Interaction of a single state with a known infinite system containing one-parameter eigenvalue band

Tomislav P. Živković

Ruđer Bošković Institute, P.O.B. 180, HR-10002 Zagreb, Croatia
E-mail: zivkovic@rudjer.irb.hr

Interaction of a quantum system $\mathcal{S}_1^a$ containing a single state $|\Theta\rangle$ with a known infinite-dimensional quantum system $\mathcal{S}_\infty^b$ containing an eigenvalue band $[\lambda_a, \lambda_b]$ is considered. A new approach for the treatment of the combined system $\mathcal{S}_\infty = \mathcal{S}_1^a \oplus \mathcal{S}_\infty^b$ is developed. This system contains embedded eigenstates $|\Psi(\varepsilon)\rangle$ with continuous eigenvalues $\varepsilon \in [\lambda_a, \lambda_b]$, and, in addition, it may contain isolated eigenstates $|\Psi_I\rangle$ with discrete eigenvalues $\varepsilon_I \notin [\lambda_a, \lambda_b]$. Exact expressions for the solution of the combined system are derived. In particular, due to the interaction with the system $\mathcal{S}_\infty^b$, eigenvalue E of the state $|\Theta\rangle$ shifts and, in addition, if $E \in [\lambda_a, \lambda_b]$ this shifted eigenvalue broadens. Exact expressions for the eigenvalue shift and for the eigenvalue distribution of the state $|\Theta\rangle$ are derived. In the case of the weak coupling this eigenvalue distribution reduces to the standard resonance curve. Also, exact expressions for the time evolution of the state $|\Theta(t)\rangle$ that is initially prepared in the state $|\Theta(0)\rangle \equiv |\Theta\rangle$ are obtained. Here again in the case of the weak coupling this time evolution reduces to the familiar exponential decay. The suggested method is exact and it applies to each coupling of the system $\mathcal{S}_1^a$ with the system $\mathcal{S}_\infty^b$, however strong. It also presents a relatively good approximation for the interaction of a nondegenerate eigenstate $|\Theta_s\rangle$ of an arbitrary system $\mathcal{S}^a$ with an infinite system $\mathcal{S}_\infty^b$ containing a single eigenvalue band, provided this eigenstate is relatively well separated from other eigenstates of $\mathcal{S}^a$ and provided the interaction between the systems $\mathcal{S}^a$ and $\mathcal{S}_\infty^b$ is not excessively strong.

1.   Introduction

The aim of this paper is to initiate the development of a general mathematical formalism for the treatment of the interaction of a finite quantum system $\mathcal{S}_\rho^a$ with an infinite quantum system $\mathcal{S}_\infty^b$. System $\mathcal{S}_\rho^a$ contains ρ discrete eigenvalues and eigenstates, while $\mathcal{S}_\infty^b$ is an arbitrary quantum system that, in addition to possible discrete eigenvalues and eigenstates, may contain one or more eigenvalue bands. We assume that the solution of the system $\mathcal{S}_\infty^b$ is known, and we concentrate on the following problem: What is the solution of a system $\mathcal{S}_\rho^a$ subject to the interaction with the system $\mathcal{S}_\infty^b$?

There are numerous problems in physics and chemistry of this type. For example, consider the interaction of an atom or a molecule with the electromagnetic field. This atom or molecule can be approximated with a system $\mathcal{S}_\rho^a$ containing finite number of discrete eigenvalues E_s and the corresponding 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 $|\Theta_p, \mathbf{k}\varpi, \mathbf{k}'\varpi'\rangle$, which in turn interact with three-photon states, etc. [1]. To a very good approximation one can ignore all states containing multiple photons, and one can associate system $\mathcal{S}_\infty^b$ 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 $|\Theta_s\rangle$ are eigenstates of the isolated molecule which are assumed to be known (at least to the very good approximation). Hence one has formally the problem of the interaction of a finite system $\mathcal{S}_\rho^a$ with the known infinite system $\mathcal{S}_\infty^b$. As another example consider the interaction of the molecule with a surface of a solid. Molecule in isolation can be again approximated with some finite-dimensional system $\mathcal{S}_\rho^a$. System $\mathcal{S}_\infty^b$ represents a solid with a surface. The solution to this system usually consists of multiple eigenvalue bands $\lambda_s(\mathbf{k})$ ($s = 1, 2, \ldots$) [2]. In addition, system $\mathcal{S}_\infty^b$ may also contain some discrete eigenvalues corresponding to the possible surface states [3]. One would like to derive properties of the molecule (system $\mathcal{S}_\rho^a$) subject to the interaction with a solid (system $\mathcal{S}_\infty^b$). Again one can assumes that the solution to the system $\mathcal{S}_\infty^b$ is known. Usually one knows only an approximate solution of this system [2]. Nevertheless, assuming this approximate solution to be good enough, the problem is to find a solution of the combined system $\mathcal{S}_\infty \equiv \mathcal{S}_\rho^a \oplus \mathcal{S}_\infty^b$ with emphasize on the subsystem $\mathcal{S}_\rho^a$.

