

Interaction of a finite quantum system with an infinite quantum system that contains a single one-parameter eigenvalue band

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Interaction of a finite quantum system \mathbf{S}_ρ^a that contains ρ eigenvalues and eigenstates with an infinite quantum system \mathbf{S}_∞^b that contains a single one-parameter eigenvalue band is considered. A new approach for the treatment of the combined system $\mathbf{S}_\infty \equiv \mathbf{S}_\rho^a \oplus \mathbf{S}_\infty^b$ is developed. This system contains embedded eigenstates $|\Psi(\varepsilon)\rangle$ with continuous eigenvalues ε , and, in addition, it may contain isolated eigenstates $|\Psi_s\rangle$ with discrete eigenvalues ε_s . Two $\rho \times \rho$ eigenvalue equations, a *generic* eigenvalue equation and a *fractional shift* eigenvalue equation are derived. It is shown that all properties of the system \mathbf{S}_ρ^a that interacts with the system \mathbf{S}_∞^b can be expressed in terms of the solutions to those two equations. The suggested method produces correct results, however strong the interaction between quantum systems \mathbf{S}_ρ^a and \mathbf{S}_∞^b . In the case of the weak interaction this method reproduces results that are usually obtained within the formalism of the perturbation expansion approach. However, if the interaction is strong one may encounter new phenomena with much more complex behavior. This is also the region where standard perturbation expansion fails. The method is illustrated with an example of a two-dimensional system \mathbf{S}_2^a that interacts with the infinite system \mathbf{S}_∞^b that contains a single one-parameter eigenvalue band. It is shown that all relevant completeness relations are satisfied, however strong the interaction between those two systems. This provides a strong verification of the suggested method.

KEY WORDS: interaction of quantum systems, time-independent perturbation, open quantum systems

1. Introduction

Consider the interaction of a finite quantum system \mathbf{S}_ρ^a that contains ρ discrete eigenvalues and eigenstates with an infinite quantum system \mathbf{S}_∞^b . System \mathbf{S}_ρ^a can be an arbitrary finite quantum system, while system \mathbf{S}_∞^b can be an arbitrary infinite system that contains eigenvalue bands and/or isolated eigenstates. We assume that the solution to the system \mathbf{S}_∞^b is known, and we concentrate on the following problem: What is the solution of a system \mathbf{S}_ρ^a subject to the

interaction with the system \mathbf{S}_∞^b ? In formal mathematical terms the solution of this problem requires determination of the eigenvalues and eigenstates of the combined system $\mathbf{S}_\infty \equiv S_\rho^a \oplus S_\infty^b$.

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 $|\Theta_p, \mathbf{k}\varpi\rangle$ where $|\mathbf{k}\varpi\rangle$ represents a state containing one-photon with momentum \mathbf{k} and polarization ϖ . States $|\Theta_p, \mathbf{k}\varpi\rangle$ 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 $|\Theta_p, \mathbf{k}\varpi\rangle$ with corresponding eigenvalues. The solution to this system is known since the states $|\mathbf{k}\varpi\rangle$ are essentially plane waves, while $|\Theta_p\rangle$ 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 dimensional 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 $\lambda_s(\mathbf{k})$ with the corresponding eigenstates $|\Phi_s(\mathbf{k})\rangle$ ($s = 1, 2, \dots$) [3]. In addition, system \mathbf{S}_∞^b may contain some discrete eigenvalues corresponding to the surface states [4]. One is usually 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, assuming this approximate solution to be good enough, the problem is to find a 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 (where \mathbf{S}_ρ^a is treated as the unperturbed system), or using some approximate semiclassical model [1–4]. If the interaction between the systems \mathbf{S}_ρ^a and \mathbf{S}_∞^b is relatively strong, convergence of the perturbation series may be very slow. In many cases of interest perturbation expansion may even diverge and the entire method fails. Also, if the interaction is relatively weak but if highly accurate results are needed, perturbation method may involve unacceptably large number of terms in order to obtain the required accuracy. Concerning various semiclassical models, those models are only approximate and they can never completely replace exact quantum treatment.

Recently a new method for the solution of those and similar problems was suggested [5–7]. 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 formulated for 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].

In a present paper the suggested method is generalized from the case $\rho = 1$ to the arbitrary case $\rho > 1$. In order to avoid possible complications that are not essential for this generalization, the system \mathbf{S}_∞^b is simplified and it is assumed that this system contains a single one-parameter eigenvalue band. Appropriate expressions for the more general case of the interaction of an arbitrary finite system \mathbf{S}_ρ^a with an arbitrary infinite system \mathbf{S}_∞^b can be obtained by combining results derived in this paper with results derived previously [8]. Also, in a present paper only a time-independent case is considered. 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 can be an arbitrary ρ -dimensional quantum system. With this system is associated ρ -dimensional space X_ρ^a . This system is described by the generalized eigenvalue equation

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

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

$$\langle \Theta_s | \mathbf{S}^a | \Theta_p \rangle = \delta_{sp}. \quad (1b)$$

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

$$\sum_s^\rho |\Theta_s\rangle \langle \Theta_s| \mathbf{S}^a = \mathbf{I}^a, \quad (1c)$$

where \mathbf{I}^a is a unite operator in X_ρ^a . We refer to the eigenstates $|\Theta_s\rangle$ of a system \mathbf{S}_ρ^a as *local* states.

The system \mathbf{S}_∞^b is an infinite quantum system that contains a single one-parameter eigenvalue band and no isolated eigenstates. With this system is associated an infinite-dimensional space X_∞^b . This system is described by the eigenvalue equation

$$\mathbf{B}|\Phi(k)\rangle = \lambda(k) |\Phi(k)\rangle, \quad k \in [k_a, k_b], \quad (2a)$$

where \mathbf{B} is a Hermitian operator in X_∞^b and where $\lambda(k)$ is continuous monotonic function of k . Without loss of generality one can assume that $\lambda(k)$ is monotonic increasing.

Eigenstates $|\Phi(k)\rangle$ of \mathbf{B} can be orthonormalized according to

$$\langle \Phi(k) | \Phi(k') \rangle = \delta(k - k'). \quad (2b)$$

Eigenvalues $\lambda(k)$ of \mathbf{B} are confined to the range $D = [\lambda_a, \lambda_b]$, where $\lambda_a = \lambda(k_a)$ is the smallest possible eigenvalue, while $\lambda_b = \lambda(k_b)$ is the largest possible eigenvalue. In the case when the system \mathbf{S}_∞^b contains a single one-parameter eigenvalue band, range D contains a single interval $[\lambda_a, \lambda_b]$. In a general case not considered here, this range may contain several overlapping and/or disjoint intervals [6–8]. We denote with \bar{D} the complement of D .

Relations (1a) and (2a) describe isolated 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. Operator \mathbf{V} can have nonvanishing matrix elements only between the states $|\Theta_s\rangle \in X_\rho^a$ and the states $|\Phi(k)\rangle \in X_\infty^b$. 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

$$\mathbf{C} |\Psi\rangle = \varepsilon \mathbf{S} |\Psi\rangle, \quad (3a)$$

where

$$\mathbf{C} = \mathbf{A} + \mathbf{B} + \beta \mathbf{V}, \quad \mathbf{S} = \mathbf{S}^a + \mathbf{I}^b, \quad (3b)$$

and where \mathbf{I}^b is a unit operator in X_∞^b . Since \mathbf{S}^a is positive definite in X_ρ^a , operator \mathbf{S} is positive definite in the combined space $X_\infty \equiv X_\rho^a \otimes X_\infty^b$. Eigenvalues ε of (3a) are hence real. Those eigenvalues can be discrete, in which case the corresponding eigenstates $|\Psi\rangle$ are normalized to unity, and they can be continuous, in which case the corresponding eigenstates $|\Psi\rangle$ are normalized to a delta function [5–7]. In analogy to (1b), this normalization should be done according to the metrics induced by the operator \mathbf{S} .

In the above formulation we have described the system \mathbf{S}_ρ^a 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 this case generalized eigenvalue equation (1a) reduces to a standard eigenvalue equation. Nevertheless, in certain cases it may be more appropriate to require $\mathbf{S}^a \neq \mathbf{I}^a$. For example, in the VB approach resonance structures are usually not orthogonal to each other. This leads to a Schrödinger equation of a type (1a) where $\mathbf{S}^a \neq \mathbf{I}^a$. Also the treatment of molecular vibrations leads to the eigenvalue equation of a type (1a) involving \mathbf{G} and \mathbf{F} matrices where $\mathbf{G} \neq \mathbf{I}^a$ and $\mathbf{F} \neq \mathbf{I}^a$ [9]. In the approach to be presented here, there is no substantial difference between the case $\mathbf{S}^a \neq \mathbf{I}^a$

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]. It is hence assumed that the system \mathbf{S}_∞^b is described by a standard eigenvalue equation (2a). If required, the suggested approach can be generalized to an arbitrary generalized eigenvalue equation [5].

Parameter β in (3b) is a coupling parameter between systems \mathbf{S}_ρ^a and \mathbf{S}_∞^b . Unlike standard perturbation method, the suggested approach does not rely on any kind of a power series expansion. There is hence no convergence problem, and resulting relations are valid for each value of β . Therefore one can simply in all relations replace $\beta \mathbf{V}$ with \mathbf{V} . Nevertheless, it is convenient to express the interaction as $\beta \mathbf{V}$ and not as \mathbf{V} . In this way the dependence on the coupling β is made explicit. In particular, it is easy to obtain results for the important case of the weak coupling, as well as the results for the other extreme of the strong coupling. To this effect it is convenient to normalize operator \mathbf{V} according to

$$\max_{\Theta \in X_\rho^a} \langle \Theta | \mathbf{V}^2 | \Theta \rangle = 1,$$

where $|\Theta\rangle \in X_\rho^a$ is normalized according to $\langle \Theta | \mathbf{S}^a | \Theta \rangle = 1$.

In the treatment of the system \mathbf{S}_ρ^a that interacts with the system \mathbf{S}_∞^b it is sometimes important to distinguish local eigenvalues $E_s \in D$ from local eigenvalues $E_s \in \bar{D}$. In order to emphasize this distinction we will denote with E_r those eigenvalues of (1a) that are contained inside the range D ($E_r \in D$) and with E_l (or E_j) those eigenvalues of (1a) that are contained outside this range ($E_l, E_j \in \bar{D}$). If this distinction is not important we will use generic notation E_s (or E_ρ). The same convention will be applied to all other quantities that refer to the range D and to its complement \bar{D} .

3. Solution of the combined system \mathbf{S}_∞

If $\rho = 1$ the combined system \mathbf{S}_∞ may contain two qualitatively different types of eigenvalues and eigenstates [5–7]. In the Appendix A.2 we show that the same applies to the case $\rho > 1$. Each ε contained in the range $D = [\lambda_a, \lambda_b]$ is an eigenvalue of this system. In addition, system \mathbf{S}_∞ may have finite number of discrete eigenvalues ε_s .

We call each discrete eigenvalue an *isolated* eigenvalue. Those isolated eigenvalues are usually contained in the complement \bar{D} of the range D . As shown in the Appendix A.2, there are at most ρ left isolated eigenvalues $\varepsilon_L < \lambda_a$

and at most ρ right isolated eigenvalues $\varepsilon_R > \lambda_b$. Since each eigenvalue $\varepsilon_I \in \bar{D}$ is discrete, the corresponding eigenstate or eigenstates $|\Psi_I\rangle$ can be normalized to unity. This normalization is done in accord with the metrics induced by the operator \mathbf{S} . In this respect isolated eigenstates $|\Psi_I\rangle$ are similar to the eigenstates $|\Theta_s\rangle \in X_\rho^a$ of the system \mathbf{S}_ρ^a .

In addition to isolated eigenvalues $\varepsilon_I \in \bar{D}$, combined system \mathbf{S}_∞ may contain some isolated eigenvalues $\varepsilon_r \in D$. As shown in the Appendix A.4.4, each such eigenvalue coincides with some *anomal point* of the combined system. We will discuss anomal and other characteristic points of the combined system in section 3.4.2.

We call each eigenvalue $\varepsilon \in D$ (that is not an isolated eigenvalue) an *embedded* eigenvalue. This eigenvalue is part of a continuous band of eigenvalues, and the corresponding eigenstates $|\Psi(\varepsilon)\rangle$ are normalized to a δ -function in accord with the metrics induced by the operator \mathbf{S} . In this respect embedded eigenstates of the combined system are similar to the eigenstates $|\Phi(k)\rangle$ of the system \mathbf{S}_∞^b that are also normalized to a δ -function.

3.1. Mathematical preliminaries

Eigenvalue equation (1a) that describes local system \mathbf{S}_ρ^a can be solved in any base $\{|\chi_s\rangle\} \in X_\rho^a$. Given this base, there is a unique operator \mathbf{K} acting in X_ρ^a such that

$$\langle \chi_s | \mathbf{K} | \chi_p \rangle = \delta_{sp}. \quad (4a)$$

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

$$\sum_s^\rho |\chi_s\rangle \langle \chi_s | \mathbf{K} = \mathbf{I}^a. \quad (4b)$$

In the base $\{|\chi_s\rangle\}$ operators \mathbf{A} and \mathbf{S}^a are $\rho \times \rho$ matrices with matrix elements A_{sp} and \mathbf{S}_{sp}^a , respectively

$$A_{sp} = \langle \chi_s | \mathbf{A} | \chi_p \rangle, \quad \mathbf{S}_{sp}^a = \langle \chi_s | \mathbf{S}^a | \chi_p \rangle, \quad s, p = 1, \dots, \rho. \quad (5)$$

In this base eigenvalue equation (1a) becomes a matrix eigenvalue equation. For the sake of simplicity we will use the same notation for operators \mathbf{A} and \mathbf{S}^a and their representations in this base.

As shown in the Appendix A, isolated and embedded solutions of the combined system can be expressed in terms of the solutions to two $\rho \times \rho$ eigenvalue equations. Those are *generic* and *fractional shift* eigenvalue equation. Besides operators \mathbf{A} and \mathbf{S}^a with matrix elements (5), those equations involve characteristic operator $\mathbf{f}(\varepsilon)$ and derived operator $\omega(\varepsilon)$. In analogy to operators \mathbf{A} and \mathbf{S}^a ,

operators $\mathbf{f}(\varepsilon)$ and $\boldsymbol{\omega}(\varepsilon)$ also act in the space X_ρ^a and in the base $\{|\chi_s\rangle\}$ they are also represented by $\rho \times \rho$ Hermitian matrices. Characteristic operator $\mathbf{f}(\varepsilon)$ incorporates essential features of the infinite system \mathbf{S}_∞^b and of the interaction of this system with the system \mathbf{S}_ρ^a . This operator vanishes in the complement \bar{D} of D and it is defined according to

$$\mathbf{f}(\varepsilon) = \frac{\mathbf{V}|\Phi(k)\rangle\langle\Phi(k)|\mathbf{V}}{d\lambda(k)/dk} \Big|_{\varepsilon=\lambda(k)} \cdot \begin{cases} 1 & \text{if } \varepsilon \in D, \\ 0 & \text{otherwise.} \end{cases} \quad (6a)$$

Matrix elements $f_{sp}(\varepsilon) = \langle\chi_s | \mathbf{f}(\varepsilon) | \chi_p\rangle$ of this operator are

$$f_{sp}(\varepsilon) = \frac{\langle\chi_s | \mathbf{V}|\Phi(k)\rangle\langle\Phi(k) | \mathbf{V} | \chi_p\rangle}{d\lambda(k)/dk} \Big|_{\varepsilon=\lambda(k)} \cdot \begin{cases} 1 & \text{if } \varepsilon \in D, \\ 0 & \text{otherwise.} \end{cases} \quad (6b)$$

Those matrix elements can be expressed in terms of ρ functions $a_s(\varepsilon)$

$$f_{sp}(\varepsilon) = a_s^*(\varepsilon)a_p(\varepsilon), \quad (6c)$$

where

$$a_s(\varepsilon) = \frac{\langle\Phi(k) | \mathbf{V} | \chi_s\rangle}{\sqrt{d\lambda(k)/dk}} \Big|_{\varepsilon=\lambda(k)} \cdot \begin{cases} 1 & \text{if } \varepsilon \in D, \\ 0 & \text{otherwise.} \end{cases} \quad s = 1, \dots, \rho. \quad (6d)$$

Right-hand sides of (6a), (6b) and (6d) are evaluated in the point k that satisfies $\varepsilon = \lambda(k)$. Since $\lambda(k)$ is an increasing function of k , derivative $d\lambda/dk$ is nonnegative and $\sqrt{d\lambda(k)/dk}$ in (6d) is real.

For each $\varepsilon \in D$ matrix $\mathbf{f}(\varepsilon)$ is either positive definite or zero. It is zero in a trivial case when all quantities $a_s(\varepsilon)$ ($s = 1, \dots, \rho$) vanish. Otherwise it is positive definite. In addition, (6c) implies that positive definite matrix $\mathbf{f}(\varepsilon)$ has rank one. Hence all eigenvalues of this matrix vanish, except of only one eigenvalue that may differ from zero. Eigenstates $|f_s(\varepsilon)\rangle$ of $\mathbf{f}(\varepsilon)$ can be arranged in such a way that they satisfy

$$\mathbf{f}(\varepsilon) |f_s(\varepsilon)\rangle = \xi_s(\varepsilon) |f_s(\varepsilon)\rangle, \quad (7a)$$

$$\xi_s(\varepsilon) = \xi_1(\varepsilon)\delta_{s1}, \quad (7b)$$

where $\xi_1(\varepsilon)$ is the eigenvalue corresponding to the eigenstate $|f_1(\varepsilon)\rangle$. Those eigenstates can be orthonormalized according to

$$\langle f_s(\varepsilon) | f_p(\varepsilon)\rangle = \delta_{sp}, \quad s, p = 1, \dots, \rho. \quad (7c)$$

Using (6) one finds

$$\xi_1(\varepsilon) = \sum_s^\rho a_s^*(\varepsilon)a_s(\varepsilon) = Tr(\mathbf{f}(\varepsilon)) \geq 0, \quad \varepsilon \in D, \quad (7d)$$

where $Tr(\mathbf{f}(\varepsilon))$ is a trace of the operator $\mathbf{f}(\varepsilon)$.

Since the system \mathbf{S}_∞^b contains a single one-parameter eigenvalue band, characteristic matrix $\mathbf{f}(\varepsilon)$ has rank at most one. In more general cases not considered here, this matrix may have any rank $\leq \rho$ and in such more general cases expressions (7b) and (7d) do not apply [8].

For the sake of generality we allow for the possibility that $\mathbf{f}(\varepsilon)$ may be discontinuous in some point or points $e_d \in D$. If this is the case there is at least one matrix element $f_{sp}(\varepsilon)$ that is discontinuous in this point. For example, if the infinite system \mathbf{S}_∞^b describes a solid, it may contain so-called van Hove singularities [3]. In such points matrix elements $f_{sp}(\varepsilon)$ may be discontinuous, or they may even diverge. We denote the set of all points $e_d \in D$ where $\mathbf{f}(\varepsilon)$ is discontinuous with Λ .

Unlike operator $\mathbf{f}(\varepsilon)$ that vanishes outside the range D , derived operator $\omega(\varepsilon)$ is nonzero in all points outside D and in almost all points inside D . This operator is expressed in terms of the characteristic operator $\mathbf{f}(\varepsilon)$ according to

$$\omega(\varepsilon) = P \int \frac{\mathbf{f}(\lambda)}{\varepsilon - \lambda} d\lambda, \tag{8a}$$

where P denotes principal Cauchy integral value [10]. If $\varepsilon \in \bar{D}$ this is a standard integral. However, if $\varepsilon \in D$ subintegral function on the right-hand side of (8a) may diverge in a point $\lambda = \varepsilon$. In this case one has to take a principal Cauchy integral value of this integral.

Matrix elements $\omega_{sp}(\varepsilon)$ of $\omega(\varepsilon)$ can be written in terms of the matrix elements $f_{sp}(\varepsilon)$ of $\mathbf{f}(\varepsilon)$ according to

$$\omega_{sp}(\varepsilon) = P \int \frac{f_{sp}(\lambda)}{\varepsilon - \lambda} d\lambda. \tag{8b}$$

Those matrix elements can be also written in a more explicit form

$$\omega_{sp}(\varepsilon) = P \int_{k_a}^{k_b} \frac{\langle \chi_s | \mathbf{V} | \Phi(k) \rangle \langle \Phi(k) | \mathbf{V} | \chi_p \rangle}{\varepsilon - \lambda(k)} dk. \tag{8c}$$

Since $\mathbf{f}(\lambda)$ is either positive definite or zero and since $\lim_{\varepsilon \rightarrow \pm\infty} \omega(\varepsilon) = 0$, one finds that for each $\varepsilon \in \bar{D}$ an arbitrary (nontrivial) state $|\Theta\rangle \in X_\rho^a$ satisfies

$$\langle \Theta | \omega(\pm\infty) | \Theta \rangle = 0, \tag{9a}$$

$$\langle \Theta | d\omega/d\varepsilon | \Theta \rangle < 0, \quad \varepsilon \in \bar{D}. \tag{9b}$$

Matrix $\omega(\varepsilon)$ is hence positive definite for each $\varepsilon \in (\lambda_b, \infty)$ and negative definite for each $\varepsilon \in (-\infty, \lambda_a)$. In other words, each nontrivial state $|\Theta\rangle \in X_\rho^a$ satisfies

$$\langle \Theta | \omega(\varepsilon) | \Theta \rangle < 0 \quad \text{if } \varepsilon \in (-\infty, \lambda_a) \quad \text{and} \quad \langle \Theta | \omega(\varepsilon) | \Theta \rangle > 0 \quad \text{if } \varepsilon \in (\lambda_b, \infty). \quad (9c)$$

If $f_{sp}(\varepsilon)$ is discontinuous in a point $e_d \in \Lambda$, matrix element $\omega_{sp}(\varepsilon)$ diverges in this point [7]. The type of the singularity in this point depends on the nature of discontinuity of $f_{sp}(\varepsilon)$. For example, if e_d is left (right) edge of the interval D and if right (left) limit value of $f_{sp}(\varepsilon)$ as one converges to this point is nonzero, $f_{sp}(\varepsilon)$ is discontinuous in this point. In this case one finds

$$\lim_{\varepsilon \rightarrow \lambda_a} \omega_{sp}(\varepsilon) = -\infty, \quad \lim_{\varepsilon \rightarrow \lambda_b} \omega_{sp}(\varepsilon) = \infty.$$

Thus if $e_d = \lambda_a$ matrix element $\omega_{sp}(\varepsilon)$ diverges to $-\infty$ in this point, while if $e_d = \lambda_b$ it diverges to $+\infty$ in this point. One also finds that in the former case left derivative $\omega_{sp}'(\varepsilon) = d\omega_{sp}(\varepsilon)/d\varepsilon$ of the corresponding matrix element converges to $-\infty$, while in a latter case right derivative of this matrix element converges to $-\infty$.

Operators \mathbf{A} and \mathbf{S}^a contain all information necessary for the description of the isolated system \mathbf{S}_ρ^a . As will be shown in following sections, characteristic operator $\mathbf{f}(\varepsilon)$ contains all additional information necessary for the description of this system subject to the interaction with the system \mathbf{S}_∞^b . In order to construct this operator it is not necessary to specify details of the infinite system \mathbf{S}_∞^b and of the interaction of this system with finite system \mathbf{S}_ρ^a . For this construction it is sufficient to know ρ functions $a_s(\varepsilon)$. There are many different systems \mathbf{S}_∞^b that may produce the same functions $a_s(\varepsilon)$. 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 \mathbf{S}_∞ .

3.2. Generic eigenvalue equation

Two equations are important for the solution of the combined system \mathbf{S}_∞ . First of those two equations is the “generic” equation

$$\left[\beta^2 \omega(\varepsilon_s) + \mathbf{A} \right] |\theta_s\rangle = \varepsilon_s \mathbf{S}^a |\theta_s\rangle. \quad (10)$$

This is a nonlinear eigenvalue equation. It may have eigenvalues $\varepsilon_I \in \bar{D}$ as well as eigenvalues $\varepsilon_r \in D$. As shown in the Appendix A.3 and in the following section, each eigenvalue $\varepsilon_I \in \bar{D}$ of this equation is an isolated eigenvalue of the combined system. In addition, eigenstate $|\theta_I\rangle \in X_\rho^a$ of (10) is proportional to the X_ρ^a -component of the corresponding isolated eigenstate $|\Psi_I\rangle$. Concerning eigenvalues $\varepsilon_r \in D$, those eigenvalues are so-called *resonant points* (see section 3.4.2) and they are related to the embedded solutions of the combined system. In some cases to be discussed later, those eigenvalues can be isolated eigenvalues of the

combined system. Generic equation (10) thus describes many important features of the combined system \mathbf{S}_∞ .

Formally, generic equation (10) is eigenvalue equation (1a) perturbed with the perturbation $\beta^2\omega(\varepsilon)$. One can consider each eigenvalue ε_s of this equation as a function of a coupling parameter β , i.e. $\varepsilon_s \equiv \varepsilon_s(\beta)$. For each local eigenvalue E_s , there is an eigenvalue $\varepsilon_s(\beta)$ that in a limit $\beta \rightarrow 0$ converges to E_s . If E_s is κ_s -degenerate, there are κ_s such eigenvalues $\varepsilon_s(\beta)$. Each such eigenvalue can be considered as the eigenvalue E_s of the isolated system \mathbf{S}_ρ^a perturbed by the interaction of this system with the infinite system \mathbf{S}_∞^b . If β is relatively small and if the operator $\omega(\varepsilon)$ is bounded in D , each eigenvalue ε_s of (10) is in this way associated with some unperturbed eigenvalue E_s . In this case there is one-to-one correspondence between eigenstates $|\Theta_s\rangle$ of the isolated system \mathbf{S}_ρ^a and eigenstates $|\theta_s\rangle$ of the generic eigenvalue equation. Hence eigenvalue equation (10) has exactly ρ eigenvalues and eigenstates. However and as emphasized in the previous section, operator $\omega(\varepsilon)$ may diverge in some points $e_d \in \Lambda$. In this case equation (10) may have some additional eigenvalues $\varepsilon_d \equiv \varepsilon_d(\beta)$, however small the coupling β (see Appendix A.6). In the limit $\beta \rightarrow 0$ each such additional eigenvalue converges to some point $e_d \in \Lambda$ where $\omega(\varepsilon)$ diverges, i.e. one has $\varepsilon_d(0) = e_d$. The point $e_d \in \Lambda$ may coincide with some local eigenvalue $E_s \in D$. If this is not the case ($e_d \notin \{E_s\}$), the point $\varepsilon_d(0) = e_d$ is not an eigenvalue of (10) in the case $\beta = 0$, though $\varepsilon_d(\beta)$ can be an eigenvalue of (10) for each $\beta > 0$, however small.

In conclusion, if the coupling β is small, each eigenvalue ε_s of (10) can be considered either as some local eigenvalue E_s perturbed by the interaction of the system \mathbf{S}_ρ^a with the infinite system \mathbf{S}_∞^b , and/or this eigenvalue may be associated with some divergent point $e_d \in \Lambda$ off $\omega(\varepsilon)$. Concerning those divergent points, of particular interest is the case when $\omega(\varepsilon)$ diverges on the left (right) edge of the range D . In this case one may have one or several isolated eigenvalues $\varepsilon_l \in \overline{D}$ as well as one or several resonant points $\varepsilon_r \in \overline{D}$ that in a limit $\beta \rightarrow 0$ converge to this edge of the range D . In section 4.1 we will give an example of such eigenvalues and corresponding eigenstates.

If the coupling β is not small, generic eigenvalue equation may have several eigenvalues that are associated with the same point $e_d \in \Lambda$. Such an example will be given in section 4.1. There may be also some additional eigenvalues that are associated neither with some the local eigenvalue E_s nor with some point e_d . This is due to the fact that generic eigenvalue equation is not linear. Hence if the coupling β is not small, the number of the eigenvalues to this equation can exceed the dimension ρ of the space X_ρ^a , even in the case when operator $\omega(\varepsilon)$ is bounded in the range D .

3.3. Isolated eigenvalues $\varepsilon_I \in \bar{D}$ and the corresponding eigenstates of the combined system

In the Appendix A.3 we show that $\varepsilon_I \in \bar{D}$ is an (isolated) eigenvalue of the combined system if and only if it is a root of the equation

$$h(\varepsilon_I) \equiv \left| \beta^2 \boldsymbol{\omega}(\varepsilon_I) + \mathbf{A} - \varepsilon_I \mathbf{S}^a \right| = 0, \quad \varepsilon_I \in \bar{D}, \quad (11)$$

where \mathbf{A} and \mathbf{S}^a are $\rho \times \rho$ matrices with matrix elements (5), while $\boldsymbol{\omega}(\varepsilon)$ is a $\rho \times \rho$ matrix with matrix elements (8b). Further, each normalized eigenstate $|\Psi_I\rangle$ corresponding to this eigenvalue is of the form

$$|\Psi_I\rangle = \frac{1}{\sqrt{Q_I}} \left[\sum_s^\rho C_s^{(I)} |\chi_s\rangle + \beta \int_{k_a}^{k_b} \frac{\sum_s^\rho \langle \Phi(k) | \mathbf{V} | \chi_s \rangle C_s^{(I)}}{\varepsilon_I - \lambda(k)} |\Phi(k)\rangle dk \right], \quad (12a)$$

where

$$Q_I = \sum_{sp}^\rho C_s^{(I)*} \mathbf{S}_{sp}^a C_p^{(I)} + \beta^2 \int_{\lambda_a}^{\lambda_b} \frac{\sum_{sp} C_s^{(I)*} f_{sp}(\lambda) C_p^{(I)}}{(\varepsilon_I - \lambda)^2} d\lambda, \quad (12b)$$

and where the coefficients $C_s^{(I)}$ are components of the vector $\mathbf{C}^{(I)}$ that is a non-trivial solution of the matrix equation

$$\left[\beta^2 \boldsymbol{\omega}(\varepsilon_I) + \mathbf{A} \right] \mathbf{C}^{(I)} = \varepsilon_I \mathbf{S}^a \mathbf{C}^{(I)}, \quad \varepsilon_I \in \bar{D}. \quad (12c)$$

Due to (4a) expression (12a) implies

$$C_s^{(I)} = \sqrt{Q_I} \langle \chi_s | \mathbf{K} | \Psi_I \rangle. \quad (12d)$$

Given an isolated eigenvalue ε_I , relation (12c) can have multiple solutions. Degeneracy of this eigenvalue equals nullity of a matrix $\mathbf{H}(\varepsilon_I) \equiv \beta^2 \boldsymbol{\omega}(\varepsilon_I) + \mathbf{A} - \varepsilon_I \mathbf{S}^a$. By definition [11], this nullity equals number of the linearly independent solutions $\mathbf{C}^{(I)}$ to the matrix equation (12c). Since this is a $\rho \times \rho$ matrix, an isolated eigenvalue ε_I can be at most ρ -degenerate.

Isolated eigenstate (12a) is normalized in accord with a metrics induced by the positive definite operator \mathbf{S} , i.e. $\langle \Psi_I | \mathbf{S} | \Psi_I \rangle = 1$. As shown in the Appendix A.3, all isolated eigenstates can be orthonormalized according to

$$\langle \Psi_I | \mathbf{S} | \Psi_J \rangle = \delta_{IJ}. \quad (13)$$

This relation is automatically satisfied if isolated eigenvalues ε_I and ε_J differ from each other, $\varepsilon_I \neq \varepsilon_J$. However, in the case of degenerate isolated eigenstates orthogonality (13) should be explicitly enforced. This can be done either

by Gram–Schmidt orthonormalization [11] or by any other orthonormalization procedure.

Above expressions produce all isolated solutions that have eigenvalues outside the range D . In order to find those solutions one has first to solve equation (11). Each solution $\varepsilon_I \in \overline{D}$ of this equation is an isolated eigenvalue. Once a particular isolated eigenvalue ε_I is found, the corresponding normalized eigenstate(s) is given by (12a) and (12b) where the coefficients $C_s^{(I)}$ are obtained as a solution of (12c).

One can write expressions (12) in a more compact form using generic eigenvalue equation. Isolated eigenstate $|\Psi_I\rangle$ is a linear combination $|\Psi_I\rangle = |\Psi_I^a\rangle + |\Psi_I^b\rangle$ where $|\Psi_I^a\rangle \in X_\rho^a$ and $|\Psi_I^b\rangle \in X_\infty^b$. Equation (12c) is an eigenvalue equation for the component $|\Psi_I^a\rangle$ of $|\Psi_I\rangle$. One easily finds that this equation is a generic eigenvalue equation (10) as written in a matrix form. According to (12a), if $\varepsilon_I \in \overline{D}$ the corresponding eigenstate $|\theta_I\rangle$ of (10) is proportional to the component $|\Psi_I^a\rangle$ of the isolated eigenstate $|\Psi_I\rangle$ of the combined system. In particular one has

$$|\Psi_I^a\rangle = \frac{1}{\sqrt{Q_I}} |\theta_I\rangle, \tag{14a}$$

where

$$Q_I = \langle \theta_I | \mathbf{S}^a | \theta_I \rangle - \beta^2 \langle \theta_I | \mathbf{d}\omega / \mathbf{d}\varepsilon_I | \theta_I \rangle. \tag{14b}$$

Eigenstate $|\theta_I\rangle$ of (10) is related to the eigenvector $\mathbf{C}^{(1)}$ of (12c) according to

$$|\theta_I\rangle = \sum_s^\rho C_s^{(I)} |\chi_s\rangle.$$

Once $\varepsilon_I \in \overline{D}$ and $|\theta_I\rangle$ are obtained as a solution of (10), one can derive $|\Psi_I^b\rangle \in X_\infty^b$ according to

$$|\Psi_I^b\rangle = \frac{\beta}{\sqrt{Q_I}} \int_{k_a}^{k_b} \frac{\langle \Phi(k) | \mathbf{V} | \theta_I \rangle}{\varepsilon_I - \lambda(k)} |\Phi(k)\rangle \, dk. \tag{14c}$$

Note that the components $|\Psi_I^a\rangle$ and $|\Psi_I^b\rangle$ of $|\Psi_I\rangle$ are not normalized in accord with a metrics induced by the operator \mathbf{S} . In this way is normalized only the complete eigenstate $|\Psi_I\rangle$.

In conclusion, each eigenvalue $\varepsilon_I \in \overline{D}$ of the generic equation is an isolated eigenvalue of the combined system. The corresponding eigenstate $|\theta_I\rangle$ determines X_ρ^a component of the isolated eigenstate $|\Psi_I\rangle$ according to (14a) and (14b). In addition, X_∞^b component of this eigenstate is determined according to (14c). In this way generic equation determines all isolated eigenvalues $\varepsilon_I \in \overline{D}$ and all the

corresponding eigenstates $|\Psi_I\rangle$. We shall discuss remaining eigenvalues $\varepsilon_r \in D$ and the corresponding eigenstates $|\theta_r\rangle$ of (10) in section 3.4.4.

3.3.1. Properties of isolated eigenvalues $\varepsilon_I \in \bar{D}$ and of the corresponding eigenstates

Consider now some characteristic properties of those solutions of (10) that are associated with the isolated eigenvalues $\varepsilon_I \in \bar{D}$. As shown in the Appendix A.2, one may have at most ρ left isolated eigenvalues $\varepsilon_I \equiv \varepsilon_L < \lambda_a$ and at most ρ right isolated eigenvalues $\varepsilon_I \equiv \varepsilon_R > \lambda_a$. Thus one may have as many as 2ρ isolated eigenvalues $\varepsilon_I \in \bar{D}$. Further, in a metrics defined by the operator \mathbf{S} , probability to find isolated eigenstate $|\Psi_I\rangle$ in a normalized state $|\Theta\rangle \in X_\rho^a$ ($\langle\Theta|\mathbf{S}^a|\Theta\rangle = 1$) is a square $|\langle\Theta|\mathbf{S}|\Psi_I\rangle|^2$ of the amplitude $\langle\Theta|\mathbf{S}|\Psi_I\rangle \equiv \langle\Theta|\mathbf{S}^a|\Psi_I^a\rangle$. According to (14a) this amplitude equals

$$\langle\Theta|\mathbf{S}|\Psi_I\rangle = \frac{\langle\Theta|\mathbf{S}^a|\theta_I\rangle}{\sqrt{Q_I}}. \quad (15)$$

In particular, probability $w_{I_s}^a = |\langle\Theta_s|\mathbf{S}|\Psi_I\rangle|^2$ to find isolate eigenstate $|\Psi_I\rangle$ in the local state $|\Theta_s\rangle \in X_\rho^a$ equals

$$w_{I_s}^a = \frac{\langle\theta_I|\mathbf{S}^a|\Theta_s\rangle\langle\Theta_s|\mathbf{S}^a|\theta_I\rangle}{\langle\theta_I|\mathbf{S}^a|\theta_I\rangle - \beta^2\langle\theta_I|\mathbf{d}\omega/\mathbf{d}\varepsilon_I|\theta_I\rangle}. \quad (16a)$$

Since local states $|\Theta_s\rangle$ form a complete set in X_ρ^a , the probability w_I^a to find isolated eigenstate $|\Psi_I\rangle$ in the system \mathbf{S}_ρ^a , that is to find this eigenstate in any of the states $|\Theta\rangle \in X_\rho^a$, equals $w_I^a = \sum_s w_{I_s}^a$. Hence and due to (1c)

$$w_I^a \equiv \sum_s w_{I_s}^a \equiv \langle\Psi_I^a|\mathbf{S}^a|\Psi_I^a\rangle = \frac{\langle\theta_I|\mathbf{S}^a|\theta_I\rangle}{\langle\theta_I|\mathbf{S}^a|\theta_I\rangle - \beta^2\langle\theta_I|\mathbf{d}\omega/\mathbf{d}\varepsilon_I|\theta_I\rangle}. \quad (16b)$$

In a similar way, probability density $\rho_I(k)$ to find isolated eigenstate $|\Psi_I\rangle$ in the state $|\Phi(k)\rangle \in X_\infty^b$ is a square of the amplitude $\langle\Phi(k)|\mathbf{S}|\Psi_I\rangle \equiv \langle\Phi(k)|\Psi_I^b\rangle$

$$\rho_I(k) = \left| \langle\Phi(k)|\Psi_I^b\rangle \right|^2. \quad (17a)$$

According to (14c) this amplitude equals

$$\langle\Phi(k)|\Psi_I^b\rangle = \frac{\beta}{\sqrt{Q_I}} \frac{\langle\Phi(k)|\mathbf{V}|\theta_I\rangle}{(\varepsilon_I - \lambda(k))}. \quad (17b)$$

Since the states $|\Phi(k)\rangle$ form a complete set in X_∞^b the probability w_I^b to find isolated eigenstate $|\Psi_I\rangle$ in the system \mathbf{S}_∞^b equals

$$w_I^b = \int \rho_I(k) dk = \frac{\beta^2}{Q_I} \int \frac{|\langle\Phi(k)|\mathbf{V}|\theta_I\rangle|^2}{(\varepsilon_I - \lambda(k))^2} dk. \quad (17c)$$

The state $|\Psi_I\rangle$ should be found with certainty either in a system \mathbf{S}_ρ^a or in a system \mathbf{S}_∞^b . Hence above probabilities must satisfy completeness requirement

$$w_I^a + \int \rho_I(k) dk = 1. \quad (18)$$

One can formally derive this expression from relations (14).

