(a)** Probability densities $\sigma_1(\varepsilon, 0.1)$ and $\sigma_2(\varepsilon, 0.1)$ are sharply localized inside the range D at positions $\varepsilon_{R1}(0.1)$ and $\varepsilon_{R2}(0.1)$, respectively. **(b)** Probability density $\sigma_1(\varepsilon, 0.1)$ and universal resonance curve $\rho_1^0(\varepsilon, 0.1)$ highly magnified. **(c)** Probability density $\sigma_2(\varepsilon, 0.1)$ and universal resonance curve $\rho_2^0(\varepsilon, 0.1)$ highly magnified. **(d)** Vertical scale in Fig. 5a highly magnified. Densities $\sigma_s(\varepsilon, 0.1)$ deviate from the ideal shape of the corresponding universal resonance curves $\rho_s^0(\varepsilon, 0.1)$

expression one finds only one real solution $\beta_c = 0.32611$. Geometrically, the point (β_c, ε_c) is on the intersection of the line $\varepsilon = \varepsilon_c$ and of the function $\varepsilon = \varepsilon_{R1}(\beta)$ (see Fig. 3). This is the only candidate for the anomalous point. Using (37) one finds that the state $|\theta_c\rangle$ which satisfies $\mathbf{h}(\varepsilon_c) |\theta_c\rangle = 0$ does not satisfy $\mathbf{f}(\varepsilon_c) |\theta_c\rangle$. The point $\varepsilon = \varepsilon_c$ is hence not an anomalous point. In conclusion, the system \mathbf{S}_∞ contains no anomalous point and hence no isolated eigenstate with the eigenvalue $\varepsilon_c \in D$.

Consider now cardinal embedded solutions of the combined system. Fractional shift equation (22a) produces all such solutions. In a 2×2 case this equation reduces to Eqs. 39 and 41. In particular, eigenvalues $X_d(\varepsilon, \beta)$ of a fractional shift eigenvalue equation are solutions to the Eq. 39. Those solutions are given in the explicit form (40). This determines eigenvalues $X_d(\varepsilon, \beta)$ of a fractional shift equation for each $\varepsilon \in D$. Once this eigenvalue is known, the corresponding X_ρ^a -component $|\Psi_d^a(\varepsilon, \beta)\rangle$ of the embedded eigenstate $|\Psi_d(\varepsilon, \beta)\rangle$ is given by expressions (41) and (24). This component determines all related properties of the open system \mathbf{S}_ρ^a . As an example, in Fig. 5 are shown eigenvalue distributions of local states $|\Theta_1\rangle$ and $|\Theta_2\rangle$ in the case $\beta = 0.1$. Those distributions corresponds to the line (a) in Fig. 3. For this value of β combined system has no isolated eigenstate and those distributions are completely determined by densities $\sigma_s(\varepsilon, 0.1) = \rho_{1,s}(\varepsilon, 0.1) + \rho_{2,s}(\varepsilon, 0.1)$ where $\rho_{d,s}(\varepsilon, 0.1) = |\langle \Theta_s | \mathbf{S} | \Psi_d(\varepsilon, 0.1) \rangle|^2$. As shown in Sect. 6.2.2, $\sigma_s(\varepsilon, \beta)$ is a probability density to find local state $|\Theta_s\rangle$

with the eigenvalue $\varepsilon \in D$. Due to the relatively weak interaction of the system \mathbf{S}_2^a with its surrounding, initial unperturbed eigenvalues $E_s \in D$ of \mathbf{S}_2^a are only slightly shifted to the new positions $\varepsilon_s(0.1)$ (see Fig. 5a). Since $\varepsilon_s(0.1) \in D$, those shifted eigenvalues are not sharp and they acquire the shape of the universal resonance curves $\rho_s^0(\varepsilon, 0.1)$ as given by expression (32b). The widths of those two resonant curves calculated according to (33a) are $\Delta\varepsilon_1(0.1) = 0.00137$ and $\Delta\varepsilon_2(0.1) = 0.00143$, respectively. Those widths are quite small and densities $\sigma_s(\varepsilon, 0.1)$ are hence well approximated with the corresponding universal resonance curves $\rho_s^0(\varepsilon, 0.1)$. In particular, density $\sigma_1(\varepsilon, 0.1)$ has a prominent resonant shape centered at the point $\varepsilon = \varepsilon_{R1}(0.1) = 0.26749$, while density $\sigma_2(\varepsilon, 0.1)$ has a prominent resonant shape centered at the point $\varepsilon = \varepsilon_{R2}(0.1) = 0.89403$. In Fig. 5b is shown density $\sigma_1(\varepsilon, 0.1)$ magnified. Approximate density $\sigma_1^0(\varepsilon, 0.1)$ is also shown. On this scale there is virtually no difference between exact density $\sigma_1(\varepsilon, 0.1)$ and approximate density $\sigma_1^0(\varepsilon, 0.1)$. In Fig. 5c are in the same way compared densities $\sigma_2(\varepsilon, 0.1)$ and $\sigma_2^0(\varepsilon, 0.1)$. Further, one finds $S_1(0.1) = \int \sigma_1(\varepsilon, 0.1)d\varepsilon = 1$ and $S_2(0.1) = \int \sigma_2(\varepsilon, 0.1)d\varepsilon = 1$. Concerning component probabilities $C_{d,s}(0.1) = \int \rho_{d,s}(\varepsilon, 0.1)d\varepsilon$, one has $C_{1,1}(0.1) = 0.94312$ and $C_{1,2}(0.1) = 0.05688$. Density $\sigma_1(\varepsilon, 0.1)$ is hence essentially density of the state $|\Theta_1\rangle$ which interacts with its surrounding. Similarly one finds $C_{2,2}(0.1) = 0.97613$ and $C_{2,1}(0.1) = 0.02387$. Density $\sigma_2(\varepsilon, 0.1)$ is hence essentially density of the state $|\Theta_2\rangle$ which interacts with its surrounding.

Densities $\sigma_1(\varepsilon, 0.1)$ and $\sigma_2(\varepsilon, 0.1)$ have only approximately the shape of the universal resonance curve. This is shown in Fig. 5d which is the same as Fig. 5a, but with vertical scale highly magnified. On this scale one can see that those densities deviate from the universal resonance curve. However, since $\beta = 0.1$ is small the difference between exact densities $\sigma_s(\varepsilon, 0.1)$ and approximate densities $\sigma_s^0(\varepsilon, 0.1)$ is in absolute scale negligible.

As another example, in Fig. 6 are shown spectral distributions of local states $|\Theta_s\rangle$ for the value $\beta = 0.4$. This value corresponds to the line (b) in Fig. 3. This is relatively strong coupling and probability densities $\sigma_s(\varepsilon, 0.4)$ do not resemble universal resonance curves situated at corresponding resonance points. For this value of β standard perturbation expansion fails. Solving fractional shift eigenvalue equation and using expressions (26–27) one finds $S_1(0.4) = \int \sigma_1(\varepsilon, 0.4)d\varepsilon = 0.99897$ and $S_2(0.4) = \int \sigma_2(\varepsilon, 0.4)d\varepsilon = 0.26610$. Unlike in the case $\beta = 0.1$, those probabilities are less than one. In the case $\beta = 0.4$ in addition to embedded eigenstates combined system contains an isolated eigenstate $|\Psi_{R2}\rangle$ with the eigenvalue $\varepsilon_{R2}(0.4) = 1.24735$ (see Fig. 3). Missing probabilities are due to this eigenstate. Using expressions (18) one finds $w_{R2,1}(0.4) = 0.00103$ and $w_{R2,2}(0.4) = 0.73390$. As required by the completeness relation (34a), those probabilities satisfy $S_1(0.4) + w_{R2,1}(0.4) = 1$ and $S_2(0.4) + w_{R2,2}(0.4) = 1$.

In two previous examples probabilities $S_1(\beta)$ and $S_2(\beta)$ for two values of the coupling parameter β ($\beta = 0.1$ and $\beta = 0.4$) were given. In Fig. 7 are shown those probabilities as functions of β for the interval $\beta \in [0, 2.2]$. In particular, in Fig. 7a is shown probability $S_1(\beta) = C_{1,1}(\beta) + C_{2,1}(\beta)$ to find local state $|\Theta_1\rangle$ in any of the embedded eigenstates of the combined system. Component probabilities $C_{d,1}(\beta) = \int |\langle \Theta_1 | \mathbf{S} | \Psi_d(\varepsilon, \beta) \rangle|^2 d\varepsilon$ are also shown. In Fig. 7b is shown probability $S_2(\beta) = C_{1,2}(\beta) + C_{2,2}(\beta)$ to find local state $|\Theta_2\rangle$ in any of the embedded eigenstates of

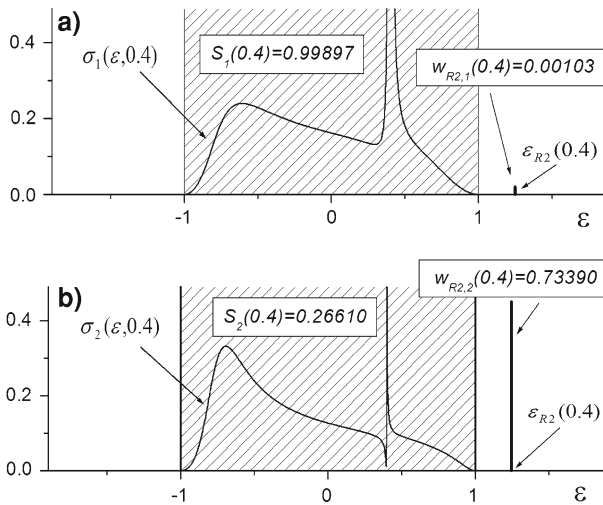


Fig. 6 Eigenvalue distributions of local states $|\Theta_1\rangle$ and $|\Theta_2\rangle$ in the case $\beta = 0.4$. Those distributions correspond to the line (b) in Fig. 3. In addition to embedded eigenstates, combined system contains an isolated eigenstate $|\Psi_{R2}(0.4)\rangle$ with eigenvalue $\varepsilon_{R2}(0.4)$. (a) Eigenvalue distribution of local state $|\Theta_1\rangle$. (b) Eigenvalue distribution of local state $|\Theta_2\rangle$

the combined system as well as corresponding component probabilities $C_{1,2}(\beta)$ and $C_{2,2}(\beta)$. If $\beta < \beta_{R2}$ combined system has no isolated eigenstates. Hence $S_1(\beta) = S_2(\beta) = 1$. In addition, if β is small each probability $S_s(\beta)$ is dominated by one of its component probabilities $C_{d,s}(\beta)$. This is the case with the point $\beta = 0.1$ analyzed in more details in Fig. 5. As β continuously increases, in the point $\beta = \beta_{R2}$ combined system obtains right isolated eigenstate $|\Psi_{R2}\rangle$. At this point probability $S_2(\beta)$ drops from the constant value $S_2(\beta) = 1$ to $S_2(\beta_{R2}+) = 0.18299$. This is compensated for by the probability $w_{R2,2}(\beta_{R2}+) = 0.81701$ to find right isolated eigenstate $|\Psi_{R2}\rangle$ in the local state $|\Theta_2\rangle$ (see Figs. 4b and 7b). However, since probability $w_{R2,1}(\beta_{R2}+) = 0.00026$ is very small, there is no noticeable drop in the probability $S_1(\beta_{R2}+)$ at this point (see Fig. 7a). If $\beta > \beta_{R2}$ standard perturbation expansion fails. This is the case with the point $\beta = 0.4$ analyzed in more details in Fig. 6. In general, probabilities $S_1(\beta)$ and $S_2(\beta)$ discontinuously change at points $\beta = \beta_{R2}$, $\beta = \beta_{L2}$, $\beta = \beta_{L1}$ and $\beta = \beta_{R1}$ where the combined system, considered as a function of β , acquires isolated eigenstates.

Completeness relations for the couplings $\beta = 0.1$ and $\beta = 0.4$ were verified in Figs. 5 and 6, respectively. Those relations are verified in a systematic way in Fig. 8. In Fig. 8a probabilities $S_1(\beta)$ to find local state $|\Theta_1\rangle$ in any of the embedded eigenstates of the combined system as well as probabilities $w_{R1,1}(\beta)$, $w_{R2,1}(\beta)$, $w_{L1,1}(\beta)$ and $w_{L2,1}(\beta)$ to find this state in various isolated eigenstates of the combined system are plotted as functions of a coupling parameter β . A sum of all those probabilities is also shown. As required by the completeness relation (34a), this sum equals one for each value of β . In Fig. 7b are in the same way plotted probabilities $S_2(\beta)$, $w_{R1,2}(\beta)$, $w_{R2,2}(\beta)$, $w_{L1,2}(\beta)$ and $w_{L2,2}(\beta)$ that correspond to the local state $|\Theta_2\rangle$. The sum of those probabilities also equals one for each value of β . Complete agreement of those

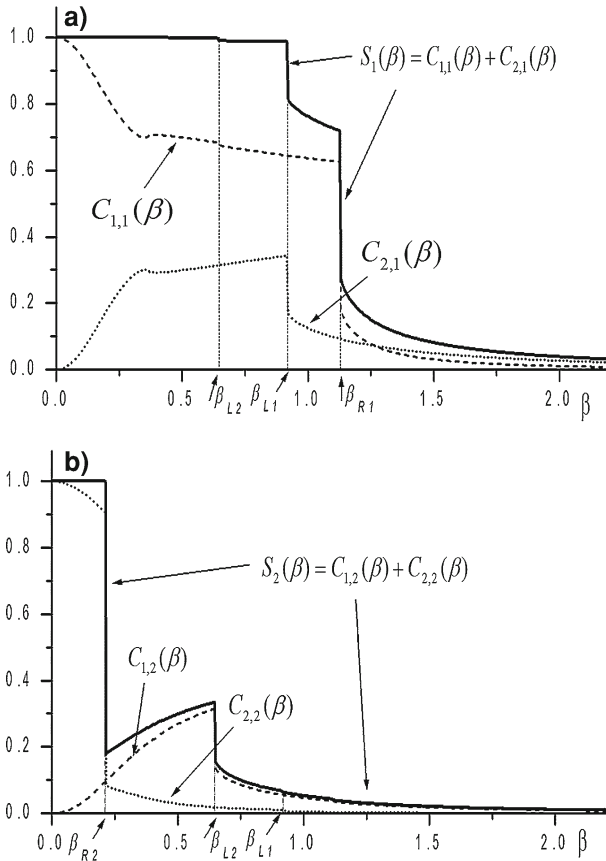


Fig. 7 Probabilities $S_s(\beta) = C_{1,s}(\beta) + C_{2,s}(\beta)$ to find local state $|\Theta_s\rangle$ in any of the embedded eigenstates of the combined system and corresponding component probabilities $C_{d,s}(\beta) = \int | \langle \Theta_s | \mathbf{S} | \Psi_d(\varepsilon, \beta) \rangle |^2 d\varepsilon$. **(a)** Probability $S_1(\beta)$ and component probabilities $C_{1,1}(\beta)$ and $C_{2,1}(\beta)$. **(b)** Probability $S_2(\beta)$ and component probabilities $C_{1,2}(\beta)$ and $C_{2,2}(\beta)$

probabilities with the requirements of the completeness relations provides a strong verification of the suggested method. However, this method can be also verified in an explicit direct way [5, 6].

9.2 Example E2

As another example consider the system \mathbf{S}_2^a characterized by matrices

$$\mathbf{A} = \begin{pmatrix} 0.5 & -0.25 \\ -0.25 & 1.6 \end{pmatrix}, \quad \mathbf{S}^a = \begin{pmatrix} 1.1 & 0.1 \\ 0.1 & 1 \end{pmatrix}, \quad (47a)$$

Those matrices are identical to matrices (42a) of the example E1, except for a single matrix element of the matrix \mathbf{A} . Eigenvalues and corresponding eigenstates of the system \mathbf{S}_2^a are now

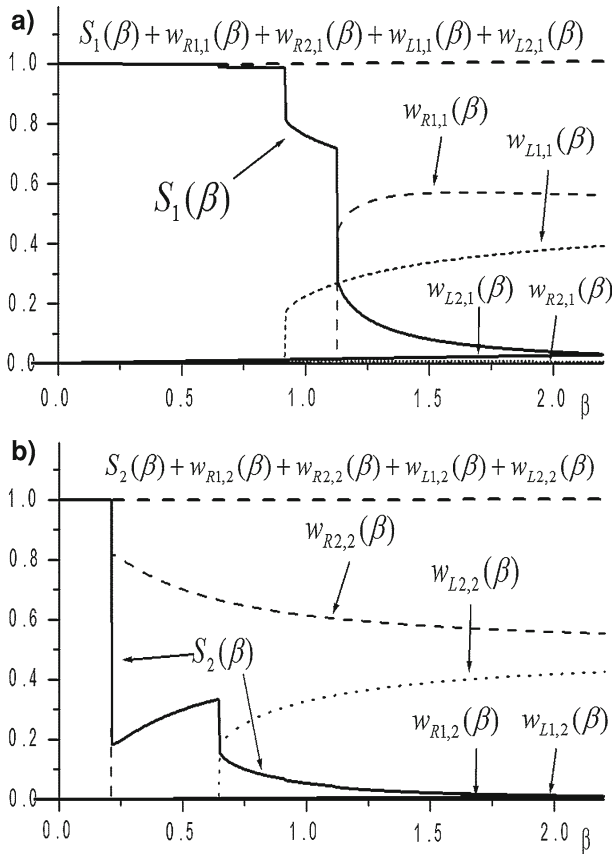


Fig. 8 (a) Verification of the completeness relation for the eigenvalue distribution of a local state $|\Theta_1\rangle$. (b) Verification of the completeness relation for the eigenvalue distribution of a local state $|\Theta_2\rangle$

$$E_1 = 0.39164, \quad E_2 = 1.72763, \tag{47b}$$

$$|\Theta_1\rangle = \begin{pmatrix} 0.91093 \\ 0.21799 \end{pmatrix}, \quad |\Theta_2\rangle = \begin{pmatrix} 0.29604 \\ -0.98064 \end{pmatrix}, \tag{47c}$$

where $|\Theta_s\rangle$ are orthonormalized according to (1b).