In this and similar cases one has formally identical situation. There is a system $\mathcal{S}_\rho^a$ that contains finite number of discrete eigenvalues E_s. With this system is associated a ρ-dimensional space X_ρ^a. Corresponding eigenstates $|\Theta_s\rangle \in X_\rho^a$ are localized, and they can be normalized to unity. There is another system $\mathcal{S}_\infty^b$ that contains an infinite number of eigenvalues and eigenstates. In addition to possible discrete eigenvalues, system $\mathcal{S}_\infty^b$ contains one or more eigenvalue bands $\lambda_s(\mathbf{k})$. With this system is associated an infinite-dimensional space X_∞^b orthogonal to the space X_ρ^a. Corresponding eigenstates $|\Phi_s(\mathbf{k})\rangle \in X_\infty^b$ can be orthonormalized to a δ-function. Functions $\lambda_s(\mathbf{k})$ and the eigenstates $|\Phi_s(\mathbf{k})\rangle$ are known, or if not exactly known, one can at least obtain a relatively reliable approximation to those quantities. Also, if there are any discrete eigenvalues of the system $\mathcal{S}_\infty^b$, those eigenvalues and the corresponding eigenstates are also known. Our ultimate goal is to describe properties of an arbitrary system $\mathcal{S}_\rho^a$ that interacts with an arbitrary system $\mathcal{S}_\infty^b$.

Standard way how one treats such problems is to use perturbation expansion [1]. Since the system $\mathcal{S}_\infty^b$ is infinite, this is usually the only method available. In particular, the only systematical method for the treatment of the interaction of a molecule with radiation is presently perturbation expansion. No other sufficiently exact and sufficiently general method is known. Though perturbation expansion is a very powerful and very general approach, in the case of strong coupling it suffers from a serious drawback of slow convergence. If the coupling is sufficiently strong, perturbation series may even diverge and the entire method fails.

We will present here a new method for the solution of such problems. This method provides exact expressions for the eigenvalues and the corresponding eigenstates of the

combined system $\mathcal{S}_\infty$. No power series expansion in terms of the coupling parameter is involved, and the results obtained are valid for each coupling. From a numerical point of view this is particularly important if the coupling between systems $\mathcal{S}_\rho^a$ and $\mathcal{S}_\infty^b$ is strong or if highly precise solution to the system $\mathcal{S}_\infty$ is required. In addition to this computational benefit, it is always advantageous to find new ways how to formulate and solve old problems. New formulations and new solutions of old problems usually carry a potential to open some previously unknown ways of looking at those problems, and they may provide some novel conceptual insights that could not be obtained otherwise.

2.   Formulation of a problem

In order to consider above problem in the most general form, one has first to solve mathematically simpler problem. The solution of this simpler problem is then used as a building block to obtain a general solution [4]. Accordingly, in the present paper we make two restrictions. First, we assume that the system $\mathcal{S}_\rho^a$ is one-dimensional ($\rho = 1$). In this case the space X_1^a that is associated with this system contains a single state $|\Theta\rangle$ with the eigenvalue E. Corresponding eigenvalue equation is

$$\mathbf{A}|\Theta\rangle = E|\Theta\rangle, \quad \langle\Theta|\Theta\rangle = 1, \tag{1}$$

where $\mathbf{A} = E|\Theta\rangle\langle\Theta|$ is a Hermitian operator and where $|\Theta\rangle$ is normalized to unity. We refer to the state $|\Theta\rangle$ as a local state.