Each isolated eigenvalue $\varepsilon_I \in \bar{D}$ can be considered as a function of the coupling β as well as a function of local eigenvalues E_s . One finds (see Appendix A.5)

$$\frac{\partial \varepsilon_I}{\partial \beta} = \frac{2\beta \langle \theta_I | \boldsymbol{\omega}(\varepsilon_I) | \theta_I \rangle}{\langle \theta_I | \mathbf{S}^a | \theta_I \rangle - \beta^2 \langle \theta_I | d\boldsymbol{\omega}/d\varepsilon_I | \theta_I \rangle}, \quad (19a)$$

$$\frac{\partial \varepsilon_I}{\partial E_s} = w_{I_s}^a \geq 0. \quad (19b)$$

Above relations give the rate of change of the isolated eigenvalue ε_I with a change of a coupling β and with a change of local eigenvalues E_s . According to (19a) and due to (9c), if the coupling β increases isolated eigenvalue ε_I moves away from the interval $D = [\lambda_a, \lambda_b]$. Thus the effect of the coupling β is to repeal each isolated eigenvalue away from this interval. According to (19b), derivative $\partial \varepsilon_I / \partial E_s$ equals probability $w_{I_s}^a = |\langle \Theta_s | \mathbf{S} | \Psi_I \rangle|^2$ to find isolate eigenstate $|\Psi_I\rangle$ in the local state $|\Theta_s\rangle \in X_\rho^a$. In particular, if a local eigenvalue E_s increases (decreases), isolated eigenvalue ε_I also increases (decreases), i.e., it moves in the same direction. In addition and due to (9b) one has $0 \leq \partial \varepsilon_I / \partial E_s < 1$. One also finds

$$w_I^a = \sum_s^\rho \frac{\partial \varepsilon_I}{\partial E_s}. \quad (19c)$$

Consider finally the case when $\mathbf{f}(\varepsilon)$ is discontinuous on the edge λ_a or λ_b of the range D . In this case $\boldsymbol{\omega}(\varepsilon)$ as well as $d\boldsymbol{\omega}/d\varepsilon$ diverges in this point [7] and by definition the edge in question is contained in the set Λ . If isolated eigenvalue ε_I is very close to this edge, $d\boldsymbol{\omega}/d\varepsilon_I$ is very large. Depending on the eigenstate $|\theta_I\rangle$ of (10), this usually implies that matrix element $\langle \theta_I | d\boldsymbol{\omega}/d\varepsilon_I | \theta_I \rangle$ has very large negative value. Probabilities $w_{I_s}^a$ and w_I^a (equations (16)) are hence extremely small. As a consequence, contributions of isolated solutions that are associated with the discontinuity of $\mathbf{f}(\varepsilon)$ on the edge of the range D to various densities is in this case negligible. In addition, as long as ε_I is close to the edge in question, derivatives $\partial \varepsilon_I / \partial \beta$ and $\partial \varepsilon_I / \partial E_s$ (equations (19)) are also extremely small. Under those conditions $\varepsilon_I \equiv \varepsilon_I(\beta)$ considered as a function of β is approximately constant, i.e. it moves very slowly away from the edge in question. In section 4 we will illustrate those properties with an example where $\lambda_a \in \Lambda$. In this case $\mathbf{f}(\varepsilon)$ is discontinuous on the left edge λ_a of the range D and $\boldsymbol{\omega}(\varepsilon)$ as well as $d\boldsymbol{\omega}/d\varepsilon$ diverge in the point $\varepsilon = \lambda_a$.

3.3.2. Isolated solutions in the weak coupling limit

Standard perturbation expansion approach treats the case when the coupling β is small [1, 2]. In this case and if $E_I \in \bar{D}$ is an interior point of the point-set \bar{D} , relation (10) has a root $\varepsilon_I \in \bar{D}$ that is close to $\varepsilon = E_I$. If E_I is non-degenerate and if $\omega(\varepsilon)$ does not diverge in a point $\varepsilon = E_I$, one finds $\varepsilon_I \approx E_I + \beta^2 \langle \Theta_I | \omega(E_I) | \Theta_I \rangle$ (see (A.32a)). This approximation has a structure of the second order perturbation correction. Since $\langle \chi_s | \mathbf{V} | \chi_p \rangle = 0$ there is no first order correction. This result is in accord with the standard perturbation expansion method that includes second order expansion terms [1, 2].

The case when $\mathbf{f}(\varepsilon)$ is discontinuous on some edge of the range D requires a special treatment. In this case for each coupling $\beta > 0$ perturbation $\beta\omega(\varepsilon)$ is on this edge infinite. Hence standard perturbation expansion fails. Examining expression (10) one finds that in this case combined system \mathbf{S}_∞ may contain an isolated eigenvalue $\varepsilon_L < \lambda_a (\varepsilon_R > \lambda_b)$, however small the coupling $\beta > 0$. For example, if $\mathbf{f}(\varepsilon)$ is discontinuous in the point $\varepsilon = \lambda_a$ and if $\lim_{\varepsilon \rightarrow \lambda_a^+} \mathbf{f}(\varepsilon) \neq 0$ is finite, one finds that for sufficiently small β generic equation (10) has eigenvalues $\varepsilon_s(\beta) \approx \lambda_a \pm A \exp(-K/\beta^2)$ where $A > 0$ and $K > 0$ are constants [8]. In particular, the eigenvalue $\varepsilon_L(\beta) \approx \lambda_a - A \exp(-K/\beta^2) < \lambda_a$ of (10) is a left isolated eigenvalue of the combined system. For small β this eigenvalue is extremely close to the point λ_a where $\mathbf{f}(\varepsilon)$ is discontinuous and according to the discussion in a previous section, one has $w_{I_s} \approx 0$. In conclusion, if $\mathbf{f}(\varepsilon)$ is discontinuous on the edge λ_a (or λ_b) of the range D and if β is sufficiently small, the probability w_{I_s} to find isolated eigenstate $|\Psi_I\rangle$ associated with this edge in the local state $|\Theta_s\rangle$ is negligible. An example of such an eigenvalue will be given in sections 4.1 and 4.2.

Note that above functions $\varepsilon_s(\beta)$ are not analytic in the point $\beta = 0$ and hence they can not be expressed as a power series expansion in this point. In fact, in the limit $\beta \rightarrow 0$ all derivatives of those functions are zero! This again demonstrates that standard perturbation expansion fails in this point. In general, standard perturbation expansion method should fail to reproduce all those eigenvalues $\varepsilon_s \equiv \varepsilon_s(\beta)$ of (10) that in a limit $\beta \rightarrow \beta_0$ converge to some point $\varepsilon_s(\beta_0) \in \Lambda$ where $\omega(\varepsilon)$ diverges. A special case of this general result is a case $\beta_0 = 0$ and $\varepsilon_s(\beta_0) = \lambda_a (= \lambda_b)$.

3.4. Embedded eigenvalues and eigenstates of the combined system

Each $\varepsilon \in D$ is an embedded eigenvalue of the combined system. The corresponding embedded eigenstate $|\Psi(\varepsilon)\rangle$ can be written as a linear combination $|\Psi(\varepsilon)\rangle = |\Psi^a(\varepsilon)\rangle + |\Psi^b(\varepsilon)\rangle$ where $|\Psi^a(\varepsilon)\rangle \in X_p^a$ and $|\Psi^b(\varepsilon)\rangle \in X_\infty^b$. In a metrics induced by the operator \mathbf{S} , those eigenstates are orthonormalized to a δ -function

according to

$$\langle \Psi(\varepsilon) | \mathbf{S} | \Psi(\varepsilon') \rangle = \delta(\varepsilon - \varepsilon'). \tag{20a}$$

In addition, embedded eigenstates are orthogonal to all isolated eigenstates

$$\langle \Psi(\varepsilon) | \mathbf{S} | \Psi_s \rangle = 0, \quad \varepsilon \in D. \tag{20b}$$

A key quantity in the treatment of embedded solutions is a fractional shift $x(\varepsilon)$ [5–7]. One finds that this quantity is well defined almost everywhere in D . There may exist only a finite number of isolated points where fractional shift is ambiguous. Those are “anomal” points and in those points combined system contains isolated eigenvalues and eigenstates (see section 3.4.2).

Fractional shift can be obtained from the eigenvalue of the fractional shift eigenvalue equation to be considered in the following section. Once fractional shift is known, one can express various quantities describing combined system \mathbf{S}_∞ in terms of a fractional shift and in terms of the corresponding eigenstate $|\psi(\varepsilon)\rangle$ of this equation. In particular, the component $|\Psi^a(\varepsilon)\rangle$ of the embedded eigenstate $|\Psi(\varepsilon)\rangle$ can be expressed in this way.

We will first define fractional shift $x(\varepsilon)$ and then we will derive fractional shift eigenvalue equation that determines this quantity. Next the solution of this equation will be considered. Using this solution, component $|\Psi^a(\varepsilon)\rangle \in X_\rho^a$ of the normalized eigenstate $|\Psi(\varepsilon)\rangle$ will be derived.

3.4.1. Fractional shift and fractional shift eigenvalue equation

One arrives at the notion of the fractional shift in the following way: Unperturbed infinite system \mathbf{S}_∞^b can be approximated to any desired degree of accuracy with a huge but finite system \mathbf{S}_n^b containing n eigenvalues λ_i and n eigenstates $|\Phi_i\rangle$. This can be done in such a way that eigenvalues λ_i are nondegenerate and locally equidistant (see Appendix A.2). For large enough n those eigenvalues are densely distributed over the interval $D = [\lambda_a, \lambda_b]$. System \mathbf{S}_n^b interacts with the finite system \mathbf{S}_ρ^a . Eigenvalues ε_k ($k = 1, \dots, n + \rho$) of the corresponding combined system $\mathbf{S}_{n+\rho} = \mathbf{S}_\rho^a \oplus \mathbf{S}_n^b$ are interlaced with the unperturbed eigenvalues λ_i according to [12]

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

Consider $(n - \rho)$ quantities

$$x(\varepsilon_k) = \frac{\varepsilon_k - \lambda_{k-1}}{\lambda_k - \lambda_{k-1}}, \quad k = \rho + 1, \rho + 2, \dots, n. \tag{22}$$

Each $x(\varepsilon_k)$ is a *fractional shift* of the perturbed eigenvalue ε_k relative to the unperturbed eigenvalue λ_{k-1} [5–7]. In particular and due to the interlacing rule (21), in the case $\rho = 1$ one has $0 \leq x(\varepsilon_k) \leq 1$ [5–7]. In the limit $n \rightarrow \infty$

discrete quantities $x(\varepsilon_k)$ converge to a function $x(\varepsilon)$ of a continuous parameter $\varepsilon \in D$. Fractional shift thus defined is the ratio of two infinitesimal quantities. One should imagine an infinite number of unperturbed eigenvalues λ_i densely distributed over the eigenvalue interval $D = [\lambda_a, \lambda_b]$. Perturbed eigenvalues ε_k are also densely distributed over this interval. For each finite n there is a small shift $\Delta\varepsilon_k = \varepsilon_k - \lambda_{k-1}$ of the perturbed eigenvalue ε_k relative to the unperturbed eigenvalue λ_{k-1} . Another small quantity is the interval $\Delta\lambda_k = \lambda_k - \lambda_{k-1}$ between two adjacent unperturbed eigenvalues. The $n \rightarrow \infty$ limit of the ratio of those two quantities is the fractional shift $x(\varepsilon)$.

As shown in the Appendix A.4.3, for each $\varepsilon \in D$, except for the so-called anomalous points $\varepsilon_a \in D$, fractional shift is well defined and it is a solution of the eigenvalue equation

$$\mathbf{H}(\varepsilon) |\psi(\varepsilon)\rangle = X(\varepsilon) \mathbf{f}(\varepsilon) |\psi(\varepsilon)\rangle, \quad (23a)$$

where

$$\mathbf{H}(\varepsilon) = \beta^2 \boldsymbol{\omega}(\varepsilon) + \mathbf{A} - \varepsilon \mathbf{S}^a, \quad (23b)$$

and where
$$X(\varepsilon) = -\pi\beta^2 \cot(\pi x(\varepsilon)), \quad \varepsilon \in D. \quad (23c)$$

We consider anomalous points and other characteristic points of the combined system in the following section.

We call equation (23a) a *fractional shift* equation. For each $\varepsilon \in D$ this is a generalized eigenvalue equation with eigenvalue(s) $X(\varepsilon)$ and with the corresponding eigenstate(s) $|\psi(\varepsilon)\rangle$. Eigenvalue $X(\varepsilon)$ of this equation determines fractional shift $x(\varepsilon)$ according to (23c). As shown in the Appendix A.4.1, fractional shift is confined to the interval $[1 - \rho, 1]$

$$1 - \rho \leq x(\varepsilon) \leq 1. \quad (24)$$

Since for each integer m one has $\cot(\pi(x(\varepsilon) + m)) = \cot(\pi x(\varepsilon))$, expression (23c) determines fractional shift up to an additive integer constant. None of other quantities to be derived in this paper is sensitive to this constant. Hence one can confine fractional shift $x(\varepsilon)$ to the interval $[0, 1)$. We will call fractional shift confined to this interval a *principal value* of a fractional shift. If required, exact value of the fractional shift can be obtained using the continuation argument, i.e. imposing the condition that fractional shift $x(\varepsilon)$ should be a continuous function of ε . This method can be generalized to include anomalous points where fractional shift is not defined [8]. Unless otherwise specified, we will assume that the fractional shift is confined to its principal value.

Consider now eigenstate $|\psi(\varepsilon)\rangle$ of the fractional shift equation. As shown in the Appendix A.4.2, in conjunction with the fractional shift $x(\varepsilon)$ this eigenstate determines X_ρ^a -component $|\Psi^a(\varepsilon)\rangle$ of the embedded eigenstate $|\Psi(\varepsilon)\rangle$

according to

$$|\Psi^a(\varepsilon)\rangle = \frac{\sin(\pi x(\varepsilon))}{\pi\beta\sqrt{\langle\psi(\varepsilon)|\mathbf{f}(\varepsilon)|\psi(\varepsilon)\rangle}}|\psi(\varepsilon)\rangle. \quad (25a)$$

Using (23c) one can express $\sin(\pi x(\varepsilon))$ in terms of the eigenvalue $X(\varepsilon)$ of the fractional shift equation

$$\sin(\pi x(\varepsilon)) = \frac{\pi\beta^2}{\sqrt{\pi^2\beta^4 + (X(\varepsilon))^2}}, \quad \varepsilon \in D. \quad (25b)$$

Component $|\Psi^a(\varepsilon)\rangle \in X_\rho^a$ of $|\Psi(\varepsilon)\rangle$ determines all properties of the system \mathbf{S}_ρ^a that interacts with the system \mathbf{S}_∞^b . Hence, as far as embedded solutions of the combined system are concerned, fractional shift equation provides complete description of the system \mathbf{S}_ρ^a that interacts with the system \mathbf{S}_∞^b .

3.4.2. Characteristic points of the combined system

In a base $\{|\chi_s\rangle\} \in X_\rho^a$ fractional shift equation (23a) is a $\rho \times \rho$ matrix eigenvalue equation (A.14a). Standard $\rho \times \rho$ eigenvalue equation involving Hermitian matrices 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. Since this operator has rank at most one, the number of linearly independent eigenstates that this equation may have substantially decreases.

According to (25a), X_ρ^a -component $|\Psi^a(\varepsilon)\rangle$ of the embedded eigenstate $|\Psi(\varepsilon)\rangle$ of the combined system is proportional to the eigenstate $|\psi(\varepsilon)\rangle$ of a fractional shift equation. It is possible for the embedded eigenstate $|\Psi(\varepsilon)\rangle$ to contain no X_ρ^a -component. In this case trivial solution $|\psi(\varepsilon)\rangle = 0$ of the fractional shift equation is allowed. However, if the eigenstate $|\psi(\varepsilon)\rangle$ of the combined system contains X_ρ^a -component, only nontrivial solutions $|\psi(\varepsilon)\rangle \neq 0$ of this equation should be considered. It is important to determine necessary and sufficient conditions for the existence of trivial solutions of the fractional shift equation.

General properties of the solutions to the fractional shift equation, such as number of those solutions and admissibility of a trivial solution, can be analyzed in terms of *characteristic points* $\varepsilon \in D$. Those are *singular*, *critical* and *resonant* points. In addition, of interest are also points $e_d \in \Lambda$ where operator $\omega(\varepsilon)$ diverges.

Singular points $\varepsilon_0 \in D$ correspond to singular solutions of the combined system. Those solutions were first defined in the case of a finite combined system $\mathbf{S}_{n+\rho}$ [12]. By definition, eigenvalue ε_k of a finite combined system $\mathbf{S}_{n+\rho}$ is *singular* if it coincides with some eigenvalue λ_i of the corresponding unperturbed system \mathbf{S}_n^b . Otherwise it is *cardinal*. As shown in the Appendix A.4.1, one can generalize the distinction between singular and cardinal solutions to the

infinite combined system \mathbf{S}_∞ [5–7]. One finds that fractional shift $x(\varepsilon) = 0$ corresponds to a singular solution, while all other (noninteger) values of fractional shift correspond to cardinal solutions. Each singular point $\varepsilon_0 \in D$ satisfies $x(\varepsilon_0) = 0$ and it describes perturbed eigenvalue that in the limit $n \rightarrow \infty$ coincides with some unperturbed eigenvalue (see Appendix A.4). According to (23c), the point $x(\varepsilon_0) = 0$ corresponds to the eigenvalue $X(\varepsilon_0) = \pm\infty$ of the fractional shift equation. This eigenvalue is not a proper eigenvalue of (23a) and singular solutions thus appear as limit quantities to “standard” solutions of the fractional shift equation. If $\lim_{\varepsilon \rightarrow \varepsilon_0} X(\varepsilon)\mathbf{f}(\varepsilon)|\psi(\varepsilon)\rangle$ is well defined and finite and if $\lim_{\varepsilon \rightarrow \varepsilon_0} X(\varepsilon) = \pm\infty$, one has a singular solution in a point $\varepsilon = \varepsilon_0$. In this way fractional shift equation, in addition to cardinal solutions, contains also singular solutions. According to (25a), in a singular point $\varepsilon_0 \in D$ one has $|\Psi^a(\varepsilon_0)\rangle = 0$, unless $\langle\psi(\varepsilon_0)|\mathbf{f}(\varepsilon_0)|\psi(\varepsilon_0)\rangle = 0$. In this latter case the correct expression is obtained as a limit $|\Psi^a(\varepsilon_0)\rangle = \lim_{\varepsilon \rightarrow \varepsilon_0} |\Psi^a(\varepsilon)\rangle$.

Second type of characteristic points are critical points $\varepsilon_c \in D$. In a critical point operator $\mathbf{f}(\varepsilon)$ vanishes, i.e. $\mathbf{f}(\varepsilon_c) = 0$. As explained in section 3.1, for almost all $\varepsilon \in D$ rank of $\mathbf{f}(\varepsilon)$ equals one. Exception are critical points (if any) where this rank equals zero and where $a_s(\varepsilon_c) = 0$ for each $s = 1, \dots, \rho$.

According to expressions (6), operator $\mathbf{f}(\varepsilon)$ incorporates essential features of the interaction between the state $|\Phi(k)\rangle \in X_\infty^b$ ($\varepsilon = \lambda(k)$) and the system \mathbf{S}_ρ^a . Since in a critical point $\varepsilon = \varepsilon_c$ one has $\mathbf{f}(\varepsilon_c) = 0$, the state $|\Phi(k_c)\rangle$ where $\varepsilon_c = \lambda(k_c)$ does not interact with any state of the system \mathbf{S}_ρ^a . This state is hence an eigenstate of the combined system \mathbf{S}_∞ . This eigenstate has no X_ρ^a component, and hence in a critical point trivial solution $|\psi(\varepsilon_c)\rangle = 0$ of the fractional shift equation is allowed. However, if ε is not a critical point, the state $|\Phi(k)\rangle$ ($\varepsilon = \lambda(k)$) interacts with at least one state in \mathbf{S}_ρ^a . In this case one finds that $|\Psi(\varepsilon)\rangle$ contains a nontrivial X_ρ^a -component. In conclusion, in a critical point trivial solution $|\psi(\varepsilon)\rangle = 0$ of the fractional shift equation is allowed. If the point ε is not critical, only nontrivial solutions of this equation are permitted.

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 nontrivial state $|\theta\rangle \in X_\rho^a$ such that $\mathbf{H}(\varepsilon_r)|\theta\rangle = 0$. We denote the set of all resonant points $\varepsilon_r \in D$ with Ξ . We also define a special type of resonant points, so-called *anomal* points. The point ε_r is anomal if there is a nontrivial state $|\theta\rangle \in X_\rho^a$ that satisfies $\mathbf{f}(\varepsilon_r)|\theta\rangle = 0$ in addition to $\mathbf{H}(\varepsilon_r)|\theta\rangle = 0$. If it is important to emphasize that resonant point $\varepsilon_r \in \Xi$ is anomal, we will denote this point with $\varepsilon_r \equiv \varepsilon_a$. We call each resonant point ε_r that is not an anomal point, a *proper* resonant point. Anomal points are important since in those points the combined system has isolated eigenstates (see Appendix A.4.4). Each degenerate resonant point is an anomal point. This follows from the fact that operator $\mathbf{f}(\varepsilon)$ has rank at most one. In more general cases not considered here, rank of $\mathbf{f}(\varepsilon)$ can assume any value $\leq \rho$ and degenerate resonant points are not necessarily anomal [8]. In

general, one finds that if the rank of $\mathbf{f}(\varepsilon_r)$ is κ_r , then each $(\kappa_r + 1)$ -degenerate resonant point must be anomalous [8].

In addition to the distinction between proper and anomalous resonant points, it is also convenient to distinguish between *active* and *passive* resonant points. By definition, resonant point ε_r is *active* if there is at least one state $|\theta\rangle \in X_\rho^a$ that satisfies $\mathbf{f}(\varepsilon_r)|\theta\rangle \neq 0$ in addition to $\mathbf{H}(\varepsilon_r)|\theta\rangle = 0$. Otherwise it is *passive*. One easily finds that each passive resonant point is anomalous. One also finds that a nondegenerate active resonant point is not anomalous, i.e. it is a proper resonant point. Significance of resonant points is discussed in more details in the following two sections.

3.4.3. General properties of the solutions to the fractional shift equation

Let us analyze general properties of the solutions to the fractional shift equation in terms of the above characteristic points. The main distinction is between resonant points $\varepsilon_r \in D$ and points $\varepsilon \in D$ that are not resonant.

Consider first the point $\varepsilon \in D$ that is not a resonant point ($\varepsilon \notin \Xi$). In such a point operator $\mathbf{H}(\varepsilon)$ is regular, and it has an inverse $\mathbf{H}^{-1}(\varepsilon)$. Equation (23a) is hence equivalent to

$$|\psi(\varepsilon)\rangle = X(\varepsilon)\mathbf{H}^{-1}(\varepsilon)\mathbf{f}(\varepsilon)|\psi(\varepsilon)\rangle, \quad (26a)$$

There are two further possibilities, the point $\varepsilon \notin \Xi$ is either a critical point or it is not a critical point. In the later case operator $\mathbf{f}(\varepsilon)$ has rank one. Since $\mathbf{H}^{-1}(\varepsilon)$ is regular the product $\mathbf{H}^{-1}(\varepsilon)\mathbf{f}(\varepsilon)$ has also rank one. Up to the normalization constant this product must be a projection operator on some state $|\zeta(\varepsilon)\rangle \in X_\rho^a$. Hence and due to (26a) eigenstate $|\psi(\varepsilon)\rangle$ of (23a) must be proportional to $|\zeta(\varepsilon)\rangle$, i.e. $|\psi(\varepsilon)\rangle \propto |\zeta(\varepsilon)\rangle$. This implies that fractional shift equation has exactly one nontrivial eigenstate. Further, since $\varepsilon \notin \Xi$ is not a critical point, trivial solution is not allowed. Assume namely $|\psi(\varepsilon)\rangle = 0$. In this case the state $|\Phi(k)\rangle \in X_\infty^b$ where $\varepsilon = \lambda(k)$ must be an eigenstate of the combined system. However, since $\mathbf{f}(\varepsilon) \neq 0$ there is an interaction between this state and the finite system \mathbf{S}_ρ^a . Hence this state can not be an eigenstate of the combined system. This proves that the assumption $|\psi(\varepsilon)\rangle = 0$ is wrong. Since $|\psi(\varepsilon)\rangle \neq 0$ expression (26a) implies $X(\varepsilon) \neq 0$ and hence $x(\varepsilon) \neq 0.5$.

Consider now critical point $\varepsilon_c \notin \Xi$. As explained in a previous section, in this point X_ρ^a -component of the embedded eigenstate $|\Psi(\varepsilon_c)\rangle$ vanishes. Hence $|\psi(\varepsilon_c)\rangle = 0$. This conclusion is consistent with fractional shift equation (23a). In a critical point one has $\mathbf{f}(\varepsilon_c) = 0$ and right-hand side of this equation equals zero. However, since $\mathbf{H}(\varepsilon_c)$ is regular, each nontrivial state $|\psi\rangle \neq 0$ ($|\psi\rangle \in X_\rho^a$) satisfies $\mathbf{H}(\varepsilon_c)|\psi\rangle \neq 0$. This implies $|\Psi(\varepsilon_c)\rangle = 0$. Since in a critical point there is no interaction between the state $|\Psi(\varepsilon_c)\rangle \in X_\infty^b$ and the system \mathbf{S}_ρ^a , fractional shift $x(\varepsilon_c)$ associated with this eigenstate must be zero. The corresponding solution is hence singular. There is also a possibility that some local eigenvalue E_s

may coincide with the critical point, $E_s = \varepsilon_c$. If this is the case, and since $|\Psi(\varepsilon_c)\rangle$ does not interact with $|\Theta_s\rangle$, eigenvalue $E_s = \varepsilon_c$ is degenerate. Degenerate eigenstates corresponding to this eigenvalue are $|\Psi(\varepsilon_c)\rangle \in X_\infty^b$ and $|\Theta_s\rangle \in X_\rho^a$.

Consider now the solution of a fractional shift equation in a resonant point $\varepsilon_r \in \Xi$. In this point there is a nontrivial state $|\theta\rangle \in X_\rho^a$ that satisfies $\mathbf{H}(\varepsilon_r)|\theta\rangle = 0$. For this state fractional shift equation (23a) reduces to

$$X(\varepsilon_r)\mathbf{f}(\varepsilon_r)|\theta\rangle = 0. \quad (26b)$$

An obvious solution to this equation is $X(\varepsilon_r) = 0$ and $|\psi(\varepsilon_r)\rangle \equiv |\theta\rangle$. The corresponding fractional shift is $x(\varepsilon_r) = 0.5$. This solution always exists. However, if the resonant point ε_r is anomalous, there is a nontrivial state $|\theta\rangle \in X_\rho^a$ that satisfies $\mathbf{f}(\varepsilon_r)|\theta\rangle = 0$ in addition to $\mathbf{H}(\varepsilon_r)|\theta\rangle = 0$. In this case fractional shift equation (23a) is satisfied with the state $|\psi(\varepsilon_r)\rangle \equiv |\theta\rangle$ with an arbitrary eigenvalue $X(\varepsilon_r)$. Hence fractional shift $x(\varepsilon_r)$ can assume any value admissible by the condition (24). Since $\langle\psi(\varepsilon_r)|\mathbf{f}(\varepsilon_r)|\psi(\varepsilon_r)\rangle = 0$ and according to the expression (25a), each noninteger fractional shift $x(\varepsilon_r)$ produces an infinite value for the component $|\Psi^a(\varepsilon_r)\rangle$. This divergence indicates the existence of the isolated eigenstate in the point ε_r [8]. In conclusion, in an anomalous point the combined system has one or several isolated eigenstates. On the other hand, if the resonant point ε_r is not anomalous, fractional shift equation has a unique solution and the corresponding fractional shift equals $x(\varepsilon_r) = 0.5$.

To summarize the above discussion, in each point $\varepsilon \in D$ that is not an anomalous point fractional shift equation has one and only one physically acceptable solution. In this case there is only one fractional shift $x(\varepsilon)$ and (up to the normalization and phase) only one eigenstate $|\psi(\varepsilon)\rangle$ of this equation. In particular, if $\varepsilon \in D$ is not resonant one has $x(\varepsilon) \neq 0.5$, while if $\varepsilon = \varepsilon_r$ is a proper resonant point one has $x(\varepsilon_r) = 0.5$. Hence fractional shift $x(\varepsilon)$, considered as a continuous function of $\varepsilon \in D$, can cross the value $x(\varepsilon) = 0.5$ only in a resonant point. Further, if ε is not a critical point, the corresponding eigenstate $|\Psi(\varepsilon)\rangle$ of the combined system has a nontrivial X_ρ^a -component $|\Psi^a(\varepsilon)\rangle \neq 0$. In this case fractional shift equation has a nontrivial solution $|\psi(\varepsilon)\rangle \neq 0$. However, if ε is a critical point ($\varepsilon = \varepsilon_c$), eigenstate $|\Psi(\varepsilon_c)\rangle$ of the combined system has no component in the space X_ρ^a . In this case fractional shift equation has only a trivial solution $|\psi(\varepsilon_c)\rangle = 0$. In addition, in a critical point one has $x(\varepsilon_c) = 0$ and the corresponding solution is singular.

Situation is different if ε_r is an anomalous point. In this case fractional shift as determined by the equation (23a) is not well defined and it can assume any value consistent with the requirement (24). As a consequence, the combined system contains one or several isolated eigenstates in this point.

3.4.4. Resonant eigenvalue equation

By definition, in the resonant point $\varepsilon_r \in D$ operator $\mathbf{H}(\varepsilon_r)$ is singular. This point is hence an eigenvalue of the eigenvalue equation

$$\left[\beta^2 \boldsymbol{\omega}(\varepsilon_r) + \mathbf{A} \right] |\theta_r\rangle = \varepsilon_r \mathbf{S}^a |\theta_r\rangle, \quad \varepsilon_r \in D. \quad (10')$$

This equation is generic eigenvalue equation (10) restricted to the range D . As shown in section 3.3, each eigenvalue $\varepsilon_I \in \bar{D}$ of the generic eigenvalue equation is an isolated eigenvalue of the combined system. This eigenvalue is contained outside the range D . The corresponding eigenstate is given by expressions (14a) and (14b). On the other hand, each eigenvalue $\varepsilon_r \in D$ of this equation is contained inside the range D . If the interaction between the systems \mathbf{S}_ρ^a and \mathbf{S}_∞^b is relatively weak, most solutions of the equation (10') have a simple physical interpretation. Let $E_r \in D$ be a nondegenerate eigenvalue of (1a). Let further E_r be an interior point in the range D , i.e. E_r is not on a boundary of this range. If the coupling β is sufficiently small, equation (10') has an eigenvalue $\varepsilon_r(\beta) \in D$ that in a limit $\beta \rightarrow 0$ converges to E_r . This eigenvalue can be identified with the eigenvalue $E_r \in D$ of the local system \mathbf{S}_ρ^a shifted to the position ε_r by the interaction of this system with the infinite system \mathbf{S}_∞^b . One finds (see section 3.4.7) that if β is sufficiently small, each active eigenvalue $\varepsilon_r(\beta) \in D$ of (10') that is associated with a nondegenerate eigenvalue $\varepsilon_r(0) = E_r$ and which in addition satisfies $E_r \notin \Lambda$ defines a universal resonance curve [13]. This curve has the maximum at $\varepsilon = \varepsilon_r$, it has a finite width $\Delta\varepsilon_r$ and the area under this curve equals unity. Similar result is obtained if E_r is κ_r -degenerate where $\kappa_r > 1$. In this case one may have as many as κ_r eigenvalues $\varepsilon_s(\beta)$ of (10') that in a limit $\beta \rightarrow 0$ converge to E_r . In general, those eigenvalues do not generate universal resonance curve and some of them may be anomal. However, each of those eigenvalues can be still considered as the eigenvalue E_r perturbed by the interaction of the system \mathbf{S}_ρ^a with the infinite system \mathbf{S}_∞^b . In view of those properties we call equation (10') where eigenvalues $\varepsilon_r \in D$ are confined to the range D a *resonant eigenvalue equation* and we call each eigenvalue $\varepsilon_r \in D$ of this equation a *resonant point* (see section 3.4.2).

As emphasized in section 3.2, if $\boldsymbol{\omega}(\varepsilon)$ is not bounded in the range D , equation (10') may have some additional eigenvalues $\varepsilon_r \in D$ that in the limit $\beta \rightarrow 0$ converge to some point $e_d \in \Lambda$ where $\boldsymbol{\omega}(\varepsilon)$ diverges. One finds that those additional eigenvalues do not generate a universal resonant curve.

If the coupling β is not small, eigenvalue distribution of the system \mathbf{S}_ρ^a in the interaction with the system \mathbf{S}_∞^b may be so distorted that any interpretation of the resonant points ε_r as the perturbed eigenvalues E_r of the system \mathbf{S}_ρ^a becomes meaningless (see section 4.3 and figure 8). Also and as emphasized in section 3.2, the combined system may contain some resonant points that are associated neither with unperturbed eigenvalues E_r , nor with some point

e_d where $\omega(\varepsilon)$ diverges. Though in the case of the strong coupling resonance interpretation of the eigenvalues ε_r of the eigenvalue equation (10') is usually inadequate, those eigenvalues and the corresponding eigenstates still play an important role in connection with the solutions of the fractional shift equation. In particular and as explained in a previous section, if ε_r is an anomalous point there is an isolated eigenstate of the combined system in this point, however strong the coupling β (see section 4.4).

3.4.5. Solution of the fractional shift equation in the base $\{|\phi_s(\varepsilon)\rangle\}$

Let us now consider in more details solution of a fractional shift equation. For the sake of simplicity and unless otherwise specified, we will assume that operator $\omega(\varepsilon)$ is bounded in D , i.e. we assume that the set Λ is empty.

One can solve equation (23a) in any base $\{|\chi_s\rangle\} \in X_\rho^a$. However, particularly convenient is the base $\{|\chi_s\rangle\} \equiv \{|\phi_s(\varepsilon)\rangle\}$ containing eigenstates of the eigenvalue equation

$$\left[\beta^2 \omega(\varepsilon) + \mathbf{A} \right] |\phi_s(\varepsilon)\rangle = \eta_s(\varepsilon) \mathbf{S}^a |\phi_s(\varepsilon)\rangle. \quad (27a)$$

Those eigenstates can be orthonormalized according to

$$\langle \phi_s(\varepsilon) | \mathbf{S}^a | \phi_p(\varepsilon) \rangle = \delta_{sp}, \quad s, p = 1, \dots, \rho. \quad (27b)$$

Eigenstates $|\phi_s(\varepsilon)\rangle$ and the corresponding eigenvalues $\eta_s(\varepsilon)$ depend on ε and on a parameter β . For each ε (and for each parameter β) there are ρ orthonormalized eigenstates $|\phi_s(\varepsilon)\rangle$ and ρ corresponding eigenvalues $\eta_s(\varepsilon)$. One can consider eigenvalue equation (27a) for each real ε . However, in connection with the embedded eigenstates of the combined system, of particular interest is the solution of this equation in the case $\varepsilon \in D$.

Eigenvalue equation (27a) is related to the generic eigenvalue equation (10). Each eigenvalue ε_r of (10) satisfies $\eta_s(\varepsilon_r) = \varepsilon_r$ for at least one $s = 1, \dots, \rho$. It is convenient to denote with Ξ_r the set of all indices s such that $\eta_s(\varepsilon_r) = \varepsilon_r$. If the eigenvalue ε_r of (10) is κ_r -degenerate, there are κ_r such indices and κ_r corresponding functions $\eta_s(\varepsilon)$. One can orthonormalize the corresponding eigenstates $|\theta_s\rangle$ of (10) in such a way that they satisfy

$$\langle \theta_s | \mathbf{S}^a | \theta_p \rangle = \delta_{sp}, \quad |\theta_s\rangle = |\phi_s(\varepsilon_r)\rangle, \quad s, p \in \Xi_r. \quad (27c)$$

Though equations (10) and (27a) are related, they are substantially different. For each ε equation (27a) is an eigenvalue equation that has ρ orthonormalized eigenstates $|\phi_s(\varepsilon)\rangle$ and ρ corresponding eigenvalues $\eta_s(\varepsilon)$. On the other hand, generic equation (10) is a nonlinear eigenvalue equation and it may have the solution only for some isolated points $\varepsilon = \varepsilon_s$. Eigenstates $|\theta_s\rangle$ of this equation are usually not orthogonal to each other and this equation may have more than ρ distinct eigenvalues and eigenstates.