Let the infinite system \mathbf{S}_∞^b that interacts with the above system \mathbf{S}_2^a contain two eigenvalue bands in the intervals $I_1 \equiv [a_1, b_1] = [-1, 1]$ and $I_2 \equiv [a_2, b_2] = [2, 3]$, respectively. Let further this system contain an isolated eigenstate $|\Phi_0\rangle$ with the eigenvalue $\lambda_0 = 1.2$. Assume that the characteristic operator $\mathbf{f}_1(\varepsilon)$ which describes the interaction of the first eigenvalue band with the system \mathbf{S}_2^a is given by matrix elements (43), while the characteristic operator $\mathbf{f}_2(\varepsilon)$ which describes the interaction of

the second eigenvalue band with the system \mathbf{S}_2^a is given by matrix elements

$$\mathbf{f}_2(\varepsilon) = \begin{pmatrix} f_{11}^{(2)}(\varepsilon) & f_{12}^{(2)}(\varepsilon) \\ f_{21}^{(2)}(\varepsilon) & f_{22}^{(2)}(\varepsilon) \end{pmatrix} \equiv \begin{pmatrix} q_{11}^{(2)}(\varepsilon) & q_{12}^{(2)}(\varepsilon) \\ q_{21}^{(2)}(\varepsilon) & q_{22}^{(2)}(\varepsilon) \end{pmatrix} \cdot \begin{cases} 1 & \text{if } \varepsilon \in I_2 \\ 0 & \text{otherwise} \end{cases} \quad (48a)$$

where $q_{sp}^{(2)}(\varepsilon)$ are polynomials

$$\begin{aligned} q_{11}^{(2)}(\varepsilon) &= (\varepsilon - 2)^2 (2\varepsilon^2 - 14\varepsilon + 25), \\ q_{22}^{(2)}(\varepsilon) &= (\varepsilon - 2)^2 (\varepsilon^2 - 8\varepsilon + 17), \\ q_{12}^{(2)}(\varepsilon) &\equiv q_{21}^{(2)}(\varepsilon) = (\varepsilon - 2)^3 (\varepsilon - 4). \end{aligned} \quad (48b)$$

Let further the characteristic matrix $\mathbf{F}(x)$ which describes the interaction of the eigenstate $|\Phi_0\rangle$ with the system \mathbf{S}_2^a be given by

$$\mathbf{F}(\varepsilon) = \begin{pmatrix} 0.5 & -0.3 \\ -0.3 & 0.2 \end{pmatrix} \cdot \delta(\varepsilon - \lambda_0). \quad (49)$$

In Fig. 9a are shown matrix elements $f_{sp}(\varepsilon)$ of the global characteristic matrix $\mathbf{f}(\varepsilon) = \mathbf{f}_1(\varepsilon) + \mathbf{f}_2(\varepsilon) + \mathbf{F}(\varepsilon)$. Local eigenvalues E_1 and E_2 are also shown. Interaction of the system \mathbf{S}_2^a with the system \mathbf{S}_∞^b described by this characteristic matrix is much more complex than in the previous example. There are several new features. First, the system \mathbf{S}_∞^b has two (nonoverlapping) eigenvalue bands in the intervals I_1 and I_2 , respectively. In particular, one has $\mathbf{f}(\varepsilon) \equiv \mathbf{f}_1(\varepsilon)$ if $\varepsilon \in I_1$ and $\mathbf{f}(\varepsilon) \equiv \mathbf{f}_2(\varepsilon)$ if $\varepsilon \in I_2$. Second, characteristic matrix $\mathbf{f}(\varepsilon)$ is not continuous in the point $\varepsilon = b_2 = 3$ on the right edge of the interval I_2 . Third, local eigenvalue $E_2 \notin D$ is outside the range $D = I_1 \cup I_2$, while in the previous example both eigenvalues of the isolated system \mathbf{S}_ρ^a were contained inside the range D . Finally, the system \mathbf{S}_∞^b has an isolated eigenvalue at the point $\varepsilon = \lambda_0 = 1.2 \notin D$ and in this point characteristic matrix $\mathbf{f}(\varepsilon)$ diverges.

Eigenvalues $\xi_1(\varepsilon)$ and $\xi_2(\varepsilon)$ of $\mathbf{f}(\varepsilon)$ are shown in Fig. 9b. As required, those eigenvalues are nonnegative and they vanish outside the range D and outside the point $\varepsilon = \lambda_0$. Rank of matrix $\mathbf{f}(\varepsilon)$ equals two for each interior point $\varepsilon \in D$, except for the critical point $\varepsilon_c = 0.38197 \in D$ where $\text{rank}(\mathbf{f}(\varepsilon_c)) = 1$. This is the same critical point as in the example E1. In addition, this rank equals two in the point $\varepsilon = \lambda_0$.

Consider next global derived matrix $\omega(\varepsilon) = \omega_1(\varepsilon) + \omega_2(\varepsilon) + \Omega(\varepsilon)$. Matrix elements of the derived matrix $\omega_1(\varepsilon)$ associated with the eigenvalue band $\nu = 1$ are given by expressions (45). Since matrix elements of the characteristic matrix $\mathbf{f}_2(\varepsilon)$ are polynomials inside the interval I_2 , one can again use expression (11) to obtain:

$$\begin{aligned} \omega_{11}^{(2)}(\varepsilon) &= q_{11}^{(2)}(\varepsilon) \ln \left| \frac{\varepsilon - 2}{\varepsilon - 3} \right| - g_{11}^{(2)}(\varepsilon), \\ \omega_{22}^{(2)}(\varepsilon) &= q_{22}^{(2)}(\varepsilon) \ln \left| \frac{\varepsilon - 2}{\varepsilon - 3} \right| - g_{22}^{(2)}(\varepsilon), \end{aligned}$$

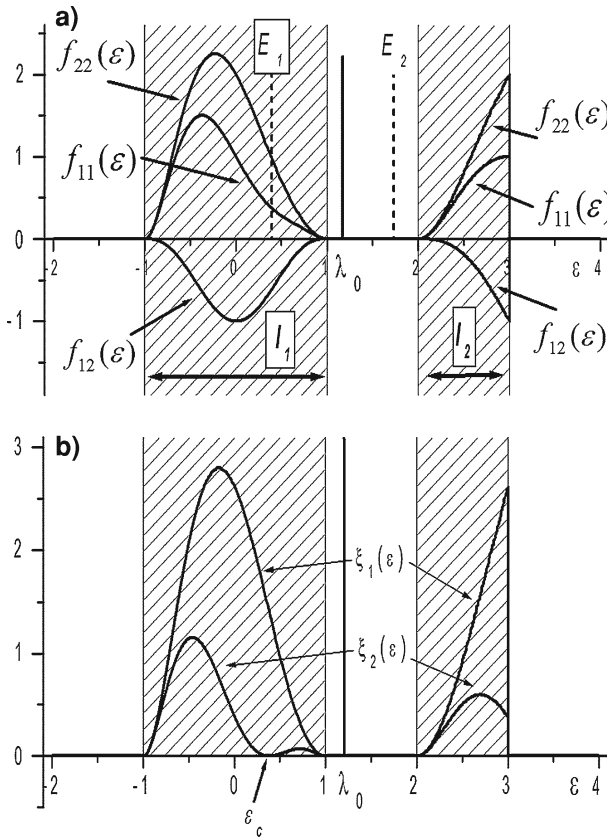


Fig. 9 Example E2. (a) Matrix elements $f_{sp}(\epsilon)$ of the characteristic matrix $\mathbf{f}(\epsilon)$. Those matrix elements vanish outside the range $D \equiv I_1 \cup I_2$ and excluding the point $\epsilon = \lambda_0$. Eigenvalue E_1 of the local system \mathbf{S}_2^a is inside the range D while eigenvalue E_2 is outside this range. (b) Eigenvalues $\xi_s(\epsilon)$ of the characteristic matrix

$$\omega_{12}^{(2)}(\epsilon) \equiv \omega_{21}^{(2)} = q_{12}^{(2)}(\epsilon) \ln \left| \frac{\epsilon - 2}{\epsilon - 3} \right| - g_{12}^{(2)}(\epsilon), \tag{50a}$$

where $q_{sp}^{(2)}(\epsilon)$ are polynomials (48b), while $g_{sp}^{(2)}(\epsilon)$ are polynomials:

$$\begin{aligned} g_{11}^{(2)}(\epsilon) &= 2\epsilon^3 - 17\epsilon^2 + \frac{140}{3}\epsilon - \frac{121}{3}, \\ g_{22}^{(2)}(\epsilon) &= \epsilon^3 - \frac{19}{2}\epsilon^2 + \frac{88}{3}\epsilon - \frac{109}{4}, \\ g_{12}^{(2)}(\epsilon) \equiv g_{21}^{(2)}(\epsilon) &= \epsilon^3 - \frac{15}{2}\epsilon^2 + \frac{52}{3}\epsilon - \frac{157}{12}. \end{aligned} \tag{50b}$$

Since $\mathbf{f}_2(\epsilon)$ is nonzero in the point $\epsilon = b_2 = 3$ on the right edge of the interval I_2 , those matrix elements diverges in this point [8]. Finally, using (12) and (49) one finds

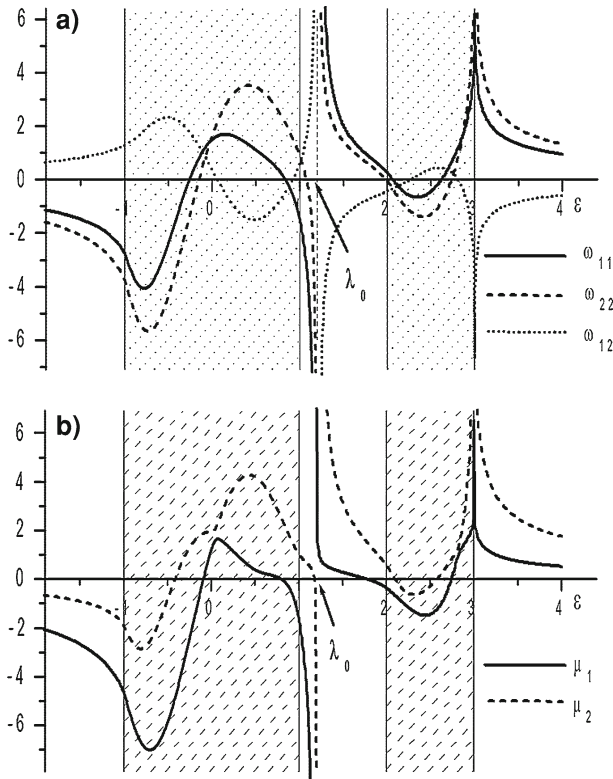


Fig. 10 Example E2. (a) Matrix elements $\omega_{sp}(\varepsilon)$ of the derived matrix $\omega(\varepsilon)$. (b) Eigenvalues $\mu_s(\varepsilon)$ of the derived matrix $\omega(\varepsilon)$

derived matrix $\Omega(\varepsilon)$

$$\Omega(\varepsilon) = \begin{pmatrix} 0.5 & -0.3 \\ -0.3 & 0.2 \end{pmatrix} \cdot \frac{1}{\varepsilon - \lambda_0} \begin{cases} 1 & \text{if } \varepsilon \neq \lambda_0 \\ 0 & \text{if } \varepsilon = \lambda_0 \end{cases} \quad (51)$$

In Fig. 10a are shown matrix elements $\omega_{sp}(\varepsilon)$ of the global derived matrix $\omega(\varepsilon) = \omega_1(\varepsilon) + \omega_2(\varepsilon) + \Omega(\varepsilon)$, while in Fig. 10b are shown eigenvalues $\mu_1(\varepsilon)$ and $\mu_2(\varepsilon)$ of this matrix. Matrix elements $\omega_{sp}(\varepsilon)$ diverge in a point $\varepsilon = b_2$ where characteristic matrix $\mathbf{f}(\varepsilon)$ is discontinuous and their $\varepsilon \rightarrow \lambda_0$ limits diverge in a point $\varepsilon = \lambda_0$ where a system \mathbf{S}_∞^b (surrounding) has an isolated eigenvalue. Eigenvalues $\mu_1(\varepsilon)$ and $\mu_2(\varepsilon)$ of $\omega(\varepsilon)$ have the same properties in those points. In accord with the requirement (14b), both eigenvalues are decreasing functions of ε for each $\varepsilon \notin D = I_1 \cup I_2$ and $\varepsilon \neq \lambda_0$. However, in the interval I_1 as well as in the interval I_2 those eigenvalues can be decreasing as well as increasing functions of ε . In the point $\varepsilon = \lambda_0$ those eigenvalues are not continuous and in this point they have the values $\mu_1(\lambda_0) = 0.27462$ and $\mu_2(\lambda_0) = 1.71374$, respectively (see Fig. 10b). The same general behavior applies to diagonal matrix elements $\omega_{11}(\varepsilon)$ and $\omega_{22}(\varepsilon)$ of the derived matrix $\omega(\varepsilon)$ (see Fig. 10a).

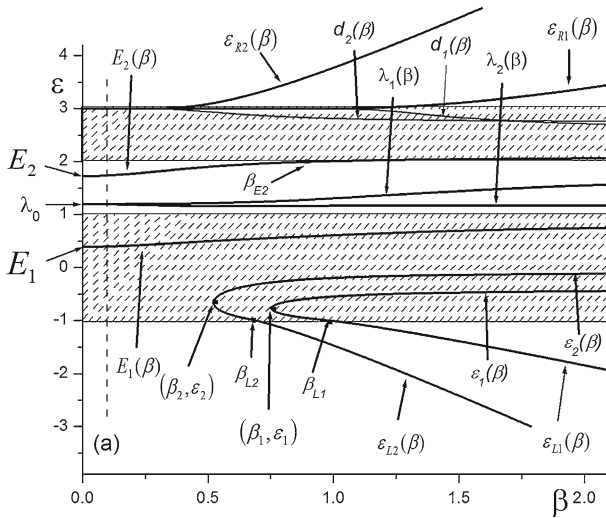


Fig. 11 Eigenvalues $\varepsilon_r(\beta)$ of the generic equation considered as functions of the coupling β . Eigenvalues inside the range D are resonant points, while eigenvalues outside this range are isolated eigenvalues of the combined system. Eigenvalue distributions of local states $|\Theta_s\rangle$ for the coupling β corresponding to the line (a) is shown in Fig. 15

Generic eigenvalue equation (15a) produces all isolated eigenstates and all resonant points of the combined system. In the case of a two dimensional system \mathbf{S}_2^a this equation reduces to the Eqs. 36 and 37. Solutions of the Eq. 36 of a type $\varepsilon = \varepsilon(\beta)$ are shown in Fig. 11. There are 12 such solutions: $\varepsilon_{R1}(\beta)$, $\varepsilon_{R2}(\beta)$, $\varepsilon_1(\beta)$, $\varepsilon_2(\beta)$, $\varepsilon_{L1}(\beta)$, $\varepsilon_{L2}(\beta)$, $\lambda_1(\beta)$, $\lambda_2(\beta)$, $E_1(\beta)$, $E_2(\beta)$, $d_1(\beta)$ and $d_2(\beta)$. If $\beta = 0$ eigenvalues of the generic equation coincide with local eigenvalues. In particular, one has $E_1(0) = E_1$ and $E_2(0) = E_2$. In addition, generic equation has two eigenvalues that in a $\beta \rightarrow 0$ limit coincide with isolated eigenvalue λ_0 of the \mathbf{S}_∞^b system. Those are eigenvalues $\lambda_1(\beta)$ and $\lambda_2(\beta)$:

$$\lim_{\beta \rightarrow 0} \lambda_1(\beta) = \lim_{\beta \rightarrow 0} \lambda_2(\beta) = \lambda_0. \tag{52}$$

Consider eigenvalues $E_1(\beta)$ and $E_2(\beta)$ in more details. Since $E_1(0) \in D$, for small β eigenvalue $E_1(\beta)$ is contained in the range D . It is hence a resonant point. Using expression (38) one finds that this is true for each β , however large. On the other hand, since $E_2(0) \notin D$ for small β one has $E_2(\beta) \notin D$. This eigenvalue is hence an isolated eigenvalue of the combined system. However, if the coupling β is as strong as $\beta > \beta_{E2}$ one has $E_2(\beta) \in D$ and this eigenvalue becomes a resonant point. In the point $\beta = \beta_{E2}$ one has $\varepsilon = a_2 = 2$. Inserting this value into (38a) one finds $\beta_{E2} = 0.92203$.

Consider next eigenvalues $\varepsilon_{L1}(\beta)$, $\varepsilon_{L2}(\beta)$, $\varepsilon_1(\beta)$ and $\varepsilon_2(\beta)$. Eigenvalues $\varepsilon_{L1}(\beta)$ and $\varepsilon_1(\beta)$ are two branches of one and the same analytic function $\beta = \beta_1(\varepsilon)$, while $\varepsilon_{L2}(\beta)$ and $\varepsilon_2(\beta)$ are two branches of another analytic function $\beta = \beta_2(\varepsilon)$. One can analyze those functions in a form $\beta = \beta_1(\varepsilon)$ and $\beta = \beta_2(\varepsilon)$ using explicit expressions

(38). Condition $d\beta_1(\varepsilon)/d\varepsilon = 0$ determines the point $(\beta_1, \varepsilon_1) = (0.75300, -0.76789)$ while condition $d\beta_2(\varepsilon)/d\varepsilon = 0$ determines the point $(\beta_2, \varepsilon_2) = (0.52241, -0.66072)$. Eigenvalues $\varepsilon_{L1}(\beta)$ and $\varepsilon_1(\beta)$ exist only if $\beta \geq \beta_1$ while eigenvalues $\varepsilon_{L2}(\beta)$ and $\varepsilon_2(\varepsilon)$ exist only if $\beta \geq \beta_2$. For each β (where defined) eigenvalues $\varepsilon_1(\beta)$ and $\varepsilon_2(\varepsilon)$ are inside the range D and hence these eigenvalues are resonant points. Concerning eigenvalues $\varepsilon_{L1}(\beta)$ and $\varepsilon_{L2}(\beta)$, for small β those eigenvalues are resonant points. However, if the coupling is as strong as $\beta > \beta_{L2}$ eigenvalue $\varepsilon_{L2}(\beta)$ becomes left isolated eigenvalue of the combined system, while if $\beta > \beta_{L1}$ eigenvalue $\varepsilon_{L1}(\beta)$ becomes another left isolated eigenvalue of the combined system. As $\beta > \beta_{L1}$ further increases, isolated eigenvalues $\varepsilon_{L1}(\beta)$ and $\varepsilon_{L2}(\beta)$ continue to decrease. This is in accord with expressions (14) and (17) that imply $\partial\varepsilon_L/\partial\beta < 0$ for each left isolated eigenvalue $\varepsilon_L < a_1 = -1$ (extreme left subinterval \bar{I}_{left} of \bar{D} is $\bar{I}_{left} = (-\infty, a_1)$). Hence for each $\beta > \beta_{L1}$ combined system has two left isolated eigenvalues. In the points β_{L1} and β_{L2} one has $\varepsilon = a_1 = -1$. In analogy to (46) one finds $\beta_{L2} = 0.69110$ and $\beta_{L1} = 0.98637$.

Concerning eigenvalues $\varepsilon_{R1}(\beta)$, $\varepsilon_{R2}(\beta)$, $d_1(\beta)$ and $d_2(\beta)$, one finds that $\varepsilon_{R1}(\beta)$ and $\varepsilon_{R2}(\beta)$ are right isolated eigenvalues while $d_1(\beta)$ and $d_2(\beta)$ are resonant points. In analogy to the left isolated eigenvalues, as β increases right isolated eigenvalues $\varepsilon_{R1}(\beta)$ and $\varepsilon_{R2}(\beta)$ monotonically increase. Hence for sufficiently big β combined system has two right isolated eigenvalues. For small β those eigenvalues asymptotically approach the value $\varepsilon = b_2 = 3$. For example, if $\beta \approx 0.94$ one has $\varepsilon_{R1}(\beta) \approx 3.001$ and $d_1(\beta) \approx 2.999$, while if β decreases to $\beta = 0.70167$ one has $\varepsilon_{R1}(\beta) \approx 3.000001$ and $d_1(\beta) \approx 2.999999$. Similarly, if $\beta \approx 0.278$ one has $\varepsilon_{R2}(\beta) \approx 3.001$ and $d_2(\beta) \approx 2.999$, while if β decreases to $\beta = 0.19069$ one has $\varepsilon_{R2}(\beta) \approx 3.000001$ and $d_2(\beta) \approx 2.999999$. This asymptotic behavior is due to the fact that matrix elements of the characteristic operator $\mathbf{f}(\varepsilon)$ are discontinuous in the point $\varepsilon = b_2 = 3$ [8].

Consider finally eigenvalues $\lambda_1(\beta)$ and $\lambda_2(\beta)$. According to (52), in a limit $\beta \rightarrow 0$ those eigenvalues converge to the isolated eigenvalue $\lambda_0 = 1.2$ of the infinite system \mathbf{S}_∞^b . Since $\lambda_0 \notin D$, for sufficiently small β those eigenvalues are isolated eigenvalues of the combined system. One finds that this is true for each β , however large. In order to illustrate a nontrivial shape of those eigenvalues, in Fig. 12 are shown those eigenvalues with amplified ε -coordinate.