Second, we assume that the system $\mathcal{S}_\infty^b$ contains only a single one-parameter eigenvalue band and no discrete eigenvalues. Corresponding eigenvalue equation is

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

where $\mathbf{B}$ is a Hermitian operator. The function $\lambda(k)$ is a continuous nondecreasing function of a parameter k. All eigenvalues of a system $\mathcal{S}_\infty^b$ are confined to the interval $[\lambda_a, \lambda_b]$, where $\lambda_a = \lambda(k_a)$ is the smallest possible eigenvalue, while $\lambda_b = \lambda(k_b)$ is the largest possible eigenvalue. Since the eigenvalue band depends only on a single parameter, eigenstates $|\Phi(k)\rangle \in X_\infty^b$ are nondegenerate. Those eigenstates can be orthonormalized to a δ-function according to

$$\big\langle\Phi(k)\big|\Phi\big(k'\big)\big\rangle = \delta\big(k - k'\big). \tag{2b}$$

Relations (1) and (2) describe systems $\mathcal{S}_1^a$ and $\mathcal{S}_\infty^b$ in isolation, that is without mutual interaction. An arbitrary interaction can be written in the form $\beta\mathbf{V}$ where $\mathbf{V}$ is a Hermitian operator that has nonvanishing matrix elements only between a state $|\Theta\rangle \in X_1^a$ and states $|\Phi(k)\rangle \in X_\infty^b$, and where β is a coupling parameter. Without loss of generality one can assume $\mathbf{V} \neq 0$ and $\beta \geqslant 0$. The eigenvalue equation describing combined system $\mathcal{S}_\infty \equiv \mathcal{S}_1^a \oplus \mathcal{S}_\infty^b$ subject to the interaction $\beta\mathbf{V}$ is

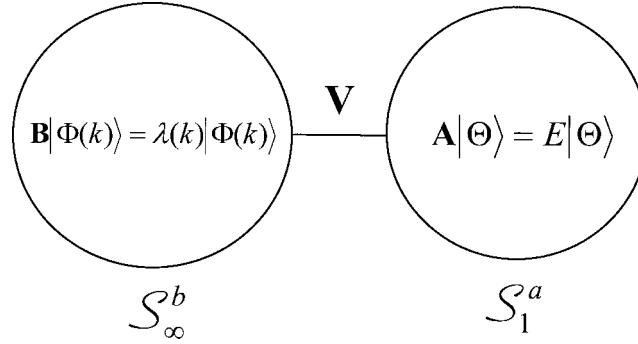$$\mathbf{H}|\Psi\rangle = \varepsilon|\Psi\rangle, \tag{3a}$$

Figure 1. Interaction of the one-dimensional system $\mathcal{S}_1^a$ with infinite-dimensional system $\mathcal{S}_\infty^b$. System $\mathcal{S}_1^a$ is described by a single eigenstate $|\Theta\rangle$ with the eigenvalue E. System $\mathcal{S}_\infty^b$ is described by the eigenvalue equation (2). Combined system $\mathcal{S}_\infty$ is described by the eigenvalue equation (3).

where

$$\mathbf{H} = \mathbf{A} + \mathbf{B} + \beta\mathbf{V}. \tag{3b}$$

We emphasize that β is not an expansion parameter. Unlike the standard perturbation approach where various results are usually expressed as a power series expansion in terms of β, we will obtain all results in a closed form. Therefore one could simply in all relations replace $\beta\mathbf{V}$ with $\mathbf{V}$. Nevertheless, it is convenient to write the interaction in the form $\beta\mathbf{V}$. In this way the dependence on the coupling strength is made explicit. Various effects can be thus directly analyzed in terms of a coupling between systems $\mathcal{S}_1^a$ and $\mathcal{S}_\infty^b$ (see figure 1).