Consider now the solution of the fractional shift equation (23a) in the base $\{|\phi_s(\varepsilon)\rangle\}$. Eigenstate $|\psi(\varepsilon)\rangle$ of this equation can be expressed as a linear combination

$$|\psi(\varepsilon)\rangle = \sum_s^\rho C_s(\varepsilon) |\phi_s(\varepsilon)\rangle. \tag{28a}$$

Orthonormality (27b) implies

$$C_s(\varepsilon) = \langle \phi_s(\varepsilon) | \mathbf{S}^a | \Psi(\varepsilon) \rangle. \tag{28b}$$

This is expression (A.14c) applied to the base $\{|\phi_s(\varepsilon)\rangle\}$.

Let us denote quantities $a_s(\varepsilon)$ and $f_{sp}(\varepsilon)$ as expressed in the base $\{|\phi_s(\varepsilon)\rangle\}$ with $\alpha_s(\varepsilon)$ and $F_{sp}(\varepsilon)$, respectively:

$$\alpha_s(\varepsilon) = \frac{\langle \Phi(k) | \mathbf{V} | \phi_s(\varepsilon) \rangle}{\sqrt{d\lambda(k)/dk}} \Big|_{\varepsilon=\lambda(k)} \cdot \begin{cases} 1 & \text{if } \varepsilon \in D, \\ 0 & \text{otherwise,} \end{cases} \tag{29a}$$

$$F_{sp}(\varepsilon) = \alpha_s^*(\varepsilon)\alpha_p(\varepsilon) \equiv \langle \phi_s(\varepsilon) | \mathbf{f}(\varepsilon) | \phi_p(\varepsilon) \rangle. \tag{29b}$$

If $\varepsilon \in D$ is not a resonant point ($\varepsilon \notin \Xi$), one has $\eta_s(\varepsilon) \neq \varepsilon$ for each $s = 1, \dots, \rho$. As shown in the Appendix A.4.3, in this case fractional shift equation has a unique solution

$$X(\varepsilon) = -\frac{1}{\sum_p^\rho \frac{\alpha_p^*(\varepsilon)\alpha_p(\varepsilon)}{\varepsilon - \eta_p(\varepsilon)}}, \quad x(\varepsilon) = \frac{1}{\pi} \text{tg}^{-1} \left(-\pi\beta \sum_p^\rho \frac{\alpha_p^*(\varepsilon)\alpha_p(\varepsilon)}{\varepsilon - \eta_p(\varepsilon)} \right), \tag{30a}$$

and

$$|\psi(\varepsilon)\rangle = \sum_s^\rho \frac{\alpha_s^*(\varepsilon)}{\varepsilon - \eta_s(\varepsilon)} |\phi_s(\varepsilon)\rangle, \quad \varepsilon \notin \Xi. \tag{30b}$$

According to (30b), if $\varepsilon \notin \Xi$ is not a critical point, one has $|\psi(\varepsilon)\rangle \neq 0$ while if $\varepsilon = \varepsilon_c$ is a critical point one has $\alpha_s(\varepsilon_c) = 0$ ($s = 1, \dots, \rho$) and fractional shift equation has only a trivial solution $|\psi(\varepsilon)\rangle = 0$. In addition, since $\eta_s(\varepsilon) \neq \varepsilon$ ($s = 1, \dots, \rho$) eigenvalue $X(\varepsilon)$ is nonzero. Hence $x(\varepsilon) \neq 0.5$. Further, if all $\eta_s(\varepsilon)$ and all $\alpha_s(\varepsilon)$ are continuous functions of ε , fractional shift $x(\varepsilon)$ is also a continuous function of ε . One also finds that the solution (30) is singular ($x(\varepsilon) = 0$) if and only if

$$\sum_p^\rho \frac{\alpha_p^*(\varepsilon)\alpha_p(\varepsilon)}{\varepsilon - \eta_p(\varepsilon)} = 0, \quad \varepsilon \notin \Xi. \tag{31}$$

In particular, in a critical point $\varepsilon = \varepsilon_c \notin \Xi$ one has a singular solution and one finds $x(\varepsilon_c) = \lim_{\varepsilon \rightarrow \varepsilon_c} x(\varepsilon) = 0$.

If $\varepsilon = \varepsilon_r$ is a resonant point ($\varepsilon_r \in \Xi$), fractional shift equation can have several solutions (see Appendix A.4.3). Among those solution there is always a “standard” solution which equals the $\varepsilon \rightarrow \varepsilon_r$ limit of the solution (30). There is also a solution that satisfies $x(\varepsilon_r) = 0.5$ which may (but need not) coincide with a standard solution. In particular, if the resonant point ε_r is active, there is at least one $p \in \Xi_r$ such that $\alpha_p(\varepsilon_r) \neq 0$, and fractional shift of a standard solution equals 0.5:

$$x(\varepsilon_r) = \lim_{\varepsilon \rightarrow \varepsilon_r} x(\varepsilon) = 0.5. \tag{32a}$$

Concerning the eigenstate (30b), this eigenstate diverges in a limit $\varepsilon \rightarrow \varepsilon_r$. However, fractional shift equation (23a) defines this eigenstate only up to the norm and phase. If one neglects this norm, one finds that the eigenstate (30b) converges to the standard eigenstate $|\psi(\varepsilon_r)\rangle$. If for each $s \in \Xi_r$ the derivative $\eta'_s(\varepsilon_r)$ of a function $\eta_s(\varepsilon)$ satisfies $\eta'_s(\varepsilon_r) \neq 1$, one finds

$$|\psi(\varepsilon_r)\rangle \propto \lim_{\varepsilon \rightarrow \varepsilon_r} |\psi(\varepsilon)\rangle \propto \sum_{s \in \Xi_r} \frac{\alpha_s^*(\varepsilon_r)}{1 - \eta'_s(\varepsilon_r)} |\phi_s(\varepsilon_r)\rangle, \quad \varepsilon_r \in \Xi, \tag{32b}$$

where \propto indicates proportionality (norm is neglected).

Since standard solution (32) satisfies $x(\varepsilon_r) = 0.5$, it corresponds to the case when perturbed eigenvalue ε_r is situated exactly in the middle between two adjacent infinitesimally close unperturbed eigenvalues. This is exactly opposite to the case $x(\varepsilon) = 0$ when the perturbed eigenvalue ε equals unperturbed eigenvalue and when the solution is singular.

If a resonant point $\varepsilon = \varepsilon_r$ is not anomalous, it is necessarily active and non-degenerate. In this case standard solution is the only solution of the fractional shift equation and up to the norm one finds

$$|\psi(\varepsilon_r)\rangle \propto \lim_{\varepsilon \rightarrow \varepsilon_r} |\psi(\varepsilon)\rangle \propto |\phi_r(\varepsilon_r)\rangle \equiv |\theta_r\rangle. \tag{33}$$

In (32) and (33) we have assumed that ε_r is active. Slightly more complicated expressions are obtained if ε_r is passive. In particular, if ε_r is passive but not critical there is at least one $s \notin \Xi_r$ such that $\alpha_s(\varepsilon_r) \neq 0$ and one finds

$$\lim_{\varepsilon \rightarrow \varepsilon_r} X(\varepsilon) = -\frac{1}{\sum_{s \notin \Xi_r} \frac{\alpha_s^*(\varepsilon_r)\alpha_s(\varepsilon_r)}{\varepsilon_r - \eta_s(\varepsilon_r)}}, \quad \lim_{\varepsilon \rightarrow \varepsilon_r} x(\varepsilon) = \frac{1}{\pi} t g^{-1} \left(\pi \beta \sum_{s \notin \Xi_r} \frac{\alpha_s^*(\varepsilon_r)\alpha_s(\varepsilon_r)}{\varepsilon_r - \eta_s(\varepsilon_r)} \right), \tag{34a}$$

while if $\varepsilon_r \equiv \varepsilon_c$ is passive and critical one has

$$\lim_{\varepsilon \rightarrow \varepsilon_c} X(\varepsilon) = X(\varepsilon_c) = \infty, \quad \lim_{\varepsilon \rightarrow \varepsilon_c} x(\varepsilon) = x(\varepsilon_c) = 0. \quad (34b)$$

In both cases as $\varepsilon \rightarrow \varepsilon_r$ fractional shift $x(\varepsilon)$ converges to a particular solution of the family of possible solutions. This is a “standard” solution. Unlike the case of active resonant points where standard solution satisfies $x(\varepsilon_r) = 0.5$, in the case of passive resonant point standard solution satisfies $x(\varepsilon_r) \neq 0.5$.

If the point ε_r is anomal, besides standard solution there are many additional solutions (see Appendix A.4.3). One finds that active resonant point is anomal if and only if it is degenerate, while passive resonant point is always anomal.

Above we have considered the solution of the fractional shift equation in a base $\{|\phi_s(\varepsilon)\rangle\}$. This base is convenient for theoretical considerations, especially for the discussion of the weak coupling limit which provides a link with a standard perturbation expansion approach (see section 3.4.7). Another convenient base for this solution is the set $\{|f_s(\varepsilon)\rangle\}$ of the orthonormalized eigenstates of the operator $\mathbf{f}(\varepsilon)$. This base is more convenient numerically. Unlike the base $\{|\phi_s(\varepsilon)\rangle\}$ that depends on the coupling β , the base $\{|f_s(\varepsilon)\rangle\}$ does not depend on β . In addition, with the choice $\{|f_s(\varepsilon)\rangle\}$ one can efficiently exploit the fact that the rank of the operator $\mathbf{f}(\varepsilon)$ is at most one. This may significantly simplify numerical aspects of the solution. For the sake of simplicity we omit the consideration of this base here [8].

3.4.6. Component $|\Psi^a(\varepsilon)\rangle \in X_\rho^a$ of the embedded eigenstate $|\Psi(\varepsilon)\rangle$

Once fractional shift $x(\varepsilon)$ and the eigenstate $|\psi(\varepsilon)\rangle$ of a fractional shift equation are known, one can obtain component $|\Psi^a(\varepsilon)\rangle \in X_\rho^a$ of the normalized eigenstate $|\Psi(\varepsilon)\rangle$ of the combined system. Inserting the solution (30) into (25) one finds

$$|\Psi^a(\varepsilon)\rangle = \sum_s^\rho |\Psi_s^a(\varepsilon)\rangle, \quad (35a)$$

where

$$|\Psi_s^a(\varepsilon)\rangle = \frac{\beta}{\sqrt{1 + \pi^2 \beta^4 \left(\sum_p^\rho \frac{F_{pp}(\varepsilon)}{\varepsilon - \eta_p(\varepsilon)} \right)^2}} \frac{\alpha_s^*(\varepsilon)}{\varepsilon - \eta_s(\varepsilon)} |\phi_s(\varepsilon)\rangle, \quad \varepsilon \notin \Xi. \quad (35b)$$

In the above expression $|\phi_s(\varepsilon)\rangle$ are eigenstates of (27a) orthonormalized according to (27b). Since $\alpha_s(\varepsilon)$ is zero outside the range D , one has $|\Psi_s^a(\varepsilon)\rangle = 0$ if $\varepsilon \notin D$. As required, component $|\Psi_a(\varepsilon)\rangle$ of the embedded eigenstate $|\Psi(\varepsilon)\rangle$ vanishes outside the range D . In addition, in a critical point $\varepsilon = \varepsilon_c \notin \Xi$ one has

$\alpha_s(\varepsilon_c) = 0$ for each $s \in 1, \dots, \rho$. Hence $|\Psi^a(\varepsilon)\rangle$ vanishes also in a critical point

$$|\Psi^a(\varepsilon_c)\rangle = \lim_{\varepsilon \rightarrow \varepsilon_c} |\Psi^a(\varepsilon)\rangle = 0, \quad \varepsilon_c \notin \Xi.$$

In all other points $\varepsilon \notin \Xi$ one has $|\Psi^a(\varepsilon)\rangle \neq 0$. This is in accord with our general discussion in section 3.4.3.

Expression (35) is valid for each $\varepsilon \in D$ that is not a resonant point. As shown in a previous section, if $\varepsilon = \varepsilon_r$ is a resonant point one may have multiple solutions. Among those solutions there is always a “standard” solution that can be obtained as the $\varepsilon \rightarrow \varepsilon_r$ limit of the solution (35). Two cases are possible; the point ε_r is either active or passive.

If ε_r is active, there is at least one $s \in \Xi_r$ such that $\alpha_s(\varepsilon_r) \neq 0$. In this case

$$\lim_{\varepsilon \rightarrow \varepsilon_r} |\Psi^a(\varepsilon)\rangle = |\Psi^a(\varepsilon_r)\rangle = \sum_{s \in \Xi_r} |\Psi_s^a(\varepsilon_r)\rangle, \quad \varepsilon_r \in \Xi, \quad (36a)$$

where

$$\lim_{\varepsilon \rightarrow \varepsilon_r} |\Psi_s^a(\varepsilon)\rangle = |\Psi_s^a(\varepsilon_r)\rangle = \frac{1}{\pi\beta \sum_{p \in \Xi_r} \frac{F_{pp}(\varepsilon_r)}{1-\eta'_p(\varepsilon_r)}} \frac{\alpha_s^*(\varepsilon_r)}{1-\eta'_s(\varepsilon_r)} |\phi_s(\varepsilon_r)\rangle \begin{cases} 1 & \text{if } s \in \Xi_r, \\ 0 & \text{otherwise.} \end{cases} \quad (36b)$$

In the above expression one assumes $\eta'_s(\varepsilon_r) \neq 1$ for each $s \in \Xi_r$. One easily derives corresponding expression for some rare cases when there is $s \in \Xi_r$ such that $\eta'_s(\varepsilon_r) = 1$.

According to (27c) each state $|\phi_s(\varepsilon_r)\rangle \equiv |\theta_s\rangle$ ($s \in \Xi_r$) is an eigenstate of the resonant eigenvalue equation (10'). Component $|\Psi^a(\varepsilon_r)\rangle$ of the standard eigenstate $|\Psi(\varepsilon_r)\rangle$ is hence a linear combination of only those eigenstates $|\theta_s\rangle$ of (10') that satisfy $s \in \Xi_r$. In particular, if the resonant point ε_r is not anomalous, standard solution is the only solution in this point. In this case ε_r must be nondegenerate and one finds

$$\lim_{\varepsilon \rightarrow \varepsilon_r} |\Psi^a(\varepsilon)\rangle = |\Psi^a(\varepsilon_r)\rangle = \frac{1}{\pi\beta\alpha_r(\varepsilon_r)} |\theta_r\rangle, \quad \varepsilon_r \in \Xi, \quad (36c)$$

where eigenstate $|\theta_r\rangle$ of (10') is normalized according to $\langle\theta_r | \mathbf{S} |\theta_r\rangle = 1$.

Above expressions apply to the case when ε_r is active. According to (32a) in this case fractional shift satisfies $x(\varepsilon_r) = 0.5$. Slightly more complicated expressions are obtained if ε_r is passive. According to (34) in this case fractional shift satisfies $x(\varepsilon_r) \neq 0.5$.

Once $|\Psi^a(\varepsilon)\rangle$ is known, one easily derives all properties of a system \mathbf{S}_ρ^a that interacts with the infinite system \mathbf{S}_∞^b . In the metrics induced by the operator \mathbf{S}

norm of the state $|\Psi_s^a(\varepsilon)\rangle$ can be defined as

$$\rho_s(\varepsilon) \equiv \langle \Psi_s^a(\varepsilon) | \mathbf{S} | \Psi_s^a(\varepsilon) \rangle = \frac{\beta^2}{1 + \pi^2 \beta^4 \left(\sum_p \frac{F_{pp}(\varepsilon)}{\varepsilon - \eta_p(\varepsilon)} \right)^2} \frac{F_{ss}(\varepsilon)}{(\varepsilon - \eta_s(\varepsilon))^2}. \quad (37a)$$

Above expression follows from (35b) and from the orthonormality (27b). One finds that norm $\rho_s(\varepsilon)$ equals probability density to find the state $|\phi_s(\varepsilon)\rangle$ in the eigenstate $|\Psi(\varepsilon)\rangle$ of the combined system:

$$\rho_s(\varepsilon) = |\langle \phi_s(\varepsilon) | \mathbf{S}^a | \Psi(\varepsilon) \rangle|^2. \quad (37b)$$

Of more practical interest are probability densities $\rho_s^a(\varepsilon)$ to find local states $|\Theta_s\rangle$ in the eigenstate $|\Psi(\varepsilon)\rangle$ of the combined system. In a metrics induced by the operator \mathbf{S}^a those probability densities equal

$$\rho_s^a(\varepsilon) = |\langle \Theta_s | \mathbf{S}^a | \Psi(\varepsilon) \rangle|^2. \quad (38a)$$

Since $|\Psi(\varepsilon)\rangle$ has the eigenvalue ε , quantity $\rho_s^a(\varepsilon)$ is a probability density to find local state $|\Theta_s\rangle$ with the eigenvalue $\varepsilon \in D$. In conjuncture with isolated eigenstates $|\Psi_I\rangle$ and corresponding probabilities $w_{I_s}^a$, density $\rho_s^a(\varepsilon)$ determines eigenvalue distribution of a state $|\Theta_s\rangle$ when the system \mathbf{S}_ρ^a is not isolated but when it interacts with the system \mathbf{S}_∞^b (see section 3.5). One finds

$$\rho_s^a(\varepsilon) = \frac{\beta^2}{1 + \pi^2 \beta^4 \left(\sum_p \frac{F_{pp}(\varepsilon)}{\varepsilon - \eta_p(\varepsilon)} \right)^2} \left| \sum_p \frac{\alpha_p^*(\varepsilon)}{\varepsilon - \eta_p(\varepsilon)} \langle \Theta_s | \mathbf{S}^a | \phi_p(\varepsilon) \rangle \right|^2, \varepsilon \notin \Xi. \quad (38b)$$

One can also consider probability density $\rho^a(\varepsilon)$ to find the system \mathbf{S}_ρ^a in the eigenstate $|\Psi(\varepsilon)\rangle$, i.e. to find any of the states $|\Theta_s\rangle \in X_\rho^a$ with the eigenvalue ε . In a metrics induced by the operator \mathbf{S} this probability density equals $\langle \Psi^a(\varepsilon) | \mathbf{S} | \Psi^a(\varepsilon) \rangle \equiv \langle \Psi(\varepsilon) | \mathbf{S}^a | \Psi(\varepsilon) \rangle$. By definition, this is the norm of the component $|\Psi^a(\varepsilon)\rangle \in X_\rho^a$ of the embedded eigenstate $|\Psi(\varepsilon)\rangle$. Since the states $|\Theta_s\rangle$ as well as the states $|\phi_s(\varepsilon)\rangle$ are orthonormalized in accord with the metrics induced by the operator \mathbf{S} , this probability density equals the sum $\sum_s \rho_s^a(\varepsilon)$ as well as the sum $\sum_s \rho_s(\varepsilon)$. Hence

$$\rho^a(\varepsilon) \equiv \sum_s \rho_s^a(\varepsilon) \equiv \sum_s \rho_s(\varepsilon) = \langle \Psi^a(\varepsilon) | \mathbf{S}^a | \Psi^a(\varepsilon) \rangle. \quad (39a)$$

Using any of the expressions (35), (37a) or (38b), in all three cases one finds

$$\rho^a(\varepsilon) = \frac{\beta^2}{1 + \pi^2 \beta^4 \left(\sum_s \frac{F_{ss}(\varepsilon)}{\varepsilon - \eta_s(\varepsilon)} \right)^2} \sum_s \frac{F_{ss}(\varepsilon)}{(\varepsilon - \eta_s(\varepsilon))^2}, \quad \varepsilon \notin \Xi. \quad (39b)$$

In particular, if and only if $\varepsilon = \varepsilon_c \notin \Xi$ is a critical point this probability density vanishes

$$\rho^a(\varepsilon_c) = \lim_{\varepsilon \rightarrow \varepsilon_c} \rho^a(\varepsilon) = 0, \quad \varepsilon_c \notin \Xi. \quad (39c)$$

Above densities apply to each $\varepsilon \in D$ that is not a resonant point. Consider now the case $\varepsilon = \varepsilon_r \in \Xi$. If ε_r is active, corresponding standard component $|\Psi^a(\varepsilon_r)\rangle$ is given by (36). Using this expression one finds standard probability densities $\rho_s(\varepsilon_r)$ and $\rho_s^a(\varepsilon_r)$

$$\lim_{\varepsilon \rightarrow \varepsilon_r} \rho_s(\varepsilon) = \rho_s(\varepsilon_r) = \frac{\frac{F_{ss}(\varepsilon_r)}{(1 - \eta'_s(\varepsilon_r))^2}}{\pi^2 \beta^2 \left(\sum_{p \in \Xi_r} \frac{F_{pp}(\varepsilon_r)}{1 - \eta'_p(\varepsilon_r)} \right)^2} \begin{cases} 1 & \text{if } s \in \Xi_r, \\ 0 & \text{if } s \notin \Xi_r, \end{cases} \quad (40a)$$

$$\lim_{\varepsilon \rightarrow \varepsilon_r} \rho_s^a(\varepsilon) = \rho_s^a(\varepsilon_r) = \frac{\frac{F_{ss}(\varepsilon_r)}{(1 - \eta'_s(\varepsilon_r))^2}}{\pi^2 \beta^2 \left(\sum_{p \in \Xi_r} \frac{F_{pp}(\varepsilon_r)}{1 - \eta'_p(\varepsilon_r)} \right)^2} \left| \sum_{p \in \Xi_r} \frac{\alpha_p^*(\varepsilon_r)}{1 - \eta'_p(\varepsilon_r)} \langle \Theta_s | \mathbf{S}^a | \phi_p(\varepsilon_r) \rangle \right|^2. \quad (40b)$$

Both expressions imply

$$\lim_{\varepsilon \rightarrow \varepsilon_r} \rho^a(\varepsilon) = \rho^a(\varepsilon_r) = \frac{\sum_{s \in \Xi_r} \frac{F_{ss}(\varepsilon_r)}{(1 - \eta'_s(\varepsilon_r))^2}}{\pi^2 \beta^2 \left(\sum_{p \in \Xi_r} \frac{F_{pp}(\varepsilon_r)}{1 - \eta'_p(\varepsilon_r)} \right)^2}, \quad \varepsilon_r \in \Xi. \quad (40c)$$

As already emphasized, expressions (40) are valid provided $\eta'_p(\varepsilon_r) \neq 1$ for each $s \in \Xi_r$.

If the resonant point ε_r is nondegenerate, above expressions reduce to

$$\rho_s(\varepsilon_r) = \frac{\delta_{s,r}}{\pi^2 \beta^2 F_{rr}(\varepsilon_r)}, \quad \rho_s^a(\varepsilon_r) = \frac{|\langle \Theta_s | \mathbf{S}^a | \phi_r(\varepsilon_r) \rangle|^2}{\pi^2 \beta^2 F_{rr}(\varepsilon_r)},$$

$$\rho^a(\varepsilon_r) = \frac{1}{\pi^2 \beta^2 F_{rr}(\varepsilon_r)}. \quad (41)$$

Since ε_r is active, this is a proper resonant point. The solution (41) is hence unique.

As explained in section 3.4.3, if the resonant point ε_r is anomalous, fractional shift $x(\varepsilon_r)$ can assume any value consistent with (24). Densities $\rho_s(\varepsilon_r)$ and $\rho_s^a(\varepsilon_r)$ in this point are hence not unique. Only one of those densities, a standard density equals the $\varepsilon \rightarrow \varepsilon_r$ limit of the solution in the neighborhood of ε_r . Remaining densities correspond to one or several isolated eigenstates in this anomalous point. Those densities have the shape of the weighted δ -function and they require a special treatment [8].

3.4.7. Component $|\Psi^a(\varepsilon)\rangle$ in the weak coupling limit

According to (35) component $|\Psi^a(\varepsilon)\rangle \in X_\rho^a$ of the embedded eigenstate $|\Psi(\varepsilon)\rangle$ is a sum of ρ states $|\Psi_s^a(\varepsilon)\rangle \in X_\rho^a$. Each state $|\Psi_s^a(\varepsilon)\rangle$ is associated with some local eigenvalue E_s and with the corresponding eigenstate $|\Theta_s\rangle$. Let us now consider this component in the case of small β . As shown in the Appendix A.6, if the state $|\Psi_s^a(\varepsilon)\rangle$ is associated with the local eigenvalue $E_s \in \bar{D}$ that is an interior point in \bar{D} and if β is sufficiently small, this state is negligible. Hence in the case of small β only those states $|\Psi_s^a(\varepsilon)\rangle$ that are associated with local eigenvalues $E_s \in D$ contribute to $|\Psi^a(\varepsilon)\rangle$. We shall now consider those states in more details.

Let $E_r \in D$ be κ_r -degenerate and let E_r be an interior point in D . In this case there are κ_r resonant points ε_s and κ_r functions $\eta_s(\varepsilon)$ that in a limit $\beta \rightarrow 0$ converge to E_r . Those resonant points and those functions are not necessarily mutually distinct and some of them may coincide. We shall write $s \in Z_r$ if $\varepsilon_s \equiv \varepsilon_s(\beta)$ satisfies $\varepsilon_s(0) = E_r$. Otherwise we shall write $s \notin Z_r$. If the operator $\omega(\varepsilon)$ does not diverge in the point $\varepsilon = E_r$ and if β is sufficiently small, each state $|\Psi_s^a(\varepsilon)\rangle$ associated with local eigenvalue E_r has the form (see Appendix A.6)

$$|\Psi_s^a(\varepsilon)\rangle \approx |\Psi_s^a(\varepsilon)\rangle^\circ = \frac{\beta}{\sqrt{1 + \pi^2 \beta^4 \left(\sum_{p \in Z_r} \frac{F_{pp}(\varepsilon_p)}{\varepsilon - \varepsilon_p} \right)^2}} \frac{\alpha_s^*(\varepsilon_s)}{\varepsilon - \varepsilon_s} |\phi_s(\varepsilon)\rangle, \quad s \in Z_r, \tag{42a}$$

where symbol (\circ) indicates that this expression is valid for small β . Note that $|\Psi_s^a(\varepsilon)\rangle \approx 0$ if $\alpha_s(\varepsilon_s) = 0$. In particular, if ε_s is passive one has $|\Psi_s^a(\varepsilon)\rangle^\circ = 0$. According to (A.33b) one has also $|\phi_s(\varepsilon)\rangle = |\Theta_s\rangle + O(\beta^2) \approx |\Theta_s\rangle$. The state $|\Psi_s^a(\varepsilon)\rangle$ is hence essentially proportional to $|\Theta_s\rangle$. We shall however retain more general form $|\phi_s(\varepsilon)\rangle$ in the above expression.

The interaction of the system \mathbf{S}_∞^b with the system \mathbf{S}_ρ^a may either completely or only partially remove the degeneracy of E_r . Hence each resonant point ε_s ($s \in Z_r$) may be still degenerate. If this is the case it is convenient instead of a single

state $|\Psi_s^a(\varepsilon)\rangle^\circ$ to consider the sum $|\Psi_{(s)}^a(\varepsilon)\rangle^\circ$ of all those states that are associated with the same degenerate resonant point ε_s

$$|\Psi_{(s)}^a(\varepsilon)\rangle^\circ = \sum_{p \in \Xi_s} |\Psi_p^a(\varepsilon)\rangle^\circ, \quad s \in Z_r. \quad (42b)$$

This state is nonzero if the resonant point ε_s is active, otherwise it is zero. If E_r is nondegenerate there is only one $\varepsilon_r(\beta)$ with a property $\varepsilon_r(0) = E_r$. In this case (42a) and (42b) reduce to

$$|\Psi_r^a(\varepsilon)\rangle \approx |\Psi_r^a(\varepsilon)\rangle^\circ \equiv |\Psi_{(r)}^a(\varepsilon)\rangle^\circ = \frac{\beta \alpha_r^*(\varepsilon_r)}{\sqrt{(\varepsilon - \varepsilon_r)^2 + \pi^2 \beta^4 F_{rr}(\varepsilon_r)^2}} |\phi_r(\varepsilon)\rangle. \quad (42c)$$

Again, $|\Psi_r^a(\varepsilon)\rangle$ is negligible if the resonant point ε_r is passive (in which case one has $\alpha_r(\varepsilon_r) = 0$).

In the above expressions it was assumed that E_r is an interior point in the range D . According to (35b) one has $|\Psi_s^a(\varepsilon)\rangle = 0$ if $\varepsilon \notin D$. However, if E_r is an interior point in D and if β is sufficiently small, those expressions satisfy $|\Psi_s^a(\varepsilon)\rangle^\circ \approx 0$ if $\varepsilon \notin D$. On the other hand, if E_r coincides with the edge of the range D ($E_r = \lambda_a$ or $E_r = \lambda_b$), each resonant point ε_s ($s \in Z_r$) in a limit $\beta \rightarrow 0$ converges to this edge and the property $|\Psi_s^a(\varepsilon)\rangle \approx 0$ if $\varepsilon \notin D$ does not follow from (42). In such (rare) cases expressions (42) are still valid, provided one includes the condition $|\Psi_s^a(\varepsilon)\rangle = 0$ ($\varepsilon \notin D$) into those expressions. However, if E_r is an interior point in D , explicit inclusion of this condition is not necessary.

According to the above discussion, if $\omega(\varepsilon)$ is everywhere bounded and if β is small, each resonant point $\varepsilon_s \equiv \varepsilon_s(\beta)$ in a limit $\beta \rightarrow 0$ converges to some local eigenvalue $E_r \in D$ and one has $\varepsilon_s(0) = E_r$. However, operator $\omega(\varepsilon)$ may diverge in some points $e_d \in \Lambda$ inside the range D , while outside this range it must be bounded. In this case generic eigenvalue equation (10) may have some additional eigenvalues $\varepsilon_d \equiv \varepsilon_d(\beta)$ that in a limit $\beta \rightarrow 0$ converge to some point $\varepsilon_d(0) \equiv e_d \in \Lambda$ where operator $\omega(\varepsilon)$ is singular. Expressions (42) hence need some corrections. Each resonant point $\varepsilon_s \equiv \varepsilon_s(\beta)$ in those expressions satisfies $\varepsilon_s(0) = E_r$. If Λ is nonempty one may have either $\varepsilon_s(0) = E_r \in \Lambda$ or $\varepsilon_s(0) = E_r \notin \Lambda$. In the former case $\omega(\varepsilon)$ diverges in E_r and expressions (42) fail [8]. However, coincidence of $\varepsilon_s(0) = E_r$ with $\varepsilon_d(0) \in \Lambda$ is rare. Hence we will not consider such cases here [8]. In the latter case expressions (42) are still valid for each $\varepsilon \in D$, except in some small intervals containing those resonant points $\varepsilon_d(\beta)$ that satisfy $\varepsilon_d(0) \in \Lambda$ and $\varepsilon_d(0) \neq E_r$. One could incorporate those corrections directly into expressions (42). However, it is more convenient to resolve this problem in another way. Instead of to associate states $|\Psi_s^a(\varepsilon)\rangle$ with local eigenvalues E_r , one can associate those states with resonant points ε_s . From this point of view there are states $|\Psi_s^a(\varepsilon)\rangle$ associated with resonant points $\varepsilon_s \equiv \varepsilon_s(\beta)$ that satisfy $\varepsilon_s(0) = E_r \notin \Lambda$, and there are also some additional states $|\Psi_d^a(\varepsilon)\rangle$

associated with resonant points $\varepsilon_d \equiv \varepsilon_d(\beta)$ that satisfy $\varepsilon_d(0) \in \Lambda$. Those additional states absorb all necessary corrections. In conclusion, with each resonant point $\varepsilon_s \equiv \varepsilon_s(\beta)$ we associate a state $|\Psi_s^a(\varepsilon)\rangle$. If this resonant point in a limit $\beta \rightarrow 0$ converges to local eigenvalue $\varepsilon_s(0) \equiv E_r \notin \Lambda$, this state is correctly given by expression (42a). However, if in this limit $\varepsilon_s \equiv \varepsilon_s(\beta)$ converges to $\varepsilon_s(0) \in \Lambda$ and if in addition $\varepsilon_s(0)$ differs from all local eigenvalues ($\varepsilon_s(0) \notin \{E_r\}$), the state $|\Psi_s^a(\varepsilon)\rangle$ is not approximated by the expression (42a) [8]. One finds that such a state is negligible for each $\varepsilon \in D$, except for those values of ε that are contained in some extremely small interval close to the point $\varepsilon_s(0) \in \Lambda$. In particular, in a limit $\beta \rightarrow 0$ integral of the norm of such a state converges to zero (see expression (47)). Hence each state $|\Psi_s^a(\varepsilon)\rangle$ that is associated with a resonant point $\varepsilon_s \equiv \varepsilon_s(\beta)$ and which satisfies $\varepsilon_s(0) \in \Lambda$ and $\varepsilon_s(0) \notin \{E_r\}$ can be neglected.

Consider now the norm $\rho_s(\varepsilon) = \langle \Psi_s^a(\varepsilon) | \mathbf{S}^a | \Psi_s^a(\varepsilon) \rangle$ of the state $|\Psi_s^a(\varepsilon)\rangle$. Expression (42a) implies

$$\rho_s(\varepsilon) \approx \rho_s^0(\varepsilon) = \frac{\beta^2}{1 + \pi^2 \beta^4 \left(\sum_{p \in Z_r} \frac{F_{pp}(\varepsilon_p)}{\varepsilon - \varepsilon_p} \right)^2} \frac{F_{ss}(\varepsilon_s)}{(\varepsilon - \varepsilon_s)^2}, \quad s \in Z_r. \quad (43a)$$

Norm $\rho_s^0(\varepsilon)$ approximates density $\rho_s(\varepsilon)$ (expression (37)) in the case of small β . Functional form of approximate density $\rho_s^0(\varepsilon)$ is quite interesting. First one finds that passive resonant points ε_p ($p \in Z_r$) do not contribute to this density. This density depends only on active resonant points ε_p ($p \in Z_r$) and on the corresponding quantities $F_{pp}(\varepsilon_p)$. Further, this density vanishes in each active resonant point ε_p that differs from ε_s . In other words one has $\rho_s^0(\varepsilon_p) = 0$ if ε_p is active and if $\varepsilon_p \neq \varepsilon_s$. As implied by (40a), this is an exact property valid for each β . In addition, between any two mutually distinct active resonant points ε_p and $\varepsilon_{p'}$ ($\varepsilon_p \neq \varepsilon_{p'}$) there is a point $\varepsilon = \varepsilon_0$ such that the sum in the denominator of (43a) vanishes. In this point one has $\rho_s^0(\varepsilon_0) = \beta^2 F_{ss}(\varepsilon_s) / (\varepsilon_0 - \varepsilon_s)^2$. Since $\varepsilon_s = E_r + O(\beta^2)$ the quantity $(\varepsilon_0 - \varepsilon_r)$ is of the order $O(\beta^2)$. This implies that $\rho_s^0(\varepsilon_0)$ is of the order $O(\beta^{-2})$. Hence if β is sufficiently small density $\rho_s^0(\varepsilon)$ has a sharp pick in the point $\varepsilon = \varepsilon_0$. One may have several mutually distinct active resonant points ε_p and several such picks between those resonant points. In conclusion, density $\rho_s^0(\varepsilon)$ may contain several picks that are spaced close to the local eigenvalue E_r .

If the resonant point ε_s is degenerate, instead of a single density (43a) it is convenient to consider total density $\rho_{(s)}(\varepsilon)$ associated with this point. One has

$$\rho_{(s)}(\varepsilon) \equiv \sum_{p \in \Xi_s} \rho_p(\varepsilon) = \left\langle \Psi_{(s)}^a \left| \mathbf{S}^a \right| \Psi_{(s)}^a(\varepsilon) \right\rangle \approx \rho_{(s)}^0(\varepsilon), \quad (43b)$$

where

$$\rho_{(s)}^0(\varepsilon) = \frac{\beta^2}{1 + \pi^2 \beta^4 \left(\sum_{p \in Z_r} \frac{F_{pp}(\varepsilon_p)}{\varepsilon - \varepsilon_p} \right)^2} \frac{\sum_{p \in \Xi_s} F_{pp}(\varepsilon_s)}{(\varepsilon - \varepsilon_s)^2}, \quad s \in Z_r. \quad (43c)$$

Density $\rho_{(s)}^0(\varepsilon)$ is associated with (in general degenerate) resonant point $\varepsilon_s \equiv \varepsilon_s(\beta)$ that in a limit $\beta \rightarrow 0$ converges to a local eigenvalue $E_r \notin \Lambda$. According to the above expression, if ε_s is passive one has $\rho_{(s)}^0(\varepsilon) = 0$. However, if ε_s is active one has $\rho_{(s)}^0(\varepsilon) \neq 0$ for each $\varepsilon \in D$, except when $\varepsilon = \varepsilon_p$ is another active resonant point that satisfies $p \in Z_r$ and $\varepsilon_p \neq \varepsilon_s$. In this latter case one has $\rho_{(s)}^0(\varepsilon_p) = 0$. In addition, the area of the density $\rho_{(s)}^0(\varepsilon)$ associated with the active resonant point equals unity [8]. Hence

$$\int \rho_{(s)}^0(\varepsilon) d\varepsilon = \begin{cases} 1 & \text{if } \varepsilon_s \text{ active,} \\ 0 & \text{otherwise,} \end{cases} \quad s \in Z_r. \quad (44a)$$

According to (44a) total area due to all densities $\rho_p(\varepsilon)$ that are associated with a local eigenvalue $E_r \in D$ equals the number of mutually distinct and active resonant points $\varepsilon_s \equiv \varepsilon_s(\beta)$ that satisfy $\varepsilon_s(0) = E_r$. Since this can not exceed degeneracy κ_r of the local eigenvalue E_r , one finds

$$\sum_{s \in Z_r} \int \rho_s^0(\varepsilon) d\varepsilon \leq \kappa_r. \quad (44b)$$

Equality in the above expression is obtained if and only if all resonant points ε_s that are associated with local eigenvalue $E_r (s \in Z_r)$ are active and non-degenerate. In this case all such resonant points are proper resonant points and there is no anomalous point associated with this local eigenvalue.