In conclusion, for sufficiently big β combined system has 6 isolated eigenvalues, $\varepsilon_{R1}(\beta)$, $\varepsilon_{R2}(\beta)$, $\varepsilon_{L1}(\beta)$, $\varepsilon_{L2}(\beta)$, $\lambda_1(\beta)$ and $\lambda_2(\beta)$. In addition, for each $\beta < \beta_{E2}$ there is isolated eigenvalue $E_2(\beta)$. Note that isolated eigenvalues $\varepsilon_{L1}(\beta)$, $\varepsilon_{L2}(\beta)$, $\varepsilon_{R1}(\beta)$ and $\varepsilon_{R2}(\beta)$ do not exist in the point $\beta = 0$. Hence no perturbation expansion method can reproduce those eigenvalues.

Once above eigenvalues are obtained as solutions to (36), one can derive corresponding isolated eigenstates according to (37) and (15b,c). Those eigenstates determine all related properties of the open system \mathbf{S}_2^a . In particular, probabilities $w_{r,s}$ and $w_r = w_{r,1} + w_{r,2}$ are given by (18). Probabilities for right and left isolated eigenstates are shown in Fig. 13. In Fig. 13a are shown probabilities $w_{R1,s} \equiv |\langle \Theta_s | \mathbf{S} | \Psi_{R1} \rangle|^2$ to find right isolated eigenstate $|\Psi_{R1}\rangle$ in a local state $|\Theta_s\rangle$, as well as global right probability $w_{R1} = w_{R1,1} + w_{R1,2}$ to find right isolated eigenstate $|\Psi_{R1}\rangle$ in a local system \mathbf{S}_2^a . Since the characteristic operator $\mathbf{f}(\varepsilon)$ is discontinuous in the point $\varepsilon = b_2$ where right isolated eigenstate $|\Psi_{R1}\rangle$ emerges, those probabilities are continuous functions of β . However, those functions are not analytic [8]. This is qualitatively different behavior

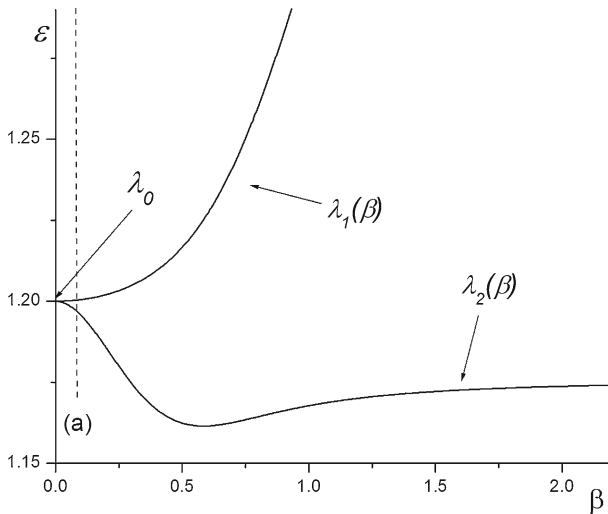


Fig. 12 Eigenvalues $\lambda_1(\beta)$ and $\lambda_2(\beta)$ from Fig. 11 highly magnified

from probabilities shown in Fig. 4 which are all identically zero for small β and which display a sudden jump from zero to a finite nonzero value at some critical point (β_{R1} , β_{R2} , β_{L1} or β_{L2}). Similar behavior applies to probabilities $w_{R2} = w_{R2,1} + w_{R2,2}$ and $w_{R2,s} = |\langle \Theta_s | S | \Psi_{R2} \rangle|^2$ associated with right isolated eigenstate $|\Psi_{R2}\rangle$ (see Fig. 13b). Those probabilities are also continuous functions of a coupling parameter β . However, probabilities associated with left isolated eigenstates $|\Psi_{L1}\rangle$ and $|\Psi_{L2}\rangle$ that emerge at the point $\varepsilon = a_1$ where characteristic operator $\mathbf{f}(\varepsilon)$ is continuous, have a sudden jump from zero to a finite nonzero value. In particular, left isolated eigenvalue $\varepsilon_{L1}(\beta)$ exists only if $\beta > \beta_{L1} = 0.98637$. As $\beta < \beta_{L1}$ continuously increases, in a point $\beta = \beta_{L1}$ probabilities $w_{L1} = w_{L1,1} + w_{L1,2}$ and $w_{L1,s} = |\langle \Theta_s | S | \Psi_{L1} \rangle|^2$ discontinuously jump from zero to a finite nonzero values $w_{L1}(\beta_{L1}+) = 0.14935$, $w_{L1,1}(\beta_{L1}+) = 0.11491$ and $w_{L1,2}(\beta_{L1}+) = 0.03444$, respectively (Fig. 13c). The same applies to another left isolated eigenstate $|\Psi_{L2}\rangle$. This eigenstate exists only if $\beta > \beta_{L2} = 0.69110$. At this point probabilities $w_{L2} = w_{L2,1} + w_{L2,2}$ and $w_{L2,s} = |\langle \Theta_s | S | \Psi_{L2} \rangle|^2$ discontinuously jump from zero to a finite nonzero values $w_{L2}(\beta_{L2}+) = 0.17876$, $w_{L2,1}(\beta_{L2}+) = 0.09566$ and $w_{L2,2}(\beta_{L2}+) = 0.08310$, respectively (see Fig. 13d).

Probabilities associated with isolated eigenstates $|\Psi_{\lambda_1}\rangle$, $|\Psi_{\lambda_2}\rangle$ and $|\Psi_{E2}\rangle$ are shown in Fig. 14. Spectral distributions of local states $|\Theta_s\rangle$ corresponding to the line (a) in this figure are shown in Fig. 15. If $\beta = 0$ eigenstates $|\Psi_{\lambda_1}\rangle$ and $|\Psi_{\lambda_2}\rangle$ coincide with isolated eigenstate $|\Phi_0\rangle$ of the infinite system \mathbf{S}_∞^b . This eigenstate has no X_2^a component and hence all corresponding probabilities vanish in a point $\beta = 0$ (see Fig. 14a and b). As β increases, eigenstate $|\Phi_0\rangle$ splits into two eigenstates $|\Psi_{\lambda_1}\rangle$ and $|\Psi_{\lambda_2}\rangle$ with nonvanishing X_2^a components. Since those probabilities are continuous functions of β , they are small if β is small. In Fig. 14a are shown probabilities $w_{\lambda_1,s} \equiv |\langle \Theta_s | S | \Psi_{\lambda_1} \rangle|^2$ to find isolated eigenstate $|\Psi_{\lambda_1}\rangle$ in a local state $|\Theta_s\rangle$, as well as global probability $w_{\lambda_1} = w_{\lambda_1,1} + w_{\lambda_1,2}$ to find isolated eigenstate $|\Psi_{\lambda_1}\rangle$ in a local system \mathbf{S}_2^a . In Fig. 14b are shown analogous probabilities for another isolated eigenstate $|\Psi_{\lambda_2}\rangle$. Probabilities

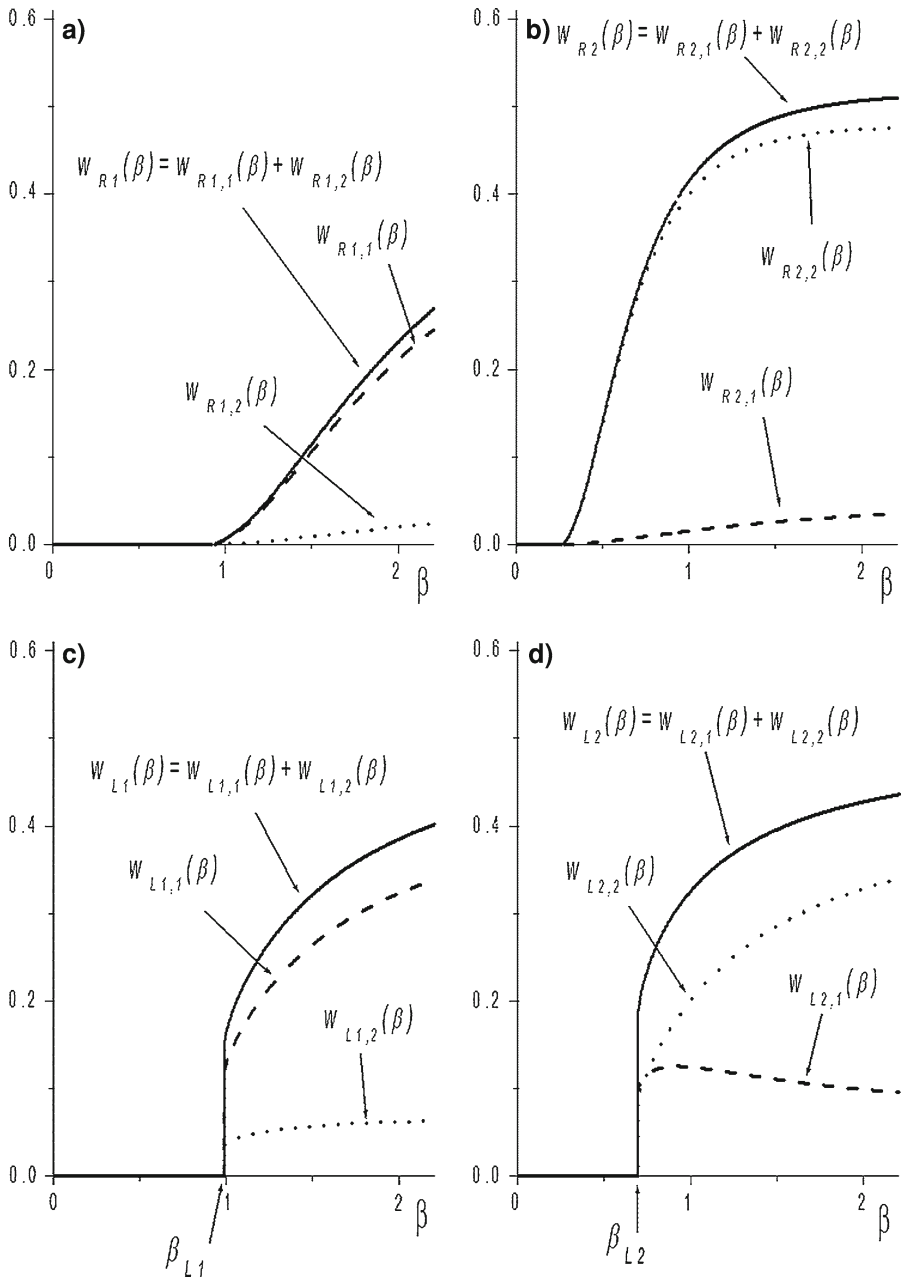


Fig. 13 Probabilities $w_{r,s}(\beta) \equiv |\langle \Theta_s | \mathbf{S} | \Psi_r \rangle|^2$ to find isolated eigenstate $|\Psi_r\rangle$ in a local state $|\Theta_s\rangle$ and probabilities $w_r = w_{r,1} + w_{r,2}$ to find this eigenstate in the system \mathbf{S}_2^a for left and right eigenstates of the combined system. **(a)** Probabilities corresponding to the eigenstate $|\Psi_{R1}\rangle$. **(b)** Probabilities corresponding to the eigenstate $|\Psi_{R2}\rangle$. **(c)** Probabilities corresponding to the eigenstate $|\Psi_{L1}\rangle$. **(d)** Probabilities corresponding to the eigenstate $|\Psi_{L2}\rangle$

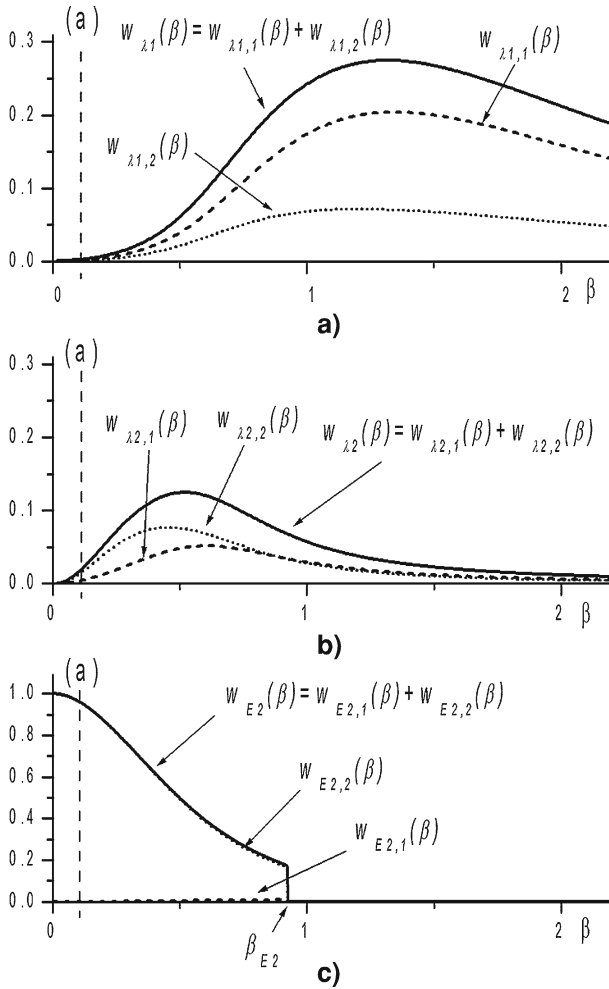


Fig. 14 Probabilities $w_{r,s}(\beta)$ for the remaining three isolated eigenstates $|\Psi_{\lambda_1}\rangle$, $|\Psi_{\lambda_2}\rangle$ and $|\Psi_{E_2}\rangle$. (a) Probabilities corresponding to the eigenstate $|\Psi_{\lambda_1}\rangle$. (b) Probabilities corresponding to the eigenstate $|\Psi_{\lambda_2}\rangle$. (c) Probabilities corresponding to the eigenstate $|\Psi_{E_2}\rangle$

$w_{E_2,s} \equiv |\langle \Theta_s | \mathbf{S} | \Psi_{E_2} \rangle|^2$ and $w_{E_2} = w_{E_2,1} + w_{E_2,2}$ associated with the isolated eigenstate $|\Psi_{E_2}\rangle$ display qualitatively different behavior (see Fig. 14c). Since for $\beta = 0$ this eigenstate coincides with local eigenstate $|\Theta_2\rangle$ with the eigenvalue $E_2(0) \equiv E_2 \notin D$, one has $w_{E_2,1}(0) = 0$, $w_{E_2,2}(0) = 1$ and $w_{E_2}(0) = 1$. Hence for small β one has $w_{E_2,1}(\beta) \approx 0$, $w_{E_2,2}(\beta) \approx 1$ and $w_{E_2}(\beta) \approx 1$. As β increases, local state $|\Theta_2\rangle$ is perturbed by the interaction with the system \mathbf{S}_∞^b , and this state transforms into the isolated eigenstate $|\Psi_{E_2}\rangle$. If the interaction is as strong as $\beta_{E_2} = 0.92203$, eigenvalue $E_2(\beta)$ enters the range D and at this point there is no more isolated eigenstate $|\Psi_{E_2}\rangle$. Accordingly, all corresponding probabilities drop to zero.

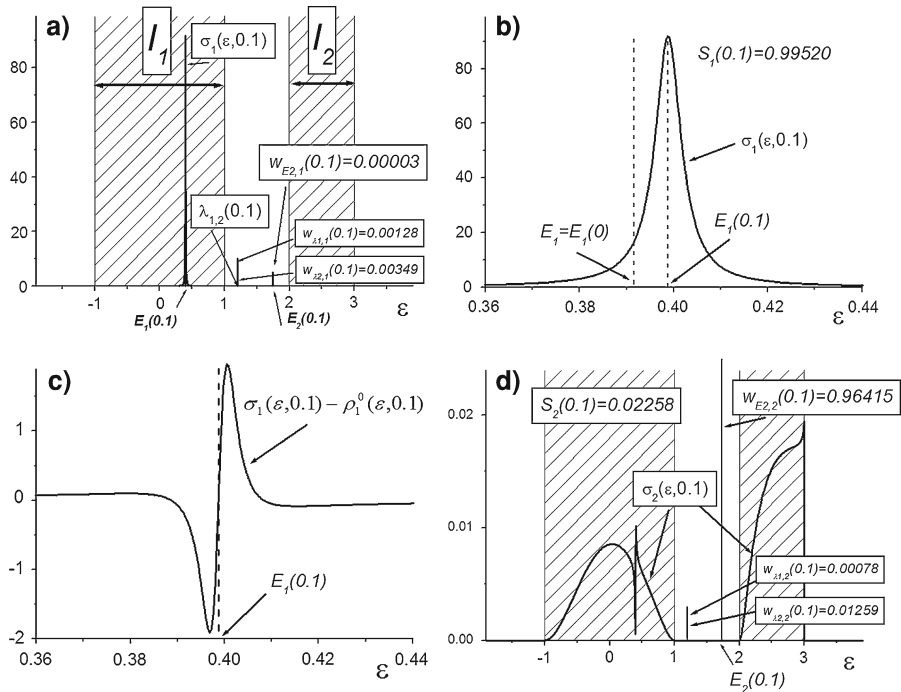


Fig. 15 Eigenvalue distributions of local states $|\Theta_1\rangle$ and $|\Theta_2\rangle$ in the case $\beta = 0.1$. Those distributions correspond to the line (a) in Figs. 11, 12 and 14. (a) Eigenvalue distribution of the state $|\Theta_1\rangle$. (b) Probability density $\sigma_1(\varepsilon, 0.1)$ highly magnified. (c) Difference between probability density $\sigma_1(\varepsilon, 0.1)$ and approximate density $\rho_1^0(\varepsilon, 0.1)$ highly magnified. (d) Spectral distribution of local state $|\Theta_2\rangle$ with probability density $\sigma_2(\varepsilon, 0.1)$ highly magnified. Probabilities not in scale

Consider now embedded solutions of the combined system. One finds eigenvalues $X_d(\varepsilon)$ and X_ρ^a -components $|\Psi_d^a(\varepsilon)\rangle$ of the embedded eigenstates $|\Psi_d(\varepsilon)\rangle$ using expressions (39–41) and (24). In Fig. 15 are shown spectral distributions of local states $|\Theta_s\rangle$ for the coupling $\beta = 0.1$. This coupling corresponds to the line (a) in Figs. 11, 12 and 14. This is relatively weak coupling and since $E_1(0.1) = 0.39872 \in D$, probability density $\sigma_1(\varepsilon, 0.1)$ to find local state $|\Theta_1\rangle$ with the eigenvalue $\varepsilon \in D$, i.e. to find this state either in the embedded eigenstate $|\Psi_1(\varepsilon, 0.1)\rangle$ or in the embedded eigenstate $|\Psi_2(\varepsilon, 0.1)\rangle$ has a prominent resonance shape at this point (Fig. 15a). Unlike in the example **E1** where total contribution from the density $\sigma_1(\varepsilon, 0.1)$ equals $S_1(0.1) = 1$, one now finds $S_1(0.1) = \int \sigma_1(\varepsilon, 0.1)d\varepsilon = 0.99520 < 1$. In the case $\beta = 0.1$ in addition to embedded eigenstates combined system has isolated eigenstates $|\Psi_{\lambda_1}(0.1)\rangle$, $|\Psi_{\lambda_2}(0.1)\rangle$ and $|\Psi_{E_2}(0.1)\rangle$ with eigenvalues $\lambda_1(0.1) = 1.20050$, $\lambda_2(0.1) = 1.19578$ and $E_2(0.1) = 1.73998$, respectively (see Fig. 11). Missing contribution is due to those isolated eigenstates. One finds $w_{\lambda_{1,1}}(0.1) = 0.00128$, $w_{\lambda_{2,1}}(0.1) = 0.00349$ and $w_{E_2,1}(0.1) = 0.00003$. The sum of all those probabilities equals one in complete agreement with the completeness relation (34a). Since $C_{1,1}(0.1) = 0.98780$ and $C_{2,1}(0.1) = 0.00758$, contribution $S_1(0.1) = C_{1,1}(0.1) + C_{2,1}(0.1)$ is mainly due to the embedded eigenstate $|\Psi_1(\varepsilon, 0.1)\rangle$ with relatively negligible contribution