Our aim is to solve the combined eigenvalue equation (3a) given the solution of the eigenvalue equation (2a). Accordingly, we will consider system $\mathcal{S}_\infty^b$ as the original unperturbed system. From this point of view, relation (3a) is a perturbed eigenvalue equation where the perturbation is represented by the interaction $\beta\mathbf{V}$ and by the operator $\mathbf{A}$ that describes the system $\mathcal{S}_1^a$. In a standard formulation of the perturbation approach, one usually considers union of systems $\mathcal{S}_1^a$ and $\mathcal{S}_\infty^b$ without mutual interaction as the unperturbed system. Moreover, in this standard approach emphasize is on the state $|\Theta\rangle \in X_1^a$ as the original unperturbed state and one usually does not consider the effect of the perturbation on the states $|\Phi(k)\rangle \in X_\infty^b$.

As already emphasized, we will solve above problem in a novel way that does not rely on the power expansion characteristic to the standard perturbation method. In the first part of the paper the solution of the eigenvalue equation (3a) will be considered. After this is done, we will generalize the obtained results to the corresponding time-dependent eigenvalue equation. In addition, we will briefly consider the solution to a more general generalized eigenvalue equation.

Though we have assumed that the system $\mathcal{S}_1^a$ is one-dimensional, the results obtained can be also applied to multi-dimensional system $\mathcal{S}_\rho^a$ in the interaction with a system $\mathcal{S}_\infty^b$. If $|\Theta_s\rangle$ is a nondegenerate eigenstate of $\mathcal{S}_\rho^a$ it interacts with other eigenstates of $\mathcal{S}_\rho^a$ only indirectly through the intermediate interaction with $\mathcal{S}_\infty^b$. If the corresponding

eigenvalue E_s is relatively well separated from other eigenvalues of $\mathcal{S}_\rho^a$ and if the interaction between $\mathcal{S}_\rho^a$ and $\mathcal{S}_\infty^b$ is not excessively strong, one can neglect all other eigenstates of $\mathcal{S}_\rho^a$. Thus to a very good approximation one has the interaction of the one-dimensional system $\mathcal{S}_1^a$ containing a single eigenstate $|\Theta_s\rangle \equiv |\Theta\rangle$ with the system $\mathcal{S}_\infty^b$. The results obtained in this paper apply to such cases as well. In addition, one can completely relax this restriction to the one-dimensional space $\mathcal{S}_1^a$ as well as another restriction to the space $\mathcal{S}_\infty^b$ containing only a single one-parameter eigenvalue band [4]. Accordingly, all results presented in this paper can be generalized to the interaction of an arbitrary finite-dimensional system $\mathcal{S}_\rho^a$ with an arbitrary infinite-dimensional system $\mathcal{S}_\infty^b$ [4].

3. Interaction of the one-dimensional system with the known finite-dimensional system

In order to solve eigenvalue equation (3a) we will utilize the known solution of the similar eigenvalue equation that instead of the infinite-dimensional system $\mathcal{S}_\infty^b$ involves a finite-dimensional system $\mathcal{S}_n^b$. The solution of the eigenvalue equation that describes combined system $\mathcal{S}_{n+1} \equiv \mathcal{S}_1^a \oplus \mathcal{S}_n^b$ can be obtained in a closed form [5]. Our general strategy is to derive an appropriate limit $n \to \infty$.

For the sake of additional flexibility, we will describe n-dimensional system $\mathcal{S}_n^b$ with a generalized eigenvalue equation

$$\mathbf{B}|\Phi_i\rangle = \lambda_i \mathbf{S}^b|\Phi_i\rangle, \quad i = 1, \ldots, n. \tag{4a}$$

The eigenstates $|\Phi_i\rangle$ of this system can be orthonormalized according to

$$\langle\Phi_i|\mathbf{S}^b|\Phi_j\rangle = \delta_{ij}. \tag{4b}$$

In the above relations $\mathbf{B}$ and $\mathbf{S}^b$ are Hermitian operators acting in the space X_n^b. In addition, operator $\mathbf{S}^b$ is positive definite. No other assumption about those operators is made. Hermiticity of these operators and positive definiteness of $\mathbf{S}^b$ ensures that the eigenvalues λ_i are real.