In the following section we will show that expression (44a) is in accord with the completeness requirements. In fact, one can derive this expression from those requirements carefully following the transition to the limit $\beta \rightarrow 0$. However, this is quite convoluted derivation of this expression.

If E_r is nondegenerate and if $F_{rr}(\varepsilon_r) \neq 0$ above expressions simplify. In this case resonant point $\varepsilon_r \equiv \varepsilon_r(\beta)$ that satisfies $\varepsilon_r(0) = E_r$ is a proper resonant point and expressions (43) reduce to

$$\rho_r(\varepsilon) \approx \rho_r^0(\varepsilon) = \frac{\beta^2 F_{rr}(\varepsilon_r)}{(\varepsilon - \varepsilon_r)^2 + \pi^2 \beta^4 F_{rr}^2(\varepsilon_r)}. \quad (45a)$$

This also follows from (42c). Density $\rho_r^0(\varepsilon)$ approximates density $\rho_r(\varepsilon)$ (equation (37)) in the case of small β and in the case when E_r is nondegenerate. Considered as a function of ε , $\rho_r^0(\varepsilon)$ is a universal resonance curve [13]. This is

a bell shaped curve with a maximum ρ_r^{\max} in a resonant point $\varepsilon = \varepsilon_r$, with the width $\Delta\varepsilon_r$, and with a unite area:

$$\rho_r^{\max} = \rho_r^0(\varepsilon_r) = \frac{1}{\pi^2 \beta^2 F_{rr}^2(\varepsilon_r)}, \quad \Delta\varepsilon_r = 2\pi\beta^2 F_{rr}(\varepsilon_r), \quad (45b)$$

$$\int \rho_r^0(\varepsilon) d\varepsilon = 1. \quad (45c)$$

Expression (45c) is a special case of the expression (44a).

Consider now quantities ε_r and $F_{ss}(\varepsilon_r)$ ($s \in \Xi_r$) that appear in the above expressions. Concerning resonant point ε_r one has $\varepsilon_r = E_s + O(\beta^2)$. In particular, if $E_r \in D$ is nondegenerate, resonant point $\varepsilon = \varepsilon_r$ can be approximated as

$$\varepsilon_r \approx E_r + \beta^2 \langle \Theta_r | \omega(E_r) | \Theta_r \rangle, \quad (46a)$$

(see Appendix A.5). Concerning quantities $F_{ss}(\varepsilon_r)$ one has

$$F_{ss}(\varepsilon_r) = \langle \Theta_s | \mathbf{f}(E_s) | \Theta_s \rangle + O(\beta^2). \quad (46b)$$

In the above expressions we have assumed that $\omega(\varepsilon)$ is regular in the point $\varepsilon = E_r$, i.e. $E_r \notin \Lambda$. If $E_r \in \Lambda$ operator $\omega(\varepsilon)$ diverges in $\varepsilon = E_r$ and in this case one can not obtain resonant point ε_r ($s \in Z_r$) by a standard perturbation expansion. In particular, approximation (46a) fails and the state $|\Psi_s^a(\varepsilon)\rangle$ is not given by expression (42a). Further, if $E_r \in \Lambda$ is nondegenerate density $\rho_r^0(\varepsilon)$ has not the shape of the universal resonance curve (45a). However, if E_r is an interior point of the range D and if it is degenerate, density $\rho_r^0(\varepsilon)$ still has a unite area and expression (45c) still holds [8]. Finally, resonant point $\varepsilon_s \equiv \varepsilon_s(\beta)$ may in the limit $\beta \rightarrow 0$ converge to the point $\varepsilon_s(0) = e_d \in \Lambda$ that differs from all local eigenvalues E_p . In this case the corresponding state $|\Psi_s^a(\varepsilon)\rangle$ may satisfy $|\Psi_s(\varepsilon)\rangle \neq 0$ in some immediate vicinity of the resonant point ε_s . However, if β is small global contribution of the corresponding density $\rho_s(\varepsilon)$ is negligible and one finds [8]

$$\int \rho_s(\varepsilon) d\varepsilon \approx 0, \quad \text{if } \lim_{\beta \rightarrow 0} \varepsilon_s(\beta) = e_d \in \Lambda \quad \text{and} \quad e_d \notin \{E_p\}. \quad (47)$$

Due to (47) one can neglect global contribution to the density $\rho^a(\varepsilon)$ of all those resonant points ε_r that are not associated with some local eigenvalue E_p . It is however feasible that in some cases those contributions, though globally negligible, might be of some interest.

Above we have considered densities $\rho_s(\varepsilon)$ in the case of small β . According to (37b) density $\rho_s(\varepsilon)$ is a probability density to find a state $|\phi_s(\varepsilon)\rangle$ in the embedded eigenstate $|\Psi(\varepsilon)\rangle$ of the combined system. More important from this density is probability density $\rho_s^a(\varepsilon) = |\langle \Theta_s | \mathbf{S}^a | \Psi(\varepsilon) \rangle|^2$ to find local state $|\Theta_s\rangle$ in the embedded eigenstate $|\Psi(\varepsilon)\rangle$. Since $|\Psi(\varepsilon)\rangle$ has the eigenvalue ε , density $\rho_s^a(\varepsilon)$

in conjuncture with probabilities $w_{I_s}^a$ determines spectral (eigenvalue) distribution of the state $|\Theta_s\rangle$ when the system \mathbf{S}_ρ^a is not isolated but when it interacts with the system \mathbf{S}_∞^b (see section 3.5). According to (A.33), if β is small one has $|\phi_s(\varepsilon)\rangle = |\Theta_s\rangle + O(\beta^2)$. Hence

$$\rho_s^a(\varepsilon) = \rho_s(\varepsilon) + O(\beta^2) \approx \rho_s(\varepsilon). \quad (48)$$

In a small coupling limit densities $\rho_s(\varepsilon)$ and $\rho_s^a(\varepsilon)$ coincide. Hence all the above expressions apply to densities $\rho_s^a(\varepsilon)$ as well as to densities $\rho_s(\varepsilon)$. In particular, if local eigenvalue E_r is nondegenerate, the interaction with the system \mathbf{S}_∞^b shifts this eigenvalue to a new position ε_r (expression (46a)). If ε_r is active this eigenvalue broadens and assumes the shape of the universal resonance curve (expression (45a)). This curve is a spectral distribution of a nondegenerate state $|\Theta_s\rangle$ that interacts with the infinite system \mathbf{S}_∞^b . This reproduces well-known result from the standard perturbation expansion method [1].

3.4.8. Emergence of resonance in the case when the coupling β is large

In a previous section it was shown that in the case when β is small density $\rho^a(\varepsilon) = \sum_s \rho_s^a(\varepsilon) = \sum_s \rho_s(\varepsilon)$ exhibits strong resonance in the neighborhood of each active resonant point $\varepsilon_s \in D$ that in a limit $\beta \rightarrow 0$ converges to some local eigenvalue E_r . In particular, if E_r is nondegenerate and if $\omega(\varepsilon)$ is not singular in this point, density $\rho^a(\varepsilon)$ has close to this point the shape of the universal resonance curve with the unit area. According to (45b), as β decreases, the height ρ_r^{\max} of this curve increases, its width $\Delta\varepsilon_r$ decreases, and overall resonance structure becomes more and more prominent. On the other hand, if β increases, resonance structure in most cases becomes less and less prominent until it is completely lost. However, there are some exceptional cases when density $\rho^a(\varepsilon)$ may still contain sharp resonant picks, even when β is not small. We will now discuss such cases.

Let $\varepsilon_r \in D$ be an active resonant point and let $\varepsilon_r \notin \Lambda$. Assume that β is not small. If $\eta'_p(\varepsilon_r) \neq 1$ for each $p \in \Xi_r$ and if ε_r is an interior point in D , one can approximate the state $|\Psi^a(\varepsilon)\rangle \in X_\rho^a$ in some small neighborhood Δ of this resonant point according to (see Appendix A.7)

$$|\Psi^a(\varepsilon)\rangle \approx |\Psi_{(r)}^a(\varepsilon)\rangle \approx \frac{\beta}{\sqrt{(\varepsilon - \varepsilon_r)^2 + \pi^2\beta^4 \left(\sum_{p \in \Xi_r} \frac{F_{pp}(\varepsilon_r)}{1 - \eta'_p(\varepsilon_r)} \right)^2}} \sum_{s \in \Xi_r} \frac{\alpha_s^*(\varepsilon_r)}{1 - \eta'_s(\varepsilon_r)} |\phi_s(\varepsilon)\rangle, \quad (49a)$$

where the state

$$|\Psi_{(r)}^a(\varepsilon)\rangle = \sum_{s \in \Xi_r} |\Psi_s^a(\varepsilon)\rangle \quad (49b)$$

is associated with a resonant point $\varepsilon = \varepsilon_r$. Probability density $\rho^a(\varepsilon)$ equals norm of the state $|\Psi^a(\varepsilon)\rangle$ and it can be approximated as

$$\rho^a(\varepsilon) \approx \rho_{(r)}^1(\varepsilon) = \frac{\beta^2}{(\varepsilon - \varepsilon_r)^2 + \pi^2 \beta^4 \left(\sum_{p \in \Xi_r} \frac{F_{pp}(\varepsilon_r)}{1 - \eta'_p(\varepsilon_r)} \right)^2} \sum_{s \in \Xi_r} \frac{F_{ss}(\varepsilon_r)}{(1 - \eta'_s(\varepsilon_r))^2}, \quad \varepsilon \in \Delta. \quad (49c)$$

Above expressions apply to an arbitrary β which may be very large. However, those expressions are valid only within a small interval Δ that contains resonant point ε_r . Within this interval one has $\alpha_s(\varepsilon) \approx \alpha_s(\varepsilon_r)$ and $\eta_s(\varepsilon) \approx \eta_s(\varepsilon_r) + \eta'_s(\varepsilon_r)(\varepsilon - \varepsilon_r)$. As $|\varepsilon - \varepsilon_r|$ decreases expressions (49) are more and more reliable and in the point $\varepsilon = \varepsilon_r$ they are exact. In particular, according to (40c) one has

$$\rho^a(\varepsilon_r) = \rho_{(r)}^1(\varepsilon_r). \quad (49d)$$

However, as $|\varepsilon - \varepsilon_r|$ increases those expressions deteriorate and if $|\varepsilon - \varepsilon_r| > \Delta$ they are no more reliable. Formally, the function $\rho_{(r)}^1(\varepsilon)$, which approximates probability density $\rho^a(\varepsilon)$ in the interval Δ , is proportional to the universal resonance curve centered at the position $\varepsilon = \varepsilon_r$ where it has its maximum value $\rho_{(r)}^1(\varepsilon_r) \equiv \rho^a(\varepsilon_r)$. At the position where $\rho_{(r)}^1(\varepsilon)$ has half of its maximum value, it has the width $\Delta\varepsilon_{(r)}$. One finds:

$$\rho_{(r)}^1(\varepsilon_r) = \frac{1}{\pi^2 \beta^2 \left(\sum_{p \in \Xi_r} \frac{F_{pp}(\varepsilon_r)}{1 - \eta'_p(\varepsilon_r)} \right)^2} \sum_{s \in \Xi_r} \frac{F_{ss}(\varepsilon_r)}{(1 - \eta'_s(\varepsilon_r))^2}, \quad (50a)$$

$$\Delta\varepsilon_{(r)} = 2\pi\beta^2 F_{(r)}(\varepsilon_r), \quad \text{where } F_{(r)}(\varepsilon_r) = \sum_{p \in \Xi_r} \frac{F_{pp}(\varepsilon_r)}{1 - \eta'_p(\varepsilon_r)}. \quad (50b)$$

If β is not small the width $\Delta\varepsilon_{(r)}$ of the universal resonance curve $\rho_{(r)}^1(\varepsilon)$ is usually much larger than the interval Δ , i.e. $\Delta\varepsilon_{(r)} \gg \Delta$. Since approximation (49c) fails if $|\varepsilon - \varepsilon_r| > \Delta$, not much can be implied about the resonance structure of the density $\rho^a(\varepsilon)$. However, if the quantity $F_{(r)}(\varepsilon_r)$ is sufficiently small one may have $\Delta\varepsilon_{(r)} < \Delta$, even in the case when the coupling β is not small. In this case in a small neighborhood Δ of the point $\varepsilon = \varepsilon_r$ density $\rho^a(\varepsilon)$ displays a prominent shape of the universal resonance curve $\rho_{(r)}^1(\varepsilon)$ with a small width $\Delta\varepsilon_{(r)}$ and with the area

$$\int \rho_{(r)}^1(\varepsilon) d\varepsilon = \frac{1}{\sum_{p \notin \Xi_r} \frac{F_{pp}(\varepsilon_r)}{1 - \eta'_p(\varepsilon_r)}} \sum_{s \in \Xi_r} \frac{F_{ss}(\varepsilon_r)}{(1 - \eta'_s(\varepsilon_r))^2}. \quad (50c)$$

According to the expressions (29), the quantity $F_{(r)}(\varepsilon_r)$ is small if in the point $\varepsilon = \varepsilon_r$ eigenstates $|\phi_s(\varepsilon_r)\rangle \equiv |\theta_s\rangle \in X_\rho^a$ ($s \in \Xi_r$) of the resonant eigenvalue equation interact very weakly with the state $|\Phi(k)\rangle \in X_\infty^b$ where $\varepsilon_r = \lambda(k)$.

In conclusion, expression (50c) makes sense only if the quantity $F_{(r)}(\varepsilon_r)$ is sufficiently small. In section (4) will be given an example of such a resonance structure.

Consider now quantities $F_{ss}(\varepsilon_r)$ and $\eta'_s(\varepsilon_r)$ that are needed in the above expressions. Using (27c), (29b) and (A.36a) one finds

$$F_{ss}(\varepsilon_r) = \langle \theta_s | \mathbf{f}(\varepsilon_r) | \theta_s \rangle, \quad \eta'_s(\varepsilon_r) = \beta^2 \langle \theta_s | \boldsymbol{\omega}'(\varepsilon_r) | \theta_s \rangle, \quad s \in \Xi_r. \quad (51)$$

According to (9b) one has $\langle \theta | \boldsymbol{\omega}'(\varepsilon) | \theta \rangle < 0$ for each $\varepsilon \notin D$ and for each nontrivial $|\theta\rangle \in X_\rho^a$. On the other hand, if $\varepsilon \in D$ one may have $\langle \theta | \boldsymbol{\omega}'(\varepsilon) | \theta \rangle < 0$ as well as $\langle \theta | \boldsymbol{\omega}'(\varepsilon) | \theta \rangle > 0$ (see figure 2b). However, in a special case when $\langle \theta | \mathbf{f}(\varepsilon) | \theta \rangle = 0$ one finds $\langle \theta | \boldsymbol{\omega}'(\varepsilon) | \theta \rangle < 0$ [8]. If $\mathbf{f}(\varepsilon)$ is reasonably smooth in the point $\varepsilon \in D$ this implies $\langle \theta | \boldsymbol{\omega}'(\varepsilon) | \theta \rangle < 0$ if $\langle \theta | \mathbf{f}(\varepsilon) | \theta \rangle$ is relatively small, i.e. if $\langle \theta | \mathbf{f}(\varepsilon) | \theta \rangle \approx 0$. Since in the above case $F_{(r)}(\varepsilon_r)$ is small, one must have $F_{ss}(\varepsilon_r) \approx 0$ ($s \in \Xi_r$). Hence $\langle \theta_s | \boldsymbol{\omega}'(\varepsilon_r) | \theta_s \rangle < 0$ for each $s \in \Xi_r$ [8]. One thus finds $\eta'_s(\varepsilon_r) < 0$ ($s \in \Xi_r$). Since $F_{pp}(\varepsilon) \geq 0$ this implies

$$\int \rho_{(r)}^1(\varepsilon) d\varepsilon < 1. \quad (50d)$$

If the resonant point $\varepsilon = \varepsilon_r$ is nondegenerate, expressions (49) and (50) reduce to

$$|\Psi^a(\varepsilon)\rangle \approx \frac{\beta \alpha_r^*(\varepsilon_r)}{\sqrt{(1-\eta'_r(\varepsilon_r))^2(\varepsilon-\varepsilon_r)^2 + \pi^2 \beta^4 (F_{rr}(\varepsilon_r))^2}} |\phi_r(\varepsilon)\rangle, \quad (52a)$$

$$\rho^a(\varepsilon) \approx \rho_{(r)}^1(\varepsilon) = \frac{\beta^2 F_{rr}(\varepsilon_r)}{(1-\eta'_r(\varepsilon_r))^2(\varepsilon-\varepsilon_r)^2 + \pi^2 \beta^4 F_{rr}(\varepsilon_r)^2}, \quad \varepsilon \in \Delta, \quad (52b)$$

$$\rho_{(r)}^1(\varepsilon_r) = \frac{1}{\pi^2 \beta^2 F_{rr}(\varepsilon_r)}, \quad \Delta\varepsilon_{(r)} = 2\pi\beta^2 \frac{F_{rr}(\varepsilon_r)}{1-\eta'_r(\varepsilon_r)}, \quad (53a)$$

$$\int \rho_{(r)}^1(\varepsilon) d\varepsilon = \frac{1}{1-\eta'_r(\varepsilon_r)} < 1. \quad (53b)$$

It is instructive to compare expressions (49–53) valid for each β with expressions (42–46) valid in the case of small β . First, note that expressions (42–46) apply to each $\varepsilon \in D$, while expressions (49–53) apply only to a small interval Δ containing active resonant point ε_r . In particular, expression (50c) for the area of the curve (49b) makes sense if and only if the width $\Delta\varepsilon_{(r)}$ of this curve as calculated according to (50b) is sufficiently small. Further, if β is small and if $E_s \in D$ is nondegenerate and active, the area associated with the corresponding resonance curve equals unity (equation (45c)), while in the case when β is not small, the area associated with nondegenerate active resonant point ε_r is less than unity (expression (53b)). Similar difference applies to a degenerate case

(compare expressions (44a) and (50d)). Mathematically, this difference is mainly due to the fact that in a small coupling limit one has $\eta'_s(\varepsilon) \approx 0$ and expressions (49–53) accordingly simplify.

One final point. Density $\rho_{(r)}^1(\varepsilon)$ is approximate norm of the state $|\Psi_{(r)}^a(\varepsilon)\rangle$ in a small interval Δ at the resonant point ε_r . In this interval the state $|\Psi_{(r)}^a(\varepsilon)\rangle$ approximates component $|\Psi^a(\varepsilon)\rangle$ of the embedded eigenstate $|\Psi(\varepsilon)\rangle$. Hence:

$$\rho_{(r)}^1(\varepsilon) \approx \rho^a(\varepsilon) = \sum_s^\rho \rho_s^a(\varepsilon) = \sum_s^\rho \rho_s(\varepsilon) \approx \sum_{s \in \Xi_r} \rho_s(\varepsilon), \quad \varepsilon \in \Delta, \quad (54)$$

where $\rho_s(\varepsilon)$ is a probability density to find eigenstate $|\phi_s(\varepsilon)\rangle$ of (27a) with the eigenvalue ε . Since β is not small this probability density differs from the probability density $\rho_s^a(\varepsilon)$ to find local state $|\Theta_s\rangle$ with the eigenvalue ε , i.e. unlike (48) one has in general $\rho_s(\varepsilon) \neq \rho_s^a(\varepsilon)$.

3.5. Eigenvalue distributions of local states $|\Theta_s\rangle \in X_\rho^a$

Each state $|\Psi(\varepsilon)\rangle$ with the eigenvalue $\varepsilon \in D$ is an embedded eigenstate of the combined system, while each state $|\Psi_I\rangle$ with the eigenvalue $\varepsilon_I \in \bar{D}$ is an isolated eigenstate of this system. If this system contains no anomalous points, those eigenstates form a complete set in the space X_∞ of the combined system. Hence an arbitrary state $|\Omega\rangle \in X_\infty$ can be written as a linear combination of those eigenstates. In particular, each state $|\Theta\rangle \in X_\rho^a$ can be written as a linear combination

$$|\Theta\rangle = \sum_I \langle \Psi_I^a | \mathbf{S}^a | \Theta \rangle |\Psi_I\rangle + \int_{\lambda_a}^{\lambda_b} \langle \Psi^a(\varepsilon) | \mathbf{S}^a | \Theta \rangle |\Psi(\varepsilon)\rangle d\varepsilon, \quad (55a)$$

where coefficients $\langle \Psi_I^a | \mathbf{S}^a | \Theta \rangle$ and $\langle \Psi^a(\varepsilon) | \mathbf{S}^a | \Theta \rangle$ can be obtained from (14) and (35), respectively. If in the combined system \mathbf{S}_∞ one measures the eigenvalue of the state $|\Theta\rangle$, one obtains the value $\varepsilon_I \in \bar{D}$ with the probability $|\langle \Theta | \mathbf{S}^a | \Psi_I^a \rangle|^2$ and the value $\varepsilon \in D$ with the probability density $|\langle \Theta | \mathbf{S}^a | \Psi^a(\varepsilon) \rangle|^2$. Those quantities define eigenvalue profile or eigenvalue (spectral) distribution of the state $|\Theta\rangle$. This state must be found with a certainty either with some eigenvalue $\varepsilon \in D$ or with some eigenvalue $\varepsilon_I \in \bar{D}$. Hence

$$\sum_I |\langle \Theta | \mathbf{S}^a | \Psi_I^a \rangle|^2 + \int |\langle \Theta | \mathbf{S}^a | \Psi^a(\varepsilon) \rangle|^2 d\varepsilon = 1. \quad (55b)$$

This expression formally follows from (55a), from the normalization $\langle \Theta | \mathbf{S}^a | \Theta \rangle = 1$ of the state $|\Theta\rangle$ and from the orthonormalities (13) and (20) of the isolated and embedded eigenstates. Of particular interest is the case when

$|\Theta\rangle = |\Theta_s\rangle$ is a local state. One is usually interested how original eigenvalues E_s and the corresponding eigenstates $|\Theta_s\rangle$ of the isolated system \mathbf{S}_ρ^a are modified by the interaction of this system with the infinite system \mathbf{S}_∞^b . Eigenvalue distribution of the local state $|\Theta_s\rangle$ that interacts with the system \mathbf{S}_∞^b is given by probabilities $w_{I_s}^a = |\langle\Theta_s | \mathbf{S}^a | \Psi_I^a\rangle|^2$ and by probability density $\rho_s^a(\varepsilon) = |\langle\Theta_s | \mathbf{S}^a | \Psi^a(\varepsilon)\rangle|^2$. In accord with (55b) one has

$$\sum_I w_{I_s}^a + \int \rho_s^a(\varepsilon) d\varepsilon = 1, \quad s = 1, \dots, \rho, \quad (56a)$$

where probabilities $w_{I_s}^a$ are given by (16a), while probability densities $\rho_s^a(\varepsilon)$ are given by (38b). Since $\rho^a(\varepsilon) = \sum_s \rho_s^a(\varepsilon)$ while $w_I^a = \sum_s w_{I_s}^a$ and since the system \mathbf{S}_ρ^a contains ρ states $|\Theta_s\rangle$, this implies

$$\sum_I w_I^a + \int \rho_a(\varepsilon) d\varepsilon = \rho, \quad (56b)$$

where probabilities w_I^a are given by expression (16b) while probability density $\rho^a(\varepsilon)$ is given by expression (39b).

Relations (56) are completeness relations. As emphasized above, those relations are valid provided the system \mathbf{S}_∞ contains no anomalous point. If this system contains some anomalous points $\varepsilon_r \equiv \varepsilon_a \in D$, expressions (56) should include additional terms. Each such additional term is due to isolated eigenstate of the combined system with the eigenvalue in the corresponding anomalous point.

3.5.1. Eigenvalue distribution of local states in the weak coupling limit

In the case when the coupling β is small eigenvalue distribution of local states $|\Theta_s\rangle$ simplifies. In this case due to the interaction with the system \mathbf{S}_∞^b each eigenvalue E_s of the system \mathbf{S}_ρ^a is only slightly shifted to a new position. This is a small shift that is at most of the order $O(\beta^2)$. Consider first the case when the system \mathbf{S}_∞ contains no anomalous points. In this case each shifted eigenvalue $\varepsilon_r \in D$ is nondegenerate and active resonant point. According to (43a) and (44a) this shifted eigenvalue is broadened and it has unit area. In particular, if the corresponding eigenvalue E_s is nondegenerate, this shifted eigenvalue assumes the shape of the universal resonance curve. On the other hand, each shifted eigenvalue $\varepsilon_I \in \bar{D}$ remains sharp. According to (16a), if β is small the corresponding probability $w_{I_s}^a$ to find local state $|\Theta_s\rangle$ in the isolated eigenstate $|\Psi_I\rangle$ (probability for $|\Theta_s\rangle$ to have eigenvalue $\varepsilon_I \in \bar{D}$) is

$$w_{I_s}^a = \frac{\langle\theta_I | \mathbf{S}^a | \Theta_s\rangle \langle\Theta_s | \mathbf{S}^a | \theta_I\rangle}{\langle\theta_I | \mathbf{S}^a | \theta_I\rangle} + O(\beta^2).$$

Since $|\theta_I\rangle = |\Theta_I\rangle + O(\beta^2)$ this implies

$$w_{I_s}^a = \delta_{I_s} + O(\beta^2).$$

If $E_s \in \bar{D}$ there is exactly one $s \equiv I$ such that $w_{I_s}^a \approx 1$ while if $E_s \in D$ one has $w_{I_s}^a \approx 0$ for each isolated eigenstate $|\Psi_I\rangle$. Further if $E_s \in \bar{D}$ one has $\rho_s^a(\varepsilon) \approx 0$ since the eigenvalues $\varepsilon_s \notin D$ of the generic equation do not contribute to the density $\rho^a(\varepsilon)$. Hence $E_s \in \bar{D}$ implies $\sum_I w_{I_s}^a + \int \rho_s^a(\varepsilon)d\varepsilon \approx 1$ in accord with completeness requirement (56a). In this case eigenvalue distribution of local state $|\Theta_s\rangle$ consists of a sharp eigenvalue at the position $\varepsilon_s \in \bar{D}$, while the contribution of eigenvalues $\varepsilon \in D$ is negligible. Another possibility is $E_s \in D$. According to (44a) in this case one has $\int \rho_s^a(\varepsilon)d\varepsilon \approx 1$. Hence one again finds $\sum_I w_{I_s}^a + \int \rho_s^a(\varepsilon)d\varepsilon \approx 1$ in accord with completeness requirement (56a). In particular, if E_s is nondegenerate eigenvalue distribution of local state $|\Theta_s\rangle$ has the shape of the universal resonance curve centered at the point $\varepsilon = \varepsilon_s$ and situated close to the corresponding unperturbed eigenvalue E_s (see equation (45)), while the contribution of isolated eigenvalues $\varepsilon_I \in \bar{D}$ is negligible. Since β is small generic equation (10) has exactly ρ eigenvalues $\varepsilon_s(\beta)$ that in a limit $\beta \rightarrow 0$ converge to local eigenvalues E_s . Hence $\sum_I w_I^a + \int \rho^a(\varepsilon)d\varepsilon \approx \rho$ in accord with completeness requirement (56b).

Above we have neglected the contribution to total probability of those resonant points ε_d that in a limit $\beta \rightarrow 0$ converge to some point $e_d \in \Lambda$ where $\omega(\varepsilon)$ diverges and where $e_d \notin \{E_s\}$. According to (47) this contribution is negligible and hence all above conclusions remain valid.

Consider now the case when the system \mathbf{S}_∞ contains some anomalous points. If $\varepsilon_r \in D$ is such a point, it is either degenerate or passive. If it is passive the contribution of the integral $\int \rho_{(r)}(\varepsilon)d\varepsilon$ to the total probability is zero (see equation (44a)). If it is degenerate, the contribution of this integral to the total probability equals one, which is less than the degeneracy of ε_r . In both cases one finds $\sum_I w_I^a + \int \rho_a(\varepsilon)d\varepsilon < \rho$ in violation of the expression (56b). The missing contribution is due to the isolated eigenstate or eigenstates that has the eigenvalue in this anomalous point [8].

4. Example

In order to illustrate the above approach, consider the interaction of a two-dimensional system \mathbf{S}_2^a with an infinite system \mathbf{S}_∞^b that contains a single one-parameter eigenvalue band. This example is quite simple, yet complex enough to illustrate key features of the suggested approach.

Let $\{|s\rangle\}$ be an orthonormalized base in X_2^a

$$\langle s | p \rangle = \delta_{sp}, \quad \sum_s |s\rangle \langle s| = \mathbf{I}^a. \tag{57}$$

Let the system \mathbf{S}_2^a in this base be characterized by the matrices

$$\mathbf{A} = \begin{pmatrix} 0.5 & -0.25 \\ -0.25 & 0.6 \end{pmatrix}, \quad \mathbf{S}^a = \begin{pmatrix} 1.1 & 0.1 \\ 0.1 & 1 \end{pmatrix}. \quad (58a)$$

For the sake of generality we assume that this system is described by a generalized eigenvalue equation (1a) where $\mathbf{S}^a \neq \mathbf{I}^a$. Eigenvalues and corresponding eigenstates of this system are

$$E_1 = 0.25474, \quad E_2 = 0.85536, \quad (58b)$$

$$|\Theta_1\rangle = \begin{pmatrix} 0.78168 \\ 0.62368 \end{pmatrix}, \quad |\Theta_2\rangle = \begin{pmatrix} 0.60561 \\ -0.79576 \end{pmatrix}, \quad (58c)$$

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

For the sake of simplicity in (58c) and in the following expressions we freely mix bracket notation with a standard vector notation. Strictly, this is not allowed and one should write, for example, $\langle 1 | \Theta_1 \rangle = 0.78168$, $\langle 2 | \Theta_1 \rangle = 0.62368$, etc. Nevertheless, with a due caution one can use slightly inaccurate notation (58c).

Let the infinite dimensional system \mathbf{S}_∞^b contain a single one-parameter eigenvalue band in the interval $D \equiv [\lambda_a, \lambda_b] = [-1, 1]$ and let the functions $a_s(\varepsilon)$ that incorporate key information about this system and about the interaction of this system with the system \mathbf{S}_2^a be given by

$$a_1(\varepsilon) = (\varepsilon^2 - 1) \cdot \begin{cases} 1 & \text{if } \varepsilon \in D, \\ 0 & \text{otherwise,} \end{cases} \quad a_2(\varepsilon) = (\varepsilon - 1) \cdot \begin{cases} 1 & \text{if } \varepsilon \in D, \\ 0 & \text{otherwise.} \end{cases} \quad (59a)$$

Those functions define characteristic matrix $\mathbf{f}(\varepsilon)$ with matrix elements $f_{sp}(\varepsilon) = \langle s | \mathbf{f}(\varepsilon) | p \rangle$

$$\mathbf{f}(\varepsilon) = \begin{pmatrix} (\varepsilon^2 - 1)^2 & (\varepsilon^2 - 1)(\varepsilon - 1) \\ (\varepsilon^2 - 1)(\varepsilon - 1) & (\varepsilon - 1)^2 \end{pmatrix} \cdot \begin{cases} 1 & \text{if } \varepsilon \in D, \\ 0 & \text{otherwise.} \end{cases} \quad (59b)$$

Orthonormalized eigenstates and corresponding eigenvalues of this matrix are

$$|f_1(\varepsilon)\rangle = \frac{1}{\sqrt{\varepsilon^2 + 2\varepsilon + 2}} \begin{pmatrix} 1 + \varepsilon \\ 1 \end{pmatrix}, \quad |f_2(\varepsilon)\rangle = \frac{1}{\sqrt{\varepsilon^2 + 2\varepsilon + 2}} \begin{pmatrix} 1 \\ 1 - \varepsilon \end{pmatrix}, \quad (60a)$$

$$\xi_1(\varepsilon) \equiv a_1(\varepsilon)^2 + a_2(\varepsilon)^2 = (\varepsilon - 1)^2(\varepsilon^2 + 2\varepsilon + 2), \quad \xi_2(\varepsilon) = 0, \quad \varepsilon \in D. \quad (60b)$$

In accord with the expression (7b), there is only one eigenvalue of $\mathbf{f}(\varepsilon)$ that may differ from zero.

In figure 1(a) are shown matrix elements $f_{sp}(\varepsilon)$ of the characteristic matrix $\mathbf{f}(\varepsilon)$. Matrix elements $f_{11}(\varepsilon)$ and $f_{12}(\varepsilon) \equiv f_{21}(\varepsilon)$ are continuous for each real ε , while matrix element $f_{22}(\varepsilon)$ is discontinuous in the point $\varepsilon = -1$ on the left

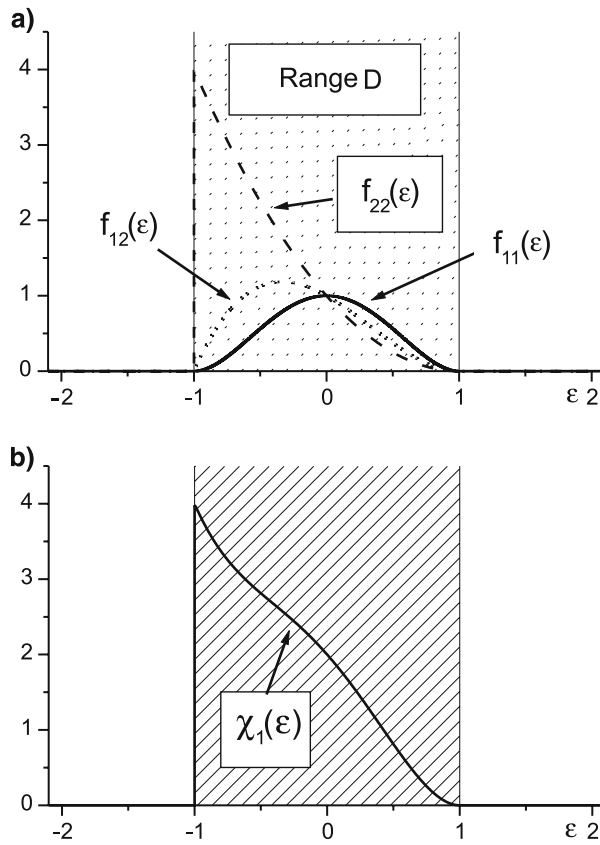


Figure 1. Characteristic matrix $\mathbf{f}(\epsilon)$ of the example combined system \mathbf{S}_∞ . In this example range D equals $D = [-1, 1]$. (a) Matrix elements $f_{sp}(\epsilon)$ of the characteristic matrix. Those matrix elements vanish outside the range D . (b) Eigenvalue $\xi_1(\epsilon)$ of the characteristic matrix.

edge of the range D . Eigenvalue $\xi_1(\epsilon)$ of $\mathbf{f}(\epsilon)$ is hence also discontinuous in this point (see figure 1(b)). By definition, the point $\lambda_a = -1$ is contained in a set Λ (see section 3.1).

According to (8b), each matrix element $\omega_{sp}(\epsilon)$ of the derived matrix $\omega(\epsilon)$ is an integral of a type

$$K(\epsilon) = P \int_a^b \frac{f(\lambda)}{\epsilon - \lambda} d\lambda. \tag{61a}$$

If $f(\lambda)$ is polynomial, there is an exact solution to this integral. In this case one finds [7]

$$K(\epsilon) = f(\epsilon) \ln \left| \frac{\epsilon - a}{\epsilon - b} \right| - g(\epsilon), \tag{61b}$$

where

$$f(\lambda) = \sum_{i=0}^n c_i \lambda^i, \quad g(\varepsilon) = \sum_{k=1}^n c_k g_k(\varepsilon), \quad (61c)$$

and where $g_k(\varepsilon) (k > 0)$ are polynomials [7]

$$g_k(\varepsilon) = \sum_{i=0}^{k-1} \frac{\varepsilon^i}{k-i} [b^{k-i} - a^{k-i}], \quad k = 1, 2, \dots \quad (61d)$$

Hence and from (59b) one finds matrix elements $\omega_{sp}(\varepsilon) = \langle s | \boldsymbol{\omega}(\varepsilon) | p \rangle$ of the derived operator $\boldsymbol{\omega}(\varepsilon)$

$$\begin{aligned} \omega_{11}(\varepsilon) &= (\varepsilon^2 - 1)^2 \ln \left| \frac{\varepsilon + 1}{\varepsilon - 1} \right| - 2\varepsilon^3 + \frac{10}{3}\varepsilon, \\ \omega_{22}(\varepsilon) &= (\varepsilon - 1)^2 \ln \left| \frac{\varepsilon + 1}{\varepsilon - 1} \right| - 2\varepsilon + 4, \\ \omega_{12}(\varepsilon) \equiv \omega_{21}(\varepsilon) &= (\varepsilon^2 - 1) (\varepsilon - 1) \ln \left| \frac{\varepsilon + 1}{\varepsilon - 1} \right| - 2\varepsilon^2 + 2\varepsilon + \frac{4}{3}. \end{aligned} \quad (62)$$

In figure 2(a) are shown those matrix elements. Since $f_{22}(\varepsilon)$ is discontinuous in the point $\varepsilon = -1 \in \Lambda$, matrix element $\omega_{22}(\varepsilon)$ diverges in this point. According to (62) this is a logarithmic type divergence. However, matrix elements $\omega_{11}(\varepsilon)$ and $\omega_{12}(\varepsilon)$ are everywhere continuous and finite. In particular one finds $\omega_{11}(-1) = -4/3$ and $\omega_{12}(-1) = -8/3$. In accord with (9c) one has $\omega_{ss}(\varepsilon) < 0$ if $\varepsilon < \lambda_a = -1$ and $\omega_{ss}(\varepsilon) > 0$ if $\varepsilon > \lambda_b = 1$. However, if $\varepsilon \in D$ those matrix elements may assume positive as well as negative values.