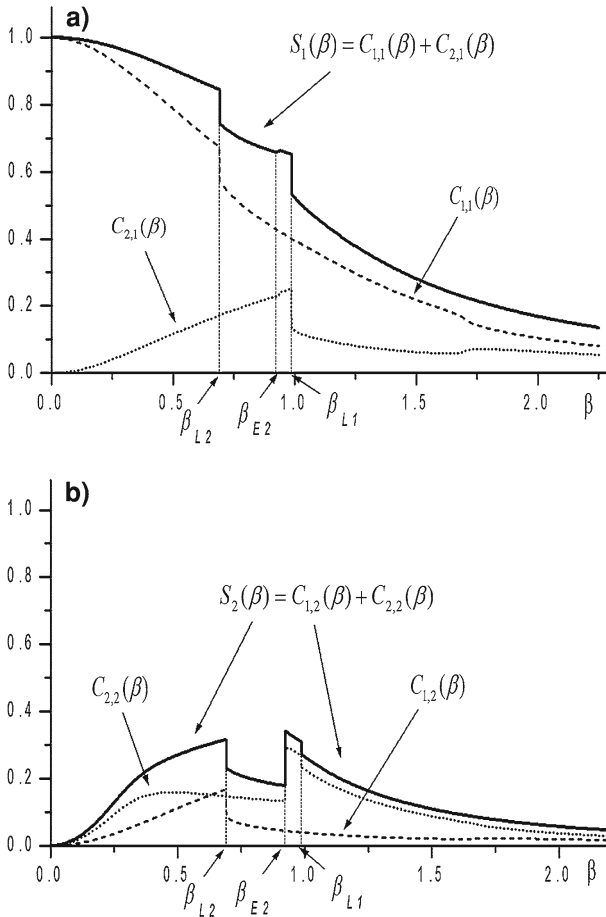


Fig. 16 Probabilities $S_s(\beta) = C_{1,s}(\beta) + C_{2,s}(\beta)$ to find local state $|\Theta_s\rangle$ in any of the embedded eigenstates of the combined system and corresponding component probabilities $C_{d,s}(\beta) = \int |\langle \Theta_s | \mathbf{S} | \Psi_d(\varepsilon, \beta) \rangle|^2 d\varepsilon$. **(a)** Probability $S_1(\beta)$ and component probabilities $C_{1,1}(\beta)$ and $C_{2,1}(\beta)$. **(b)** Probability $S_2(\beta)$ and component probabilities $C_{1,2}(\beta)$ and $C_{2,2}(\beta)$

from embedded eigenstate $|\Psi_2(\varepsilon, 0.1)\rangle$. Resonant shape $\sigma_1(\varepsilon, 0.1)$ is made manifest in Fig. 15b where density $\sigma_1(\varepsilon, 0.1)$ is shown magnified. In Fig. 15c is shown the difference $\sigma_1(\varepsilon, 0.1) - \rho_1^0(\varepsilon, 0.1)$ between this density and universal resonance curve $\rho_1^0(\varepsilon, 0.1)$ as given by (32b). This difference is relatively small and density $\sigma_1(\varepsilon, 0.1)$ is hence well approximated with this universal resonance curve.

In Fig. 15d is shown eigenvalue distribution of another local state $|\Theta_2\rangle$. Concerning probability $S_2(0.1)$ to find this state in any of the embedded eigenstates, one finds $S_2(0.1) = \int \sigma_2(\varepsilon, 0.1) d\varepsilon = 0.02258$. This probability is rather small since the eigenvalue $E_2(0.1) = 1.73995 \notin D$ of the perturbed eigenstate $|\Psi_{E2}\rangle$ is outside the range D . Corresponding density $\sigma_2(\varepsilon, 0.1)$ has no resemblance to the universal resonance curve (see Fig. 15d). Spectral distribution of the local state $|\Theta_2\rangle$ is essentially repre-

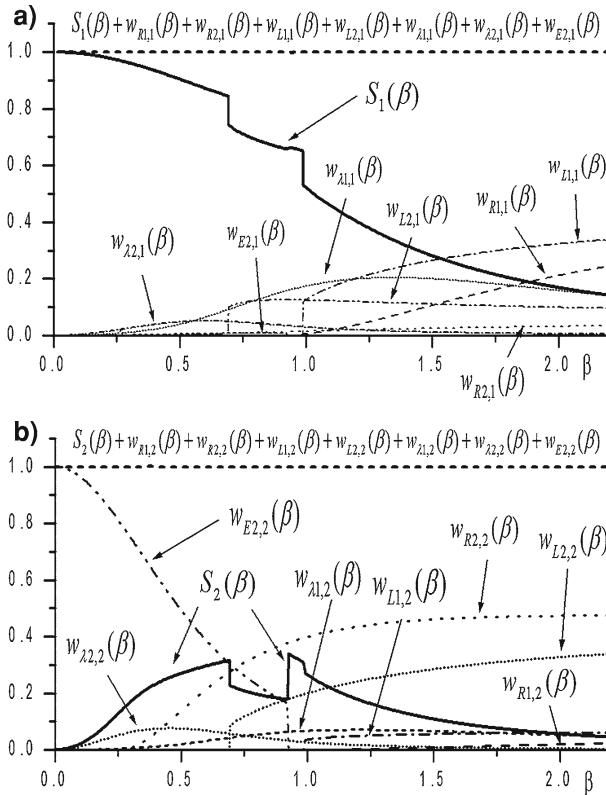


Fig. 17 (a) Verification of the completeness relation for the eigenvalue distribution of a local state $|\Theta_1\rangle$. (b) Verification of the completeness relation for the eigenvalue distribution of a local state $|\Theta_2\rangle$

sented by the isolated eigenstate $|\Psi_{R2}(0.1)\rangle$ with the eigenvalue $E_2(0.1) \notin D$ and with the corresponding probability $w_{E2,2}(0.1) = 0.96415 < 1$. This distribution, in addition to a dominant contribution from the isolated eigenstate $|\Psi_{E2}(0.1)\rangle$ and to a contribution $S_2(0.1)$ from embedded eigenstates, contains also some minor contributions from isolated eigenstates $|\Psi_{\lambda 1}(0.1)\rangle$ and $|\Psi_{\lambda 2}(0.1)\rangle$. One finds $w_{\lambda 1,2}(0.1) = 0.00078$ and $w_{\lambda 2,2}(0.1) = 0.01259$. As required by the completeness relation, the sum of all those contributions equals one.

In Fig. 16 are shown probabilities $S_d(\beta) = C_{d,1}(\beta) + C_{d,2}(\beta)$ associated with embedded eigenstates $|\Psi_d(\varepsilon, \beta)\rangle$ as functions of β for the interval $\beta \in [0, 2.2]$. Component probabilities $C_{d,s}(\beta)$ are also shown. Those quantities are discontinuous in the points $\beta = \beta_{L2}$, $\beta = \beta_{L1}$ and $\beta = \beta_{E2}$ where the combined system, considered as a function of β , either acquires or loses isolated eigenstates. Since $E_1 \in D$ while $E_2 \notin D$, for small β one has $S_1(\beta) \approx 1$ and $S_2(\beta) \approx 0$. This is the region where perturbation expansion can be applied. However for large β , especially for $\beta > \beta_{L2}$, perturbation expansion breaks.

Completeness relations are verified in Fig. 17. In Fig. 17a probabilities $S_1(\beta)$, $w_{R1,1}(\beta)$, $w_{R2,1}(\beta)$, $w_{L1,1}(\beta)$, $w_{L2,1}(\beta)$, $w_{\lambda 1,1}(\beta)$, $w_{\lambda 2,1}(\beta)$ and $w_{E2,1}(\beta)$ associated with

a local state $|\Theta_1\rangle$ are plotted as functions of a coupling parameter β . A sum of all those probabilities is also shown. As required by the completeness relation, this sum equals one for each value of β . In Fig. 17b are in the same way analyzed probabilities associated with the local state $|\Theta_2\rangle$.

10 Conclusions

Exact nonperturbative method for the description of an open quantum system \mathbf{S}_ρ^a that interacts with the surrounding (an infinite quantum system \mathbf{S}_∞^b) is presented. System \mathbf{S}_ρ^a is an arbitrary finite-dimensional quantum system that contains ρ eigenvalues E_s and ρ corresponding eigenstates $|\Theta_s\rangle$. Those eigenstates span the space X_ρ^a . System \mathbf{S}_∞^b is an arbitrary infinite-dimensional quantum system. In general, this system may contain discrete eigenvalues λ_i as well as several eigenvalue bands in intervals $I_v = [a_v, b_v]$ (including the possibility $b_v = \infty$). The union $D = \cup_v I_v$ of all those intervals contains all continuous eigenvalues of \mathbf{S}_∞^b . Discrete eigenvalues λ_i of \mathbf{S}_∞^b may be contained in D as well as in its complement \bar{D} . The set of all eigenstates of \mathbf{S}_∞^b spans an infinite dimensional space X_∞^b .

In order to describe properties of the open system \mathbf{S}_ρ^a it is sufficient to know only X_ρ^a -components of the properly normalized eigenstates of the combined system $\mathbf{S}_\infty \equiv \mathbf{S}_\rho^a \oplus \mathbf{S}_\infty^b$. X_∞^b -components of those eigenstates are not required. One finds that combined system \mathbf{S}_∞ contains two qualitatively different types of eigenvalues and eigenstates. This system may contain *isolated* eigenvalues ε_r with the corresponding eigenstates $|\Psi_r\rangle$ as well as *embedded* eigenvalues ε with the corresponding eigenstates $|\Psi(\varepsilon, \dots)\rangle$.

There are two types of isolated eigenvalues ε_r and corresponding eigenstates. If ε_r differs from all discrete eigenvalues of \mathbf{S}_∞^b ($\varepsilon_r \notin \{\lambda_j\}$) it is *cardinal*, otherwise ($\varepsilon_r \in \{\lambda_j\}$) it is *singular*. Most important and usually most numerous are isolated cardinal eigenstates. Those eigenstates contribute to the properties of the open system \mathbf{S}_ρ^a . On the other hand, isolated singular eigenstates do not contribute to those properties, except for the so called *weakly singular* eigenstates which are quite rare.

In addition to isolated eigenstates with isolated eigenvalues ε_r , each $\varepsilon \in D$ is also an eigenvalue of the combined system. This eigenvalue is a part of a continuous band of eigenvalues and the corresponding eigenstates $|\Psi(\varepsilon, \dots)\rangle$ are normalized to a δ -function. Those are *embedded* eigenstates of the combined system. With each embedded eigenstate is associated a *fractional shift* $x(\varepsilon)$. This quantity satisfies $x(\varepsilon) \in [1 - \rho, 1]$. However, fractional shift can be confined to the interval $[0, 1]$ which is a *principal value* of fractional shift. Embedded eigenstates can be also singular and cardinal. One finds that embedded singular eigenstates have fractional shift $x(\varepsilon) = 0$, while embedded cardinal eigenstates have fractional shift $x(\varepsilon) \neq 0$. For each $\varepsilon \in D$ combined system may have an infinite number of embedded singular eigenstates, while the number of embedded cardinal eigenstates is at most ρ . Embedded cardinal eigenstates can be hence labeled with discrete index d as $|\Psi_d(\varepsilon)\rangle$ where for each $\varepsilon \in D$ this index can assume at most ρ values. To the properties of the open system \mathbf{S}_ρ^a contribute only embedded cardinal eigenstates. In conclusion, in order to describe open quantum

system \mathbf{S}_ρ^a it is sufficient to know X_ρ^a -components of all isolated and of all embedded cardinal eigenstates of the combined system.

Two eigenvalue equations, generic eigenvalue equation and fractional shift eigenvalue equation are derived. Both are $\rho \times \rho$ eigenvalue equations and they both act in the ρ -dimensional space X_ρ^a associated with the system \mathbf{S}_ρ^a . First equation determines all isolated cardinal eigenvalues and all X_ρ^a -components of the corresponding eigenstates of the combined system. Second equation determines all X_ρ^a -components of the embedded cardinal eigenstates of the combined system. In almost all cases those two equations provide a complete description of the open system \mathbf{S}_ρ^a .

Generic equation is a nonlinear eigenvalue equation. Each eigenvalue $\varepsilon_r \notin D$ of this equation is an isolated cardinal eigenvalue of the combined system. Once this eigenvalue is known, one easily obtains the corresponding isolated eigenstate $|\Psi_r\rangle$. Concerning eigenvalues $\varepsilon_r \in D$ of this equation, those eigenvalues are *resonant* points. A special type of resonant points, so-called *anomal* points are shown to be also isolated eigenvalues of the combined system. Generic eigenvalue equation thus provides all isolated cardinal eigenvalues and eigenstates of the combined system.

For each $\varepsilon \in D$ fractional shift equation is a linear eigenvalue equation. This equation is related to embedded cardinal solutions of the combined system. In particular, X_ρ^a -component $|\Psi_d^a(\varepsilon)\rangle$ of embedded cardinal eigenstate $|\Psi_d(\varepsilon)\rangle$ is given in terms of the solution to this equation.

Since the suggested method produces correct results however strong the interaction between quantum systems \mathbf{S}_ρ^a and \mathbf{S}_∞^b , it can be applied to all those cases where the standard perturbation expansion fails. If this interaction is weak, one obtains standard results known from the perturbation expansion approach. In particular, due to the interaction with the infinite system \mathbf{S}_∞^b , each eigenvalue $E_s \notin D$ of the system \mathbf{S}_ρ^a that is contained outside the eigenvalue range D of this infinite system moves to a new position $\varepsilon_s(\beta)$, and it remains sharp. Each eigenvalue $E_s \in D$ of the system \mathbf{S}_ρ^a that is contained inside this eigenvalue range also moves to a new position $\varepsilon_s(\beta)$. However, since $E_s \in D$ this shifted eigenvalue is usually not sharp and it acquires a finite width. In particular, if E_s is nondegenerate shifted eigenvalue $\varepsilon_s \in D$ usually acquires the shape of the universal resonance curve with a finite width $\Delta\varepsilon_s$. Only in a special case when $\varepsilon_s = \varepsilon_a$ is an *anomal* point, the width $\Delta\varepsilon_s$ drops to zero, and in this case one has one or several isolated solutions in this point [8]. If the interaction between the systems \mathbf{S}_ρ^a and \mathbf{S}_∞^b is strong this simple picture is destroyed, and one has much more complex behavior. Various density distributions in the case of a strong interaction have no resemblance to the universal resonance curve. In addition, in this case combined system usually has some isolated eigenstates which can not be interpreted as perturbed eigenstates of \mathbf{S}_ρ^a or as perturbed eigenstates of \mathbf{S}_∞^b . In the case of such strong interactions standard perturbation expansion fails.

The suggested method is illustrated with two examples. In the first example infinite system \mathbf{S}_∞^b contains a single eigenvalue band in the interval $I_1 \equiv [-1, 1]$. In the second example which is much more complex infinite system \mathbf{S}_∞^b contains two eigenvalue bands, one eigenvalue band in the interval $I_1 \equiv [-1, 1]$ and another eigenvalue band in the interval $I_2 \equiv [2, 3]$. In addition, this system contains an isolated eigenstate with the eigenvalue $\lambda_0 = 1.2$. It is shown that all relevant probabilities and density

distributions satisfy completeness relation (34a). This relation is verified for a wide range of a parameter β , including very weak as well as extremely strong interactions. The agreement of those probabilities and density distributions with the completeness relation provides a strong verification of the suggested method.

Appendices

A Solution of a finite combined system $\mathbf{S}_{n+\rho}$

Let \mathbf{S}_n^b be n -dimensional quantum system described by the eigenvalue equation

$$\mathbf{B} |\Phi_i\rangle = \lambda_i |\Phi_i\rangle, \quad i = 1, \dots, n, \tag{A1a}$$

where \mathbf{B} is a Hermitian operator acting in the n -dimensional space X_n^b . Eigenstates $|\Phi_i\rangle \in X_n^b$ of \mathbf{B} can be orthonormalized according to

$$\langle \Phi_i | \Phi_j \rangle = \delta_{ij}. \tag{A1b}$$

Let the system \mathbf{S}_n^b interact with the system \mathbf{S}_ρ^a described by the eigenvalue equation (1a). This interaction can be written in the form $\beta \mathbf{V}$ where \mathbf{V} is a Hermitian operator that connects the states $|\Theta_s\rangle \in X_\rho^a$ with the states $|\Phi_i\rangle \in X_n^b$ and where $\beta \geq 0$ is a coupling parameter. Combined system $\mathbf{S}_{n+\rho} \equiv \mathbf{S}_\rho^a \oplus \mathbf{S}_n^b$ that includes this interaction is described by the generalized eigenvalue equation

$$\mathbf{C} |\Psi_k\rangle = \varepsilon_k \mathbf{S} |\Psi_k\rangle, \quad k = 1, \dots, n + \rho, \tag{A2a}$$

where

$$\mathbf{C} = \mathbf{A} + \mathbf{B} + \beta \mathbf{V}, \quad \mathbf{S} = \mathbf{S}^a + \mathbf{I}^b. \tag{A2b}$$

and where \mathbf{I}^b is a unit operator in X_n^b .

Eigenstates $|\Psi_k\rangle$ of the eigenvalue equation (A2a) can be orthonormalized according to

$$\langle \Psi_k | \mathbf{S} | \Psi_l \rangle = \delta_{kl}, \tag{A3a}$$

Each such eigenstate is a linear combination

$$|\Psi_k\rangle = |\Psi_k^a\rangle + |\Psi_k^b\rangle, \tag{A3b}$$

where

$$|\Psi_k^a\rangle \in X_\rho^a, \quad |\Psi_k^b\rangle \in X_\infty^b. \tag{A3c}$$

If the solution to the system \mathbf{S}_n^b is known, the solution to the combined system $\mathbf{S}_{n+\rho}$ can be obtained in a compact form that does not require diagonalization of a huge $(n + \rho) \times (n + \rho)$ eigenvalue equation (A2a) [9].

Define Hermitian operator $\mathbf{\Omega}(\varepsilon)$ [9]

$$\mathbf{\Omega}(\varepsilon) = \sum_{i(\lambda_i \neq \varepsilon)}^n \frac{\mathbf{V} |\Phi_i\rangle \langle \Phi_i| \mathbf{V}}{\varepsilon - \lambda_i}, \quad (\text{A4a})$$

The summation in this expression is performed over all indices i such that $\lambda_i \neq \varepsilon$. If ε differs from all unperturbed eigenvalues λ_i ($\varepsilon \notin \{\lambda_j\}$), this summation contains all n terms.

Operator $\mathbf{\Omega}(\varepsilon)$ incorporates essential features of the interaction of the system \mathbf{S}_n^b with the system \mathbf{S}_ρ^a . However, this operator has nonvanishing matrix elements only in the space X_ρ^a . In particular, in the base $\{|s\rangle\} \in X_\rho^a$ this operator is a $\rho \times \rho$ Hermitian matrix with matrix elements $\Omega_{sp}(\varepsilon)$

$$\Omega_{sp}(\varepsilon) = \sum_{i(\lambda_i \neq \varepsilon)}^n \frac{\langle s | \mathbf{V} | \Phi_i \rangle \langle \Phi_i | \mathbf{V} | p \rangle}{\varepsilon - \lambda_i}, \quad s, p = 1, \dots, \rho. \quad (\text{A4b})$$

It is convenient to distinguish *cardinal* ($\varepsilon_k \notin \{\lambda_i\}$) and *singular* ($\varepsilon_k \in \{\lambda_i\}$) eigenvalues and corresponding eigenstates of the combined system $\mathbf{S}_{n+\rho}$ [9].