The interaction between systems $\mathcal{S}_1^a$ and $\mathcal{S}_n^b$ is introduced by the Hermitian operators $\beta\mathbf{V}$ and $\beta\mathbf{P}$, and the eigenvalue equation describing the combined system $\mathcal{S}_{n+1}$ subject to the interaction $(\beta\mathbf{V}, \beta\mathbf{P})$ is

$$\mathbf{H}|\Psi_r\rangle = \varepsilon_r \mathbf{S}|\Psi_r\rangle, \quad r = 1, \ldots, n+1, \tag{5a}$$

where

$$\mathbf{H} = \mathbf{A} + \mathbf{B} + \beta\mathbf{V}, \qquad \mathbf{S} = |\Theta\rangle\langle\Theta| + \mathbf{S}^b + \beta\mathbf{P}. \tag{5b}$$

In order to guarantee the reality of the eigenvalues ε_r operator $\mathbf{S}$ is required to be positive definite. One finds that $\mathbf{S}$ is positive definite if and only if operator $\mathbf{P}$ satisfies [5]

$$\beta^2 \sum_i^n \langle\Theta|\mathbf{P}|\Phi_i\rangle\langle\Phi_i|\mathbf{P}|\Theta\rangle < 1. \tag{6}$$

There is no condition on the operator $\mathbf{V}$, except that this operator should be Hermitian and that it should connect the state $|\Theta\rangle \in X_1^a$ with the states $|\Phi_i\rangle \in X_n^b$.

In analogy to (4b) eigenstates $|\Psi_r\rangle$ can be orthonormalized according to

$$\langle\Psi_r|\mathbf{S}|\Psi_p\rangle = \delta_{rp}. \tag{5c}$$

It is convenient to distinguish *cardinal* and *singular* eigenvalues and eigenstates of the combined system [5]. By definition, an eigenvalue ε_r of (5a) is cardinal if it differs from all the eigenvalues λ_i of (4a), otherwise it is singular [5]. In other words, each cardinal eigenvalue ε_r satisfies $\varepsilon_r \notin \{\lambda_i\}$, where $\{\lambda_i\}$ is the set of all the eigenvalues of the system $\mathcal{S}_n^b$. Cardinal solutions are by far the most important. Singular solutions usually result as a consequence of some symmetry or as a consequence of some other special condition.

Concerning cardinal solutions one finds [5]: $\varepsilon_r \notin \{\lambda_i\}$ is an eigenvalue of the perturbed eigenvalue equation (5) if and only if it is a root of the function $h(\varepsilon)$:

$$h(\varepsilon) \equiv \beta^2\Omega(\varepsilon) + E - \varepsilon = 0, \tag{7a}$$

where

$$\Omega(\varepsilon) = \sum_i^n \frac{\langle\Theta|\mathbf{V} - \varepsilon\mathbf{P}|\Phi_i\rangle\langle\Phi_i|\mathbf{V} - \varepsilon\mathbf{P}|\Theta\rangle}{\varepsilon - \lambda_i}. \tag{7b}$$

Once a particular perturbed eigenvalue ε_r is found as a root of $h(\varepsilon) = 0$, the corresponding normalized eigenstate is [5]

$$|\Psi_r\rangle = \frac{1}{Q_r^{1/2}}\left[|\Theta\rangle + \beta\sum_i^n \frac{\langle\Phi_i|\mathbf{V} - \varepsilon_r\mathbf{P}|\Theta\rangle}{\varepsilon_r - \lambda_i}|\Phi_i\rangle\right], \tag{8a}$$

where

$$Q_r = 1 + \beta^2\sum_i^n \frac{|\langle\Phi_i|\mathbf{V} - \lambda_i\mathbf{P}|\Theta\rangle|^2}{(\varepsilon_r - \lambda_i)^2} - \beta^2\sum_i^n \left|\langle\Theta|\mathbf{P}|\Phi_i\rangle\right|^2. \tag{8b}$$

There is only one eigenvector $|\Psi_r\rangle$ associated with each eigenvalue $\varepsilon_r \notin \{\lambda_i\}$, i.e., each cardinal eigenvalue is nondegenerate. Similar expressions are obtained for singular solutions of the perturbed eigenvalue equation. However, singular eigenvalues may be degenerate [5].