For completeness in figure 2(b) are shown derivatives $\omega_{sp}'(\varepsilon)$ of the above matrix elements. In accord with (9b) one has $\omega_{ss}'(\varepsilon) < 0$ for each $\varepsilon \in \bar{D}$ while for $\varepsilon \in D$ those derivatives may assume any value. Note that in addition to the derivative $\omega_{22}'(\varepsilon)$, derivative $\omega_{12}'(\varepsilon)$ also diverges in a point $\varepsilon = -1$. This is due to the fact that $f_{12}(\varepsilon)$ has zero of the first order in this point [7].

One has now all necessary information for the description of the system \mathbf{S}_2^a that interacts with the infinite system \mathbf{S}_∞^b .

4.1. Solution of the generic eigenvalue equation

Isolated eigenvalues and eigenstates of the combined system as well as resonant points are solutions of the generic equation (10). This equation has a non-trivial solution if and only if the determinant of the system vanishes. In a 2×2 case condition $|\mathbf{H}(\varepsilon)| = 0$ implies

$$|\mathbf{H}(\varepsilon)| \equiv h_{11}(\varepsilon)h_{22}(\varepsilon) - h_{12}(\varepsilon)h_{21}(\varepsilon) = 0, \quad (63a)$$

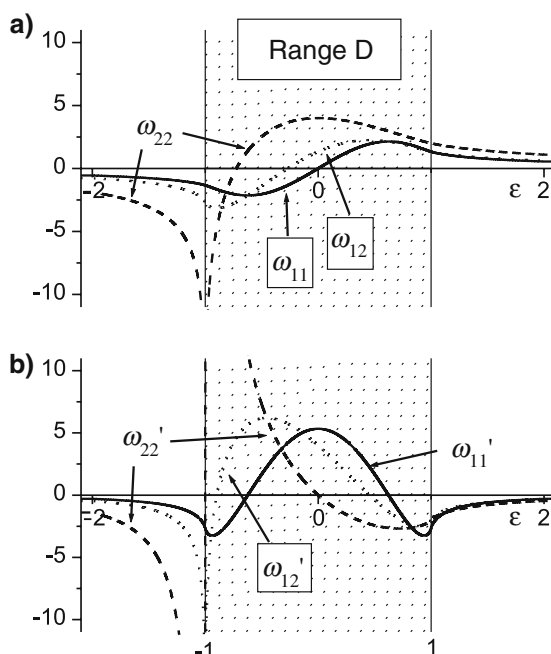


Figure 2. Derived matrix $\omega(\varepsilon)$. (a) matrix elements $\omega_{sp}(\varepsilon)$ of $\omega(\varepsilon)$. Matrix element $\omega_{22}(\varepsilon)$ diverges in the point $\varepsilon = -1$. (b) Derivatives $\omega_{sp}'(\varepsilon)$ of matrix elements $\omega_{sp}(\varepsilon)$. Derivatives $\omega_{22}'(\varepsilon)$ and $\omega_{12}'(\varepsilon)$ diverge in the point $\varepsilon = -1$.

where

$$h_{sp}(\varepsilon) \equiv \beta^2 \omega_{sp}(\varepsilon) + A_{sp} - \varepsilon \mathbf{S}_{sp}^a. \tag{63b}$$

Hence

$$\beta^4 |\omega(\varepsilon)| + \beta^2 \{ \omega_{11}(\varepsilon) (A_{22} - \varepsilon \mathbf{S}_{22}^a) + \omega_{22}(\varepsilon) (A_{11} - \varepsilon \mathbf{S}_{11}^a) - 2\omega_{12}(\varepsilon) (A_{12} - \varepsilon \mathbf{S}_{12}^a) \} + |\mathbf{A} - \varepsilon \mathbf{S}^a| = 0, \tag{63c}$$

where $\omega_{sp}(\varepsilon)$ are given by (62) and where $|\omega(\varepsilon)|$ and $|\mathbf{A} - \varepsilon \mathbf{S}^a|$ are determinants of matrices $\omega(\varepsilon)$ and $(\mathbf{A} - \varepsilon \mathbf{S}^a)$, respectively. In our case one has $\omega_{12}(\varepsilon) \equiv \omega_{21}(\varepsilon)$ which slightly simplifies expression (63c). Since $\mathbf{H}(\varepsilon)$ is hermitian one has in general $h_{12}(\varepsilon) \equiv h_{21}^*(\varepsilon)$ and $\omega_{12}(\varepsilon) \equiv \omega_{21}^*(\varepsilon)$.

One can solve (63c) for β to obtain solutions of a type $\beta = \beta(\varepsilon)$ and for ε to obtain solutions of a type $\varepsilon = \varepsilon(\beta)$. In the former case note that (63c) is quadratic in $x = \beta^2$. Hence and since $\beta \geq 0$ there are two analytic solutions of a type $\beta = \beta(\varepsilon)$ that can be obtained in a closed form. Only real solutions are admitted since β can not assume complex values. In the latter case each solution $\varepsilon = \varepsilon(\beta)$ to (63c) is an eigenvalue of the generic eigenvalue equation. Those

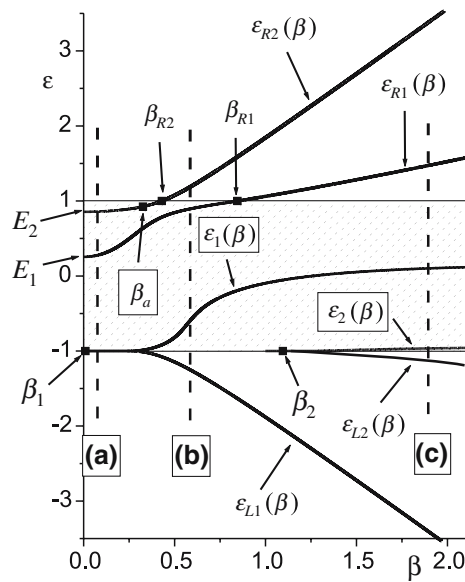


Figure 3. Eigenvalues of the generic equation considered as functions of the coupling β . Eigenvalues inside the range D are resonant points, while eigenvalues outside this range are isolated eigenvalues of the combined system. Eigenvalue distributions of local states $|\Theta_s\rangle$ for the coupling β corresponding to the lines (a), (b) and (c) are shown in figures 6, 7 and 8, respectively.

For details see text.

solutions are shown in figure 3. Considered as a function of β there are six such solutions, $\varepsilon_{R1}(\beta)$, $\varepsilon_{R2}(\beta)$, $\varepsilon_1(\beta)$, $\varepsilon_2(\beta)$, $\varepsilon_{L1}(\beta)$ and $\varepsilon_{L2}(\beta)$.

If $\beta = 0$ eigenvalues of the generic equation coincide with local eigenvalues. In particular, one has $\varepsilon_{R1}(0) = E_1 = 0.25474$ and $\varepsilon_{R2}(0) = E_2 = 0.85536$. 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 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 $\beta > \beta_{R1}$ increases, isolated eigenvalues $\varepsilon_{R1}(\beta)$ and $\varepsilon_{R2}(\beta)$ continue to increase. This is in accord with expressions (9c) and (19a) that imply $\partial\varepsilon_R/\partial\beta > 0$ for each right isolated eigenvalue $\varepsilon_R > \lambda_b$. Hence for each $\beta > \beta_{R1}$ combined system has two right isolated eigenvalues. This is maximum number of right isolated eigenvalues that combined system with $\rho = 2$ may have.

Points β_{R1} and β_{R2} can be obtained from the requirement that in those points one must have $\varepsilon = \lambda_b = 1$. Inserting this value into (63c) and using expressions

(62) that imply $\omega_{11}(1) = 4/3$, $\omega_{22}(1) = 2$ and $\omega_{12}(1) = 4/3$, one finds

$$\frac{8}{9} \cdot \beta^4 - 0.8 \cdot \beta^2 + 0.1175 = 0.$$

This is quadratic equation in the unknown $x = \beta^2$. Since $\beta \geq 0$ there are two solutions, $\beta_{R2} = 0.42992$ and $\beta_{R1} = 0.84567$.

Consider now remaining four eigenvalues $\varepsilon_{L1}(\beta)$, $\varepsilon_{L2}(\beta)$, $\varepsilon_1(\beta)$ and $\varepsilon_2(\beta)$. Those eigenvalues are also continuous functions of β and they emerge from the point $\varepsilon = \lambda_a = -1 \in \Lambda$ on the left edge of the range D . The emergence of those eigenvalues is due to the divergence of the operator $\omega(\varepsilon)$ in this point. In order to analyze behavior of those eigenvalues close to the point $\varepsilon = -1$, consider determinant $|\mathbf{H}(\varepsilon)|$ where $\varepsilon = -1 + h$ and where $h \neq 0$ is a small quantity. For each $h \neq 0$, however small, this determinant is a continuous function of β . Since (63c) is quadratic in $x = \beta^2$, this function crosses the value $|\mathbf{H}(-1 + h)| = 0$ in at most two points, $\beta = \beta_1(h)$ and $\beta = \beta_2(h)$. By definition, if $h > 0$ in a point $\beta = \beta_1(h)$ one has a resonant point, while if $h < 0$ in this point one has an isolated eigenvalue. In figure 3 those two values of small quantity h correspond to the resonant point $\varepsilon_1(\beta)$ and to the left isolated eigenvalue $\varepsilon_{L1}(\beta)$, respectively. Similarly for each $h \neq 0$, however small, in a point $\beta = \beta_2(h)$ one has resonant point $\varepsilon_2(\beta)$ if $h > 0$ and one has isolated eigenvalue $\varepsilon_{L2}(\beta)$ if $h < 0$. As absolute value of h decreases $\beta_1(h)$ converges to $\beta_1 = 0$, while $\beta_2(h)$ converges to a finite value $\beta_2 > 0$. Due to a divergence of $\omega_{22}(\varepsilon)$ in a point $\varepsilon = -1$, in a limit $h \rightarrow 0$ determinant $|\mathbf{H}(-1 + h)|$ diverges for each β , except for $\beta = 0$ and for $\beta = \beta_2$.

Let us now determine the point $\beta = \beta_2$. In order to find this point one has to find that value of β for which determinant $|\mathbf{H}(-1 + h)|$ does not diverge in a limit $h \rightarrow 0$. Expressions (62) imply

$$\begin{aligned} \omega_{11}(-1 + h) &= -\frac{4}{3} + O(h), & \omega_{12}(-1 + h) \equiv \omega_{21}(-1 + h) &= \frac{8}{3} + O(h), \\ \omega_{22}(-1 + h) &= (2 - h)^2 \ln \left| \frac{h}{2 - h} \right| + 6 - 2h = 4 \ln \left| \frac{h}{2 - h} \right| + O(1), \end{aligned} \quad (64a)$$

where $O(x)$ is a small quantity of the order x . Hence

$$\begin{aligned} h_{11}(-1 + h) &= -\frac{4}{3}\beta^2 + 1.6 + O(h), & h_{12}(-1 + h) &= -\frac{8}{3}\beta^2 - 0.15 + O(h), \\ h_{22}(-1 + h) &= 4\beta^2 \ln \left| \frac{h}{2 - h} \right| + O(1). \end{aligned} \quad (64b)$$

Since for each $\beta > 0$ matrix element $h_{22}(-1 + h)$ diverges in a limit $h \rightarrow 0$ while other matrix elements are in this limit finite, determinant (63a) does not diverge in this limit if and only if $h_{11}(-1) = 0$. Only in this case the product $h_{11}(-1 + h)h_{22}(-1 + h)$ can be finite in a limit $h \rightarrow 0$. This condition implies

$\beta_2 = \sqrt{1.2} = 1.09545$. If $\beta > \beta_2$ combined system contains left isolated eigenvalue $\varepsilon_{L2}(\beta) < \lambda_a = -1$ as well as a resonant point $\varepsilon_2(\beta) \in D$. If $\beta < \beta_2$ those quantities do not exist, and they both emerge at the point $\beta = \beta_2$. Hence

$$\lim_{\beta \rightarrow \beta_2^+} \varepsilon_{L2}(\beta) = -1 \in \Lambda \text{ and } \lim_{\beta \rightarrow \beta_2^+} \varepsilon_2(\beta) = -1 \in \Lambda.$$

Above analysis shows that for each $\beta \neq 0$ the combined system has an isolated eigenvalue $\varepsilon_{L1}(\beta) < -1$ as well as a resonant point $\varepsilon_1(\beta) > -1$. Though in this example generic equation (10) is a 2×2 eigenvalue equation, nevertheless it has at least four eigenvalues, however small $\beta > 0$. In a limit $\beta \rightarrow 0$ eigenvalues $\varepsilon_{R1}(\beta)$ and $\varepsilon_{R2}(\beta)$ converge to local eigenvalues E_1 and E_2 , respectively. The remaining two eigenvalues $\varepsilon_{L1}(\beta)$ and $\varepsilon_1(\beta)$ in this limit converge to the point $\varepsilon = -1 \in \Lambda$ where characteristic matrix $\mathbf{f}(\varepsilon)$ is discontinuous and where the derived matrix $\omega(\omega)$ diverges. Similarly, however close $\beta > \beta_2$ to the point $\beta = \beta_2$, the combined system has an additional isolated eigenvalue $\varepsilon_{L2}(\beta) < -1$ as well as an additional resonant point $\varepsilon_2(\beta) > -1$. In a limit $\beta \rightarrow \beta_2$ those two eigenvalues also converge to the point $\varepsilon = -1$ where matrix $\omega(\varepsilon)$ diverges. Thus for each $\beta > \beta_2$ a 2×2 generic eigenvalue equation has as many as six eigenvalues. If $\beta > 0$ is relatively small, eigenvalues $\varepsilon_{L1}(\beta)$ and $\varepsilon_1(\beta)$ are extremely close to the left edge $\varepsilon = \lambda_a = -1$ of the range D . Similarly, if $\beta > \beta_2$ is relatively close to $\beta = \beta_2$, eigenvalues $\varepsilon_{L2}(\beta)$ and $\varepsilon_2(\beta)$ are extremely close to $\varepsilon = -1$. For example, if $h = \pm 10^{-2}$ one finds $|\mathbf{H}(-1+h)| = 0$ for $\beta = 0.3126$ and for $\beta = 1.3790 > \beta_2$, if $h = \pm 10^{-5}$ one finds $|\mathbf{H}(-1+h)| = 0$ for $\beta = 0.1909$ and for $\beta = 1.1802 > \beta_{L2}$, while if $h = \pm 10^{-10}$ one finds $|\mathbf{H}(-1+h)| = 0$ for $\beta = 0.1331$ and for $\beta = 1.1337 > \beta_{L2}$. Hence at $\beta \approx 0.13$ isolated eigenvalue $\varepsilon_{L1}(\beta)$ and resonant point $\varepsilon_1(\beta)$ differ from the line $\varepsilon = -1$ as little as $h \approx \pm 10^{-10}$. If the coupling increases to $\beta \approx 0.19$ this difference is still as small as $h \approx \pm 10^{-5}$, while if the coupling is as strong as $\beta \approx 0.31$ this difference increases to $h \approx \pm 10^{-2}$. As explained in section 3.3.2, if β is small, isolated eigenvalue $\varepsilon_{L1}(\beta)$ and resonant point $\varepsilon_1(\beta)$ are approximately given by the expression $\lambda_a \pm A \exp(-K/\beta^2)$. Reasonably good fit to the above data is obtained with the expression $\varepsilon_{\pm}(\beta) = -1 \pm 0.5369 \cdot \exp(-0.3969/\beta^2)$ where (+) refers to $\varepsilon_1(\beta)$ while (-) refers to $\varepsilon_{L1}(\beta)$. In a similar way can be analysed resonant point $\varepsilon_2(\beta)$ and isolated eigenvalue $\varepsilon_{L2}(\beta)$ (see figure 3). As explained in section 3.3.1, initial closeness of those curves to the line $\varepsilon = -1$ is due to the discontinuity of the characteristic matrix $\mathbf{f}(\varepsilon)$ in the point $\varepsilon = -1$.

Above analysis determines main qualitative features of the isolated and resonant solutions of the combined system. It remains to find out whether this system contains some anomalous point. In those points, if any, the combined system \mathbf{S}_{∞} has isolated eigenvalues. Since each anomalous point is also a resonant point, those anomalous points may exist only on the curves $\varepsilon_1(\beta)$ and $\varepsilon_2(\beta)$ as well as on the curve $\varepsilon_{R1}(\beta)$ in the interval $\beta \in (0, \beta_{R1})$ and on the curve $\varepsilon_{R2}(\beta)$ in the interval $\beta \in (0, \beta_{R2})$. By definition, in the anomalous point $\varepsilon = \varepsilon_a$ there exists a non-trivial state $|\theta\rangle$ that satisfies simultaneously two conditions, $\mathbf{f}(\varepsilon)|\theta\rangle = 0$ and also

$\mathbf{H}(\varepsilon)|\theta\rangle = 0$. First condition implies that $|\theta\rangle$ must be an eigenstate of the characteristic operator $\mathbf{f}(\varepsilon)$ with the eigenvalue zero. According to (60) this implies $|\theta\rangle = |f_2(\varepsilon)\rangle$. The second condition now reads $\mathbf{H}(\varepsilon)|f_2(\varepsilon)\rangle = 0$. Hence one finds that at an anomalous point $\varepsilon = \varepsilon_a$ one should have

$$\beta^2 |fa(\varepsilon_a)\rangle = |fb(\varepsilon_a)\rangle, \tag{65a}$$

where

$$|fa(\varepsilon)\rangle = \omega(\varepsilon)|f_2(\varepsilon)\rangle, \quad |fb(\varepsilon)\rangle = (\varepsilon\mathbf{S}^a - \mathbf{A})|f_2(\varepsilon)\rangle. \tag{65b}$$

Using (58a) and (62) one can obtain an explicit analytic expression for functions $|fa(\varepsilon)\rangle$ and $|fb(\varepsilon)\rangle$. According to (65a), in the anomalous point those functions are mutually proportional. One finds that this proportionality condition implies $\varepsilon_a = 0.92515$. Once $\varepsilon = \varepsilon_a$ is known, expression (65a) implies $\beta_a = 0.32603$. System \mathbf{S}_∞ hence contains a single anomalous point at the position $\varepsilon = \varepsilon_a$. This anomalous point exists if and only if the coupling equals $\beta = \beta_a$. As shown in figure 3, this point lies on the curve $\varepsilon_{R2}(\beta)$.

In conclusion, system \mathbf{S}_∞ may contain at most two right and at most two left isolated eigenvalues. Left isolated eigenvalue $\varepsilon_{L1}(\beta)$ exists for each $\beta > 0$, right isolated eigenvalue $\varepsilon_{R2}(\beta)$ exists for each $\beta > \beta_{R2} = 0.42992$, another right isolated eigenvalue $\varepsilon_{R1}(\beta)$ exists for each $\beta > \beta_{R1} = 0.84567$, while another left isolated eigenvalue $\varepsilon_{L2}(\beta)$ exists for each $\beta > \beta_2 = 1.09543$. Hence for $\beta > \beta_2$ the system \mathbf{S}_∞ contains maximum possible number of $2\rho = 4$ isolated eigenvalues and eigenstates. Further, this system contains an anomalous point that lies on the curve $\varepsilon_{R2}(\beta)$ at the position $\varepsilon = \varepsilon_a = 0.92515$ and $\beta = \beta_a = 0.32603$. Hence this system contains an isolated eigenstate with the eigenvalue $\varepsilon_r \equiv \varepsilon_a = 0.92515 \in D$. This eigenstate exists if and only if the coupling β is exactly $\beta = \beta_a$.

4.2. Isolated solutions of the combined system

Once isolated eigenvalue $\varepsilon_I(\beta) \in \bar{D}$ is obtained as a root of the generic eigenvalue equation, one easily finds the corresponding isolated eigenstate $|\Psi_I\rangle$. Eigenstate $|\theta_s\rangle$ of a 2×2 generic eigenvalue equation (10) equals

$$|\theta_s\rangle = h_{12}(\varepsilon_s)|1\rangle - h_{11}(\varepsilon_s)|2\rangle, \tag{66}$$

where ε_s is the corresponding eigenvalue. In particular, if $\varepsilon_s \equiv \varepsilon_I \in \bar{D}$ the corresponding eigenstate $|\theta_I\rangle$ determines components $|\Psi_I^a\rangle \in X_\rho^a$ and $|\Psi_I^b\rangle \in X_\infty^b$ of the isolated eigenstate $|\Psi_I\rangle$ according to the expressions (14). Thus, once isolated eigenvalue $\varepsilon_I \in \bar{D}$ is known, derivation of the corresponding eigenstate $|\Psi_I\rangle$ is straightforward.

Concerning properties of isolated eigenstate $|\Psi_I\rangle$, of particular interest are probabilities $w_{I_s}^a = |\langle \Theta_s | \mathbf{S}^a |\Psi_I\rangle|^2$ to find this eigenstate in local states $|\Theta_s\rangle$ ($s = 1, 2$), as well as probability $w_I^a = \sum_s w_{I_s}^a$ to find this eigenstate in the system \mathbf{S}_ρ^a . Those probabilities are given by expressions (16) where the state $|\theta_I\rangle$ is given by (66). In figure 4 are shown those probabilities for the right isolated eigenstates $|\Psi_{R1}\rangle$ and $|\Psi_{R2}\rangle$. In particular, in figure 4(a) are shown probabilities $w_{R1,s}^a$ as well as probability $w_{R1}^a = w_{R1,1}^a + w_{R1,2}^a$ for the right isolated eigenstate $|\Psi_{R1}\rangle$. Since right isolated eigenvalue $\varepsilon_{R1}(\beta)$ exists only if $\beta > \beta_{R1} = 0.84567$, those probabilities vanish if $\beta \leq \beta_{R1}$. As β continuously increases, in a point $\beta = \beta_{R1}$ probabilities $w_{R1,1}^a$, $w_{R1,2}^a$ and w_{R1}^a discontinuously jump from zero to $w_{R1,1}^a(\beta_{R1}) = 0.11008$, $w_{R1,2}^a(\beta_{R1}) = 0.53733$ and $w_{R1}^a(\beta_{R1}) = 0.64741$, respectively. In figure 4(b) are shown corresponding probabilities for another right isolated eigenstate $|\Psi_{R2}\rangle$. Those probabilities vanish if $\beta \leq \beta_{R2} = 0.42992$. As β continuously increases, in a point $\beta = \beta_{R2}$ those probabilities discontinuously jump from zero to $w_{R2,1}^a(\beta_{R2}) = 0.13067$, $w_{R2,2}^a(\beta_{R2}) = 0.71062$ and $w_{R2}^a(\beta_{R2}) = 0.84129$, respectively.

In figure 5 are shown probabilities for left isolated eigenstates $|\Psi_{L1}\rangle$ and $|\Psi_{L2}\rangle$. Since left isolated eigenvalue $\varepsilon_{L1}(\beta)$ exists for each $\beta > \beta_1 = 0$, probabilities $w_{L1,s}^a$ and $w_{L1}^a = w_{L1,1}^a + w_{L1,2}^a$ are nonzero for each $\beta > 0$. As explained in a previous section, if the coupling is relatively weak, left isolated eigenvalue $\varepsilon_{L1}(\beta)$ is extremely close to the left edge $\lambda_a = -1 \in \Lambda$ of the range D (see figure 3). As discussed in section 3.3.1, corresponding probabilities are negligible (see figure 5(a)). In figure 5(b) are shown probabilities associated with left isolated eigenstate $|\Psi_{L2}\rangle$. Since left isolated eigenvalue $\varepsilon_{L2}(\beta)$ exist only if $\beta > \beta_2 = 1.09545$, those probabilities vanish if $\beta \leq \beta_2$. In addition, if $\beta > \beta_2$ is relatively close to the point β_2 , left isolated eigenvalue $\varepsilon_{L2}(\beta)$ is extremely close to the left edge $\lambda_a = -1$ of the range D and the corresponding probabilities are hence negligible.

In the case of right isolated eigenstates there is a sudden change in the corresponding probabilities as the coupling β assumes a critical value β_{R1} or β_{R2} (see figure 4), while in the case of left isolated eigenstates there is a very smooth change of those probabilities as the coupling β assumes a critical value β_1 or β_2 (see figure 5). This difference is due to the continuity (discontinuity) of the characteristic operator $\mathbf{f}(\varepsilon)$ in the corresponding boundary point [7]. Thus in the point $\lambda_b = 1$ all matrix elements $f_{sp}(\varepsilon)$ of $\mathbf{f}(\varepsilon)$ have zero of the second order. As a result matrix elements $\langle \theta | \mathbf{f}(\varepsilon) | \theta \rangle$ where $|\theta\rangle$ are the corresponding eigenstates of the generic eigenvalue equation have also zero of the second order in the point $\varepsilon = 1$. This implies that matrix element $\langle \theta | d\omega/d\varepsilon_I | \theta \rangle$ is finite in this point. Hence and according to (16a), the corresponding probabilities abruptly increase from zero to a finite nonzero value as one crosses a critical value of the interaction β . However, in a point $\lambda_a = -1$ operator $\mathbf{f}(\varepsilon)$ is discontinuous and derived operator $\omega(\varepsilon)$ as well as its derivative diverge. Hence and according to (16a) probability $w_{I_s}^a$ is extremely small if ε_I is close to the point $\varepsilon = -1$ and in a limit $\varepsilon \rightarrow -1$ it is zero. Therefore there is continuous and a very smooth

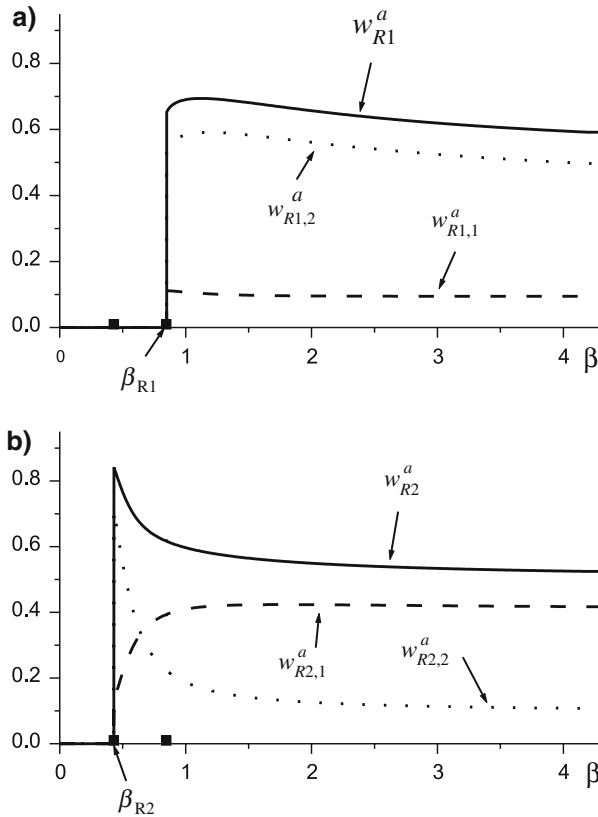


Figure 4. Probabilities $w_{Ri,s}^a$ to find right isolated eigenstates $|\Psi_{R1}\rangle$ and $|\Psi_{R2}\rangle$ in local states $|\Theta_s\rangle$ and probabilities $w_{Ri}^a = w_{Ri,1}^a + w_{Ri,2}^a$ to find those eigenstates in the system \mathbf{S}_2^a . (a) Probabilities corresponding to the eigenstate $|\Psi_{R1}\rangle$. (b) Probabilities corresponding to the eigenstate $|\Psi_{R2}\rangle$.

change of related probabilities considered as a function of coupling parameter β [7].

4.3. Embedded solutions of the combined system and eigenvalue distributions of local states

In a 2×2 case one can obtain an exact solution of the fractional shift equation (23a). In this case one finds

$$X(\varepsilon) = \frac{|\mathbf{H}(\varepsilon)|}{h_{11}(\varepsilon)f_{22}(\varepsilon) + h_{22}(\varepsilon)f_{11}(\varepsilon) - h_{12}(\varepsilon)f_{21}(\varepsilon) - h_{21}(\varepsilon)f_{12}(\varepsilon)}, \quad (67a)$$

$$|\psi(\varepsilon)\rangle = [h_{12}(\varepsilon) - X(\varepsilon)f_{12}(\varepsilon)] |1\rangle - [h_{11}(\varepsilon) - X(\varepsilon)f_{11}(\varepsilon)] |2\rangle, \quad \varepsilon \in D. \quad (67b)$$

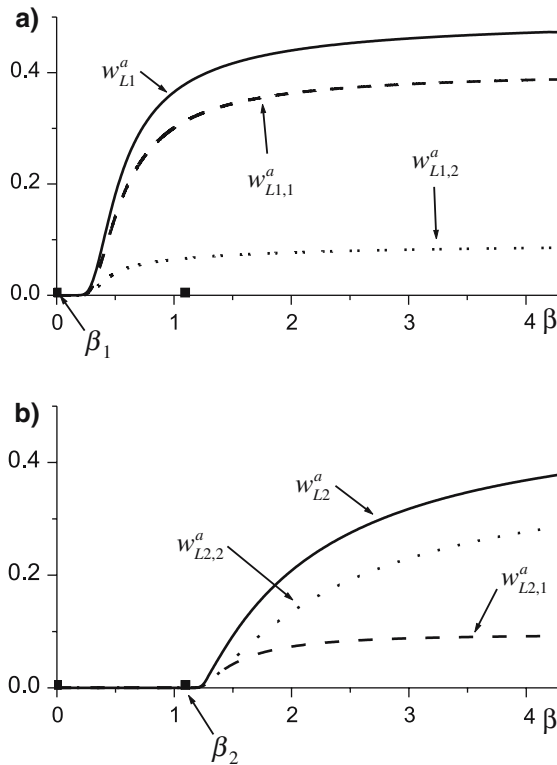


Figure 5. Probabilities $w_{Li,s}^a$ to find left isolated eigenstates $|\Psi_{L1}\rangle$ and $|\Psi_{L2}\rangle$ in local states $|\Theta_s\rangle$ and probabilities $w_{Li}^a = w_{Li,1}^a + w_{Li,2}^a$ to find those eigenstates in the system \mathbf{S}_2^a . (a) Probabilities corresponding to the eigenstate $|\Psi_{L1}\rangle$. (b) Probabilities corresponding to the eigenstate $|\Psi_{L2}\rangle$.

In particular, in a resonant point $\varepsilon = \varepsilon_r \in D$ one has $|\mathbf{H}(\varepsilon_r)| = 0$ and hence $X(\varepsilon_r) = 0$. In this case eigenstate $|\Psi(\varepsilon_r)\rangle$ reduces to the eigenstate (66) of a 2×2 generic eigenvalue equation.

Solution (67) can be inserted into (25) to obtain an explicit expression for the component $|\Psi^a(\varepsilon)\rangle \in X_\rho^a$ of the embedded eigenstate $|\Psi(\varepsilon)\rangle$. Once $|\Psi^a(\varepsilon)\rangle$ is known, one can obtain all related properties of the system \mathbf{S}_2^a that interacts with the system \mathbf{S}_∞^b .

An important quantity is probability density $\rho_s^a(\varepsilon) = |\langle \Theta_s | \mathbf{S}^a | \Psi^a(\varepsilon) \rangle|^2$ to find local state $|\Theta_s\rangle$ with the eigenvalue $\varepsilon \in D$. In conjuncture with probabilities $w_{I_s}^a$ to find this state in the isolated eigenstates $|\Psi_I\rangle$, this probability density determines eigenvalue distribution of $|\Theta_s\rangle$. We will consider such eigenvalue distributions for three characteristic values of the coupling β : weak coupling $\beta = 0.1$, intermediate coupling $\beta = 0.6$ and extremely strong coupling $\beta = 1.9$. Those values correspond to lines (a), (b) and (c), respectively, in figure 3. We will also consider eigenvalue distribution in the anomal point $\beta = \beta_a$ as well as very close

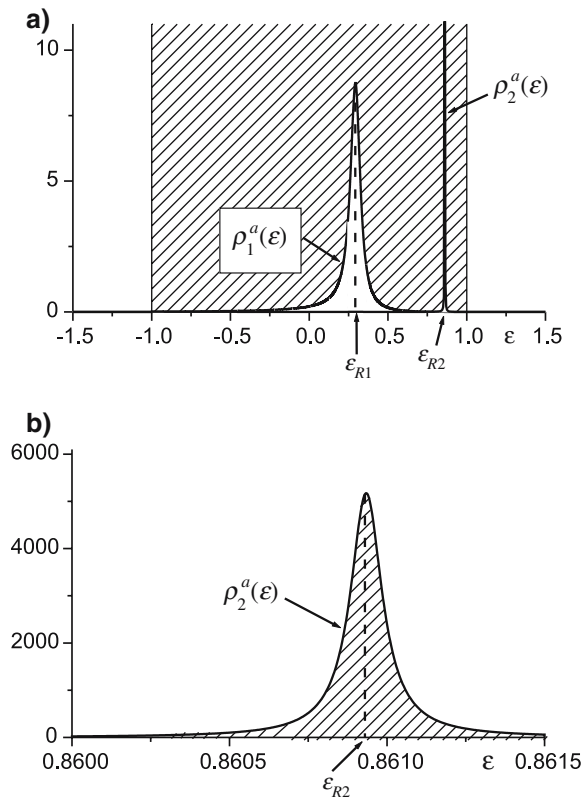


Figure 6. Eigenvalue distributions of local states $|\Theta_1\rangle$ and $|\Theta_2\rangle$ in the case $\beta = 0.1$. Those distributions correspond to the line (a) in figure 3. (a) Probability densities $\rho_1^a(\varepsilon)$ and $\rho_2^a(\varepsilon)$. (b) Probability density $\rho_2^a(\varepsilon)$ highly magnified. The shape of the universal resonant curve is manifest.

to this point in order to illustrate the emergence of the isolated eigenstate in this point.

The case $\beta = 0.1$ is considered in figure 6. This value corresponds to the line (a) in figure 3. As shown in a previous section, for each $\beta > 0$ the combined system \mathbf{S}_∞ contains left isolated eigenstate $|\Psi_{L1}\rangle$. However, if β is as small as $\beta = 0.1$, probabilities $w_{L1,s}^a(0.1)$ are negligible (see figure 5(a)). Since in the case $\beta = 0.1$ the combined system contains no other isolated eigenstate, spectral distributions of local states $|\Theta_1\rangle$ and $|\Theta_2\rangle$ reduce to probability densities $\rho_1^a(\varepsilon)$ and $\rho_2^a(\varepsilon)$, respectively.

Those probability densities are shown in figure 6(a). Due to the interaction with the system \mathbf{S}_∞ unperturbed eigenvalue $E_1 = 0.25474$ shifts to a position $\varepsilon_{R1}(0.1) = 0.29227$ while unperturbed eigenvalue $E_2 = 0.85536$ shifts to a position $\varepsilon_{R2}(0.1) = 0.86093$. Approximate expression (46a) that is valid in a weak coupling limit yields $\varepsilon_{R1}(0.1) \approx 0.29160$ and $\varepsilon_{R2}(0.1) \approx 0.86087$. Those

values are quite close to the exact values for $\varepsilon_{R1}(0.1)$ and $\varepsilon_{R2}(0.1)$, respectively. In the neighborhood of the resonant point $\varepsilon = \varepsilon_{R1}(0.1)$ probability density $\rho_1^a(\varepsilon)$ has the shape of a universal resonance curve with a relatively small width $\Delta\varepsilon_{R1}(0.1)$. Using (45b) one finds $\Delta\varepsilon_{R1}(0.1) = 0.0775$. One also finds $w_{C1}^a(0.1) = \int \rho_1^a(\varepsilon)d\varepsilon = 1$. This implies $w_{C1}^a(0.1) + w_{L1,1}^a(0.1) = 1$ in accord with the completeness requirement. Concerning probability density $\rho_2^a(\varepsilon)$, it is situated at the position $\varepsilon = \varepsilon_{R2}(0.1)$. This density has also the shape of the universal resonance curve with a unite area, $w_{C2}^a(0.1) = \int \rho_2^a(\varepsilon)d\varepsilon = 1$. Since the contribution $w_{L1,2}^a(0.1)$ of the isolated eigenstate $|\Psi_{L1}\rangle$ to the local state $|\Theta_2\rangle$ is negligible, one again finds $w_{C2}^a(0.1) + w_{L1,2}^a(0.1) = 1$. Unlike density $\rho_1^a(\varepsilon)$, probability density $\rho_2^a(\varepsilon)$ is extremely sharp and expression (45b) yields $\Delta\varepsilon_{R2}(0.1) = 0.00015$. This density is shown highly amplified in figure 6(b).