A.1 Cardinal solutions of $\mathbf{S}_{n+\rho}$

Eigenvalue $\varepsilon_k \notin \{\lambda_i\}$ is a (cardinal) eigenvalue of the combined system if and only if it is an eigenvalue of the eigenvalue equation [9]

$$\left[\beta^2 \mathbf{\Omega}(\varepsilon_k) + \mathbf{A} \right] |\theta_k\rangle = \varepsilon_k \mathbf{S}^a |\theta_k\rangle, \quad \varepsilon_k \notin \{\lambda_i\}, \quad (\text{A5a})$$

In the base $\{|s\rangle\}$ eigenvalue equation (A5a) is a $\rho \times \rho$ matrix eigenvalue equation. This equation has a nontrivial solution ($|\theta_k\rangle \neq 0$) if and only if determinant of the system vanishes:

$$|\mathbf{H}(\varepsilon_k)| = 0, \quad (\text{A5b})$$

where

$$\mathbf{H}(\varepsilon) \equiv \beta^2 \mathbf{\Omega}(\varepsilon) + \mathbf{A} - \varepsilon \mathbf{S}^a. \quad (\text{A5c})$$

and where \mathbf{A} and \mathbf{S}^a are $\rho \times \rho$ matrices with matrix elements $A_{sp} = \langle s | \mathbf{A} | p \rangle$ and $S_{sp}^a = \langle s | \mathbf{S}^a | p \rangle$, respectively, while $\mathbf{\Omega}(\varepsilon)$ is a $\rho \times \rho$ matrix with matrix elements (A4b).

Expression (A5b) produces all cardinal eigenvalues of the combined system. Once eigenvalue ε_k is obtained as a solution of (A5b), component $|\Psi_k^a\rangle \in X_\rho^a$ of the corresponding eigenstate $|\Psi_k\rangle$ equals

$$|\Psi_k^a\rangle = \frac{1}{\sqrt{Q_k}} |\theta_k\rangle, \tag{A6a}$$

where

$$Q_k = \langle \theta_k | \mathbf{S}^a | \theta_k \rangle + \beta^2 \sum_i^n \frac{\langle \theta_k | \mathbf{V} | \Phi_i \rangle \langle \Phi_i | \mathbf{V} | \theta_k \rangle}{(\varepsilon_k - \lambda_i)^2}, \tag{A6b}$$

and where $|\theta_k\rangle$ is an eigenstate of (A5a) corresponding to the eigenvalue ε_k . Component $|\Psi_k^a\rangle$ determines the corresponding X_n^b -component $|\Psi_k^b\rangle$ according to

$$|\Psi_k^b\rangle = \beta \sum_i^n \frac{\langle \Phi_i | \mathbf{V} | \Psi_k^a \rangle}{\varepsilon_k - \lambda_i} |\Phi_i\rangle. \tag{A6c}$$

Normalization constant Q_k ensures that the eigenstate $|\Psi_k\rangle$ is normalized according to the metrics induced by the operator $\mathbf{S} = \mathbf{S}^a + \mathbf{I}^b$. Hence $\langle \Psi_k | \mathbf{S} | \Psi_k \rangle = 1$ in accord with (A3a). Concerning the property $\langle \Psi_k | \mathbf{S} | \Psi_l \rangle = 0$ ($k \neq l$), this is automatically satisfied if $\varepsilon_k \neq \varepsilon_l$ [9]. However, if $\varepsilon_k = \varepsilon_l$ corresponding eigenstates are degenerate and in this case expression (A3a) should be enforced by some standard procedures such as Gram–Schmidt orthonormalization [10].

Expressions (A5) and (A6) produce all cardinal solutions of the eigenvalue equation (A2).

A.2 Singular solutions of $\mathbf{S}_{n+\rho}$

Let λ_j be η_j -degenerate eigenvalue of the system \mathbf{S}_n^b and let $|\Phi_{jm}\rangle$ ($m = 1, \dots, \eta_j$) be the corresponding eigenstates orthonormalized according to (A1b). Projection operator on the η_j -dimensional space $X_{\eta_j}^{bj}$ spanned by those eigenstates is

$$\mathbf{P}^{bj} = \sum_m^{\eta_j} |\Phi_{jm}\rangle \langle \Phi_{jm}|. \tag{A7}$$

Eigenvalue $\varepsilon_k \equiv \lambda_j$ is a (singular) eigenvalue of the combined system if and only if it satisfies [9]

$$\mathbf{H}(\lambda_j) |\theta^{aj}\rangle = -\beta \mathbf{V} \mathbf{P}^{bj} |\phi^{bj}\rangle, \tag{A8a}$$

$$\mathbf{P}^{bj} \mathbf{V} |\theta^{aj}\rangle = 0. \tag{A8b}$$

Since operator $\mathbf{H}(\lambda_j)$ acts in the space X_ρ^a while \mathbf{P}^{bj} is a projection operator on the space $X_{\eta_j}^{bj}$, one has $|\theta^{aj}\rangle \in X_\rho^a$ and $|\phi^{bj}\rangle \in X_{\eta_j}^{bj}$.

In the base $\{|s\rangle, |\Phi_{jm}\rangle\}$ ($s = 1, \dots, \rho; m = 1, \dots, \eta_j$) Eq. (A8) combine to a single $(\rho + \eta_j) \times (\rho + \eta_j)$ matrix equation. This equation has a nontrivial solution if and only if determinant of the system vanishes:

$$\begin{vmatrix} \mathbf{H}(\lambda_j) & \beta \mathbf{V} \mathbf{P}^{bj} \\ \beta \mathbf{P}^{bj} \mathbf{V} & \mathbf{0} \end{vmatrix} = 0, \quad (\text{A9a})$$

where $\mathbf{H}(\lambda_j)$ is a $\rho \times \rho$ matrix defined by (A5c), $\mathbf{W}^{(j)} \equiv \mathbf{V} \mathbf{P}^{bj}$ is a $\rho \times \eta_j$ matrix with matrix elements

$$W_{sm}^{(j)} = \langle s | \mathbf{V} | \Phi_{jm} \rangle, \quad s = 1, \dots, \rho, \quad m = 1, \dots, \eta_j. \quad (\text{A9b})$$

while $\mathbf{0}$ is a $\eta_j \times \eta_j$ null matrix. Since \mathbf{V} and \mathbf{P}^{bj} are Hermitian, one has $\mathbf{P}^{bj} \mathbf{V} = (\mathbf{V} \mathbf{P}^{bj})^+ = \mathbf{W}^{(j)+}$.

If λ_j satisfies (A9a), there is at least one nontrivial solution to (A8). In this case X_ρ^a -component of the corresponding normalized eigenstate $|\Psi^j\rangle = |\Psi^{aj}\rangle + |\Psi^{bj}\rangle$ equals [9]

$$|\Psi^{aj}\rangle = \frac{1}{\sqrt{Q}} |\theta^{aj}\rangle, \quad (\text{A10a})$$

where

$$Q = \langle \theta^{aj} | \mathbf{S}^a | \theta^{aj} \rangle + \langle \phi^{bj} | \phi^{bj} \rangle + \beta^2 \sum_{i(\lambda_i \neq \lambda_j)}^n \frac{\langle \theta^{aj} | \mathbf{V} | \Phi_i \rangle \langle \Phi_i | \mathbf{V} | \theta^{aj} \rangle}{(\lambda_j - \lambda_i)^2}, \quad (\text{A10b})$$

Corresponding X_n^b -component equals

$$|\Psi^{bj}\rangle = \frac{1}{\sqrt{Q}} \left[|\phi^{bj}\rangle + \beta \sum_{i(\lambda_i \neq \lambda_j)} \frac{\langle \Phi_i | \mathbf{V} | \theta^{aj} \rangle}{\lambda_j - \lambda_i} |\Phi_i\rangle \right]. \quad (\text{A10c})$$

Expressions (A8) and (A10) produce all singular solutions of the eigenvalue equation (A2).

It is convenient to distinguish two kinds of singular eigenstates. We call each singular eigenstate that satisfies $|\theta^{aj}\rangle = 0$ *strongly* singular, otherwise it is *weakly* singular.

A.2.1 Strongly singular solutions of $\mathbf{S}_{n+\rho}$

According to (A8) and (A10), each strongly singular eigenstate with the eigenvalue $\varepsilon_k \equiv \lambda_j$ is given by

$$|\Psi^j\rangle \equiv |\Psi^{bj}\rangle = \frac{1}{\sqrt{\langle \phi^{bj} | \phi^{bj} \rangle}} |\phi^{bj}\rangle. \tag{A11a}$$

where $|\phi^{bj}\rangle \in X_n^b$ satisfies

$$\mathbf{VP}^{bj} |\phi^{bj}\rangle = 0. \tag{A11b}$$

The number of such eigenstates depends on the properties of a $\rho \times \eta_j$ matrix $\mathbf{W}^{(j)} \equiv \mathbf{VP}^{bj}$. In a base $\{|s\rangle, |\Phi_{jm}\rangle\}$ expression (A11b) is a homogenous set of ρ linear equations in η_j unknowns:

$$\sum_m^{\eta_j} c_m \langle s | \mathbf{V} | \Phi_{jm} \rangle = 0, \quad s = 1, \dots, \rho, \tag{A11c}$$

where

$$|\phi^{bj}\rangle = \sum_m^{\eta_j} c_m |\Phi_{jm}\rangle. \tag{A11d}$$

and where c_m are unknown coefficients.

Let r_j be rank [10] of $\mathbf{W}^{(j)}$. One has $r_j \leq \rho$ and $r_j \leq \eta_j$ [10]. If $\eta_j > r_j$ expression (A11c) has $(\eta_j - r_j)$ linearly independent solutions and in this case combined system has $(\eta_j - r_j)$ strongly singular eigenstates $|\Psi^j\rangle$ with the eigenvalue λ_j . In particular, if $\eta_j > \rho$ combined system has at least $(\eta_j - \rho)$ strongly singular eigenstates. However, if $\eta_j = r_j$ combined system has no strongly singular eigenstate with this eigenvalue.

The set of all strongly singular eigenstates with the eigenvalue λ_j spans a $(\eta_j - r_j)$ -dimensional space $X_{\eta_j - r_j}^{bj-}$, subspace of $X_{\eta_j}^{bj}$. According to (A11b), this space is a nullspace [10] of $\mathbf{W}^{(j)}$. Let $X_{r_j}^{bj+}$ be a complement of $X_{\eta_j - r_j}^{bj-}$ in $X_{\eta_j}^{bj}$. This space is r_j -dimensional and it contains all vectors in $X_{\eta_j}^{bj}$ that are orthogonal to $X_{\eta_j - r_j}^{bj-}$. By definition, this is a column space [10] of $\mathbf{W}^{(j)}$. Those two spaces satisfy

$$X_{\eta_j - r_j}^{bj-} \oplus X_{r_j}^{bj+} = X_{\eta_j}^{bj}, \tag{A12a}$$

The space $X_{r_j}^{bj+}$ is an *active* subspace of $X_{\eta_j}^{bj}$. Each state in this space interacts with the system \mathbf{S}_ρ^a (i.e. it interacts with at least one state in X_ρ^a). On the other hand, $X_{\eta_j - r_j}^{bj-}$ is a *passive* subspace of $X_{\eta_j}^{bj}$. This space contains no state that interacts with \mathbf{S}_ρ^a .

In addition to active and passive spaces $X_{r_j}^{bj+}$ and $X_{\eta_j-r_j}^{bj-}$ which are associated with the eigenvalue λ_j , one can consider global active space $X^{b+} = \oplus_j X_{r_j}^{bj+}$ (orthogonal sum of all active spaces $X_{r_j}^{bj+}$) as well as global passive space $X^{b-} = \oplus_j X_{\eta_j-r_j}^{bj-}$ (orthogonal sum off all passive spaces $X_{\eta_j-r_j}^{bj-}$). Orthogonal sum of those two spaces is n -dimensional space X_n^b :

$$X_n^b = X^{b+} \oplus X^{b-}. \quad (\text{A12b})$$

Passive space X^{b-} is the largest linear space, subspace of the space X_n^b , which contains only those states which do not interact with the system \mathbf{S}_ρ^a . On the other hand, active space X^{b+} is the smallest linear space, subspace of the space X_n^b , which contains all those states that interact with this system. All strongly singular eigenstates of the combined system are contained in the passive space X^{b-} .

A.2.2 Weakly singular solutions of $\mathbf{S}_{n+\rho}$

By definition, each weakly singular eigenstate satisfies $|\theta^{aj}\rangle \neq 0$. Further, each such eigenstate must be orthogonal to all strongly singular eigenstates which span passive subspace $X_{\eta_j-r_j}^{bj-}$ of $X_{\eta_j}^{bj}$. Component $|\phi^{bj}\rangle$ of weakly singular eigenstate is hence contained in the active space $X_{r_j}^{bj+}$:

$$|\phi^{bj}\rangle \in X_{r_j}^{bj+}. \quad (\text{A13})$$

If $|\theta^{aj}\rangle \neq 0$ satisfies (A8a), the corresponding state $|\phi^{bj}\rangle \in X_{r_j}^{bj+}$ that satisfies this equation is unique. Assume namely that there are two different states $|\phi_1^{bj}\rangle \in X_{r_j}^{bj+}$ and $|\phi_2^{bj}\rangle \in X_{r_j}^{bj+}$ which satisfy (A8a) (with the same state $|\theta^{aj}\rangle$). In this case the state $|\phi^{bj}\rangle = |\phi_1^{bj}\rangle - |\phi_2^{bj}\rangle \neq 0$ satisfies (A11b) and hence $|\phi^{bj}\rangle \in X_{\eta_j-r_j}^{bj-}$. Since $X_{r_j}^{bj+}$ is a linear space this contradicts the assumption $|\phi_1^{bj}\rangle, |\phi_2^{bj}\rangle \in X_{r_j}^{bj+}$. X_n^b -component $|\Psi^{bj}\rangle$ of each weakly singular eigenstate $|\Psi^j\rangle$ is hence uniquely determined by its X_ρ^a -component $|\Psi^{aj}\rangle$. Since X_ρ^a is ρ -dimensional, combined system may have at most ρ linearly independent weakly singular eigenstates.

Weakly singular eigenstates are very rare. According to (A8b), the state $|\theta^{aj}\rangle \neq 0$ is contained in the left nullspace [10] $X_{r_j}^{aj-} \subseteq X_\rho^a$ of $\mathbf{W}^{(j)} \equiv \mathbf{V}^{\mathbf{P}bj}$ (since Hermitian conjugate of $\mathbf{W}^{(j)}$ is $\mathbf{P}^{bj}\mathbf{V}$). Dimension of this nullspace equals rank of $\mathbf{W}^{(j)}$, i.e. it equals r_j . On the other hand, according to (A8a) the state $\mathbf{H}(\lambda_j) |\theta^{aj}\rangle$ is contained in the space $X_{\rho-r_j}^{aj+} \subseteq X_\rho^a$. Since the space X_ρ^a is ρ -dimensional and since $\mathbf{W}^{(j)}$ has rank r_j , this space has dimension (at most) $\rho - r_j$. Accordingly, the state $|\theta^{aj}\rangle \neq 0$ has to satisfy simultaneously two conditions: $|\theta^{aj}\rangle \in X_{r_j}^{aj-} \subseteq X_\rho^a$ and $\mathbf{H}(\lambda_j) |\theta^{aj}\rangle \in X_{\rho-r_j}^{aj+} \subseteq X_\rho^a$. Since X_ρ^a is ρ -dimension, it is highly unlikely that those

two conditions will be satisfied in any particular case. In conclusion, combined system $\mathbf{S}_{n+\rho}$ only exceptionally may contain some weakly singular solutions.

One can distinguish two kinds of weakly singular eigenstates depending on whether $\mathbf{H}(\lambda_j) |\theta^{aj}\rangle \neq 0$ or $\mathbf{H}(\lambda_j) |\theta^{aj}\rangle = 0$. In the former case weakly singular eigenstate has a nonvanishing $X_{\eta_j}^b$ component $|\phi^{bj}\rangle \neq 0$. This component is contained in the active subspace $X_{r_j}^{bj+}$ of $X_{\eta_j}^b$. Such weakly singular eigenstate is hence of a general type (A10) where $|\theta^{aj}\rangle \neq 0$ and $|\phi^{bj}\rangle \neq 0$. In addition $|\phi^{bj}\rangle$ satisfies $|\phi^{bj}\rangle \in X_{r_j}^{bj+}$. Another possibility is $\mathbf{H}(\lambda_j) |\theta^{aj}\rangle = 0$. Each weakly singular eigenstate that satisfies this condition is an *anomal* eigenstate. According to (A8), an anomal eigenstate with the eigenvalue $\varepsilon = \lambda_j$ exists if and only if there is a nontrivial state $|\theta^{aj}\rangle \in X_{\rho}^a$ that satisfies

$$\mathbf{H}(\lambda_j) |\theta^{aj}\rangle = 0, \quad \mathbf{P}^{bj} \mathbf{V} |\theta^{aj}\rangle = 0. \tag{A14}$$

Since (A8a) implies $\mathbf{V} \mathbf{P}^{bj} |\phi^{bj}\rangle = 0$ and due to (A13), the state $|\phi^{bj}\rangle$ must vanish. Each anomal eigenstate with the eigenvalue $\varepsilon_k \equiv \lambda_j$ is hence of a general type (A10) where $|\theta^{aj}\rangle \neq 0$ and $|\phi^{bj}\rangle = 0$. This is formally almost identical to a general type (A6) of cardinal eigenstates.

A.3 Cardinal versus singular solutions of $\mathbf{S}_{n+\rho}$

There are important qualitative differences between cardinal and singular solutions. According to (A5a) each cardinal eigenvalue $\varepsilon_k \notin \{\lambda_i\}$ is at most ρ -degenerate, while according to (A8) each singular eigenvalue $\varepsilon_k \equiv \lambda_j \in \{\lambda_i\}$ is at most $(\rho + \eta_j)$ -degenerate. If the degeneracy η_j of the unperturbed eigenvalue λ_j is large, degeneracy of the singular eigenvalue $\varepsilon_k \equiv \lambda_j$ may be much bigger than the degeneracy of any cardinal eigenvalue. In particular, if $\eta_j > \rho$ combined system contains at least $\eta_j - \rho$ strongly singular eigenstates associated with the eigenvalue $\varepsilon_k \equiv \lambda_j$. On the other hand, however large η_j , this system may contain at most ρ weakly singular eigenstates associated with the eigenvalue $\varepsilon_k \equiv \lambda_j$. As emphasized in a previous section, even that much is quite unlikely and combined system only exceptionally may contain some weakly singular eigenstates. In addition, X_{ρ}^a -component $|\Psi_k^a\rangle$ of cardinal eigenstate $|\Psi_k\rangle$ uniquely determines X_n^b -component $|\Psi_k^b\rangle$ of this eigenstate (see A6c). Weakly singular eigenstates are in that respect similar to cardinal eigenstates. X_{ρ}^a -component of each weakly singular eigenstate also uniquely determines the corresponding X_n^b -component. However, this is not the case with strongly singular eigenstates which have no X_{ρ}^a -component.

A.4 Interlacing rule

In addition to the above expressions concerning cardinal and singular solutions, eigenvalues ε_k of $\mathbf{S}_{n+\rho}$ satisfy the interlacing rule [9].

Let the unperturbed eigenvalues λ_i be arranged in the nondecreasing order. Let the perturbed eigenvalues ε_k be also arranged in the nondecreasing order. Eigenvalues λ_i and ε_k thus arranged satisfy [9]

$$\varepsilon_i \leq \lambda_i \leq \varepsilon_{i+\rho}, \quad i = 1, \dots, n, \quad (\text{A15a})$$

In particular

$$\lambda_1 \leq \varepsilon_{\rho+1}, \quad \varepsilon_n \leq \lambda_n. \quad (\text{A15b})$$

Above rule applies to all eigenvalues of the combined system. If the particular eigenvalue ε_k is cardinal, corresponding inequality (\leq) should be replaced with strict inequality ($<$).