Densities $\rho_1^a(\varepsilon)$ and $\rho_2^a(\varepsilon)$ in figure 6(a) are well separated, they have both the shape of the universal resonance curve, and the area under each of those densities equals one. Density $\rho_1^a(\varepsilon)$ represents shifted eigenvalue E_1 while density $\rho_2^a(\varepsilon)$ represents shifted eigenvalue E_2 . As discussed in section 3.4.7, this is the case of the relatively weak coupling that can be successfully treated within the formalism of the standard perturbation expansion approach. The above results are typical results usually obtained within this approach. Note that in the case $\beta = 0.1$ the combined system has a third resonant point $\varepsilon_1(0.1)$ at the position $\varepsilon_1(0.1) \approx -1$. However, this resonant point is associated with the point $\varepsilon = -1$ where $\omega(\varepsilon)$ diverges and, as explained in section 3.4.7, the contribution of this resonant point to probability densities $\rho_s^a(\varepsilon)$ is negligible (see expression (47)).

In figure 7 are shown eigenvalue distributions of local states $|\Theta_1\rangle$ and $|\Theta_2\rangle$ for the case $\beta = 0.6$. This coupling corresponds to the line (b) in figure 3. Interaction is now much stronger and in addition to the left isolated eigenstate $|\Psi_{L1}\rangle$ that is always present, the system \mathbf{S}_∞ contains right isolated eigenstate $|\Psi_{R1}\rangle$. Approximate expression (46a) valid in the weak coupling limit yields $\varepsilon_{R1}(0.6) \approx 1.5820$ and $\varepsilon_{R2}(0.6) \approx 1.05385$. Both values are outside the range D . This indicated the failure of the perturbation expansion approach for this value of β . Exact values obtained as roots of (63c) are $\varepsilon_{R1}(0.6) = 0.90157$ and $\varepsilon_{R2}(0.6) = 1.20747$. Only $\varepsilon_{R2}(0.6)$ is an isolated eigenvalue, while $\varepsilon_{R1}(0.6) \in D$ is a resonant point. Using expression (50b) for the estimation of the uncertainty $\Delta\varepsilon_{R1}(0.6)$ one finds $\Delta\varepsilon_{R1}(0.6) = 0.0268$. This uncertainty is quite small and, as explained in section 3.4.8, densities $\rho_s(\varepsilon)$ and $\rho_s^a(\varepsilon)$ should have a prominent resonant feature at the position $\varepsilon_{R1}(0.6)$. As shown in figure 7 there is indeed a visible resonant structure at this point.

In addition to the right isolated eigenvalue $\varepsilon_{R2}(0.6)$, the system \mathbf{S}_∞ contains a left isolated eigenvalue $\varepsilon_{L1}(0.6) = -1.26961$ that is also obtained as a root of (63c). This eigenvalue is relatively far from the range D and the contribution of the corresponding eigenstate to spectral distributions can not be neglected. In conclusion, if $\beta = 0.6$ to the spectral distributions of local states

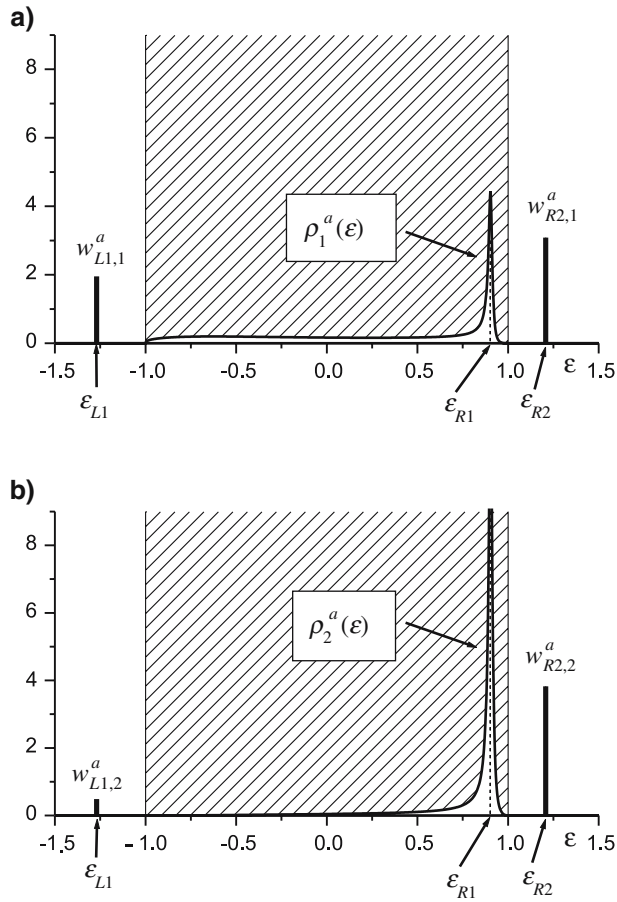


Figure 7. Eigenvalue distributions of local states $|\Theta_1\rangle$ and $|\Theta_2\rangle$ in the case $\beta = 0.6$. Those distributions correspond to the line (b) in figure 3. Probabilities $w_{L1,s}^a$ and $w_{R2,s}^a$ ($s = 1, 2$) of isolated eigenstates are shown in relative scale. (a) Eigenvalue distribution of local state $|\Theta_1\rangle$. (b) Eigenvalue distribution of local state $|\Theta_2\rangle$.

$|\Theta_1\rangle$ and $|\Theta_2\rangle$ contribute both isolated eigenstates as well as all embedded eigenstates $|\Psi(\varepsilon)\rangle$ ($\varepsilon \in D$).

In figure 7(a) is shown spectral distribution of the local state $|\Theta_1\rangle$. Probability density $\rho_1^a(\varepsilon)$ has a sharp pick at the position $\varepsilon_{R1}(0.6) = 0.90157$. However, unlike probability densities in figure 6, this probability density has significant value in the entire range D and not only close to the point $\varepsilon_{R1}(0.6)$. In addition one finds $w_{C1}^a(0.6) = \int \rho_1^a(\varepsilon)d\varepsilon = 0.49594 < 1$. Hence $\rho_1^a(\varepsilon)$ can not be reproduced by a standard perturbation expansion method. Concerning contributions of isolated eigenstates, one finds $w_{R2,1}^a(0.6) = 0.30867$ and

$w_{L1,1}^a(0.6) = 0.19539$. In accord with the completeness requirement, those probabilities satisfy $w_{L1,1}^a(0.6) + w_{R2,1}^a(0.6) + w_{C1}^a(0.6) = 1$.

In figure 7(b) is shown spectral distribution of the local state $|\Theta_2\rangle$. One again finds that a probability density $\rho_2^a(\varepsilon)$ has a sharp pick at the position $\varepsilon_{R1}(0.6)$. This pick is significantly higher than the pick associated with the density distribution $\rho_1^a(\varepsilon)$. One also finds $w_{R2,2}^a(0.6) = 0.38232$, $w_{L1,2}^a(0.6) = 0.04879$ and $w_{C2}^a(0.6) = \int \rho_2^a(\varepsilon)d\varepsilon = 0.56889$. Those probabilities again satisfy completeness requirement $w_{R2,2}^a(0.6) + w_{L1,2}^a(0.6) + w_{C2}^a(0.6) = 1$.

Though the coupling $\beta = 0.6$ is relatively large, both densities $\rho_1^a(\varepsilon)$ and $\rho_2^a(\varepsilon)$ have a sharp pick at the position $\varepsilon_{R1}(0.6)$. As explained in section 3.4.8, this is due to the fact that the width $\Delta\varepsilon_{R1}(0.6)$ as calculated according to (50b) is relatively small. Hence in a small neighborhood Δ at the point $\varepsilon = \varepsilon_{R1}(0.6)$ density $\rho^a(\varepsilon) = \rho_1^a(\varepsilon) + \rho_2^a(\varepsilon)$ is very well approximated with the universal resonance curve (52b). Note that in addition to resonant point $\varepsilon_{R1}(0.6)$ the system \mathbf{S}_∞ has another resonant point at $\varepsilon_1(0.6) = -0.55401$. Using expression (50b) one finds $\Delta\varepsilon_1(0.6) > 1$ which is bigger than the entire range D . This indicates that at the resonant point $\varepsilon_1(0.6)$ no significant resonant structure should be formed. Accordingly, in figure 7 no resonance can be noticed at this position.

In figure 8 are shown eigenvalue distributions of local states $|\Theta_1\rangle$ and $|\Theta_2\rangle$ for the case $\beta = 1.9$. This value corresponds to the line (c) in figure 3. Interaction is now extremely strong and the system \mathbf{S}_∞ contains maximum number of two left and two right isolated eigenvalues and eigenstates. Those eigenvalues are $\varepsilon_{R1}(1.9) = 3.38873$, $\varepsilon_{R2}(1.9) = 1.47546$, $\varepsilon_{L1}(1.9) = -3.41405$ and $\varepsilon_{L2}(1.9) = -1.14456$. Spectral distribution of a local state $|\Theta_1\rangle$ is shown in figure 8. One finds probabilities $w_{L1,1}^a(1.9) = 0.36034$, $w_{L2,1}^a(1.9) = 0.06962$, $w_{R1,1}^a(1.9) = 0.09588$, $w_{R2,1}^a(1.9) = 0.42344$ and $w_{C1}^a(1.9) = 0.05072$. Those probabilities are again in accord with the completeness requirement. Spectral distribution of a local state $|\Theta_2\rangle$ is shown in figure 8(b). This spectral distribution is characterized by values $w_{L1,2}^a(1.9) = 0.07611$, $w_{L2,2}^a(1.9) = 0.12052$, $w_{R1,2}^a(1.9) = 0.56568$, $w_{R2,2}^a(1.9) = 0.12833$ and $w_{C2}^a(1.9) = 0.10935$. Those values also satisfy completeness requirement. Densities $\rho_1^a(\varepsilon)$ and $\rho_2^a(\varepsilon)$ in figure 8 have no resemblance to the universal resonance curve and small coupling approximation completely fails. Those results can not be reproduced by the standard perturbation expansion approach.

4.4. Anomal point

As emphasized in section 3.5, expressions for the component $|\Psi^a(\varepsilon)\rangle \in X_\rho^a$ of the eigenstate $|\Psi(\varepsilon)\rangle$ and for related densities $\rho_s^a(\varepsilon)$ and $\rho_s(\varepsilon)$ are valid for each $\varepsilon \in D$, except for anomal points. As shown in section 4.1, the system \mathbf{S}_∞ has an anomal point at the position $\varepsilon_a = 0.92515$ and $\beta_a = 0.32603$ (see figure 3). Eigenvalue distributions of local states $|\Theta_1\rangle$ and $|\Theta_2\rangle$ for the

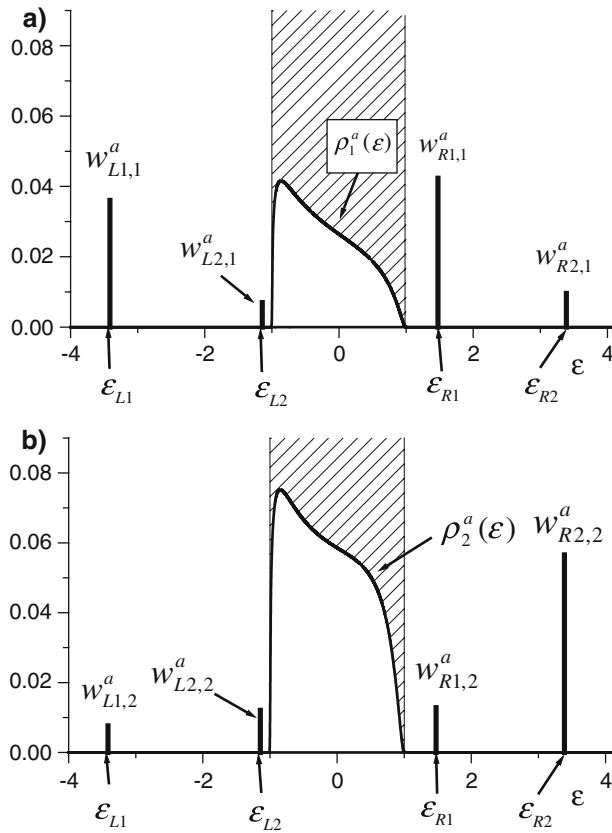


Figure 8. Eigenvalue distributions of local states $|\Theta_1\rangle$ and $|\Theta_2\rangle$ in the case $\beta = 1.9$. Those distributions correspond to the line (c) in figure 3. Probabilities $w_{Ls,p}^a$ and $w_{Rs,p}^a$ ($s, p = 1, 2$) of isolated eigenstates are shown in relative scale. (a) Eigenvalue distribution of local state $|\Theta_1\rangle$. (b) Eigenvalue distribution of local state $|\Theta_2\rangle$.

coupling $\beta = \beta_a$ are shown in figure 9(a) and (b), respectively. For this coupling the system \mathbf{S}_∞ contains only one isolated eigenstate $|\Psi_{L1}\rangle$ with the eigenvalue $\varepsilon_{L1} = -1.01406$. Corresponding probabilities are $w_{L1,1}^a(\beta_a) = 0.02612$ and $w_{L1,2}^a(\beta_a) = 0.01146$. Concerning contributions of probability densities $\rho_s^a(\varepsilon)$ to total probability one finds $w_{C1}^a(\beta_a) = \int \rho_1^a(\varepsilon)d\varepsilon = 0.94009$ and $w_{C2}^a(\beta_a) = \int \rho_2^a(\varepsilon)d\varepsilon = 0.08252$. Hence $w_{L1,1}^a(\beta_a) + w_{C1}^a(\beta_a) = 0.96620 < 1$ and $w_{L1,2}^a(\beta_a) + w_{C2}^a(\beta_a) = 0.09399 < 1$. Both expressions violate the completeness requirement (56a) and both spectral distributions are hence in error. There is obviously something missing in those expressions.

In order to understand the reason for the failure of those expressions, consider a continuous change $\beta \rightarrow \beta_a$. As long as $\beta \neq \beta_a$ all expressions are correct.

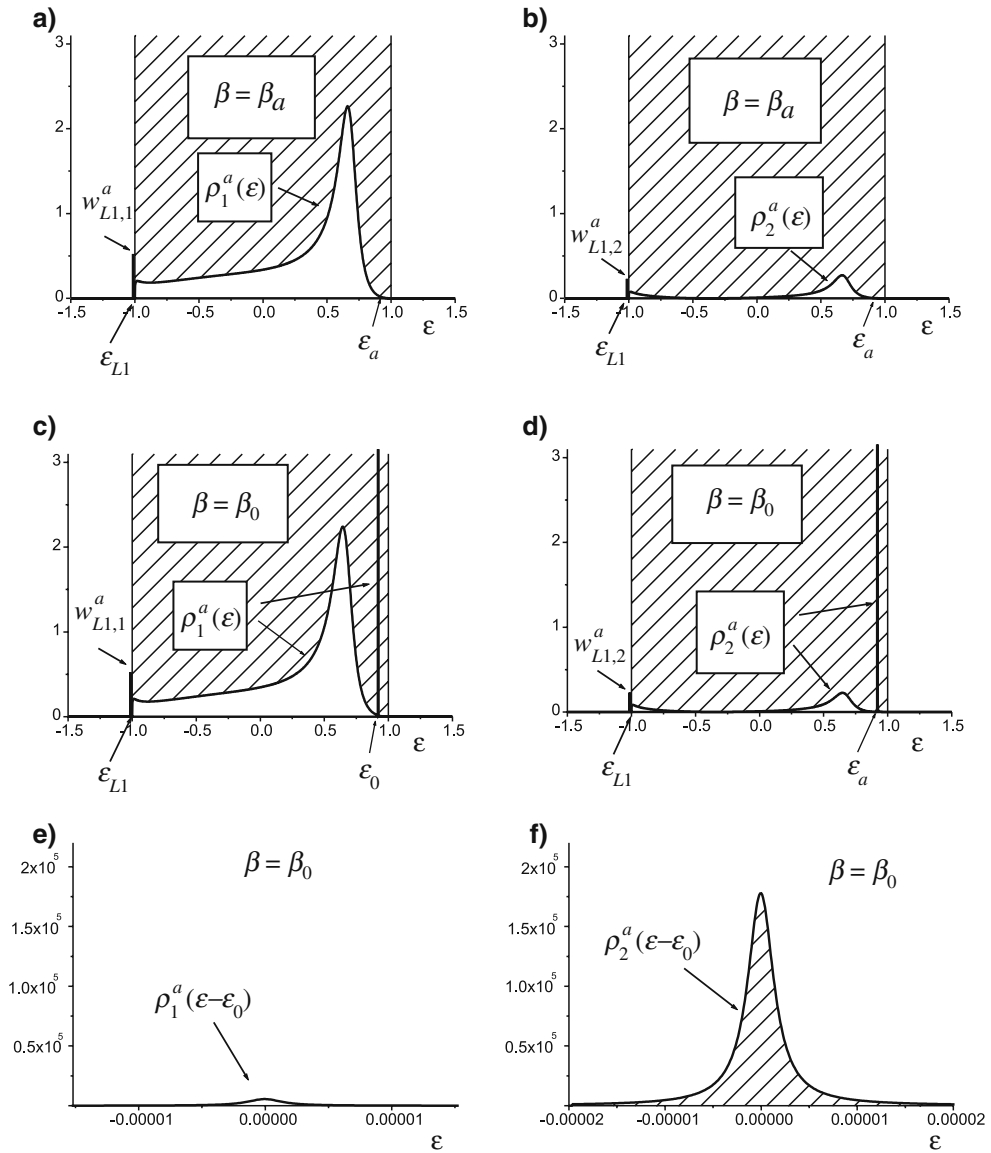


Figure 9. Eigenvalue distributions of local states $|\Theta_1\rangle$ and $|\Theta_2\rangle$ in the anomalous point $\beta = \beta_a$ and in the point $\beta_0 = \beta_a - 0.01$ close to the anomalous point. Probabilities $w_{L1,s}^a$ ($s = 1, 2$) are shown in relative scale. (a) Eigenvalue distribution of local state $|\Theta_1\rangle$ in the anomalous point. (b) Eigenvalue distribution of local state $|\Theta_2\rangle$ in the anomalous point. (c) Eigenvalue distribution of local state $|\Theta_1\rangle$ in the point $\beta_0 = \beta_a - 0.01$. (d) Eigenvalue distribution of local state $|\Theta_2\rangle$ in the point $\beta = \beta_a - 0.01$. (e) Eigenvalue distribution from figure 9(c) in the neighborhood of the point $\varepsilon = \varepsilon_0 \equiv \varepsilon_{R2}(\beta_0)$ highly amplified. (f) Eigenvalue distribution from figure 9(d) in the neighborhood of the point $\varepsilon = \varepsilon_0 \equiv \varepsilon_{R2}(\beta_0)$ highly amplified.

For physical reasons, if the coupling continuously changes, all relevant quantities should also continuously change. Hence correct expressions for those quantities in the anomalous point can be obtained as an appropriate limit of a process $\beta \rightarrow \beta_a$.

Consider the coupling $\beta = \beta_0 = \beta_a - h$ where $h = 0.01$ is relatively small quantity. In figure 9(c) and (d) are shown corresponding spectral distributions for the local states $|\Theta_1\rangle$ and $|\Theta_2\rangle$, respectively. Since $\beta_0 \neq \beta_a$ those spectral distributions are correct. One finds $w_{C_1}^a(\beta_0) = 0.97872$ and $w_{L_{1,1}}(\beta_0) = 0.02128$. Hence $w_{C_1}^a(\beta_0) + w_{L_{1,1}}(\beta_0) = 1$ in agreement with the completeness relation (figure 9(c)). One also finds $w_{C_2}^a(\beta_0) = 0.99032$ and $w_{L_{1,2}}^a(\beta_0) = 0.00968$ which implies $w_{C_2}^a(\beta_0) + w_{L_{1,2}}(\beta_0) = 1$ which also satisfies completeness requirement (figure 9(d)). Comparing figure 9(a) and (b) with figure 9(c) and (d), one can see an important difference. In figure 9(c) at the position $\varepsilon = \varepsilon_0 = \varepsilon_{R2}(\beta_0)$ close to the anomalous point $\varepsilon = \varepsilon_a$ there is a sharp pick which is absent in figure 9(a). In figure 9(d) at the same position there is a similar sharp pick which is absent in the corresponding figure 9(b). Those two picks are shown highly amplified in figure 9(e) and (f), respectively. Both picks have the shape of the universal resonance curve, they are both centered at the resonant point $\varepsilon_0 \equiv \varepsilon_{R2}(\beta_0) = 0.92004$ close to the anomalous point ($\varepsilon_a = 0.92515$) and they are both extremely narrow. Those two picks differ in their heights, first pick has the height $\approx 5.547 \times 10^3$ (figure 9(e)), while the second pick is as high as $\approx 1.778 \times 10^5$ (figure 9(f)). The existence of such a prominent resonant feature is due to the fact that in a resonant point $\varepsilon = \varepsilon_0$ the quantity $F_0(\varepsilon_0)$ is very small (see equation (50b)). One finds $F_0(\varepsilon_0) \approx 5.23 \times 10^{-6}$ and hence $\Delta\varepsilon_0 \approx 3.28 \times 10^{-6}$. The picks shown in figure 10(e,f) correspond to the value $h = 0.01$. As h decreases center of those picks slowly shifts to the anomalous point $\varepsilon_{R2}(\beta_a) = \varepsilon_a$, their width decreases to zero, while their height increases to infinity. Simultaneously the area under the first pick converges to $w_{a1}^a = 0.03381$ while the area under the second pick converges to $w_{a2}^a = 0.90601$. This is the missing contribution in the anomalous point. Since ε_a is nondegenerate, this contribution can be obtained from the expression (52) in a limit $\beta \rightarrow \beta_a$. One finds $w_{L_{1,1}}^a(\beta_a) + w_{C_1}^a(\beta_a) + w_{a1}^a = 1$ and $w_{L_{1,2}}^a(\beta_a) + w_{C_2}^a(\beta_a) + w_{a2}^a = 1$ in accord with the completeness requirement. Thus in a limit $h \rightarrow 0$ those picks contribute the missing density to the spectral distributions of local states $|\Theta_1\rangle$ and $|\Theta_2\rangle$. In conclusion, if $\beta = \beta_a$ density $\rho_s^a(\varepsilon)$ has in a point $\varepsilon = \varepsilon_a$ the shape of a delta function $w_{a,s}^a \delta(\varepsilon - \varepsilon_a)$ and one has to add this contribution to the density $\rho_s^a(\varepsilon)$ in order to obtain the correct result. This δ -like contribution to density is a characteristic fingerprint of the isolated eigenstate. In general, in an anomalous point combined system may have several isolated eigenstates [8]. Unlike isolated eigenstates discussed in section 3.3 that are associated with eigenvalues contained outside the range D , isolated eigenstates associated with anomalous points are embedded in this range. Following carefully the process $\beta \rightarrow \beta_a$ one can obtain exact expressions for those eigenstates and related probabilities [8].

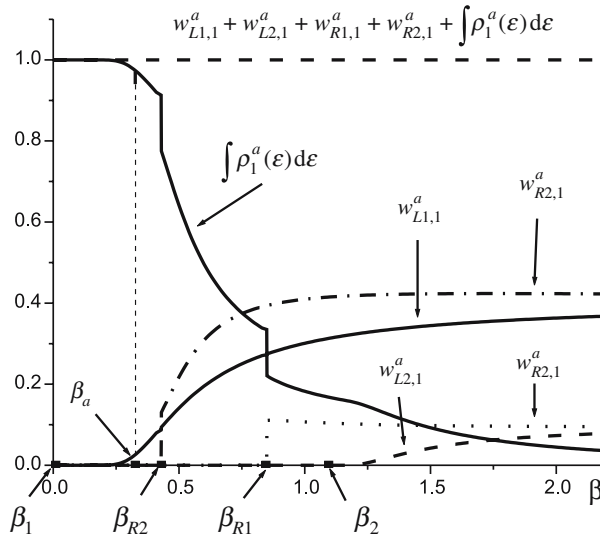


Figure 10. Verification of the completeness relation for the eigenvalue distribution of a local state $|\Theta_1\rangle$. Probabilities $w_{I,1}^a$ as well as probability $w_{C1}^a = \int \rho_1^a(\epsilon)d\epsilon$ and a total probability $\sum_I w_{I,1}^a + w_{C1}^a$ are plotted as a function of a coupling parameter β . For details see text.

4.5. Verification of completeness relations

In section 4.3 we have verified completeness relations for the values $\beta = 0.1$, $\beta = 0.6$ and $\beta = 1.9$. In a previous section we have analyzed failure of those relations in the anomalous point $\beta = \beta_a$ and we have shown that this failure is due to the existence of the isolated eigenstate $|\Psi_a\rangle$ with the eigenvalue $\epsilon_a \in D$. In figures 10 and 11 completeness relations are verified in a more systematic way. In particular, in figure 10 are shown probabilities $w_{R1,1}^a(\beta)$, $w_{R2,1}^a(\beta)$, $w_{L1,1}^a(\beta)$, $w_{L2,1}^a(\beta)$ and $w_{C1}^a(\beta) = \int \rho_1^a(\epsilon)d\epsilon$ associated with the eigenvalue distribution of the local state $|\Theta_1\rangle$. Total probability $w_{all,1}(\beta) = \sum_I w_{I,1}^a(\beta) + w_{C1}^a(\beta)$ is also shown. All those probabilities are given as a function of a coupling β for the relatively large interval $\beta \in [0, 2.2]$. This interval includes the case of the weak coupling as well as the case of the extremely strong coupling. According to the completeness requirement one should have $w_{all,1}(\beta) = 1$ for each β . One finds that this is true for each β , except for the anomalous point $\beta = \beta_a$. In this point contribution of embedded eigenstates $w_{C1}^a(\beta)$ has a sudden drop and hence $w_{all,1}(\beta)$ discontinuously decreases from the required value $w_{all,1}(\beta) = 1$ to the value $w_{all,1}(\beta_a) = 0.96620$. As discussed in a previous section, this is due to the existence of the isolated eigenstate $|\Psi_a\rangle$ with the sharp eigenvalue $\epsilon_a = 0.92515 \in D$. This eigenstate exists if and only if $\beta = \beta_a \in D$. In this respect it differs qualitatively from isolated eigenstates that are not embedded in the range D . Those

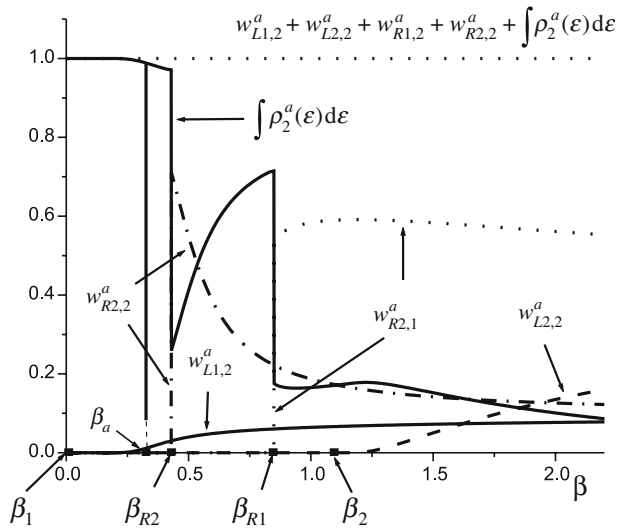


Figure 11. Verification of the completeness relation for the eigenvalue distribution of a local state $|\Theta_2\rangle$. Probabilities $w_{I,2}^a$ as well as probability $w_{C_2}^a = \int \rho_2^a(\epsilon) d\epsilon$ and a total probability $\sum_I w_{I,2}^a + w_{C_2}^a$ are plotted as a function of a coupling parameter β . For details see text.

latter eigenstates exist not only for a particular value of β , but rather for each β that is larger than some critical value.

In figure 11 are shown probabilities $w_{R1,2}^a(\beta)$, $w_{R2,2}^a(\beta)$, $w_{L1,2}^a(\beta)$, $w_{L2,2}^a(\beta)$ and $w_{C_2}^a(\beta) = \int \rho_2^a(\epsilon) d\epsilon$ associated with the eigenvalue distribution of the local state $|\Theta_2\rangle$. Corresponding total probabilities $w_{all,2}(\beta) = \sum_I w_{I,2}^a(\beta) + w_{C_2}^a(\beta)$ are also shown. Again one finds $w_{all,2}(\beta) = 1$ for each β , except for the anomalous point $\beta = \beta_a$. In this point contribution of embedded eigenstates $w_{C_2}^a(\beta)$ has a sudden drop and $w_{all,2}(\beta)$ decreases from $w_{all,2}(\beta) = 1$ to the value $w_{all,2}(\beta_a) = 0.09399$.

Probabilities shown in figures 10 and 11 display a lot of structure. Particularly interesting is the contribution $w_{C_s}^a(\beta) = \int \rho_s^a(\epsilon) d\epsilon$ of all embedded eigenstates to the total probability associated with a local state $|\Theta_s\rangle$. This contribution is the probability to find this state in any of the embedded eigenstates $|\Psi(\epsilon)\rangle$ ($\epsilon \in D$). For example, consider probability $w_{C_2}^a(\beta)$ shown in figure 11. For each $\beta > 0$ the combined system \mathbf{S}_∞ contains isolated eigenstate $|\Psi_{L1}\rangle$ with the eigenvalue $\epsilon_{L1} < -1$. If $\beta < \beta_{R2}$ this is the only isolated eigenstate contained in the combined system. However, for small enough β the contribution $w_{L1,2}^a(\beta)$ of this eigenstate to the total probability $w_{all,2}(\beta) = 1$ is negligible (see section 4.2 and figure 5(a)). Hence $w_{C_2}^a(\beta) \approx 1$. As β increases, $w_{L1,2}^a(\beta)$ increases and hence $w_{C_2}^a(\beta)$ slightly decreases. In the anomalous point $\beta = \beta_a$ probability $w_{C_2}^a(\beta)$ abruptly decreases to a very low value. This is due to the existence of the isolated eigenstate in this point (see section 4.4). As β further

increases, this probability initially reassumes its former value and then it continues to decrease. As β crosses the point $\beta = \beta_{R2}$ combined system acquires right isolated eigenstate $|\Psi_{R2}\rangle$ with the eigenvalue $\varepsilon_{R2} > 1$. The corresponding probability $w_{R2,2}^a$ abruptly jumps from zero to $w_{R2,2}^a(\beta_{R2}+) = 0.71062$. Hence probability $w_{C2}^a(\beta)$ abruptly decreases for the same amount. As the coupling β further increases until the point $\beta = \beta_{R1}$, the probability $w_{C2}^a(\beta_{R2})$ slowly increases. After β crosses this point the combined system acquires another right isolated eigenstate $|\Psi_{R1}\rangle$ with the eigenvalue ε_{R1} . The corresponding probability $w_{R1,2}^a$ again abruptly jumps from zero to $w_{R1,2}^a(\beta_{R1}+) = 0.53733$. Hence probability $w_{C2}^a(\beta)$ abruptly decreases for the same amount. With the further increase of β this probability continuously changes. First it slowly decreases, then it increases, and when the contribution $w_{L2,2}^a$ of the left isolated eigenstate $|\Psi_{L2}\rangle$ becomes relatively significant, it starts again to decrease.

In conclusion, the probability $w_{C2}^a(\beta)$, considered as a function of the coupling parameter β , exhibits a very complex behavior. No power series expansion in a point $\beta = 0$ can reproduce this behavior beyond the first critical point. In the above example this is anomalous point $\beta = \beta_a$ and especially the point $\beta = \beta_{R2}$ where $w_{C2}^a(\beta)$ is discontinuous. Standard perturbation expansion approach can not predict the existence of the isolated eigenstate $|\Psi_a\rangle$ in the anomalous point $\beta = \beta_a$ and it can not reproduce probability $w_{C2}^a(\beta)$ for $\beta > \beta_{R2}$. The same applies to all other quantities shown in figures 10 and 11. In fact, the situation is even worse than that. For each $\beta > 0$ combined system \mathbf{S}_∞ contains isolated eigenvalue ε_{L1} that can not be obtained by the perturbation expansion. Hence, strictly, perturbation expansion fails for each $\beta > 0$. However, if β is small the contribution of the corresponding eigenstate $|\Psi_{L1}\rangle$ to the density $\rho^a(\varepsilon)$ is negligible (see expression (47)). Hence perturbation expansion has still (limited) validity in the case of such small β .

5. Conclusion

Exact nonperturbative method [5–7] for the treatment of the interaction of a single state with the infinite quantum system \mathbf{S}_∞^b is generalized to the interaction of an arbitrary finite quantum system \mathbf{S}_ρ^a with the infinite quantum system \mathbf{S}_∞^b . In order to emphasize the generalization $\mathbf{S}_1^a \rightarrow \mathbf{S}_\rho^a$, in a present paper it is assumed that the system \mathbf{S}_∞^b contains only a single one-parameter eigenvalue band. All eigenvalues of this system are hence contained in the range $D = [\lambda_a, \lambda_b]$ consisting of a single interval. Generalization $\mathbf{S}_1^a \rightarrow \mathbf{S}_\rho^a$ is a key step toward a final goal to develop a general mathematical formalism for the description of an arbitrary finite quantum system \mathbf{S}_ρ^a that interacts with an arbitrary infinite quantum system \mathbf{S}_∞^b [8].

It is shown that the combined system $\mathbf{S}_\infty \equiv \mathbf{S}_\rho^a \oplus \mathbf{S}_\infty^b$ usually contains two qualitatively different types of eigenvalues and eigenstates. First, the system

\mathbf{S}_∞ may contain finite number of discrete eigenvalues ε_s with the corresponding eigenstates. Those discrete eigenvalues are *isolated* eigenvalues. The corresponding isolated eigenstates $|\Psi_s\rangle$ are normalized to unity. Combined system \mathbf{S}_∞ may contain at most ρ left isolated eigenvalues $\varepsilon_I \equiv \varepsilon_L < \lambda_a$ and at most ρ right isolated eigenvalues $\varepsilon_I \equiv \varepsilon_R > \lambda_b$. Concerning isolated eigenvalues $\varepsilon_r \in D$, those eigenvalues may exist only in the so-called “anomal” points. The number and type of such points depends on the details of the interaction of the system \mathbf{S}_ρ^a with the system \mathbf{S}_∞^b . In addition to isolated eigenvalues, 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 $|\Psi(\varepsilon)\rangle$ are normalized to a δ -function. Those eigenvalues and the corresponding eigenstates are *embedded* eigenvalues and eigenstates.

Isolated and embedded solutions of the combined system are described by two key equations derived in this paper, a generic equation (10) and a fractional shift equation (23a). Both are $\rho \times \rho$ eigenvalue equations and they both act in the space X_ρ^a associated with the system \mathbf{S}_ρ^a .

Generic equation (10) is a nonlinear eigenvalue equation. Hence it may have more than ρ distinct eigenvalues and eigenstates. Each eigenvalue $\varepsilon_I \notin D$ of this equation is an isolated eigenvalue of the combined system. Once this eigenvalue is known, one easily obtains the corresponding isolated eigenstate $|\Psi_I\rangle$. In particular, eigenstate $|\theta_I\rangle$ of this equation is proportional to the X_ρ^a -component $|\Psi_I^a\rangle$ of isolated eigenstate $|\Psi_I\rangle$. Concerning eigenvalues $\varepsilon_r \in D$ of this equation, those eigenvalues are so called *resonant* points. A special type of resonant points, so-called *anomal* points are shown to be isolated eigenvalues of the combined system. The corresponding eigenstates determine related isolated eigenstates $|\Psi_r\rangle$ [8]. Thus generic eigenvalue equation provides all isolated solutions of the combined system.

For each $\varepsilon \in D$ fractional shift equation is a linear eigenvalue equation. This equation is related to embedded solutions of the combined system. In particular, X_ρ^a -component $|\Psi^a(\varepsilon)\rangle$ of embedded eigenstate $|\Psi(\varepsilon)\rangle$ is according to the expression (25a) given in terms of the solution to this equation. As far as embedded solutions are considered, this component determines all properties of the system \mathbf{S}_ρ^a that interacts with the system \mathbf{S}_∞^b . Thus generic equation (10) and fractional shift equation (23a) provide a key information for the description of the system \mathbf{S}_ρ^a that is not isolated but which interacts with surrounding media (system \mathbf{S}_∞^b). This is an exact description and no power series expansion is involved. As emphasized above, in the present paper the system \mathbf{S}_∞^b is restricted to have only a single one-parameter eigenvalue band and no isolated eigenstates. However, this method can be generalized to arbitrary quantum systems \mathbf{S}_∞^b [8]. When this is done one finds that the structure and the interpretation of the generic and fractional shift equation remains essentially unchanged [8].

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_I of the finite system \mathbf{S}_ρ^a that is contained outside the eigenvalue range D of this infinite system moves to a new position ε_I , and it remains sharp. Each eigenvalue E_r of the finite system \mathbf{S}_ρ^a that is contained inside this eigenvalue range also moves to a new position ε_r . However, since $E_r \in D$ this shifted eigenvalue is usually not sharp and it acquires a finite width. In particular, if E_r is nondegenerate shifted eigenvalue $\varepsilon_r \in D$ usually acquires the shape of the universal resonance curve with a finite width $\Delta\varepsilon_r$. Only in a special case when $\varepsilon_r = \varepsilon_a$ is an anomalous point the width $\Delta\varepsilon_r$ drops to zero and in this case one has one or several isolated solutions associated with this point [8]. If the interaction between the systems \mathbf{S}_ρ^a and \mathbf{S}_∞^b becomes strong this simple picture is destroyed, and one may have much more complex behavior. In particular, various density distributions inside the range D in a case of a relatively strong interaction have no resemblance to the universal resonance curve. This is also the region where standard perturbation expansion fails.

The method is illustrated with an example of a two-dimensional system \mathbf{S}_2^a that interacts with the infinite system \mathbf{S}_∞^b . This infinite system contains a single one-parameter eigenvalue band in the interval $D \equiv [-1, 1]$. It is shown that all relevant probabilities and density distributions satisfy completeness relations (56). Those relations are verified for a very 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 relations provides a powerful verification of the suggested method.

Acknowledgments

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Appendix A

A.1. Solution of a finite combined system $\mathbf{S}_{n+\rho}$

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

$$\mathbf{B}|\Phi_i\rangle = \lambda_i|\Phi_i\rangle, \quad i = 1, \dots, n, \quad (\text{A.1a})$$

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

$$\langle \Phi_i | \Phi_j \rangle = \delta_{ij}. \tag{A.1b}$$

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

$$\mathbf{C} |\Psi_k\rangle = \varepsilon_k \mathbf{S} |\Psi_k\rangle, \quad k = 1, \dots, n + \rho, \tag{A.2a}$$

where

$$\mathbf{C} = \mathbf{A} + \mathbf{B} + \beta \mathbf{V}, \quad \mathbf{S} = \mathbf{S}^a + \mathbf{I}^b. \tag{A.2b}$$

and where \mathbf{I}^b is a unit operator in X_n^b . The solution to the finite combined system $\mathbf{S}_{n+\rho}$ can be obtained in the closed form [12]. This system may contain singular eigenvalues $\varepsilon_k \in \{\lambda_i\}$ and cardinal eigenvalues $\varepsilon_k \notin \{\lambda_i\}$ [12].

Let $\{|\chi_s\rangle\}$ be an arbitrary base in X_ρ^a . There is a unique operator \mathbf{K} such that representation of \mathbf{K} in this base is a unit matrix (see equation (4a)). Solutions of the eigenvalue equation (A.2) can be expressed in this base. Concerning cardinal eigenvalues one finds [12]:

(a) $\varepsilon_k \notin \{\lambda_i\}$ is an eigenvalue of $\mathbf{S}_{n+\rho}$ if and only if it is a root of the function $h(\varepsilon)$:

$$h(\varepsilon) \equiv \left| \beta^2 \boldsymbol{\Omega}(\varepsilon) + \mathbf{A} - \varepsilon \mathbf{S}^a \right| = 0, \tag{A.3a}$$

where \mathbf{A} and \mathbf{S}^a are $\rho \times \rho$ Hermitian matrices with matrix elements (5), while $\boldsymbol{\Omega}(\varepsilon)$ is a $\rho \times \rho$ Hermitian matrix with matrix elements $\Omega_{sp}(\varepsilon)$

$$\Omega_{sp}(\varepsilon) = \sum_i^n \frac{\langle \chi_s | \mathbf{V} | \Phi_i \rangle \langle \Phi_i | \mathbf{V} | \chi_p \rangle}{\varepsilon - \lambda_i}, \quad s, p = 1, \dots, \rho. \tag{A.3b}$$

(b) If $\varepsilon_k \notin \{\lambda_i\}$ is an eigenvalue of the system $\mathbf{S}_{n+\rho}$, each normalized eigenstate corresponding to this eigenvalue is of the form [12]

$$|\Psi_k\rangle = \frac{1}{\sqrt{Q_k}} \left[\sum_s^\rho C_s^{(k)} |\chi_s\rangle + \beta \sum_i^n \frac{\sum_s^\rho \langle \Phi_i | \mathbf{V} | \chi_s \rangle C_s^{(k)}}{\varepsilon_k - \lambda_i} |\Phi_i\rangle \right], \tag{A.4a}$$

where

$$Q_k = \sum_{s,p}^\rho C_s^{(k)*} S_{sp}^a C_p^{(k)} + \beta^2 \sum_i^n \frac{\left| \sum_s^\rho \langle \Phi_i | \mathbf{V} | \chi_s \rangle C_s^{(k)} \right|^2}{(\varepsilon_k - \lambda_i)^2}, \tag{A.4b}$$

and where coefficients $C_s^{(k)}$ are components of a column vector $\mathbf{C}^{(k)}$ which is a nontrivial solution of a matrix equation

$$\left[\beta^2 \boldsymbol{\Omega}(\varepsilon_k) + \mathbf{A} \right] \mathbf{C}^{(k)} = \varepsilon_k \mathbf{S}^a \mathbf{C}^{(k)}. \tag{A.4c}$$

Eigenstates $|\Psi_k\rangle$ are normalized according to the metrics induced by the operator $\mathbf{S} = \mathbf{S}^a + \mathbf{I}^b$, that is one has $\langle \Psi_k | \mathbf{S} | \Psi_k \rangle = 1$. More generally, those eigenstates can be orthonormalized according to

$$\langle \Psi_k | \mathbf{S} | \Psi_l \rangle = \delta_{kl}. \tag{A.5}$$

If $\varepsilon_k \neq \varepsilon_l$ relation (A.5) is automatically satisfied [12]. However, if $\varepsilon_k = \varepsilon_l$ this relation can be enforced by any of the standard procedures such as Gram–Schmidt orthonormalization [11].

Expressions (A.3) and (A.4) produce all cardinal solutions of the combined system $\mathbf{S}_{n+\rho}$. There are analogous expressions for singular solutions of this system [12]. However, cardinal solutions are most important and most numerous. In particular, if all eigenvalues λ_i of the unperturbed system \mathbf{S}_n^b are nondegenerate, rather special conditions are required in order for the system $\mathbf{S}_{n+\rho}$ to have singular solutions [12].

In addition to the above expressions, we need the interlacing rule [12].

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 [12]

$$\varepsilon_i \leq \lambda_i \leq \varepsilon_{i+\rho}, \quad i = 1, \dots, n. \tag{A.6a}$$

In particular

$$\lambda_1 \leq \varepsilon_{\rho+1}, \quad \varepsilon_n \leq \lambda_n. \tag{A.6b}$$

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 ($<$).

Eigenvalue equations (1a) and (A.2) are generalized eigenvalue equations involving operators \mathbf{S}^a and \mathbf{S} that may satisfy $\mathbf{S}^a \neq \mathbf{I}^a$ and $\mathbf{S} \neq \mathbf{I}_{n+\rho} \equiv \mathbf{I}^a + \mathbf{I}^b$. One has to be careful how to define probabilities in systems \mathbf{S}_ρ^a and $\mathbf{S}_{n+\rho}$ in the case of such generalized eigenvalue equations. Consider system \mathbf{S}_ρ^a that is described by the eigenvalue equation (1a). Let $|\Theta\rangle \in X_\rho^a$ be an arbitrary state in X_ρ^a and let w_s be probability to find this state in the local state $|\Theta_s\rangle$ ($s = 1, \dots, \rho$). Those local states form a complete set in X_ρ^a and they are mutually exclusive eigenstates of the system \mathbf{S}_ρ^a . Hence one should have

$$\sum_s^\rho w_s = 1. \tag{A.7a}$$

Standard definition $w_s = |\langle \Theta | \Theta_s \rangle|^2$ does not satisfy this condition. One finds that in order to satisfy (A.7a) for each state $|\Theta\rangle \in X_\rho^a$ one has to define probabilities w_s according to

$$w_s = |\langle \Theta | \mathbf{S}^a | \Theta_s \rangle|^2, \quad s = 1, \dots, \rho, \tag{A.7b}$$

where local states $|\Theta_s\rangle$ are orthonormalized according to (1b) and where the state $|\Theta\rangle$ is normalized according to

$$\langle \Theta | \mathbf{S}^a | \Theta \rangle = 1. \tag{A.7c}$$

This follows from the expression (1c). Using this expression one easily proves that probabilities w_s defined according to (A.7b) satisfy requirement (A.7a) for each state $|\Theta\rangle \in X_\rho^a$. Those probabilities are defined in accord with the metrics induced by the operator \mathbf{S}^a . In a similar way and in accord with a metrics induced by the operator \mathbf{S} are defined probabilities in the combined system $\mathbf{S}_{n+\rho}$.

A.2. System \mathbf{S}_∞ as the $n \rightarrow \infty$ limit of finite-dimensional systems $\mathbf{S}_{n+\rho}$

In order to solve eigenvalue equation (3), we approximate system \mathbf{S}_∞^b with a finite dimensional system \mathbf{S}_n^b containing n eigenvalues and n eigenstates. As shown in a previous section, the solution to the corresponding combined system $\mathbf{S}_{n+\rho}$ can be obtained in the closed form. Our general strategy is to derive an appropriate $n \rightarrow \infty$ limit of this solution. Provided this limit is well defined, it represents the solution to the system \mathbf{S}_∞ .

Let $\lambda(k)$ be continuous function of k in the interval $[k_a, k_b]$. Let further this function be monotonic increasing in this interval. Partition this interval into n subintervals of equal length $\Delta k = (k_b - k_a)/n$. Midpoints of those subintervals are $k_i = k_a + (i - 1/2) \Delta k$ ($i = 1, \dots, n$). Replace function $\lambda(k)$ with n values $\lambda_i \equiv \lambda(k_i)$ sampled at those midpoints. Those n values are eigenvalues of the finite unperturbed system \mathbf{S}_n^b that approximates unperturbed system \mathbf{S}_∞^b . Since $\lambda(k)$ is an increasing function of k , each λ_i is a nondegenerate eigenvalue of \mathbf{S}_n^b . Next, replace each function $\langle \chi_s | \mathbf{V} | \Phi(k) \rangle$ ($s = 1, \dots, \rho$) with n values $\langle \chi_s | \mathbf{V} | \Phi_i \rangle$ ($i = 1, \dots, n$) sampled at midpoints k_i [5]

$$\langle \chi_s | \mathbf{V} | \Phi_i \rangle = \langle \chi_s | \mathbf{V} | \Phi(k_i) \rangle \sqrt{\Delta k}, \quad i = 1, \dots, n. \tag{A.8a}$$

Proportionality constant ($\sqrt{\Delta k}$) follows from the normalization condition

$$\int |\Phi(k)\rangle \langle \Phi(k)| dk \Leftrightarrow \sum_i |\Phi_i\rangle \langle \Phi_i|. \tag{A.8b}$$

According to (A.3) and (A.4), cardinal solutions of the combined system $\mathbf{S}_{n+\rho}$ (eigenvalues and eigenstates) can be expressed in terms of the unperturbed

eigenvalues λ_i , in terms of matrix elements $\langle \chi_s | \mathbf{V} | \Phi_i \rangle$, and in terms of matrices \mathbf{A} and \mathbf{S}^a . The above procedure determines eigenvalues λ_i and matrix elements $\langle \chi_s | \mathbf{V} | \Phi_i \rangle$, while matrices \mathbf{A} and \mathbf{S}^a are known since they describe isolated system \mathbf{S}_ρ^a . Hence this procedure effectively approximates infinite-dimensional system \mathbf{S}_∞ with $(\rho + n)$ -dimensional system $\mathbf{S}_{n+\rho}$. As n increases, system $\mathbf{S}_{n+\rho}$ converges to the system \mathbf{S}_∞ and the solution of the former system converges to the solution of the latter system. In addition to cardinal solutions, system $\mathbf{S}_{n+\rho}$ may contain singular solutions. However, more detailed analyses shows that one can always approximate infinite system \mathbf{S}_∞ to any desired degree of accuracy with a finite system $\mathbf{S}_{n+\rho}$ that contains no singular solutions. Relations (A.3) and (A.4) are hence sufficient for the derivation of the required $n \rightarrow \infty$ limit, and explicit relations for the singular solutions are not needed.

Interlacing rule (A.6) implies that in a limit $n \rightarrow \infty$ one can have two qualitatively different solutions of the combined system \mathbf{S}_∞ . Eigenvalues $\lambda_i \equiv \lambda(k_i)$ of the finite unperturbed system \mathbf{S}_n^b are confined to the interval $D = [\lambda_a, \lambda_b]$ where $\lambda_a = \lambda(k_a)$ and $\lambda_b = \lambda(k_b)$. As n increases, $\lambda_1 > \lambda_a$ converges to λ_a while $\lambda_n < \lambda_b$ converges to λ_b . In a limit $n \rightarrow \infty$ unperturbed eigenvalues λ_i are dense in D . Due to the interlacing rule, perturbed eigenvalues $\varepsilon_{\rho+1}, \dots, \varepsilon_n$ are also dense in this interval. Hence in a limit $n \rightarrow \infty$ each $\varepsilon \in D$ is a perturbed eigenvalue. We call such eigenvalues of the combined system *embedded* eigenvalues [5–7]. Each embedded eigenvalue is a part of a continuous band of eigenvalues, and the corresponding eigenstates $|\Psi(\varepsilon)\rangle$ are normalized to a δ -function in accord with the metrics defined by the operator \mathbf{S} .

In addition to the embedded eigenvalues, there are 2ρ perturbed eigenvalues that in a process $n \rightarrow \infty$ may (but need not) escape the interval D . According to (A.6b) those are ρ perturbed eigenvalues $\varepsilon_1, \dots, \varepsilon_\rho$ that may satisfy $\varepsilon_k < \lambda_a$, and ρ perturbed eigenvalues $\varepsilon_{n+1}, \dots, \varepsilon_{n+\rho}$ that may satisfy $\varepsilon_k > \lambda_b$. Let \bar{D} be a complement of D . We call each perturbed eigenvalue $\varepsilon_I \in \bar{D}$ of \mathbf{S}_∞ an *isolated* eigenvalue. Since this eigenvalue is outside the eigenvalue band D , it is discrete. The corresponding eigenstate $|\Psi_I\rangle$ can be hence normalized to unity. In this respect isolated eigenstates $|\Psi_I\rangle$ of \mathbf{S}_∞ are similar to local states $|\Theta_s\rangle \in X_\rho^a$ that are also normalized to unity. There are at most ρ left isolated eigenvalues (and corresponding eigenstates) $\varepsilon_L < \lambda_a$ and at most ρ right isolated eigenvalues (and corresponding eigenstates) $\varepsilon_R > \lambda_b$.

It will be shown in the following sections that the range D may contain some characteristic points $\varepsilon_r \in D$ in which the process $n \rightarrow \infty$ leads to the creation of isolated eigenvalues and eigenstates. Hence, in addition to the isolated eigenvalues $\varepsilon_I \in \bar{D}$, the system \mathbf{S}_∞ may also contain some isolated eigenvalues $\varepsilon_r \in D$.

A.3. Isolated eigenvalues $\varepsilon_I \in \bar{D}$ and corresponding eigenstates

Since isolated eigenvalue $\varepsilon_I \in \bar{D}$ is outside the range D , it is relatively easy to obtain the $n \rightarrow \infty$ limit of relations (A.3) and (A.4). In particular, using expression (A.8b) summation over i in (A.3b) is replaced with an integral according to

$$\Omega_{sp}(\varepsilon) \rightarrow \omega_{sp}(\varepsilon) = \int_{k_a}^{k_b} \frac{\langle \chi_s | \mathbf{V} | \Phi(k) \rangle \langle \Phi(k) | \mathbf{V} | \chi_p \rangle}{\varepsilon - \lambda(k)} dk, \quad \varepsilon \in \bar{D}.$$

Hence and from (A.3) one derives (11) where matrix elements $\omega_{sp}(\varepsilon)$ of the operator $\omega(\varepsilon)$ are given by (8b) or by the equivalent expression (8c). In a similar way one derives all remaining relations concerning isolated eigenvalues $\varepsilon_I \in \bar{D}$ and the corresponding eigenstates. In particular, orthonormality (A.5) of the eigenstates of a finite combined system $\mathbf{S}_{n+\rho}$ implies orthonormality (13) of isolated eigenstates $|\Psi_I\rangle$ of the combined system \mathbf{S}_∞ . Generic eigenvalue equation (10) for the case $\varepsilon_s \notin D$ is also derived in this way.

A.4. Embedded eigenvalues and eigenstates

Concerning embedded eigenvalues and eigenstates, one has to be more careful. Each $\varepsilon \in D$ is an embedded eigenvalue of the combined system \mathbf{S}_∞ and the transition to the limit $n \rightarrow \infty$ of the relations (A.3) and (A.4) is not so simple. For the special case $\rho = 1$ this transition was done elsewhere [5, 6]. In order to derive correct $n \rightarrow \infty$ limit for the case $\rho \neq 1$, we will use the same general approach. Only the main points of this approach will be outlined. For more detailed discussion the reader may consult reference [5].

A.4.1. Derivation of the fractional shift equation

Consider the system $\mathbf{S}_{n+\rho}$ for some huge n . Define $(n - \rho)$ quantities $x(\varepsilon_k)$ according to (22). Each $x(\varepsilon_k)$ is a *fractional shift* of the perturbed eigenvalue $\varepsilon_k \in D$ relative to the unperturbed eigenvalue $\lambda_{k-1} \in D$ [5, 6]. Interlacing rule (A.6) implies

$$\frac{\lambda_{k-\rho} - \lambda_{k-1}}{\lambda_k - \lambda_{k-1}} \leq x(\varepsilon_k) \leq 1. \tag{A.9a}$$

In particular, in the case $\rho = 1$ one has $0 \leq x(\varepsilon_k) \leq 1$ [5].

Let the finite system $\mathbf{S}_{n+\rho}$ approximate infinite system \mathbf{S}_∞ as described in section A.2. If functions $\lambda(k)$ and $\langle \chi_s | \mathbf{V} | \Phi(k) \rangle$ are reasonably smooth, one can

expand those functions in the point $k = k_k$ to obtain

$$\lambda_{k+j} \equiv \lambda(k_{k+j}) = \lambda(k_k) + (d\lambda/dk)_k j \Delta k + O(j^2/n^2), \tag{A.10a}$$

$$\langle \chi_s | \mathbf{V} | \Phi(k_{k+j}) \rangle = \langle \chi_s | \mathbf{V} | \Phi(k_k) \rangle + O(j/n), \quad s = 1, \dots, \rho, \tag{A.10b}$$

where $(d\lambda/dk)_k$ is a derivative of a function $\lambda(k)$ in a point $k = k_k$ and where $O(x)$ is small quantity of the order x . In particular, (A.10a) implies

$$\Delta\lambda_{k+j} \equiv \lambda_{k+j} - \lambda_{k+j-1} = (d\lambda/dk)_k \Delta k + O(j^2/n^2). \tag{A.10c}$$

If $(d\lambda/dk)_k \neq 0$ intervals $\Delta\lambda_{k+j}$ between two adjacent unperturbed eigenvalues are of the order $O(n^{-1})$. Since for sufficiently big n one has $O(\rho^2/n^2) = O(n^{-2})$, relations (A.9a) and (A.10a) imply

$$1 - \rho + O(n^{-1}) \leq x(\varepsilon_k) \leq 1. \tag{A.9b}$$

Fractional shift is thus confined to the well-defined finite interval. According to (22), if $x(\varepsilon_k) = 1$ one has $\varepsilon_k = \lambda_k$, while if $x(\varepsilon_k) = 0$ one has $\varepsilon_k = \lambda_{k-1}$. In both cases perturbed eigenvalue ε_k equals some unperturbed eigenvalue λ_i and ε_k is hence a singular eigenvalue of the combined system $\mathbf{S}_{n+\rho}$. Neglecting terms of the order $O(n^{-1})$, the same applies to all other integer values $x(\varepsilon_k)$. Hence in a limit $n \rightarrow \infty$ integer values of the fractional shift $x(\varepsilon)$ correspond to the singular eigenvalue of the combined system, while all other values correspond to cardinal eigenvalues of this system. In addition and according to (A.9b), in this limit fractional shift $x(\varepsilon)$ satisfies (24).

Let $\varepsilon_k \notin \{\lambda_i\}$ be a cardinal eigenvalue of a finite system $\mathbf{S}_{n+\rho}$ and let this eigenvalue be embedded in the range D . Consider the $n \rightarrow \infty$ limit of a matrix $\Omega(\varepsilon_k)$. Each matrix element $\Omega_{sp}(\varepsilon_k)$ of this matrix can be written as a sum of two components

$$\Omega_{sp}(\varepsilon_k) = \Omega_{sp}^{(0)}(\varepsilon_k) + \Omega_{sp}^{(1)}(\varepsilon_k), \tag{A.11a}$$

where

$$\Omega_{sp}^{(0)}(\varepsilon_k) = \sum_{j=-N(n)}^{N(n)} \frac{\langle \chi_s | \mathbf{V} | \Phi_{k+j} \rangle \langle \Phi_{k+j} | \mathbf{V} | \chi_p \rangle}{\varepsilon_k - \lambda_{k+j}}, \tag{A.11b}$$

$$\Omega_{sp}^{(1)}(\varepsilon_k) = \sum_{j < -N(n)} \frac{\langle \chi_s | \mathbf{V} | \Phi_{k+j} \rangle \langle \Phi_{k+j} | \mathbf{V} | \chi_p \rangle}{\varepsilon_k - \lambda_{k+j}} + \sum_{j > N(n)} \frac{\langle \chi_s | \mathbf{V} | \Phi_{k+j} \rangle \langle \Phi_{k+j} | \mathbf{V} | \chi_p \rangle}{\varepsilon_k - \lambda_{k+j}}. \tag{A.11c}$$

Choose $N(n) = \lfloor n^{1/3} \rfloor$ to be 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 .

Consider component $\Omega_{sp}^{(0)}(\varepsilon_k)$. Since $|j| < n^{1/3}$ and according to (A.10b), for large enough n one has $\langle \chi_s | \mathbf{V} | \Phi(k_{k+j}) \rangle \approx \langle \chi_s | \mathbf{V} | \Phi(k_k) \rangle$ and hence $\langle \chi_s | \mathbf{V} | \Phi_{k+j} \rangle \approx \langle \chi_s | \mathbf{V} | \Phi_k \rangle$. Thus one can factor out constant term $\langle \chi_s | \mathbf{V} | \Phi_k \rangle \langle \Phi_k | \mathbf{V} | \chi_p \rangle$ under the summation sign in (A.11b). Using relations (A.8a) and (A.10) as well as the definition (22) of a fractional shift one finds

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

With the identity [14]

$$\frac{1}{x} + \sum_{j=1}^{\infty} \left(\frac{1}{x-j} + \frac{1}{x+j} \right) = \pi \cot(\pi x). \tag{A.12}$$

this implies

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

As n increases this approximation improves and in a limit $n \rightarrow \infty$ it is exact [5]. Since $\lambda(k_k) \approx \varepsilon_k$ one has

$$\frac{\langle \chi_s | \mathbf{V} | \Phi(k_k) \rangle \langle \Phi(k_k) | \mathbf{V} | \chi_p \rangle}{(d\lambda/dk)_k} \rightarrow \frac{\langle \chi_s | \mathbf{V} | \Phi(k) \rangle \langle \Phi(k) | \mathbf{V} | \chi_p \rangle}{d\lambda/dk} \Big|_{\varepsilon=\lambda(k)} = f_{sp}(\varepsilon). \tag{A.13}$$

Hence in the limit $n \rightarrow \infty$ component $\Omega_{sp}^{(0)}(\varepsilon_k)$ of $\Omega_{sp}(\varepsilon_k)$ should be replaced according to

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

In a similar way one finds that in this limit component $\Omega_{sp}^{(1)}(\varepsilon_k)$ should be replaced according to [5]

$$\Omega_{sp}^{(1)}(\varepsilon_k) \rightarrow \omega_{sp}(\varepsilon) = P \int_{k_a}^{k_b} \frac{\langle \chi_s | \mathbf{V} | \Phi(k) \rangle \langle \Phi(k) | \mathbf{V} | \chi_p \rangle}{\varepsilon - \lambda(k)} dk, \quad \varepsilon \in D,$$

where P denotes principal Cauchy integral value [10].

Using expression (6b), functions $\omega_{sp}(\varepsilon)$ can be expressed in terms of functions $f_{sp}(\varepsilon)$ according to (8b). This implies (8a). Further, in a limit $n \rightarrow \infty$ components $C_s^{(k)} \equiv C_s(\varepsilon_k)$ of $\mathbf{C}^{(k)} \equiv \mathbf{C}(\varepsilon_k)$ become continuous functions of ε ,

i.e. $C_s^{(k)} \rightarrow C_s(\varepsilon)$. Combining all those results one finds that in a limit $n \rightarrow \infty$ matrix equation (A.4c) translates into

$$\sum_p^\rho \left[\beta^2 \omega_{sp}(\varepsilon) + A_{sp} - \varepsilon S_{sp}^a \right] C_p(\varepsilon) = X(\varepsilon) \sum_p^\rho f_{sp}(\varepsilon) C_p(\varepsilon), \quad s = 1, \dots, \rho, \quad (\text{A.14a})$$

where

$$X(\varepsilon) = -\pi\beta^2 \cot(\pi x(\varepsilon)). \quad (\text{A.14b})$$

Expression (A.14a) is a generalized eigenvalue equation with the eigenvalue $X(\varepsilon)$ and with the corresponding eigenvector(s) $\mathbf{C}(\varepsilon)$. Since in a limit $n \rightarrow \infty$ one has $C_s^{(k)} \rightarrow C_s(\varepsilon)$, expressions (4a) and (A.4a) imply $C_s(\varepsilon) \propto \langle \chi_s | \mathbf{K} | \Psi(\varepsilon) \rangle$ where $|\Psi(\varepsilon)\rangle$ is embedded eigenstate of the combined system. Hence one finds that this matrix eigenvalue equation is equivalent to the eigenvalue equation (23) and that components $C_s(\varepsilon)$ of $\mathbf{C}(\varepsilon)$ are connected to the eigenstate $|\psi(\varepsilon)\rangle$ of (23) according to

$$C_s(\varepsilon) = \langle \chi_s | \mathbf{K} | \psi(\varepsilon) \rangle. \quad (\text{A.14c})$$

Eigenstate $|\psi(\varepsilon)\rangle$ of (23a) is hence proportional to the X_ρ^a -component $|\Psi^a(\varepsilon)\rangle$ of the eigenstate $|\Psi(\varepsilon)\rangle$ of the combined system. Proportionality constant will be derived in the next section.

Note the difference between eigenvalue equation (A.14a) derived above and the original eigenvalue equation (A.4c) that applies to a finite system $\mathbf{S}_{n+\rho}$. Solutions to (A.4c) are perturbed eigenvalues ε_k and the corresponding eigenvectors $\mathbf{C}^{(k)}$. As n increases eigenvalues ε_k ($k = \rho + 1, \dots, n$) become dense in the interval D , and in a limit $n \rightarrow \infty$ each $\varepsilon \in D$ becomes an eigenvalue of the combined system. There is hence no information contained in the particular eigenvalue $\varepsilon \in D$. According to (A.14b) this information about eigenvalues is in the equation (A.14a) 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. Accordingly, we call eigenvalue equation (A.14) a *fractional shift* equation. This is our key equation for the description of the embedded solutions of a combined system.

A.4.2. Derivation of the X_ρ^a -component of the normalized eigenstate $|\Psi(\varepsilon)\rangle$

In order to derive component $|\Psi^a(\varepsilon)\rangle \in X_\rho^a$ of the normalized eigenstate $|\Psi(\varepsilon)\rangle = |\Psi^a(\varepsilon)\rangle + |\Psi^b(\varepsilon)\rangle$ of the infinite combined system \mathbf{S}_∞ , we again consider finite combined system $\mathbf{S}_{n+\rho}$ and analyze X_ρ^a -component of the corresponding eigenstates $|\Psi_k\rangle$ in a limit $n \rightarrow \infty$.

Normalized eigenstate (A.4a) of a finite system $\mathbf{S}_{n+\rho}$ can be written as a sum of three terms

$$|\Psi_k\rangle = \frac{1}{\sqrt{Q_k}} \left[|Z_k\rangle + \beta \left| \Psi_k^{(0)} \right\rangle + \beta \left| \Psi_k^{(1)} \right\rangle \right], \quad (\text{A.15a})$$

where

$$|Z_k\rangle = \sum_s^\rho C_s^{(k)} |\chi_s\rangle \in X_\rho^a, \quad (\text{A.15b})$$

$$\left| \Psi_k^{(0)} \right\rangle = \sum_{j=-M(n)}^{M(n)} \frac{\langle \Phi_{k+j} | \mathbf{V} | Z_k \rangle}{\varepsilon_k - \lambda_{k+j}} |\Phi_{k+j}\rangle \in X_n^b, \quad (\text{A.15c})$$

$$\left| \Psi_k^{(1)} \right\rangle = \sum_{j < -M(n)} \frac{\langle \Phi_{k+j} | \mathbf{V} | Z_k \rangle}{\varepsilon_k - \lambda_{k+j}} |\Phi_{k+j}\rangle + \sum_{j > M(n)} \frac{\langle \Phi_{k+j} | \mathbf{V} | Z_k \rangle}{\varepsilon_k - \lambda_{k+j}} |\Phi_{k+j}\rangle \in X_n^b, \quad (\text{A.15d})$$

and where

$$Q_k = \langle Z_k | \mathbf{S}^a | Z_k \rangle + \beta^2 \left\langle \Psi_k^{(0)} \left| \Psi_k^{(0)} \right\rangle + \beta^2 \left\langle \Psi_k^{(1)} \left| \Psi_k^{(1)} \right\rangle. \quad (\text{A.15e})$$

In the above expressions choose $M(n) = \lfloor n^{2/3} \rfloor$ to be the largest integer smaller than $n^{2/3}$. With this choice function $\left| \Psi_k^{(0)} \right\rangle$ contains contributions to the perturbed eigenstate $|\Psi_k\rangle$ from approximately $2n^{2/3}$ unperturbed states $|\Phi_{k+j}\rangle \in X_n^b$ whose eigenvalues λ_{k+j} are close to ε_k , while function $\left| \Psi_k^{(1)} \right\rangle$ contains contributions from approximately $(n - 2n^{2/3}) \approx n$ remaining states $|\Phi_{k+j}\rangle \in X_n^b$.

Let us estimate quantity Q_k that determines normalization of the eigenstate $|\Psi_k\rangle$. One has

$$\langle Z_k | \mathbf{S}^a | Z_k \rangle = \sum_{s,p}^\rho C_s^{(k)*} S_{sp}^a C_p^{(k)}, \quad (\text{A.16a})$$

$$\left\langle \Psi_k^{(0)} \left| \Psi_k^{(0)} \right\rangle = \sum_{j=-M(n)}^{M(n)} \frac{\langle Z_k | \mathbf{V} | \Phi_{k+j} \rangle \langle \Phi_{k+j} | \mathbf{V} | Z_k \rangle}{(\varepsilon_k - \lambda_{k+j})^2}, \quad (\text{A.16b})$$

$$\left\langle \Psi_k^{(1)} \left| \Psi_k^{(1)} \right\rangle = \sum_{j < -M(n)} \frac{\langle Z_k | \mathbf{V} | \Phi_{k+j} \rangle \langle \Phi_{k+j} | \mathbf{V} | Z_k \rangle}{(\varepsilon_k - \lambda_{k+j})^2} + \sum_{j > M(n)} \frac{\langle Z_k | \mathbf{V} | \Phi_{k+j} \rangle \langle \Phi_{k+j} | \mathbf{V} | Z_k \rangle}{(\varepsilon_k - \lambda_{k+j})^2}. \quad (\text{A.16c})$$

Matrix element $\langle Z_k | \mathbf{S}^a | Z_k \rangle$ is of the order $O(1)$. Concerning $\left\langle \Psi_k^{(0)} \left| \Psi_k^{(0)} \right\rangle$, note that all terms under summation sign in (A.16b) satisfy $|j| \leq n^{2/3}$. Hence $\langle Z_k | \mathbf{V} | \Phi_{k+j} \rangle \approx \langle Z_k | \mathbf{V} | \Phi_k \rangle$ and relations (A.8a), (A.10a) and (22) imply [5]

$$\left\langle \Psi_k^{(0)} \left| \Psi_k^{(0)} \right\rangle \approx \frac{1}{\Delta \lambda_k} \frac{\langle Z_k | \mathbf{V} | \Phi(k_k) \rangle \langle \Phi(k_k) | \mathbf{V} | Z_k \rangle}{(d\lambda/dk)_k} \sum_{j=-M(n)}^{M(n)} \frac{1}{(x(\varepsilon_k) - j)^2}.$$

As n increases above expression is more and more exact. Since $M(n) \approx n^{2/3}$ one can in a limit $n \rightarrow \infty$ extend summation over j to the interval $j \in (-\infty, \infty)$. Further, if one takes derivation of (A.12) with respect to x one finds

$$\sum_{j=-\infty}^{\infty} \frac{1}{(x-j)^2} = \frac{\pi^2}{\sin^2(\pi x)}.$$

Hence for sufficiently big n one has

$$\langle \Psi_k^{(0)} | \Psi_k^{(0)} \rangle \approx \frac{1}{\Delta \lambda_k} \frac{\langle Z_k | \mathbf{V} | \Phi(k_k) \rangle \langle \Phi(k_k) | \mathbf{V} | Z_k \rangle}{(d\lambda/dk)_k} \frac{\pi^2}{\sin^2(\pi x(\varepsilon_k))}. \quad (\text{A.17a})$$

Intervals $\Delta \lambda_k$ scale as $O(n^{-1})$. This implies that if $\lim_{n \rightarrow \infty} \langle Z_k | \mathbf{V} | \Phi(k_k) \rangle \neq 0$ the quantity $\langle \Psi_k^{(0)} | \Psi_k^{(0)} \rangle$ scales at least as $O(n)$. Similar analyzes shows that $\langle \Psi_k^{(1)} | \Psi_k^{(1)} \rangle$ scales not faster than $O(n^{2/3})$ [5]. Hence, provided in a limit $n \rightarrow \infty$ one has $\langle Z_k | \mathbf{V} | \Phi(k_k) \rangle \neq 0$, one can in this limit neglect $\langle \Psi_k^{(1)} | \Psi_k^{(1)} \rangle$ and $\langle Z_k | \mathbf{S}^a | Z_k \rangle$ relative to $\langle \Psi_k^{(0)} | \Psi_k^{(0)} \rangle$. In this case

$$Q_k \approx \beta^2 \langle \Psi_k^{(0)} | \Psi_k^{(0)} \rangle. \quad (\text{A.17b})$$

In analogy to (A.7b), probability to find the state $|\Theta\rangle \in X_\rho^a$ in the state $|\Psi_k\rangle$ equals $w_k = |\langle \Theta | \mathbf{S} | \Psi_k \rangle|^2 \equiv |\langle \Theta | \mathbf{S}^a | \Psi_k \rangle|^2$ where $|\Theta\rangle$ is normalized according to $\langle \Theta | \mathbf{S}^a | \Theta \rangle = 1$. Expression (A.4a) implies $\langle \Theta | \mathbf{S}^a | \Psi_k \rangle = \langle \Theta | \mathbf{S}^a | Z_k \rangle / \sqrt{Q_k}$. Hence and from (A.17)

$$w_k \approx \Delta \lambda_k \frac{|\langle \Theta | \mathbf{S}^a | Z_k \rangle|^2 (d\lambda/dk)_k}{\beta^2 \langle Z_k | \mathbf{V} | \Phi(k_k) \rangle \langle \Phi(k_k) | \mathbf{V} | Z_k \rangle} \frac{\sin^2(\pi x(\varepsilon_k))}{\pi^2}.$$

Using (A.13) and (A.15b) this equals

$$w_k \approx \Delta \lambda_k \frac{\left| \sum_s \langle \Theta | \mathbf{S}^a | \chi_s \rangle C_s^{(k)} \right|^2}{\beta^2 \sum_{sp} C_s^{(k)*} f_{sp}(\varepsilon_k) C_p^{(k)}} \frac{\sin^2(\pi x(\varepsilon_k))}{\pi^2}. \quad (\text{A.18})$$

Let $|\Psi(\varepsilon)\rangle$ be an eigenstate of the infinite system \mathbf{S}_∞ corresponding to the eigenvalue ε . In the limit $n \rightarrow \infty$ one has $\Delta \lambda_k \rightarrow d\lambda$, $\Delta \varepsilon_k \rightarrow d\varepsilon$ and $C_s^{(k)} \equiv C_s(\varepsilon_k) \rightarrow C_s(\varepsilon)$. In this limit discrete probabilities w_k are replaced with the probabilities $|\langle \Theta | \mathbf{S}^a | \Psi(\varepsilon) \rangle|^2 d\varepsilon$ to find the state $|\Theta\rangle$ in the eigenstate $|\Psi(\varepsilon)\rangle$ and in

the eigenvalue interval $d\varepsilon$. By definition, $\rho_{\Theta}(\varepsilon) = |\langle \Theta | \mathbf{S}^a | \Psi(\varepsilon) \rangle|^2$ is a probability density to find a state $|\Theta\rangle$ in the eigenstate $|\Psi(\varepsilon)\rangle$. One can further show that in a limit $n \rightarrow \infty$ almost for each ε one has $d\lambda = d\varepsilon$ [5]. Hence and from (A.18)

$$\rho_{\Theta}(\varepsilon) = \frac{|\sum_s \langle \Theta | \mathbf{S}^a | \chi_s \rangle C_s(\varepsilon)|^2 \sin^2(\pi x(\varepsilon))}{\beta^2 \sum_{sp} C_s^*(\varepsilon) f_{sp}(\varepsilon) C_p(\varepsilon) \pi^2}.$$

Density $\rho_{\Theta}(\varepsilon)$ determines probability amplitude $\langle \Theta | \mathbf{S}^a | \Psi(\varepsilon) \rangle$ up to an arbitrary phase. One can always adjust the phase of $|\Psi(\varepsilon)\rangle$ in such a way as to satisfy

$$\langle \Theta | \mathbf{S}^a | \Psi(\varepsilon) \rangle = \frac{\sum_s \langle \Theta | \mathbf{S}^a | \chi_s \rangle C_s(\varepsilon) \sin(\pi x(\varepsilon))}{\beta \sqrt{\sum_{sp} C_s^*(\varepsilon) f_{sp}(\varepsilon) C_p(\varepsilon)} \pi}. \tag{A.19}$$

This expression is valid for each $|\Theta\rangle \in X_{\rho}^a$. Hence it determines $\mathbf{S}^a | \Psi(\varepsilon) \rangle$. Since $\mathbf{S}^a | \Psi(\varepsilon) \rangle \in X_{\rho}^a$ and since \mathbf{S}^a is regular in X_{ρ}^a , this determines X_{ρ}^a -component $|\Psi^a(\varepsilon)\rangle$ of the eigenstate $|\Psi(\varepsilon)\rangle$. Explicit form of this component can be obtained using relations (4b) and (A.14c). One thus derives expression (25a). This is our key expression that gives component $|\Psi^a(\varepsilon)\rangle \in X_{\rho}^a$ of the normalized eigenstate $|\Psi(\varepsilon)\rangle$ of \mathbf{S}_{∞} in terms of the fractional shift $x(\varepsilon)$ and in terms of the eigenstate $|\psi(\varepsilon)\rangle$ of a fractional shift equation.