B Solution of the infinite combined system \mathbf{S}_∞

General strategy in the derivation of correct expressions for the description of open system \mathbf{S}_ρ^a that interacts with an infinite system \mathbf{S}_∞^b is to approximate infinite combined system $\mathbf{S}_\infty = \mathbf{S}_\rho^a \oplus \mathbf{S}_\infty^b$ with a finite combined system $\mathbf{S}_{n+\rho} = \mathbf{S}_\rho^a \oplus \mathbf{S}_n^b$ that contains $n + \rho$ eigenvalues and eigenstates. This can be done by replacing infinite-dimensional system \mathbf{S}_∞^b with n -dimensional system \mathbf{S}_n^b . As n increases, the corresponding finite-dimensional combined system $\mathbf{S}_{n+\rho}$ should converge to \mathbf{S}_∞ . The solution to this finite system is given in Sect. A. One now investigates the $n \rightarrow \infty$ limit of this solution. Provided \mathbf{S}_∞ is approximated by finite systems $\mathbf{S}_{n+\rho}$ in an appropriate way, this limit is well defined and in this way one derives corresponding expressions for the infinite combined system \mathbf{S}_∞ [5–8].

B.1 Isolated solutions of the combined system \mathbf{S}_∞

Each isolated eigenvalue ε_r of the combined system \mathbf{S}_∞ can be contained either in the range D or in its complement \overline{D} . In the case of isolated eigenvalues that satisfy $\varepsilon_r \in \overline{D}$ and which are cardinal ($\varepsilon_r \notin \{\lambda_j\}$), it is relatively easy to obtain the above $n \rightarrow \infty$ limit. For example, if the system \mathbf{S}_∞^b contains a single one-parameter eigenvalue band summation over i in (A4b) is replaced with an integral, and one finds

$$\Omega_{sp}(\varepsilon) \rightarrow \int \frac{\langle s | \mathbf{V} | \Phi(k) \rangle \langle \Phi(k) | \mathbf{V} | p \rangle}{\varepsilon - \lambda(k)} dk = \int \frac{f_{sp}(\lambda)}{\varepsilon - \lambda} d\lambda = \omega_{sp}(\varepsilon), \quad \varepsilon \in \overline{D}.$$

One thus derives expressions (15) [8]. In a similar way one derives those expressions in the general case when \mathbf{S}_∞^b contains several multiparameter eigenvalue bands and/or several isolated eigenstates. This proves expressions (15) which produce all isolated cardinal solutions of the combined system that satisfy $\varepsilon_r \in \overline{D}$.

In addition to the isolated solutions in the range \overline{D} , combined system may contain some isolated solutions in the complement \overline{D} of D . Those isolated solutions also sat-

isfy expressions (15), but in addition eigenstate $|\theta_r\rangle$ of (15a) satisfies (16). One obtains those solutions as an appropriate limit of embedded solutions [5–8] (see Sect. 6.2.3).

Concerning isolated singular solutions, in analogy to Sect. A.2 one finds that if the discrete eigenvalue λ_j of \mathbf{S}_∞^b is highly degenerate, combined system contains a large number of strongly singular eigenstates $|\Psi^j\rangle$ with the eigenvalue $\varepsilon_k \equiv \lambda_j$. However, only exceptionally this system may contain some weakly singular eigenstate with this eigenvalue (see Sect. A.3).

Consider now the distribution of the isolated eigenvalues $\varepsilon_r \in \overline{D}$. Let the range D contain two adjacent disconnected intervals $D_\mu = [a_\mu, b_\mu]$ and $D_\nu = [a_\nu, b_\nu]$ where $b_\mu < a_\nu$. Assume further that unperturbed system \mathbf{S}_∞^b contains t isolated eigenvalues in the interval $\overline{D}_{\mu\nu} = [b_\mu, a_\nu]$. In this case interlacing relations (A12) imply that the combined system \mathbf{S}_∞ may have at most $t + \rho$ isolated eigenvalues in this interval. In addition, if $t > \rho$ the combined system has at least $t - \rho$ isolated eigenvalues in this interval. The same applies to the extreme left and to the extreme right intervals in \overline{D} . In conclusion, in each subinterval of \overline{D} that is limited by adjacent intervals $D_\mu \subseteq D$ and $D_\nu \subseteq D$ (where in the case of extreme left subinterval its left edge equals $-\infty$, while in the case of extreme right subinterval its right edge equals $+\infty$) the interaction of the system \mathbf{S}_ρ^a with the system \mathbf{S}_∞^b may change (decrease or increase) the number of the initial isolated eigenvalues λ_i at most by ρ .

B.2 Embedded solutions of the combined system \mathbf{S}_∞

The case of embedded solutions with eigenvalues $\varepsilon \in D$ is more complex. Let us first see how the limit $n \rightarrow \infty$ can be obtained in the case when the system \mathbf{S}_∞^b contains a single one-parameter eigenvalue band and no isolated eigenvalues [8].

Case (a) The system \mathbf{S}_∞^b contains a single one-parameter eigenvalue band and no isolated eigenvalues. In this case expressions (2–4) reduce to

$$\mathbf{B} |\Phi(k)\rangle = \lambda(k) |\Phi(k)\rangle, \tag{B1a}$$

$$\langle \Phi(k) | \Phi(k') \rangle = \delta(k - k'), \tag{B1b}$$

$$\int |\Phi(k)\rangle \langle \Phi(k)| dk = \mathbf{I}^b, \quad k, k' \in [k_a, k_b]. \tag{B1c}$$

The range D contains a single interval $D = [a, b]$ where $a = \lambda(k_a)$ and $b = \lambda(k_b)$. Since there is a single one-parameter eigenvalue band and no isolated eigenstates, expressions (9) that define characteristic operator $\mathbf{f}(\varepsilon)$ reduce to

$$\mathbf{f}_{sp}(\varepsilon) \equiv \langle s | \mathbf{f}(\varepsilon) | p \rangle = \frac{\langle s | \mathbf{V} | \Phi(k) \rangle \langle \Phi(k) | \mathbf{V} | p \rangle}{d\lambda(k)/dk} \Big|_{k=\lambda^{-1}(\varepsilon)} \cdot \begin{cases} 1 & \text{if } \varepsilon \in D \\ 0 & \text{if } \varepsilon \notin D \end{cases} \tag{B2}$$

The corresponding derived operator $\omega(\varepsilon)$ is given in terms of this characteristic operator according to (13b).

One can now approximate infinite system \mathbf{S}_∞ by a finite-dimensional system $\mathbf{S}_{n+\rho} = \mathbf{S}_\rho^a \oplus \mathbf{S}_n^b$. First, approximate continuous eigenvalue function $\lambda(k)$ with n discrete eigenvalues $\lambda_i = \lambda(k_i)$ where k_i are equidistant and (in a limit $n \rightarrow \infty$) dense over the interval $[k_a, k_b]$:

$$k_i = k_a + (i - 0.5) \cdot \Delta k, \quad \Delta k = (k_b - k_a)/n, \quad i = 1, \dots, n. \tag{B3a}$$

Next, approximate continuous matrix elements $\langle s | \mathbf{V} | \Phi(k) \rangle$ with discrete matrix elements $\langle s | \mathbf{V} | \Phi(k_i) \rangle$ sampled at n points $k = k_i$. Due to the normalization condition

$$\int |\Phi(k)\rangle \langle \Phi(k)| dk = \mathbf{I}^b \Leftrightarrow \sum_i |\Phi_i\rangle \langle \Phi_i|$$

one has

$$\langle s | \mathbf{V} | \Phi(k) \rangle \rightarrow \langle s | \mathbf{V} | \Phi_i \rangle = \langle s | \mathbf{V} | \Phi(k_i) \rangle \sqrt{\Delta k}, \quad i = 1, \dots, n. \tag{B3b}$$

Above procedure [8] approximates infinite dimensional system \mathbf{S}_∞ with a finite dimensional system $\mathbf{S}_{n+\rho}$. Eigenvalues $\varepsilon_k (k = 1, \dots, n + \rho)$ of this finite system are interlaced with the unperturbed eigenvalues λ_i according to (A15a). Expression (A5a) produces all cardinal solutions of this finite system while expressions (A8) produce all singular solutions of this system. Next one should investigate $n \rightarrow \infty$ limit of those expressions. Due to the interlacing rule (A15a), in this limit all eigenvalues ε_k become dense in the interval $[a, b]$, except possibly at most 2ρ eigenvalues ε_k which may escape this interval and which become isolated eigenvalues of the combined system.

Using (B3), matrix elements $\Omega_{sp}(\varepsilon_k)$ of the operator $\Omega(\varepsilon_k)$ can be written as a sum [8]

$$\Omega_{sp}(\varepsilon_k) = \Omega_{sp}^{(0)}(\varepsilon_k) + \Omega_{sp}^{(1)}(\varepsilon_k), \tag{B4a}$$

where

$$\Omega_{sp}^{(0)}(\varepsilon_k) = \sum_{j=-N(n)}^{N(n)} \frac{\langle s | \mathbf{V} | \Phi(k_{k+j}) \rangle \langle \Phi(k_{k+j}) | \mathbf{V} | p \rangle}{\varepsilon_k - \lambda_{k+j}} \Delta k, \tag{B4b}$$

$$\begin{aligned} \Omega_{sp}^{(1)}(\varepsilon_k) &= \sum_{j < -N(n)} \frac{\langle s | \mathbf{V} | \Phi(k_{k+j}) \rangle \langle \Phi(k_{k+j}) | \mathbf{V} | p \rangle}{\varepsilon_k - \lambda_{k+j}} \Delta k \\ &+ \sum_{j > N(n)} \frac{\langle s | \mathbf{V} | \Phi(k_{k+j}) \rangle \langle \Phi(k_{k+j}) | \mathbf{V} | p \rangle}{\varepsilon_k - \lambda_{k+j}} \Delta k. \end{aligned} \tag{B4c}$$

In the above expressions $N(n) = \lfloor n^{1/3} \rfloor$ is the largest integer smaller than $n^{1/3}$. With this choice component $\Omega_{sp}^{(0)}(\varepsilon_k)$ contains contributions to the matrix element $\Omega_{sp}(\varepsilon_k)$ from approximately $2n^{1/3}$ unperturbed eigenvalues λ_{k+j} that are close to the perturbed eigenvalue ε_k , while component $\Omega_{sp}^{(1)}(\varepsilon_k)$ contains contributions from approximately $(n - 2n^{1/3}) \approx n$ remaining unperturbed eigenvalues λ_{k+j} that are relatively far from the perturbed eigenvalue ε_k . Since matrix elements $\langle s | \mathbf{V} | \Phi(k) \rangle$ are continuous functions of k , in the expression (B4b) one can approximate matrix elements $\langle s | \mathbf{V} | \Phi(k_{k+j}) \rangle$ with matrix elements $\langle s | \mathbf{V} | \Phi(k_k) \rangle$ to obtain [8]

$$\Omega_{sp}^{(0)}(\varepsilon_k) \approx \frac{\langle s | \mathbf{V} | \Phi(k_k) \rangle \langle \Phi(k_k) | \mathbf{V} | p \rangle}{(d\lambda/dk)_k} \sum_{j=-N(n)}^{N(n)} \frac{1}{x(\varepsilon_k) - j}.$$

where

$$x(\varepsilon_k) = \frac{\varepsilon_k - \lambda_{k-1}}{\lambda_k - \lambda_{k-1}}, \quad k = \rho + 1, \rho + 2, \dots, n. \tag{B5a}$$

With the identity [15]

$$\frac{1}{x} + \sum_{j=1}^{\infty} \left(\frac{1}{x - j} + \frac{1}{x + j} \right) = \pi \cot(\pi x).$$

One finds [8]

$$\Omega_{sp}^{(0)}(\varepsilon_k) \approx \pi \frac{\langle s | \mathbf{V} | \Phi(k_k) \rangle \langle \Phi(k_k) | \mathbf{V} | p \rangle}{(d\lambda/dk)_k} \cot(\pi x(\varepsilon_k)). \tag{B5b}$$

In this last step it is crucial that matrix elements $\langle s | \mathbf{V} | \Phi(k_{k+j}) \rangle$ smoothly change as index j continuously increases. This property follows from the fact that $\langle s | \mathbf{V} | \Phi(k) \rangle$ is a smooth function of k . Without this property transition from (B4b) to (B5b) is not possible [8].

Each $x(\varepsilon_k)$ is a *fractional shift* of the perturbed eigenvalue ε_k relative to the unperturbed eigenvalue λ_{k-1} [5–8]. In the limit $n \rightarrow \infty$ discrete quantities $x(\varepsilon_k)$ converge to a continuous function $x(\varepsilon)$ of a continuous parameter $\varepsilon \in D$. As n increases, approximation (B5b) improves and in a limit $n \rightarrow \infty$ it is exact [5,8]. One thus finds

$$\Omega_{sp}^{(0)}(\varepsilon_k) \rightarrow \pi f_{sp}(\varepsilon) \cot(\pi x(\varepsilon)), \quad \varepsilon \in D. \tag{B6a}$$

where matrix elements $f_{sp}(\varepsilon)$ are given by (B2). In a similar way one finds that in this limit component $\Omega_{sp}^{(1)}(\varepsilon_k)$ should be replaced according to [5,8]

$$\begin{aligned} \Omega_{sp}^{(1)}(\varepsilon_k) &\rightarrow P \int \frac{\langle s | \mathbf{V} | \Phi(k) \rangle \langle \Phi(k) | \mathbf{V} | p \rangle}{\varepsilon - \lambda(k)} dk = P \int \frac{f_{sp}(\lambda)}{\varepsilon - \lambda} d\lambda \\ &= \omega_{sp}(\varepsilon), \quad \varepsilon \in D, \end{aligned} \tag{B6b}$$

where P denotes principal Cauchy integral value [11]. Inserting expressions (B6) into (A5a) one derives fractional shift eigenvalue equation (22). In a similar way one derives expression (24a) [8].

Note the difference between fractional shift eigenvalue equation (22) that applies to an infinite combined system \mathbf{S}_∞ and eigenvalue equation (A5a) that applies to a finite combined system $\mathbf{S}_{n+\rho}$. Solutions to (A5a) are eigenvalues ε_k and the corresponding eigenstates $|\theta_k\rangle$. As n increases eigenvalues ε_k ($k = \rho + 1, \dots, n$) become dense in the range D , and in a limit $n \rightarrow \infty$ each $\varepsilon \in D$ becomes an eigenvalue of the combined system. There is hence no information content in the particular eigenvalue $\varepsilon \in D$. According to (22), this information about eigenvalues is replaced with the information about the fractional shift $x(\varepsilon)$. For almost each $\varepsilon \in D$ this quantity is well defined and it contains a nontrivial information about the embedded eigenstates of the combined system.

Above derivation of expressions (22) and (24) involves some assumptions which are not always satisfied [5–8]. More detailed analyze shows that those expressions are valid for each $\varepsilon \in D$, except for the anomalous points $\varepsilon_a \in D$ where the combined system may contain isolated eigenstates. By definition, $\varepsilon_a \in D$ is an anomalous point if there is a nontrivial state $|\varphi\rangle$ that satisfies $\mathbf{f}(\varepsilon_a)|\varphi\rangle = 0$ as well as $\mathbf{h}(\varepsilon_a)|\varphi\rangle = 0$ [8]. If this is the case, any value of $X(\varepsilon)$ is formally an eigenvalue of a fractional shift equation (22a).

Since the unperturbed system \mathbf{S}_∞^b contains a single one-parameter eigenvalue band, rank of the characteristic operator $\mathbf{f}(\varepsilon)$ in the range $D \equiv [a, b]$ is one, with a possible exception of few isolated points where this rank vanishes [8]. As a consequence, if $\mathbf{h}(\varepsilon)$ is regular in a point $\varepsilon \in D$ and if $\mathbf{f}(\varepsilon)$ has rank one, fractional shift eigenvalue equation (22a) has exactly one eigenstate $|\varphi(\varepsilon)\rangle$ and one corresponding eigenvalue $X(\varepsilon)$. The same is true if $\mathbf{h}(\varepsilon)$ is singular in some point $\varepsilon = \varepsilon_0 \in D$, provided no eigenstate of $\mathbf{h}(\varepsilon_0)$ satisfies at the same time $\mathbf{h}(\varepsilon_0)|\varphi(\varepsilon_0)\rangle = 0$ and $\mathbf{f}(\varepsilon_0)|\varphi(\varepsilon_0)\rangle = 0$, i.e. provided $\varepsilon = \varepsilon_0 \in D$ is not an anomalous point [8].

Above approach produces all embedded cardinal solutions of the combined system. In a similar way one finds embedded singular solutions of this system. First, one has to approximate infinite combined system \mathbf{S}_∞ with a finite dimensional system $\mathbf{S}_{n+\rho} = \mathbf{S}_\rho^a \oplus \mathbf{S}_n^b$. Instead of expression (A5a), one has now expressions (A8). According to the definition (A4b), from the summation that determines matrix elements $\Omega_{sp}(\varepsilon_k)$ ($\varepsilon_k \equiv \lambda_j$) one has to exclude all terms that satisfy $\lambda_i = \lambda_j$. One finds that in a limit $n \rightarrow \infty$ component $\Omega_{sp}^{(0)}(\varepsilon_k)$ of $\Omega_{sp}(\varepsilon_k)$ vanishes. Hence in this limit $\Omega_{sp}(\varepsilon_k) \rightarrow \omega_{sp}(\varepsilon)$ where $\omega_{sp}(\varepsilon)$ is given by (B6b). One thus derives expressions (19) where \mathbf{P}^ε is a projection on a subspace $X^{b\varepsilon}$ associated with the unperturbed eigenvalue $\lambda = \varepsilon$. Since X_∞^b contains a single one-parameter eigenvalue band, this projection operator equals

$$\mathbf{P}^\varepsilon = |\Phi(k)\rangle \langle \Phi(k)|, \quad k = \lambda^{-1}(\varepsilon). \quad (\text{B7})$$

In the case of finite combined system $\mathbf{S}_{n+\rho}$ singular solutions satisfy expressions (A8). Since each $\lambda(k)$ is nondegenerate, conditions (A11c) for the existence of strongly singular eigenstates reduce to $\langle s | \mathbf{V} | \Phi(k_i) \rangle = 0$ ($s = 1, \dots, \rho$). If \mathbf{V} is nontrivial, this

condition is very unlikely to be satisfied. According to the discussion in Sect. A.1.1., the same applies to the weakly singular solutions. As a result, combined system $\mathbf{S}_{n+\rho}$ may have only a small number of singular solutions, however large n . In a limit $n \rightarrow \infty$ the number of those solutions is negligible in comparison to the number of cardinal solutions (which are in this limit infinite in number).

One derives the same conclusion directly using expressions (19) where \mathbf{P}^ε is given by (B7). Since \mathbf{S}_∞^b contains a single one-parameter eigenvalue band, solutions of those expressions are of a general type $|\varphi(\varepsilon)\rangle \in X_\rho^a$ and $|\phi(\varepsilon)\rangle \in X_\infty^b$ with a single parameter $\varepsilon \in D$ and no additional parameters. In the case of strongly singular solutions that satisfy $|\varphi(\varepsilon)\rangle = 0$, those expressions reduce to $\mathbf{VP}^\varepsilon |\phi(\varepsilon)\rangle = 0$. Since each unperturbed eigenvalue $|\Phi(k)\rangle$ is nondegenerate this implies $\langle s | \mathbf{V} | \Phi(k)\rangle = 0$ ($s = 1, \dots, \rho$) where $k = \lambda^{-1}(\varepsilon)$. This requirement is equivalent to $\mathbf{f}(\varepsilon) = 0$. Characteristic operator $\mathbf{f}(\varepsilon)$ can vanish only in some isolated points $\varepsilon_c \in D$ and the number of strongly singular solutions is hence very limited. This number is negligible in comparison to the (c-infinite) number of cardinal solutions. Concerning weakly singular solutions, those solutions satisfy $|\varphi(\varepsilon)\rangle \neq 0$. Both conditions in (19) are hence nontrivial. In analogy to a finite case one again finds that combined system only exceptionally may contain some embedded weakly singular solutions. In particular, those solutions can exist only in some isolated points $\varepsilon_0 \in D$.