In a previous section we have derived fractional shift equation (A.14) as the $n \rightarrow \infty$ limit of the eigenvalue equation (A.4c). In this section we have derived expression (25a) as the $n \rightarrow \infty$ limit of the X_{ρ}^a -component of the normalized eigenstate (A.4a). Derivation of both expressions involves some assumptions that are not always satisfied. For example, in the derivation of the expression (25a) via expressions (A.17) and (A.19), we have assumed that in a limit $n \rightarrow \infty$ one has $\langle \mathbf{Z}_k | \mathbf{V} | \Phi(k_k) \rangle \neq 0$. In terms of the eigenstate $|\psi(\varepsilon)\rangle$ of the fractional shift equation, this translates into the requirement $\langle \psi(\varepsilon) | \mathbf{V} | \Phi(k) \rangle|_{\varepsilon=\lambda(k)} \neq 0$, which implies $\mathbf{f}(\varepsilon) |\psi(\varepsilon)\rangle \neq 0$. More detailed analysis shows that key expressions (A.14) and (A.19) are valid almost everywhere in the range D , with possible exception of characteristic points $\varepsilon \in D$ that are defined in section 3.4.2. With an appropriate interpretation, those expressions are valid in most of those characteristic points. Exceptions are so called *anomal* points $\varepsilon_a \in D$ where the combined system may contain isolated eigenstates. By definition, $\varepsilon_a \in D$ is an anomal point if there is a nontrivial state $|\theta\rangle \in X_{\rho}^a$ that satisfies $\mathbf{H}(\varepsilon_a) |\theta\rangle = 0$ and also $\mathbf{f}(\varepsilon_a) |\theta\rangle = 0$.

Finally a general comment. Expressions (10) and (23) valid in the case of the infinite dimensional space X_{∞}^b are derived from the expressions that apply to the finite dimensional space X_n^b . This derivation is possible due to two crucial characteristics of the equations that describe the interaction of the local system \mathbf{S}_{ρ}^a with the finite-dimensional system \mathbf{S}_n^b . First, key expression (A.4c) is a $\rho \times \rho$ (nonlinear) eigenvalue equation, however large the system \mathbf{S}_n^b . Hence the process

$n \rightarrow \infty$ does not change the dimension ρ of this equation. Second, expressions (A.3.4) are exact. There is hence no deterioration of the obtained results (due to the gradual accumulation of error) in the process $n \rightarrow \infty$. Both properties are crucial for the successful transition to the limit $n \rightarrow \infty$. In particular, standard perturbation methods are inappropriate to achieve this goal.

A.4.3. Solution of the fractional shift equation in the base $\{|\phi_s(\varepsilon)\rangle\}$

One can obtain an exact solution of the fractional shift equation in the base $\{|\phi_s(\varepsilon)\rangle\}$ of the eigenstates of the eigenvalue equation (27a). Those eigenstates can be orthonormalized according to (27b). Eigenstate $|\Psi(\varepsilon)\rangle$ of a fractional shift equation can be expressed as a linear combination (28a). Inserting this expression into (23a), multiplying from left by $\langle\phi_s(\varepsilon)|$ and using (27b) one finds

$$X(\varepsilon)\alpha_s^*(\varepsilon)\sum_p^{\rho}\alpha_p(\varepsilon)C_p(\varepsilon)=(\eta_s(\varepsilon)-\varepsilon)C_s(\varepsilon), \quad s=1,\dots,\rho, \quad \varepsilon\in D. \quad (\text{A.20})$$

where functions $\alpha_s(\varepsilon)$ are given by (29a) while unknown coefficients $C_s(\varepsilon)$ satisfy (28b).

In terms of the characteristic points (section 3.4.2) one finds that the point $\varepsilon = \varepsilon_c$ is critical if and only if $\alpha_s(\varepsilon_c) = 0$ ($s = 1, \dots, \rho$) while the point $\varepsilon = \varepsilon_r$ is resonant ($\varepsilon_r \in \Xi$) if and only if there is at least one function $\eta_s(\varepsilon)$ such that $\eta_s(\varepsilon_r) = \varepsilon_r$. It is convenient to define Ξ_r as the set of all indices s such that $\eta_s(\varepsilon_r) = \varepsilon_r$. Using this definition one finds that resonant point $\varepsilon = \varepsilon_r$ is active if and only if there is at least one function $\alpha_s(\varepsilon)$ ($s \in \Xi_r$) such that $\alpha_s(\varepsilon_r) \neq 0$. Otherwise it is passive.

Let us now analyze expression (A.20) in terms of characteristic points. Consider first the case when $\varepsilon \in D$ is not a resonant point:

(a) *The point $\varepsilon \in D$ is not a resonant point ($\varepsilon \notin \Xi$):*

If $\varepsilon \in D$ is not a resonant point, $\mathbf{H}(\varepsilon)$ is regular and hence $\eta_s(\varepsilon) \neq \varepsilon$ for each $s = 1, \dots, \rho$. One can divide both sides of (A.20) with $(\eta_s(\varepsilon) - \varepsilon)$ ($s = 1, \dots, \rho$) to obtain

$$C_s(\varepsilon) = K(\varepsilon)\frac{\alpha_s^*(\varepsilon)}{\varepsilon - \eta_s(\varepsilon)}, \quad s = 1, \dots, \rho, \quad (\text{A.21a})$$

where

$$K(\varepsilon) = -X(\varepsilon)\sum_p^{\rho}\alpha_p(\varepsilon)C_p(\varepsilon). \quad (\text{A.21b})$$

As shown in section 3.4.3, if ε is not a critical point, trivial solution of a fractional shift equation is not allowed. Hence (A.21a) implies $K(\varepsilon) \neq 0$, since

otherwise $C_s(\varepsilon) = 0$ ($s = 1, \dots, \rho$) which is a trivial solution. Inserting (A.21a) into (A.21b) and canceling out $K(\varepsilon) \neq 0$ one derives (30a). This implies $x(\varepsilon) \neq 0.5$. Further, since $K(\varepsilon) \neq 0$ one can without loss of generality normalize eigenstate $|\psi(\varepsilon)\rangle$ with $K(\varepsilon) = 1$. This implies (30b). Thus if ε is not a critical point, fractional shift equation has a unique solution (30) and fractional shift $x(\varepsilon)$ satisfies $x(\varepsilon) \neq 0.5$.

Consider now a critical point $\varepsilon = \varepsilon_c \notin \Xi$. In a critical point one has $\alpha_s(\varepsilon_c) = 0$ ($s = 1, \dots, \rho$). Hence (A.21a) implies $C_s(\varepsilon) = 0$ ($s = 1, \dots, \rho$). Thus in a critical point only a trivial eigenstate $|\psi(\varepsilon_c)\rangle = 0$ is possible. This also follows from (30b). Concerning the corresponding eigenvalue, this eigenvalue is not fixed by the expression (A.21). However and as explained in section 3.4.3, in a critical point one should have $x(\varepsilon_c) = 0$. Since expression (30a) implies $\lim_{\varepsilon \rightarrow \varepsilon_c} x(\varepsilon) = 0$, the value $x(\varepsilon_c) = 0$ is consistent with the continuity of the function $x(\varepsilon)$ in a critical point.

In conclusion, if $\varepsilon \notin \Xi$ there is a unique fractional shift $x(\varepsilon)$ and (up to the normalization and phase) unique eigenstate $|\psi(\varepsilon)\rangle$ of a fractional shift equation. This eigenstate is trivial in a critical point and nontrivial otherwise. In addition, if $\varepsilon \notin \Xi$ one has $x(\varepsilon) \neq 0.5$. Those conclusions are in accord with a general discussion in section 3.4.3. Expressions (30a) also imply that, provided $\alpha_s(\varepsilon)$ and $\eta_s(\varepsilon)$ ($s = 1, \dots, \rho$) are continuous functions of ε , fractional shift $x(\varepsilon)$ is also continuous function of ε . Thus fractional shift $x(\varepsilon)$, considered as a continuous function of ε , may cross the value $x(\varepsilon) = 0.5$ only in some resonant point $\varepsilon_r \in \Xi$.

Let us clarify implications of the above requirement $K(\varepsilon) \neq 0$ when ε is not a critical point. According to (A.21b), this requirement seems to imply conditions $X(\varepsilon) \neq 0$ and $\sum_p \alpha_p(\varepsilon)C_p(\varepsilon) \neq 0$. According to (30a) and since $\eta_s(\varepsilon) \neq \varepsilon$ ($s = 1, \dots, \rho$), first condition $X(\varepsilon) \neq 0$ is automatically satisfied. However, the second condition is not strictly required. Assume namely $\sum_p \alpha_p(\varepsilon_0)C_p(\varepsilon_0) = 0$ for some $\varepsilon = \varepsilon_0$. Since in a limit $\varepsilon \rightarrow \varepsilon_0$ one has $\sum_p \alpha_p(\varepsilon)C_p(\varepsilon) \rightarrow 0$ and since $K(\varepsilon_0) \neq 0$, in this limit one must have $X(\varepsilon) \rightarrow \infty$ which implies $x(\varepsilon_0) = 0$. The point $\varepsilon = \varepsilon_0$ is hence a singular point. This shows that the solution in the point $\varepsilon_0 \notin \Xi$ is singular if and only if this point satisfies (31). In addition, each critical point $\varepsilon_c \notin \Xi$ satisfies this condition and it is hence also a singular point. This is in accord with a general discussion in section 3.4.3.

(b) *The point $\varepsilon = \varepsilon_r$ is a resonant point ($\varepsilon_r \in \Xi$):*

If $\varepsilon = \varepsilon_r \in D$ is resonant, $\mathbf{H}(\varepsilon_r)$ is singular and hence there is at least one $\eta_s(\varepsilon_r)$ such that $\eta_s(\varepsilon_r) = \varepsilon_r$. The set Ξ_r is hence nonempty. There are two possibilities, the point ε_r is either active or passive.

(b1) *Resonant point $\varepsilon_r \in \Xi$ is active:*

If ε_r is active, there is at least one $s \in \Xi_r$ such that $\alpha_s(\varepsilon_r) \neq 0$. One finds that in this case (A.20) has always a solution that satisfies $X(\varepsilon_r) = 0$. General

type of this solution is:

$$X(\varepsilon_r) = 0, \quad x(\varepsilon_r) = 0.5, \tag{A.22a}$$

$$C_s(\varepsilon_r) = \begin{cases} 0 & \text{if } s \notin \Xi_r, \\ \text{arbitrary} & \text{if } s \in \Xi_r. \end{cases} \tag{A.22b}$$

Above expressions define a family of solutions if ε_r is degenerate and they define a single solution if ε_r is nondegenerate.

In addition, if ε_r is degenerate there is a nontrivial set $\{C_s(\varepsilon_r) : s \in \Xi_r\}$ such that $\sum_s \alpha_s(\varepsilon_r)C_s(\varepsilon_r) = 0$. This follows from the fact that there is at least one $p \in \Xi_r$ such that $\alpha_p(\varepsilon_r) \neq 0$. In this case fractional shift equation has in addition to (A.22) another family of solutions:

$$X(\varepsilon_r) \text{ arbitrary}, \tag{A.23a}$$

$$C_s(\varepsilon_r) = 0 \quad \text{if } s \notin \Xi_r, \quad \sum_{p \in \Xi_r} \alpha_p(\varepsilon_r)C_p(\varepsilon_r) = 0. \tag{A.23b}$$

If ε_r is nondegenerate this family of solutions does not exist. Hence in a nondegenerate active resonant point fractional shift equation has only one solution. One easily finds that such a point is necessarily a proper resonant point. However if the resonant point ε_r is degenerate, there is a nontrivial family of solutions (A.23) in addition to the family of solutions (A.22). In this case there is always a nontrivial state $|\theta\rangle \in X_\rho^a$ such that $\mathbf{H}(\varepsilon_r)|\theta\rangle = \mathbf{f}(\varepsilon_r)|\theta\rangle = 0$. The point ε_r is hence anomal. In conclusion, if a resonant point ε_r is active and nondegenerate, it is a proper resonant point and there is a unique solution (A.22) with a fractional shift $x(\varepsilon_r) = 0.5$. However, if this point is degenerate, it is anomal and there are additional solutions (A.23) with arbitrary fractional shift consistent with the requirement (24).

Consider now the $\varepsilon \rightarrow \varepsilon_r$ limit of the solution (30) where ε_r is active. Let $\varepsilon = \varepsilon_r + h$ where $h \neq 0$ is an infinitesimal quantity. For each $s \in \Xi_r$ one has

$$\varepsilon - \eta_s(\varepsilon) = (1 - \eta'_s(\varepsilon_r))h + O(h^2). \tag{A.24}$$

Expression $\varepsilon - \eta_s(\varepsilon)$ is hence at most of the order $O(h)$. Since ε_r is active, (30a) implies

$$\lim_{\varepsilon \rightarrow \varepsilon_r} X(\varepsilon) = 0, \quad \lim_{\varepsilon \rightarrow \varepsilon_r} x(\varepsilon) = 0.5. \tag{A.25a}$$

In conjuncture with (A.22a) this implies (32a). Concerning corresponding eigenstate (30b), this eigenstate formally diverges in a limit $\varepsilon \rightarrow \varepsilon_r$. However, norm of this eigenstate is of no significance and this eigenstate can be renormalized in such a way as to obtain finite result. If $\eta'_s(\varepsilon_r) \neq 1$ for each $s \in \Xi_r$ and due to (A.24), expression (30b) implies

$$\lim_{\varepsilon \rightarrow \varepsilon_r} h |\psi(\varepsilon)\rangle = \sum_{s \in \Xi_r} \frac{\alpha_s^*(\varepsilon_r)}{1 - \eta'_s(\varepsilon_r)} |\phi_s(\varepsilon_r)\rangle, \quad \varepsilon_r \in D. \tag{A.25b}$$

Slightly more complicated expression is obtained if for some $s \in \Xi_r$ one has $\eta'_s(\varepsilon_r) = 1$.

Solution (A.22) in the active resonant point contains as a special case solution (A.25) that is the $\varepsilon \rightarrow \varepsilon_r$ limit of the solution (30). This proves (32). We call this limit solution a *standard* solution. If the active resonant point ε_r is not degenerate, it is a proper resonant point. In this case standard solution is the only solution in this point. In particular one finds (33).

(b2) *Resonant point $\varepsilon_r \in \Xi$ is passive:*

If ε_r is passive one has $\alpha_s(\varepsilon_r) = 0$ for each $s \in \Xi_r$. This point is hence anomalous. In addition, according to (A.20) in this point all coefficients $C_s(\varepsilon_r)$ ($s \in \Xi_r$) are arbitrary, while coefficients $C_s(\varepsilon_r)$ ($s \notin \Xi_r$) satisfy the condition

$$C_s(\varepsilon_r) = \frac{\alpha_s^*(\varepsilon_r)}{\eta_s(\varepsilon_r) - \varepsilon_r} X(\varepsilon_r) \sum_{p \notin \Xi_r} \alpha_p(\varepsilon_r) C_p(\varepsilon_r), \quad s \notin \Xi_r. \tag{A.26}$$

One family of solutions that satisfies this condition is:

$$X(\varepsilon_r) \text{ arbitrary}, \tag{A.27a}$$

$$C_s(\varepsilon_r) = \begin{cases} \text{arbitrary} & \text{if } s \in \Xi_r, \\ 0 & \text{if } s \notin \Xi_r. \end{cases} \tag{A.27b}$$

This is not a most general solution in a passive resonant point. In particular, in this point one may have some additional solutions that satisfy $C_s(\varepsilon_r) \neq 0$ for at least some $s \notin \Xi_r$. However, solution (A.27) of a fractional shift equation is general enough to demonstrate that in a passive resonant point one should have isolated solution(s) of the combined system.

Consider now the $\varepsilon \rightarrow \varepsilon_r$ limit of the solution (30) where ε_r is passive. Since $\alpha_s(\varepsilon_r) = 0$ and $\eta_s(\varepsilon_r) = \varepsilon_r$ for each $s \in \Xi_r$, one has $\alpha_s(\varepsilon) = O(h)$ and $\alpha_s^*(\varepsilon)\alpha_s(\varepsilon) = O(h^2)$ ($\varepsilon = \varepsilon_r + h$) for each $s \in \Xi_r$. It follows that, unless $\eta'_s(\varepsilon_r) = 1$ for some $s \in \Xi_r$, in a limit $\varepsilon \rightarrow \varepsilon_r$ one has $\alpha_s^*(\varepsilon)\alpha_s(\varepsilon)/(\varepsilon - \eta_s(\varepsilon)) \rightarrow 0$ for each $s \in \Xi_r$. Further, if ε_r is not a critical point there is at least one $s \notin \Xi_r$ such that $\alpha_s(\varepsilon_r) \neq 0$. In this case relation (30a) implies (34a). However, if $\varepsilon_r \equiv \varepsilon_c$ is a critical point one has $\alpha_s(\varepsilon_c) = 0$ for each $s = 1, \dots, \rho$. In this case one finds (34b).

A.4.4. Component $|\Psi^a(\varepsilon)\rangle \in X^a_\rho$ of the eigenstate $|\Psi(\varepsilon)\rangle$

Inserting above expressions for a fractional shift $x(\varepsilon)$ and for the eigenstate $|\psi(\varepsilon)\rangle$ into relation (25a) one obtains the corresponding expression for the component $|\Psi^a(\varepsilon)\rangle$ of the embedded eigenstate $|\Psi(\varepsilon)\rangle$ of the combined system. If $\varepsilon \in D$ is not a resonant point, one has a unique component $|\Psi^a(\varepsilon)\rangle$ of $|\Psi(\varepsilon)\rangle$. However, in a resonant point $\varepsilon = \varepsilon_r$ there is a possibility of the multiple solutions. If this point is nondegenerate and active, i.e. if it is a proper resonant point, fractional shift equation has a unique solution. Otherwise this

point is anomalous and in this case fractional shift equation has multiple solutions. In particular, according to expressions (A.23) and (A.27), if ε_r is degenerate and/or passive, fractional shift $x(\varepsilon_r)$ can assume any value consistent with the requirement (24). Hence one may choose $x(\varepsilon_r)$ such that $\sin(\pi(x(\varepsilon_r))) \neq 0$. At the same time those expressions imply that $|\psi(\varepsilon_r)\rangle$ can be chosen such that $\langle \psi(\varepsilon_r) | \mathbf{f}(\varepsilon_r) | \psi(\varepsilon_r) \rangle \equiv \left| \sum_s \alpha_s(\varepsilon_r) C_s(\varepsilon_r) \right|^2 = 0$. According to (25a) this choice produces divergent solutions for $|\Psi^a(\varepsilon_r)\rangle$. The corresponding density $\rho^a(\varepsilon_r)$ is hence also divergent. Divergence of the component $|\Psi^a(\varepsilon)\rangle$ in an anomalous resonant point indicates existence of isolated eigenstate(s) [8]. In order to treat correctly anomalous points one has to include in the expressions for various quantities such as densities $\rho^a(\varepsilon)$, $\rho_s(\varepsilon)$ and $\rho_s^a(\varepsilon)$ additional δ -like contributions [8].

A.5. Properties of eigenvalue equations (1a), (10) and (27a)

Generalized eigenvalue equations (1a), (10) and (27a) are equivalent to standard eigenvalue equations

$$\mathbf{A}^{(1)} \left| \Theta_s^{(1)} \right\rangle = E_s \left| \Theta_s^{(1)} \right\rangle, \tag{A.28a}$$

$$\left[\beta^2 \boldsymbol{\omega}^{(1)}(\varepsilon_s) + \mathbf{A}^{(1)} \right] \left| \theta_s^{(1)} \right\rangle = \varepsilon_s \left| \theta_s^{(1)} \right\rangle, \tag{A.28b}$$

$$\left[\beta^2 \boldsymbol{\omega}^{(1)}(\varepsilon) + \mathbf{A}^{(1)} \right] \left| \phi_s^{(1)}(\varepsilon) \right\rangle = \eta_s(\varepsilon) \left| \phi_s^{(1)}(\varepsilon) \right\rangle, \quad s = 1, \dots, \rho, \tag{A.28c}$$

where

$$\left| \Theta_s^{(1)} \right\rangle = (\mathbf{S}^a)^{1/2} \left| \Theta_s \right\rangle, \quad \left| \theta_s^{(1)} \right\rangle = (\mathbf{S}^a)^{1/2} \left| \theta_s \right\rangle, \tag{A.29a}$$

$$\left| \phi_s^{(1)}(\varepsilon) \right\rangle = (\mathbf{S}^a)^{1/2} \left| \phi_s(\varepsilon) \right\rangle, \quad \varepsilon \in D, \quad s = 1, \dots, \rho, \tag{A.29b}$$

$$\mathbf{A}^{(1)} = (\mathbf{S}^a)^{-1/2} \mathbf{A} (\mathbf{S}^a)^{-1/2}, \quad \boldsymbol{\omega}^{(1)}(\varepsilon) = (\mathbf{S}^a)^{-1/2} \boldsymbol{\omega}(\varepsilon) (\mathbf{S}^a)^{-1/2} \tag{A.29c}$$

are transformed eigenstates and transformed operators. Since \mathbf{S}^a is positive definite, $(\mathbf{S}^a)^{-1/2}$ is regular. Operators $\mathbf{A}^{(1)}$ and $\boldsymbol{\omega}^{(1)}(\varepsilon)$ are hence Hermitian. This implies that eigenvalues E_s , ε_s and $\eta_s(\varepsilon)$ are real.

Equation (A.28b) is a nonlinear eigenvalue equation since the eigenvalue ε_s is an argument of the operator $\boldsymbol{\omega}^{(1)}(\varepsilon_s)$ on the left-hand side of this equation. The corresponding eigenstates are hence not required to be orthogonal to each other. As a consequence, generic eigenvalue equation (10) may have more than ρ distinct eigenvalues and eigenstates. Unlike equation (A.28b), equations (A.28a) and (A.28c) are linear eigenvalue equations. Hence the transformed eigenstates $\left| \Theta_s^{(1)} \right\rangle$ and $\left| \phi_s^{(1)}(\varepsilon) \right\rangle$ can be orthonormalized in a standard way

$$\left\langle \Theta_s^{(1)} \left| \Theta_p^{(1)} \right\rangle = \delta_{sp}, \quad \left\langle \phi_s^{(1)}(\varepsilon) \left| \phi_p^{(1)}(\varepsilon) \right\rangle = \delta_{sp}, \quad s, p = 1, \dots, \rho. \tag{A.30}$$

This implies (1b) and (27b), respectively. In addition, relations (A.28) and (A.29) imply

$$\mathbf{A}^{(1)} = \sum_p^\rho \left| \Theta_p^{(1)} \right\rangle E_p \left\langle \Theta_p^{(1)} \right|, \tag{A.31a}$$

$$\sum_p^\rho \left| \phi_p(\varepsilon) \right\rangle \left\langle \phi_p(\varepsilon) \right| \mathbf{S}^a = \mathbf{I}^a, \tag{A.31b}$$

where \mathbf{I}^a is a projection operator on the space X_ρ^a .

If the operator $\omega(\varepsilon)$ is bounded in some neighborhood of the point $\varepsilon = E_s$ one can apply perturbation expansion to the expressions (A.28b) and (A.28c). In this case one finds that eigenvalues ε_s as well as eigenvalues $\eta_s(\varepsilon)$ differ from the corresponding local eigenvalue E_s by a small quantity of the order $O(\beta^2)$. In particular, if this local eigenvalue is nondegenerate one finds

$$\varepsilon_s = E_s + \beta^2 \langle \Theta_s | \omega(E_s) | \Theta_s \rangle + O(\beta^4), \tag{A.32a}$$

$$\eta_s(\varepsilon) = E_s + \beta^2 \langle \Theta_s | \omega(\varepsilon) | \Theta_s \rangle + O(\beta^4). \tag{A.32b}$$

One also finds

$$|\theta_s\rangle = |\Theta_s\rangle + O(\beta^2), \quad |\Psi_I\rangle = |\Theta_I\rangle + O(\beta^2), \tag{A.33a}$$

$$|\phi_s(\varepsilon)\rangle = |\theta_s\rangle + O\left(\beta^2(\varepsilon - \varepsilon_s)\right) = |\Theta_s\rangle + O(\beta^2). \tag{A.33b}$$

Consider equation (A.28b) from another point of view. This equation implies $\left\langle \theta_s^{(1)} \right| \beta^2 \omega^{(1)}(\varepsilon_s) + \mathbf{A}^{(1)} - \varepsilon_s \left| \theta_s^{(1)} \right\rangle = 0$. Variation of this expression with the imposed condition $\left\langle \delta \theta_s^{(1)} \right| \theta_s^{(1)} \rangle = 0$ that is required in order to conserve normalization of $\left| \theta_s^{(1)} \right\rangle$ leads to

$$\begin{aligned} & 2\beta \left\langle \theta_s^{(1)} \right| \omega^{(1)}(\varepsilon_s) \left| \theta_s^{(1)} \right\rangle d\beta + \left\langle \theta_s^{(1)} \right| \beta^2 d\omega^{(1)} / d\varepsilon_s - 1 \left| \theta_s^{(1)} \right\rangle d\varepsilon_s \\ & + \left\langle \theta_s^{(1)} \right| d\mathbf{A}^{(1)} \left| \theta_s^{(1)} \right\rangle \equiv 2\beta \langle \theta_s | \omega(\varepsilon_s) | \theta_s \rangle d\beta \\ & + \left\langle \theta_s \right| \beta^2 d\omega / d\varepsilon_s - \mathbf{S}^a | \theta_s \rangle d\varepsilon_s + \left\langle \theta_s^{(1)} \right| d\mathbf{A}^{(1)} \left| \theta_s^{(1)} \right\rangle = 0. \end{aligned} \tag{A.34a}$$

Assume that $d\mathbf{A}^{(1)}$ involves only variations dE_p of local eigenvalues E_p and no variations of $|\Theta_p^{(1)}\rangle$. In this case expression (A.31a) implies

$$\begin{aligned} \langle \theta_s^{(1)} | d\mathbf{A}^{(1)} | \theta_s^{(1)} \rangle &= \sum_p^{\rho} \langle \theta_s^{(1)} | \Theta_p^{(1)} \rangle dE_p \langle \Theta_p^{(1)} | \theta_s^{(1)} \rangle \\ &= \sum_p^{\rho} \langle \theta_s | \mathbf{S}^a | \Theta_p \rangle \langle \Theta_p | \mathbf{S}^a | \theta_s \rangle dE_p. \end{aligned} \quad (\text{A.34b})$$

From the expressions (A.34) one now derives

$$\frac{\partial \varepsilon_s}{\partial \beta} = \frac{2\beta \langle \theta_s | \boldsymbol{\omega}(\varepsilon_s) | \theta_s \rangle}{\langle \theta_s | \mathbf{S}^a | \theta_s \rangle - \beta^2 \langle \theta_s | d\boldsymbol{\omega}/d\varepsilon_s | \theta_s \rangle}, \quad (\text{A.35a})$$

$$\frac{\partial \varepsilon_s}{\partial E_p} = \frac{\langle \theta_s | \mathbf{S}^a | \Theta_p \rangle \langle \Theta_p | \mathbf{S}^a | \theta_s \rangle}{\langle \theta_s | \mathbf{S}^a | \theta_s \rangle - \beta^2 \langle \theta_s | d\boldsymbol{\omega}/d\varepsilon_s | \theta_s \rangle}. \quad (\text{A.35b})$$

Those relations give the rate of change of the eigenvalues ε_s with a change of the coupling β and with a change of local eigenvalues E_p . In the case $\varepsilon_s \equiv \varepsilon_I \in \bar{D}$ relations (A.35) reduce to expressions (19). In the case $\varepsilon_s \equiv \varepsilon_r \in D$ those relations imply similar expressions involving resonant points $\varepsilon_r \in D$.

In a similar way eigenvalue equation (A.28c) implies

$$\frac{\partial \eta_s}{\partial \varepsilon} = \beta^2 \langle \phi_s(\varepsilon) | d\boldsymbol{\omega}(\varepsilon)/d\varepsilon | \phi_s(\varepsilon) \rangle, \quad (\text{A.36a})$$

$$\frac{\partial \eta_s}{\partial \beta} = 2\beta \langle \phi_s(\varepsilon) | \boldsymbol{\omega}(\varepsilon) | \phi_s(\varepsilon) \rangle. \quad (\text{A.36b})$$

where $|\phi_s(\varepsilon)\rangle$ are orthonormalized according to (27b). Further, if $\eta_s(\varepsilon)$ and $\alpha_s(\varepsilon)$ ($s \in \Xi_r$) are reasonably smooth in the resonant point $\varepsilon = \varepsilon_r$ one can expand those functions in this point to obtain

$$\varepsilon - \eta_s(\varepsilon) = (1 - \eta'_s(\varepsilon_r)) (\varepsilon - \varepsilon_r) [1 + O(\varepsilon - \varepsilon_r)], \quad (\text{A.37a})$$

$$\alpha_s(\varepsilon) = \alpha_s(\varepsilon_r) + O(\varepsilon - \varepsilon_r), \quad (\text{A.37b})$$

$$F_{ss}(\varepsilon) = F_{ss}(\varepsilon_r) + O(\varepsilon - \varepsilon_r), \quad (\text{A.37c})$$

where $O(x)$ is a small quantity of the order x . Since $F_{ss}(\varepsilon) \geq 0$ for each $\varepsilon \in D$, close to a passive resonant point $\varepsilon = \varepsilon_r$ expression (A.37c) should be replaced with stronger requirement

$$F_{ss}(\varepsilon) = O((\varepsilon - \varepsilon_r)^2), \quad s \in \Xi_r. \quad (\text{A.37d})$$

A.6. Weak coupling limit

Consider component $|\Psi^a(\varepsilon)\rangle \in X_\rho^a$ of the embedded eigenstate $|\Psi(\varepsilon)\rangle$ (equation (35)) in the case of small β . Assume first that $\omega(\varepsilon)$ is bounded in D . According to (35) component $|\Psi^a(\varepsilon)\rangle$ is a linear combination of ρ states $|\Psi_s^a(\varepsilon)\rangle \in X_\rho^a$. Since $\omega(\varepsilon)$ is bounded in D there is $K < \infty$ such that $|\omega(\varepsilon)^{(1)}| < K$ for each $\varepsilon \in D$. Hence expression (A.28c) implies that in a limit $\beta \rightarrow 0$ each eigenvalue $\eta_s(\varepsilon)$ of (27a) converges to some local eigenvalue E_r . If E_r is κ_r -degenerate there are κ_r functions $\eta_s(\varepsilon)$ that in this limit converge to E_r . Define Z_r such that $s \in Z_r$ if $\eta_s(0) = E_r$ and $s \notin Z_r$ if $\eta_s(0) \neq E_r$. If $s \in Z_r$ one has $|\eta_s(\varepsilon) - E_r| < \beta^2 K$ for each $\varepsilon \in D$. However, if $s \notin Z_r$ there is $M > 0$ such that $|\eta_s(\varepsilon) - E_r| > M$ for each $\varepsilon \in D$. In a similar way one can associate eigenvalue $\eta_s(\varepsilon)$ of (27a) with eigenvalue ε_s of a generic eigenvalue equation (10). One thus finds

$$|\eta_s(\varepsilon) - \varepsilon_s| < \beta^2 L, \quad \varepsilon \in D, \tag{A.38}$$

where $L < \infty$ is some finite constant that does not depend on ε . Hence, provide β is sufficiently small, one has $\eta_s(\varepsilon) = \varepsilon_s + O(\beta^2) \approx \varepsilon_s$ for each $\varepsilon \in D$. Inserting into (35b) one finds that for sufficiently small β the state $|\Psi_s^a(\varepsilon)\rangle$ ($s \in Z_r$) is mainly concentrated in some neighborhood of $\varepsilon_s \approx E_r$ and the norm of this state becomes negligible if $|\varepsilon - \varepsilon_s|$ is large. According to (36a) if $\varepsilon_s \approx E_r$ ($s \in Z_r$) is active the state $|\Psi_s^a(\varepsilon_r)\rangle$ is of the order $O(\beta^{-1})$. However, according to (35b) if $\varepsilon \neq \varepsilon_s \approx E_r$ the state $|\Psi_s^a(\varepsilon)\rangle$ is of the order $O(\beta)$. Hence for sufficiently small β this state must be concentrated in some small neighborhood of E_r . Since $|\Psi_s^a(\varepsilon)\rangle = 0$ if $\varepsilon \notin D$, this implies that each state $|\Psi_s^a(\varepsilon)\rangle$ that is associated with eigenvalue $\varepsilon_s \notin D$ can be neglected if β is sufficiently small. In other words, $|\Psi_s^a(\varepsilon)\rangle \approx 0$ if $s \in Z_r$ and if $E_r \in \bar{D}$. Further and due to (A.37) and (A.38), in the expression (35b) one can substitute $\varepsilon - \eta_s(\varepsilon) \approx (\varepsilon - \varepsilon_r)$, $F_{ss}(\varepsilon) \approx F_{ss}(\varepsilon_r)$ and $\alpha_s(\varepsilon) \approx \alpha_s(\varepsilon_r)$ for each $s \in Z_r$. However, if $s \notin Z_r$ the corresponding terms in the denominator of (35b) can be neglected. Hence one derives expression (42a).

Above we have assumed that $\omega(\varepsilon)$ is bounded in D . However, operator $\omega(\varepsilon)$ may diverge in some point $e_d \in \Lambda$. If $\omega(\varepsilon)$ diverges in a point $\varepsilon = E_r$ expression (42a) fails. However, if $\omega(\varepsilon)$ does not diverges in this point expression (42a) is still mainly correct. In this case estimate (A.38) applies to each $\varepsilon \in D$, except to those values of ε that are contained in some small neighborhood of each point $e_d \in \Lambda$ where $\omega(\varepsilon)$ diverges. Accordingly, expression (42a) applies to each $\varepsilon \in D$, except of those values of ε that are in the immediate vicinity of some point $e_d \in \Lambda$ where $\omega(\varepsilon)$ is singular. Instead of to have some special treatment for each ε that is close to some point $e_d \in \Lambda$, it is more convenient to consider expressions (42a) correct for each $\varepsilon \in D$ and to incorporate all deviations in some additional functions $|\Psi_d^a(\varepsilon)\rangle$. Each function $|\Psi_d^a(\varepsilon)\rangle$ is associated with a resonant point $\varepsilon_d \equiv \varepsilon_d(\varepsilon)$ that satisfies $\varepsilon_d(0) = e_d \in \Lambda$ and it is concentrated mainly

in the immediate vicinity of the point $e_d \in \Lambda$. According to this point of view we associate each function $|\Psi_s^a(\varepsilon)\rangle$ with some resonant point $\varepsilon_s(\beta)$ instead of with a local eigenvalue E_r . One finds that if $\varepsilon_s(0) = E_r \notin \Lambda$ the corresponding state $|\Psi_s^a(\varepsilon)\rangle$ is given by (35b). However, if $\varepsilon_s(0) \in \Lambda$ the corresponding state $|\Psi_s^a(\varepsilon)\rangle$ is given by a completely different expression [8]. In particular, if $\varepsilon_s(0) \in \Lambda$ and if at the same time $\varepsilon_s(0) \notin \{E_p\}$ one derives expression (47) [8].

A.7. The state $|\Psi_s^a(\varepsilon)\rangle$ close to a resonant point $\varepsilon = \varepsilon_r$

In a previous section the case of small β was considered. Assume now that β is not small and consider the state $|\Psi_s^a(\varepsilon)\rangle$ in some small neighborhood Δ of the resonant point $\varepsilon = \varepsilon_r$. Let ε_r be a κ_r -degenerate resonant point. Consider the state (35b) in the immediate vicinity of this point. There are κ_r functions $\eta_s(\varepsilon)$ ($s \in \Xi_r$) that satisfy $\eta_s(\varepsilon_r) = \varepsilon_r$. Using expansion (A.37) one finds

$$|\Psi_s^a(\varepsilon)\rangle \approx \frac{\beta}{\sqrt{(\varepsilon - \varepsilon_r)^2 + \pi^2 \beta^4 \left(\sum_{p \in \Xi_r} \frac{F_{pp}(\varepsilon_r)}{1 - \eta'_p(\varepsilon_r)} \right)^2}} \frac{\alpha_s^*(\varepsilon_r)}{\varepsilon - \eta'_s(\varepsilon_r)} |\phi_s(\varepsilon)\rangle, \quad s \in \Xi_r. \quad (\text{A.39})$$

On the other hand, if $s \notin \Xi_r$ expression (35b) implies $|\Psi_s^a(\varepsilon_r)\rangle = 0$. Hence (49a) where $|\Psi_{(r)}^a(\varepsilon)\rangle$ is a sum of all κ_r states $|\Psi_s^a(\varepsilon)\rangle$ that are associated with a resonant point ε_r .

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