Our task here is to generalize the validity of the expressions (19), (22) and (24) from the above case when the system \mathbf{S}_∞^b contains a single one-parameter eigenvalue band to the general case when this system is described by the expressions (2) and (3). This will be done in few steps. Only most important points of this generalization will be given.

Case (b) The system \mathbf{S}_∞^b contains a single eigenvalue band with a continuous parameter k and with an additional parameter m that may have $\eta \leq \rho$ discrete values $1, \dots, \eta$. In this case expressions (B1) generalize to

$$\mathbf{B} |\Phi_m(k)\rangle = \lambda(k) |\Phi_m(k)\rangle, \tag{B8a}$$

$$\langle \Phi_m(k) | \Phi_{m'}(k') \rangle = \delta_{mm'} \delta(k - k'), \tag{B8b}$$

$$\sum_m^\eta \int |\Phi_m(k)\rangle \langle \Phi_m(k)| dk = \mathbf{I}^b, \quad k \in [k_a k_b], \quad m, m' = 1, \dots, \eta. \tag{B8c}$$

Range D again contains a single interval $D = [a, b]$ where $a = \lambda(k_a)$ and $b = \lambda(k_b)$. Characteristic operator $\mathbf{f}(\varepsilon)$ has matrix elements

$$\mathbf{f}_{sp}(\varepsilon) \equiv \langle s | \mathbf{f}(\varepsilon) | p \rangle = \frac{\sum_m^\eta \langle s | \mathbf{V} | \Phi_m(k)\rangle \langle \Phi_m(k) | \mathbf{V} | p \rangle}{d\lambda(k)/dk} \Bigg|_{k=\lambda^{-1}(\varepsilon)} \cdot \begin{cases} 1 & \text{if } \varepsilon \in D \\ 0 & \text{if } \varepsilon \notin D \end{cases} \tag{B9}$$

Most important difference between this case and previous case is that in a previous case rank of matrix $\mathbf{f}(\varepsilon)$ could be at most one, while in the present case this rank can be as large as η . In order to show this, write matrix elements $\mathbf{f}_{sp}(\varepsilon)$ in a form

$$\mathbf{f}_{sp}(\varepsilon) = \sum_m^\eta a_{sm}(\varepsilon) a_{pm}^*(\varepsilon)$$

where

$$a_{sm}(\varepsilon) = \frac{\langle s | \mathbf{V} | \Phi_m(k) \rangle}{\sqrt{d\lambda(k)/dk}} \Big|_{k=\lambda^{-1}(\varepsilon)}$$

Consider η column vectors $\mathbf{V}_m(\varepsilon) = (a_{1m}(\varepsilon), a_{2m}(\varepsilon), \dots, a_{\rho m}(\varepsilon))^T$ ($m=1, \dots, \eta$) where T denotes vector transpose. Each $\mathbf{V}_m(\varepsilon)$ is a ρ -dimensional column vector. Let $\mathbf{C}_l(\varepsilon)$ be l -th column of a matrix $\mathbf{f}(\varepsilon)$. This column can be written as a linear combination

$$\mathbf{C}_l(\varepsilon) = \sum_m^\eta a_{lm}^*(\varepsilon) (a_{1m}(\varepsilon), a_{2m}(\varepsilon), \dots, a_{\rho m}(\varepsilon))^T \equiv \sum_m^\eta a_{lm}^*(\varepsilon) \mathbf{V}_m(\varepsilon)$$

Each column of $\mathbf{f}(\varepsilon)$ is a linear combination of η vectors $\mathbf{V}_m(\varepsilon)$ and hence $\mathbf{f}(\varepsilon)$ has at most η linearly independent columns. This proves that the rank of $\mathbf{f}(\varepsilon)$ is at most η . Depending on linear dependence or independence of column vectors $\mathbf{V}_m(\varepsilon)$, this rank can assume any value smaller or equal to η . In conclusion, one has $\text{rank}(\mathbf{f}(\varepsilon)) \leq \eta$. In particular, if the system \mathbf{S}_∞^b contains a single one-parameter eigenvalue band (the case a) above, one has $\text{rank}(\mathbf{f}(\varepsilon)) \leq 1$.

One can now proceed in analogy to the case (a). First, approximate continuous eigenvalue function $\lambda(k)$ with n discrete eigenvalues $\lambda_i = \lambda(k_i)$ where k_i are given by (B3a). Concerning matrix elements $\langle s | \mathbf{V} | \Phi_m(k) \rangle$ one has

$$\sum_m^\eta \int |\Phi_m(k) \langle \Phi_m(k) | dk = \mathbf{I}^b \Leftrightarrow \sum_i |\Phi_i \rangle \langle \Phi_i|.$$

Those matrix elements should be sampled at n discrete points $k = k_i$ in such a way that in a limit $n \rightarrow \infty$ for each $m = 1, \dots, \eta$ one has dense sampling over entire range D . This can be done according to

$$\langle s | \mathbf{V} | \Phi_m(k) \rangle \rightarrow \langle s | \mathbf{V} | \Phi_i \rangle = \langle s | \mathbf{V} | \Phi_{i \bmod \eta}(k_i) \rangle \sqrt{\Delta k}, \quad i = 1, \dots, n, \quad (\text{B10})$$

where $i \bmod \eta$ is i modulo η . For each $s = 1, \dots, \rho$ the sequence $\langle s | \mathbf{V} | \Phi_{i \bmod \eta}(k_i) \rangle$ ($i = 1, \dots, n$) contains η subsequences. First of those subsequences contains matrix elements: $\langle s | \mathbf{V} | \Phi_1(k_{1+j\eta}) \rangle$ ($j = 1, 2, \dots$), second of those subsequences contains matrix elements $\langle s | \mathbf{V} | \Phi_2(k_{2+j\eta}) \rangle$ ($j = 1, 2, \dots$), etc. In a limit $n \rightarrow \infty$ each of those subsequences is a smooth function of a parameter k . This property is the main reason

for the particular sampling method (B10). Matrix elements $\Omega_{sp}(\varepsilon_k)$ of the operator $\Omega_{sp}(\varepsilon_k)$ can be now written as a sum (B4a) where

$$\begin{aligned} \Omega_{sp}^{(0)}(\varepsilon_k) &= \sum_{j=-N(n)}^{N(n)} \frac{\langle s | \mathbf{V} | \Phi_{(k+j) \bmod \eta}(k_{k+j}) \rangle \langle \Phi_{(k+j) \bmod \eta}(k_{k+j}) | \mathbf{V} | p \rangle}{\varepsilon_k - \lambda_{k+j}} \Delta k, \\ \Omega_{sp}^{(1)}(\varepsilon_k) &= \sum_{j < -N(n)} \frac{\langle s | \mathbf{V} | \Phi_{(k+j) \bmod \eta}(k_{k+j}) \rangle \langle \Phi_{(k+j) \bmod \eta}(k_{k+j}) | \mathbf{V} | p \rangle}{\varepsilon_k - \lambda_{k+j}} \Delta k \\ &+ \sum_{j > N(n)} \frac{\langle s | \mathbf{V} | \Phi_{(k+j) \bmod \eta}(k_{k+j}) \rangle \langle \Phi_{(k+j) \bmod \eta}(k_{k+j}) | \mathbf{V} | p \rangle}{\varepsilon_k - \lambda_{k+j}} \Delta k \end{aligned}$$

Due to the smoothness property of each subsequences of the sequence (B10), one can in analogy to (B5b) approximate component $\Omega_{sp}^{(0)}(\varepsilon_k)$ as

$$\Omega_{sp}^{(0)}(\varepsilon_k) \approx \pi \frac{\sum_m^d \langle s | \mathbf{V} | \Phi_m(k_k) \rangle \langle \Phi_m(k_k) | \mathbf{V} | p \rangle}{(d\lambda/dk)_k} \cot(\pi x(\varepsilon_k)).$$

In a limit $n \rightarrow \infty$ one derives (B6a) where matrix elements $f_{sp}(\varepsilon)$ are given by (B9). In a similar way one finds that in this limit component $\Omega_{sp}^{(1)}(\varepsilon_k)$ should be replaced according to

$$\begin{aligned} \Omega_{sp}^{(1)}(\varepsilon_k) &\rightarrow P \int \frac{\sum_m^\eta \langle s | \mathbf{V} | \Phi_m(k) \rangle \langle \Phi_m(k) | \mathbf{V} | p \rangle}{\varepsilon - \lambda(k)} dk = P \int \frac{f_{sp}(\lambda)}{\varepsilon - \lambda} d\lambda \\ &= \omega_{sp}(\varepsilon), \quad \varepsilon \in D. \end{aligned}$$

Inserting into (A5a) one again derives fractional shift eigenvalue equation (22). In a similar way one derives expression (24a).

There is an important new feature in this case. As emphasized above, for each $\varepsilon \in D$ rank of the characteristic operator $\mathbf{f}(\varepsilon)$ can be as large as η . Hence for each $\varepsilon \in D$ fractional shift eigenvalue equation (22a) may have as many as η eigenstates $|\varphi_d(\varepsilon)\rangle$ and η eigenvalues $X_d(\varepsilon)$, i.e. η corresponding fractional shifts $x_d(\varepsilon)$. In particular, if $\mathbf{h}(\varepsilon)$ is regular in a point $\varepsilon \in D$, fractional shift eigenvalue equation has exactly $r(\varepsilon) = \text{rank}(\mathbf{f}(\varepsilon))$ solutions in this point.

Case (c) This case is a generalization of a previous case to the case when η can assume any value, including the possibility $\eta = \infty$. In this case the system \mathbf{S}_∞^b is again described by expressions (B8), but without the restriction $\eta \leq \rho$.

For each $\varepsilon \in D$ the corresponding η -dimensional space $X_\eta^{b\varepsilon}$ is spanned by orthonormalized base $B(\varepsilon) \equiv \{|\Phi_m(k)\rangle : k = \lambda^{-1}(\varepsilon); m = 1, \dots, \eta\}$. Instead of this base, consider *interaction adopted base* $B^*(\varepsilon) \equiv \{|\Phi_m^*(k)\rangle : k = \lambda^{-1}(\varepsilon); m = 1, \dots, \eta\}$ that has the following property: first $r(\varepsilon) \leq \eta$ vectors of this base form a base $B^+(\varepsilon) \equiv \{|\Phi_m^*(k)\rangle : k = \lambda^{-1}(\varepsilon); m = 1, \dots, r(\varepsilon)\}$ of the active subspace $X_{r(\varepsilon)}^{b\varepsilon+}$ of the space

$X_\eta^{b\varepsilon}$. Each vector in $X_{r(\varepsilon)}^{b\varepsilon+}$ interacts with the space X_ρ^a . In general, dimension $r(\varepsilon)$ of $X_{r(\varepsilon)}^{b\varepsilon+}$ may depend on ε , but it can not exceed dimension ρ of the space X_ρ^a . Remaining $\eta - r(\varepsilon)$ vectors form a base $B^-(\varepsilon) \equiv \{|\Phi_m^*(k)\rangle: k = \lambda^{-1}(\varepsilon); m = r(\varepsilon) + 1, \dots, \eta\}$ of the passive subspace $X_{\eta-r(\varepsilon)}^{b\varepsilon-}$ of the space $X_\eta^{b\varepsilon}$. No vector in $X_{\eta-r(\varepsilon)}^{b\varepsilon-}$ interacts with the space X_ρ^a . Accordingly, all those vectors are strongly singular eigenstates of the combined system.

Cardinal solutions of the combined system can be now obtained in the same way as in the previous case, with the only difference that all relations should be expressed in the active base $B^+(\varepsilon)$, that is in terms of active vectors $|\Phi_m^*(k)\rangle$ instead of in terms of initial vectors $|\Phi_m(k)\rangle$. However, since

$$P^\varepsilon \equiv \sum_m^\eta |\Phi_m(k)\rangle \langle \Phi_m(k)| \equiv \sum_m^\eta |\Phi_m^*(k)\rangle \langle \Phi_m^*(k)|, \quad k = \lambda^{-1}(\varepsilon).$$

one can again express all those relations in the old base. For example, due to this identity one has

$$\left. \frac{\sum_m^\eta \langle s | \mathbf{V} | \Phi_m^*(k)\rangle \langle \Phi_m^*(k) | \mathbf{V} | p \rangle}{d\lambda(k)/dk} \right|_{\varepsilon=\lambda(k)} = \left. \frac{\sum_m^\eta \langle s | \mathbf{V} | \Phi_m(k)\rangle \langle \Phi_m(k) | \mathbf{V} | p \rangle}{d\lambda(k)/dk} \right|_{\varepsilon=\lambda(k)} = \mathbf{f}_{sp}(\varepsilon)$$

which proves (B9). In this way one again derives expressions (22) and (24) for the cardinal solutions of the combined system \mathbf{S}_∞ . One similarly derives expressions (19) for the singular solutions of this system. Unlike in the case (a) above, in this more general case combined system may contain a huge number of singular solutions. In particular, each strongly singular eigenstate that has eigenvalue ε is a linear combination

$$|\phi(k)\rangle = \sum_m^\eta c_m |\Phi_m(k)\rangle, \quad k = \lambda^{-1}(\varepsilon),$$

where coefficients c_m satisfy

$$\sum_m^\eta c_m \langle s | \mathbf{V} | \Phi_m(k)\rangle = 0, \quad s = 1, \dots, \rho.$$

If $\eta > \rho$, for each $\varepsilon \in D$ one has at least $(\eta - \rho)$ such eigenstates. All those eigenstates are contained in the passive subspace $X_{\eta-r(\varepsilon)}^{b\varepsilon-}$ of the space $X_\eta^{b\varepsilon}$. If η is large the number of such strongly singular eigenstates can be substantial. Concerning weakly singular eigenstates, one again finds that the combined system may contain only a limited number of such eigenstates.

Case (d) The system \mathbf{S}_∞^b contains a single eigenvalue band with the parameter k and with an additional continuous parameter l . In this case expressions (B1) generalize to

$$\mathbf{B} |\Phi(k, l)\rangle = \lambda(k) |\Phi(k, l)\rangle, \tag{B11a}$$

$$\langle \Phi(k, l) | \Phi(k', l') \rangle = \delta(k - k') \delta(l - l'), \tag{B11b}$$

$$\int |\Phi(k, l)\rangle \langle \Phi(k, l)| dk dl = \mathbf{I}^b, \quad k \in [k_a, k_b]. \tag{B11c}$$

In general, parameter l can assume each value in some interval $L(\varepsilon)$, where this interval may depend on $\varepsilon = \lambda(k)$. Range D again contains a single interval $D = [a, b]$, where $a = \lambda(k_a)$ and $b = \lambda(k_b)$. Characteristic operator $\mathbf{f}(\varepsilon)$ has matrix elements

$$f_{sp}(\varepsilon) \equiv \langle s | \mathbf{f}(\varepsilon) | p \rangle = \frac{\int \langle s | \mathbf{V} | \Phi(k, l) \rangle \langle \Phi(k, l) | \mathbf{V} | p \rangle dl}{d\lambda(k)/dk} \Big|_{k=\lambda^{-1}(\varepsilon)} \cdot \begin{cases} 1 & \text{if } \varepsilon \in D \\ 0 & \text{if } \varepsilon \notin D \end{cases}$$

This case is similar to the previous one. The only difference is that the discrete parameter m is replaced with continuous parameter l . As a consequence, for each $\varepsilon \in D$ one has a base $B(\varepsilon) \equiv \{|\Phi(k, l)\rangle : k = \lambda^{-1}(\varepsilon); l \in L(\varepsilon)\}$. Since l is continuous, the corresponding space $X_\infty^{b\varepsilon}$ spanned by this base is infinite-dimensional. One can again consider active and passive subspaces of the space $X_\infty^{b\varepsilon}$. In the same way as in the previous case one finds that the dimension $r(\varepsilon)$ of the active subspace $X_{r(\varepsilon)}^{b\varepsilon+}$ of the ∞ -dimensional space $X_\infty^{b\varepsilon}$ is finite and at most ρ . On the other hand, passive subspace $X_\infty^{b\varepsilon-}$ of $X_\infty^{b\varepsilon}$ is infinite-dimensional. Using active base one again derives expressions (22) and (24). Concerning passive base, the corresponding space $X_\infty^{b\varepsilon-}$ contains all strongly singular eigenstates of the combined system that have eigenvalue ε .

Above results can be easily generalized to the case when the system \mathbf{S}_∞^b contains a single multiparameter eigenvalue band that may depend on several discrete parameters m as well as on several continuous parameters l .

Case (e) System \mathbf{S}_∞^b contains several eigenvalue bands.

In this case system \mathbf{S}_∞^b is described by expressions (2a) and (2b). The only restriction on the generality of those expressions is that this system contains no isolated eigenvalues and eigenstates.

If no two bands overlap, generalization from a previous case to this case is rather straightforward. Since intervals I_ν are mutually disjoint, one can treat each such interval in the same way as in the previous case when the system \mathbf{S}_∞^b contains a single eigenvalue band [6, 7]. Characteristic function $\mathbf{f}(\varepsilon)$ is just a sum of band characteristic functions $\mathbf{f}_\nu(\varepsilon)$, and one again derives expressions (19), (22) and (24).

Slightly more complex is the case when some bands overlap. The main strategy in this case is described elsewhere [6, 7]. Consider the simplest case when the system \mathbf{S}_∞^b contains two bands ν and μ that partially or completely overlap. With the band

ν is associated eigenvalue function $\lambda_\nu(k)$ where $k \in [k_{a\nu}, k_{b\nu}]$ and with the band μ is associated eigenvalue function $\lambda_\mu(k)$ where $k \in [k_{a\mu}, k_{b\mu}]$. All eigenvalues of the first band are contained in the interval $I_\nu = [\lambda_\nu(k_{a\nu}), \lambda_\nu(k_{b\nu})]$ while all eigenvalues of the second band are contained in the interval $I_\mu = [\lambda_\mu(k_{a\mu}), \lambda_\mu(k_{b\mu})]$. Consider the interval $I_{\mu\nu} = I_\nu \cup I_\mu$. In general, this interval is a union of three subintervals of which only the subinterval $I = I_\mu \cap I_\nu$ which is the intersection of I_μ and I_ν contains elements of both bands. Hence those two overlapping eigenvalue bands can be formally treated as three eigenvalue bands of which only eigenvalue band corresponding to the intersection interval I requires some special treatment. With an appropriate rescaling of eigenvalue functions $\lambda_\nu(k)$ and $\lambda_\mu(k)$ within this interval one can transform both eigenvalue functions to the same eigenvalue function $\lambda(k)$ [6]. The interval I can be hence treated as if it contains a single (multiparameter) eigenvalue band. The problem of overlapping bands is thus reduced to the previous problem of nonoverlapping bands and following this prescription one again derives expressions (22) and (24).

Case (f) General case. System \mathbf{S}_∞^b is an arbitrary infinite-dimensional system containing several multiparameter eigenvalue bands and several isolated eigenstates.

After previous case is solved, one has only to add several isolated eigenstates to \mathbf{S}_∞^b . The entire derivation of expressions (22) and (24) is the same, except for the redefinition of characteristic operator $\mathbf{f}(\varepsilon)$ which is now defined in slightly more general way in order to include the effect of those additional isolated eigenstates.

The same applies to expressions (19) which describe embedded singular eigenstates. In particular one finds that (depending on the system \mathbf{S}_∞^b) for each $\varepsilon \in D$ combined system may contain a huge number of embedded strongly singular eigenstates. All those eigenstates are contained in the passive subspace $X^{b\varepsilon-}$ of the space $X^{b\varepsilon}$. Since those eigenstates do not have X_ρ^a -component, they do not contribute to the properties of the open system \mathbf{S}_ρ^a . Concerning embedded weakly singular eigenstates, the number of those eigenstates is limited. First note that for each $\varepsilon \in D$ one may have at most ρ such eigenstates, however large dimension of the space $X^{b\varepsilon}$. Next, since those eigenstates satisfy $|\varphi(\varepsilon, \dots)\rangle \neq 0$ and $|\phi(\varepsilon, \dots)\rangle \in X^{b\varepsilon+}$, one finds that conditions (19) can be satisfied only for some isolated points $\varepsilon_0 \in D$. As a result those eigenstates do not contribute to the properties of the open system \mathbf{S}_ρ^a (excluding anomalous eigenstates which are however isolated and not embedded eigenstates).

C Derivation of completeness relations (34)

Let $\{|\Psi_r\rangle\}$ be the set of all isolated eigenstates of \mathbf{S}_∞ , let $\{|\Psi_d(\varepsilon)\rangle\}$ be the set of all embedded cardinal eigenstates of \mathbf{S}_∞ and let $\{|\Psi(\varepsilon, \dots)\rangle\}$ be the set of all embedded singular eigenstates of \mathbf{S}_∞ . Those eigenstates form a complete set in X_∞ and hence

$$\sum_r |\Psi_r\rangle \langle \Psi_r| \mathbf{S} + \sum_d \int |\Psi_d(\varepsilon)\rangle \langle \Psi_d(\varepsilon)| \mathbf{S} d\varepsilon + \sum_{(\dots)} \int |\Psi(\varepsilon, \dots)\rangle \langle \Psi(\varepsilon, \dots)| \mathbf{S} d\varepsilon = \mathbf{I}, \quad (\text{C1a})$$

where $\mathbf{I} = \mathbf{I}^a + \mathbf{I}^b$ is a unit operator in X_∞ . First term involves summation over all isolated eigenstates $|\Psi_r\rangle$ of the combined system, second term involves integration of all embedded cardinal eigenstates $|\Psi_d(\varepsilon)\rangle$ over $\varepsilon \in D$ and summation over all such eigenstates, while third term involves integration of all embedded singular eigenstates $|\Psi(\varepsilon, \dots)\rangle$ over $\varepsilon \in D$ as well as summation and integration over all additional parameters, if any. Multiply expression (C1a) from the right by projection operator \mathbf{I}^a . Since strongly singular eigenstates have no X_ρ^a -component, as a result all such eigenstates contained in the third term of (C1a) vanish. Concerning weakly singular eigenstates, those eigenstates have nonvanishing X_ρ^a -component. However, weakly singular eigenstates that correspond to anomalous points are not embedded but rather isolated eigenstates. Those eigenstates are taken care in the first term of the above expression. Remaining embedded weakly singular eigenstates can exist only in some isolated points $\varepsilon = \varepsilon_0 \in D$. Hence the integration over ε in the above third term produces zero. Thus one finds

$$\sum_r |\Psi_r\rangle \langle \Psi_r^a | \mathbf{S}^a + \sum_d \int |\Psi_d(\varepsilon)\rangle \langle \Psi_d^a(\varepsilon) | \mathbf{S}^a d\varepsilon = \mathbf{I}^a,$$

Multiplying from left by \mathbf{I}^a this implies:

$$\sum_r |\Psi_r^a\rangle \langle \Psi_r^a | \mathbf{S}^a + \sum_d \int |\Psi_d^a(\varepsilon)\rangle \langle \Psi_d^a(\varepsilon) | \mathbf{S}^a d\varepsilon = \mathbf{I}^a. \tag{C1b}$$

Let $|\Theta\rangle \in X_\rho^a$ be an arbitrary state contained in the space X_ρ^a and let this state be normalized according to $\langle \Theta | \mathbf{S}^a | \Theta \rangle = 1$. In this case

$$\sum_r \langle \Theta | \mathbf{S}^a | \Psi_r^a \rangle \langle \Psi_r^a | \mathbf{S}^a | \Theta \rangle + \sum_d \int \langle \Theta | \mathbf{S}^a | \Psi_d^a(\varepsilon) \rangle \langle \Psi_d^a(\varepsilon) | \mathbf{S}^a | \Theta \rangle d\varepsilon = 1. \tag{C1c}$$

In particular, one can choose $|\Theta\rangle$ to be a local state $|\Theta_s\rangle$:

$$\sum_r \langle \Theta_s | \mathbf{S}^a | \Psi_r^a \rangle \langle \Psi_r^a | \mathbf{S}^a | \Theta_s \rangle + \sum_d \int \langle \Theta_s | \mathbf{S}^a | \Psi_d^a(\varepsilon) \rangle \langle \Psi_d^a(\varepsilon) | \mathbf{S}^a | \Theta_s \rangle d\varepsilon = 1, \tag{C2a}$$

Physically, $\langle \Theta_s | \mathbf{S}^a | \Psi_r^a \rangle \langle \Psi_r^a | \mathbf{S}^a | \Theta_s \rangle \equiv |\langle \Theta_s | \mathbf{S} | \Psi_r \rangle|^2 = w_{r,s}$ is a probability to find isolated eigenstate $|\Psi_r\rangle$ of a combined system in a local state $|\Theta_s\rangle$. Similarly, $\langle \Theta_s | \mathbf{S}^a | \Psi_d^a(\varepsilon) \rangle \langle \Psi_d^a(\varepsilon) | \mathbf{S}^a | \Theta_s \rangle \equiv |\langle \Theta_s | \mathbf{S} | \Psi_d(\varepsilon) \rangle|^2 = \rho_{d,s}(\varepsilon)$ is a probability density to find embedded cardinal eigenstate $|\Psi_d(\varepsilon)\rangle$ of a combined system in a local state $|\Theta_s\rangle$. In view of (27), this proves (34a). Summing over s and using (1c) one finds

$$\sum_r \langle \Psi_r^a | \mathbf{S}^a | \Psi_r^a \rangle + \sum_d \int \langle \Psi_d^a(\varepsilon) | \mathbf{S}^a | \Psi_d^a(\varepsilon) \rangle d\varepsilon = \rho, \tag{C2b}$$

which proves (34b).

D Derivation of the expression (11)

Consider integral

$$K(\varepsilon) \equiv P \int_a^b \frac{f(\lambda)}{\varepsilon - \lambda} d\lambda.$$

where P denotes principal integral value. This integral is defined as a limit

$$K(\varepsilon) \equiv \lim_{h \rightarrow 0} \left\{ \int_a^{\varepsilon-h} \frac{f(\lambda)}{\varepsilon - \lambda} d\lambda + \int_{\varepsilon+h}^b \frac{f(\lambda)}{\varepsilon - \lambda} d\lambda \right\}.$$

Expanding $f(\lambda)$ in the point $\varepsilon = \lambda$ and inserting this expansion in the above expression one finds

$$\begin{aligned} K(\varepsilon) &= - \lim_{h \rightarrow 0} \left\{ \int_a^{\varepsilon-h} \sum_{i=0}^{\infty} \frac{f^{(i)}(\varepsilon)}{i!} (\lambda - \varepsilon)^{i-1} d\lambda + \int_{\varepsilon+h}^b \sum_{i=0}^{\infty} \frac{f^{(i)}(\varepsilon)}{i!} (\lambda - \varepsilon)^{i-1} d\lambda \right\} \\ &= - \lim_{h \rightarrow 0} \left\{ f(\varepsilon) \left[\int_a^{\varepsilon-h} \frac{d\lambda}{\lambda - \varepsilon} + \int_{\varepsilon+h}^b \frac{d\lambda}{\lambda - \varepsilon} \right] \right. \\ &\quad \left. + \sum_{i=1}^{\infty} \frac{f^{(i)}(\varepsilon)}{i!} (\lambda - \varepsilon)^i \left[\int_a^{\varepsilon-h} + \int_{\varepsilon+h}^b \right] \right\} \\ &= f(\varepsilon) \ln \left| \frac{a - \varepsilon}{b - \varepsilon} \right| - \sum_{i=1}^{\infty} \frac{f^{(i)}(\varepsilon)}{i!} \left[(b - \varepsilon)^i - (a - \varepsilon)^i \right] \end{aligned}$$

This proves expressions (11).

E Expressions (17), (30) and (31)

Consider generic eigenvalue equation (15a). If one increases β by an infinitesimal amount $d\beta$, eigenvalue ε_r increases by $d\varepsilon_r$, while eigenstate $|\theta_r\rangle$ changes to $|\theta_r + \delta\theta_r\rangle$:

$$\left[(\beta + d\beta)^2 \boldsymbol{\omega}(\varepsilon_r + d\varepsilon_r) + \mathbf{A} - (\varepsilon_r + d\varepsilon_r) \mathbf{S}^a \right] |\theta_r + \delta\theta_r\rangle = 0.$$

Since $d\beta$ is infinitesimal this implies:

$$\left[\left(\beta^2 + 2\beta d\beta \right) \left(\boldsymbol{\omega}(\varepsilon_r) + \frac{d\boldsymbol{\omega}}{d\varepsilon_r} d\varepsilon_r \right) + \mathbf{A} - (\varepsilon_r + d\varepsilon_r) \mathbf{S}^a \right] |\theta_r + \delta\theta_r\rangle = 0.$$

Multiplying from left by $\langle \theta_r |$ and using (15a) one finds

$$d\varepsilon_r \left\langle \theta_r \left| \beta^2 \frac{d\boldsymbol{\omega}}{d\varepsilon_r} - \mathbf{S}^a \right| \theta_r + \delta\theta_r \right\rangle + 2\beta d\beta \langle \theta_r | \boldsymbol{\omega}(\varepsilon_r) | \theta_r + \delta\theta_r \rangle = 0.$$

Since $|\delta\theta_r\rangle$ is infinitesimal this implies (17).

Expression (30)

Consider fractional shift eigenvalue equation (22a). Increase ε by an infinitesimal amount $d\varepsilon$ to obtain

$$\left[\beta^2 \boldsymbol{\omega}(\varepsilon + d\varepsilon) + \mathbf{A} - (\varepsilon + d\varepsilon)\mathbf{S}^a \right] |\varphi_d(\varepsilon + d\varepsilon, \beta)\rangle = X_d(\varepsilon + d\varepsilon, \beta) \mathbf{f}(\varepsilon + d\varepsilon) |\varphi_d(\varepsilon + d\varepsilon, \beta)\rangle$$

For clarity, in the above and in the following expressions is explicitly emphasized the dependence of the eigenstate $|\varphi_d(\varepsilon)\rangle \equiv |\varphi_d(\varepsilon, \beta)\rangle$ and of the corresponding eigenvalue $X_d(\varepsilon) \equiv X_d(\varepsilon, \beta)$ on the coupling parameter β .

If $\mathbf{f}(\varepsilon)$ is analytic in the point $\varepsilon \in D$, $\boldsymbol{\omega}(\varepsilon)$ is also analytic in this point. If in addition $X_d(\varepsilon, \beta)$ is nondegenerate, one finds that $|\varphi_d(\varepsilon, \beta)\rangle$ and $X_d(\beta, \varepsilon)$ are also analytic in this point. One can hence expand those quantities in the point $\varepsilon \in D$ to obtain

$$\begin{aligned} & \left[\beta^2 \left(\boldsymbol{\omega}(\varepsilon) + \frac{d\boldsymbol{\omega}}{d\varepsilon} d\varepsilon \right) + \mathbf{A} - (\varepsilon + d\varepsilon)\mathbf{S}^a \right] |\varphi_d(\varepsilon + d\varepsilon, \beta)\rangle \\ & = \left(X_d(\varepsilon, \beta) + \frac{\partial X_d}{\partial \varepsilon} d\varepsilon \right) \left(\mathbf{f}(\varepsilon) + \frac{d\mathbf{f}}{d\varepsilon} d\varepsilon \right) |\varphi_d(\varepsilon + d\varepsilon, \beta)\rangle \end{aligned}$$

Multiplying from left by $\langle \varphi_d(\varepsilon, \beta) |$ using (22a) and neglecting higher order terms one finds

$$\begin{aligned} \left\langle \varphi_d(\varepsilon, \beta) \left| \left[\beta^2 \frac{d\boldsymbol{\omega}}{d\varepsilon} - \mathbf{S}^a \right] \right| \varphi_d(\varepsilon, \beta) \right\rangle &= X_d(\varepsilon, \beta) \left\langle \varphi_d(\varepsilon, \beta) \left| \frac{d\mathbf{f}}{d\varepsilon} \right| \varphi_d(\varepsilon, \beta) \right\rangle \\ &+ \frac{\partial X_d}{\partial \varepsilon} \langle \varphi_d(\varepsilon, \beta) | \mathbf{f}(\varepsilon) | \varphi_d(\varepsilon, \beta) \rangle \end{aligned}$$

This implies expression (30).

Expression (31) and anomal points

Let the unperturbed eigenvalue E_s be contained in the range $D(E_s \in D)$ and let this eigenvalue be nondegenerate. In this case there is one and only one eigenvalue $\varepsilon_s \equiv \varepsilon_s(\beta)$ of a generic eigenvalue equation (15a) such that $\varepsilon_s(0) = E_s$. Let the corresponding eigenstate $|\theta_s(\beta)\rangle$ satisfy $\mathbf{f}(E_s) |\theta_s(0)\rangle \equiv \mathbf{f}(E_s) |\Theta_s\rangle \neq 0$. As emphasized in Sect. 6.2, there is an embedded eigenstate $|\varphi_s(\varepsilon, \beta)\rangle$ of the fractional shift eigenvalue equation such that $X_s(\varepsilon_s(\beta), \beta) = 0$ and (up to the norm and phase) $|\varphi_s(\varepsilon_s(\beta), \beta)\rangle = |\theta_s(\beta)\rangle$. Note that fractional shift corresponding to the eigenvalue $X_s(\varepsilon_s(\beta), \beta) = 0$ equals $x_s(\varepsilon_s(\beta), \beta) = 0.5$. This fractional shift describes embedded eigenstate with the eigenvalue ε which is exactly in the middle between two adjacent infinitesimally

close unperturbed eigenvalues λ . If $\mathbf{f}(\varepsilon)$ is smooth in a point $\varepsilon = E_s \in D$ and in some small neighborhood of this point, one has

$$\begin{aligned}\mathbf{f}(\varepsilon) &\approx \mathbf{f}(\varepsilon_s), \quad |\varphi_s(\varepsilon, \beta)\rangle \approx |\varphi_s(\varepsilon_s(\beta), \beta)\rangle \propto |\theta_s(\beta)\rangle, \\ X_s(\varepsilon, \beta) &\approx (\partial X_s(\varepsilon_r, \beta)/\partial \varepsilon_r)(\varepsilon - \varepsilon_s(\beta)).\end{aligned}$$

Above approximations are reliable if $|\varepsilon - \varepsilon_s(\beta)|$ is sufficiently small, i.e. if $\varepsilon \in \Delta(\varepsilon_s)$ where $\Delta(\varepsilon_s)$ is some small neighborhood of the point $\varepsilon_s(\beta)$. For each β those expressions are exact in a point $\varepsilon = \varepsilon_s(\beta)$. Hence, provided $\varepsilon \in \Delta(\varepsilon_s)$, one can approximate (24b) as (31). If the width $\Delta\varepsilon_s(\beta)$ of the corresponding universal resonance curve as calculated by (33a) is as small as $\Delta\varepsilon_s(\beta) < \Delta(\varepsilon_s)$, component $|\Psi_s^a(\varepsilon, \beta)\rangle$ of the embedded eigenstate $|\Psi_s(\varepsilon, \beta)\rangle$ displays a prominent resonance feature at the resonant point $\varepsilon = \varepsilon_s(\beta)$. Since $\Delta\varepsilon_s(\beta)$ is proportional to the square of the interaction parameter β , this condition is satisfied if β is sufficiently small. This justifies approximation (31) in the case of small β . However, in some cases $\Delta\varepsilon_s(\beta)$ may be small even when β is not small. In particular, if matrix element $\langle \theta_s(\beta) | \mathbf{f}(\varepsilon_s(\beta)) | \theta_s(\beta) \rangle$ is sufficiently small, $\Delta\varepsilon_s(\beta)$ may be small even for large β . One has such an extreme case in the anomalous point ($\beta = \beta_a$, $\varepsilon = \varepsilon_s(\beta_a) \equiv \varepsilon_a$) where $\langle \theta_s(\beta_a) | \mathbf{f}(\varepsilon_a) | \theta_s(\beta_a) \rangle = 0$. One can not directly analyze such a point, since in this point the method by which fractional shift equation was derived as the $n \rightarrow \infty$ limit of expressions (A5a) breaks [8]. However one can analyze this point as the limit $\beta \rightarrow \beta_a$. In this limit $\langle \theta_s(\beta) | \mathbf{f}(\varepsilon_s(\beta)) | \theta_s(\beta) \rangle \rightarrow 0$. If $X_s(\varepsilon_a, \beta_a)$ is nondegenerate, as long as $\langle \theta_s(\beta) | \mathbf{f}(\varepsilon_s(\beta)) | \theta_s(\beta) \rangle \neq 0$, however small, one has at the point $\varepsilon = \varepsilon_s(\beta)$ resonant structure described by universal resonance curve (32b). In a limit $\beta \rightarrow \beta_a$ this curve becomes infinitely narrow and infinitely high with the exact area (33c). This is a δ -function $w_s^0(\beta_a)\delta(\varepsilon - \varepsilon_a)$. Accordingly, in this limit ($\beta \rightarrow \beta_a$) one has an isolated eigenstate at the anomalous point $\varepsilon = \varepsilon_a$. More rigorous treatment shows that in an anomalous point combined system may have one or several isolated eigenstates [8]. In particular, one finds that in a point $\beta = \beta_a$, X_ρ^a -component $|\Psi_\rho^a\rangle$ of the corresponding isolated solutions is given by expressions (15b) and (15c). This is implied by formal equality of probabilities (18b) and (33c).

Acknowledgements This work was supported in part by Grant No. 098-0982915-2942 of the Ministry of Science, Education and Sports of Croatia.

References

1. A. Messiah, *Quantum Mechanics* (North-Holland, Amsterdam, 1965) Third Printing
2. P.W. Atkins, R.S. Friedman, *Molecular Quantum Mechanics*, 3rd edn. (Oxford University Press, 1997)
3. N.W. Ashcroft, N.D. Mermin, *Solid State Physics* (Harcourt Brace College Publishers, 1976)
4. A. Zangwill, *Physics at Surfaces* (Cambridge University Press, 1988)
5. T.P. Živković, J. Math. Chem. **32**, 99 (2002)
6. T.P. Živković, J. Math. Chem. **39**, 151 (2006); *ibid* **39**, 295 (2006)
7. T.P. Živković, Croat. Chem. Acta. **77**, 279 (2004)
8. T.P. Živković, J. Math. Chem. **43**, 518 (2008)
9. T.P. Živković, J. Math. Chem. **32**, 39 (2002)
10. H. Anton, *Elementary Linear Algebra* (John Wiley & Sons, Inc., 1987)

11. J. Mathews, R.L. Walker, *Mathematical Methods of Physics* (W.A. Benjamin, Inc., Menlo Park, CA, 1970)
12. E.H. Wichmann, *Quantum Physics, Berkeley Physics Course*, vol. 4 (McGraw-Hill Company, 1971)
13. M.P. Silverman, *More than One Mystery* (Springer-Verlag, 1995)
14. W.H. Press, S.A. Teukolsky, W.T. Vetterling, B.P. Flannery, *Numerical Recipes in C, The Art of Scientific Computing* (Cambridge University Press, 1994)
15. C.-E. Fröberg, *Numerical Mathematics, Theory and Computer Applications* (The Benjamin/Cumming Publishing Company, 1985)