Relations (4a) and (5a) are generalized eigenvalue equations where $\mathbf{S}^b$ is an arbitrary positive definite operator in X_n^b and where $\mathbf{P}$ is an arbitrary Hermitian operator that connects X_1^a with X_n^b and that satisfies condition (6). Most important is the case $\mathbf{P} = 0$ and $\mathbf{S}^b = \mathbf{I}^b$ where $\mathbf{I}^b$ is the projection operator on the space X_n^b. In this case eigenvalue equations (4a) and (5a) reduce to simple eigenvalue equations. The solution (7) and (8) of the eigenvalue equation (5a) accordingly simplifies. We will mainly consider only this case since it corresponds to the eigenvalue equations (2a) and (3a) of our problem. There are, however, some more general problems that require either $\mathbf{S}^b \neq \mathbf{I}^b$ and/or $\mathbf{P} \neq 0$. In

order to be able to treat such more general problems, we need a general solution (7) and (8).

In addition to the explicit expressions (7) and (8) that provide all cardinal solutions to the perturbed eigenvalue equation (5a), we also need interlacing rule according to which perturbed eigenvalues ε_r are interlaced with the unperturbed eigenvalues λ_i:

- Arrange the perturbed eigenvalues ε_r as well as unperturbed eigenvalues λ_i in the nondecreasing order. Perturbed and unperturbed eigenvalues thus arranged satisfy the interlacing rule [5]

$$\varepsilon_1 \leqslant \lambda_1 \leqslant \varepsilon_2 \leqslant \lambda_2 \leqslant \cdots \leqslant \lambda_n \leqslant \varepsilon_{n+1}. \tag{9}$$

Interlacing rule applies to many similar problems where the original system $\mathcal{S}_n^b$ is perturbed by a finite rank perturbation. Thus one may consider molecular vibrations in the harmonic approximation. One finds that in this approximation vibrational frequencies of two molecules that differ from each other by an isotopic substitution are interlaced according to this rule and its simple generalization [6].

The main idea in solving eigenvalue equation (3a) that describes combined system $\mathcal{S}_\infty$ is to approximate infinite-dimensional system $\mathcal{S}_\infty^b$ with an n-dimensional system $\mathcal{S}_n^b$. This is done by replacing infinite-dimensional space X_∞^b with an n-dimensional subspace X_n^b. Cardinal eigenvalues and eigenstates of the corresponding combined system $\mathcal{S}_{n+1} \equiv \mathcal{S}_1^a \oplus \mathcal{S}_n^b$ are given by relations (7) and (8). Taking an appropriate limit $n \to \infty$ one can obtain the required solution to the system $\mathcal{S}_\infty$.

It is important to note that the limit $n \to \infty$ can be taken in such a way that in each step (i.e., in the case of each n involved) one can avoid singular solutions. Namely, if the eigenvalue equation (5a) has some singular solutions, there is always an infinitesimal variation of the matrix elements of the operators $\mathbf{B}$ and $\mathbf{V}$ such that the resulting eigenvalue equation has no singular solutions. This follows from the fact that each eigenvalue λ_i of the unperturbed eigenvalue equation (4a) is a continuous function of the matrix elements of the matrix $\mathbf{B}$, while each eigenvalue ε_r of a perturbed eigenvalue equation (5a) is a continuous function of the matrix elements of matrices $\mathbf{B}$ and $\mathbf{V}$. Thus for each finite n all singular solutions can be eliminated with an arbitrarily small variation of matrices involved. However, if two eigenvalue equations refer to the same finite-dimensional space, and if the respective matrices differ from each other by an arbitrary small amount, then those two equations describe two physical systems that also differ from each other by an arbitrary small amount. Moreover, we consider the case where in a limit $n \to \infty$ unperturbed eigenvalues λ_i form an eigenvalue band. If n is big enough those eigenvalues become very close to each other. An infinitesimal variation of those eigenvalues does not change a physical content of the corresponding system. Therefore, one can safely assume that for each finite n one can approximate eigenvalue equation (3a) with an eigenvalue equation of a type (5a) that contains no singular solutions. Expressions (7) and (8) are hence sufficient in order to obtain a correct transition $n \to \infty$. However, though each $(n + 1)$-dimensional system $\mathcal{S}_{n+1}$ that approximates infinite-dimensional system $\mathcal{S}_\infty$ contains only cardinal solutions, as a limit of a process

$n \to \infty$ one obtains all solutions of a system $\mathcal{S}_\infty$. This property is analogous to the well-known fact that an infinite sequence of rational numbers may converge to any real number, rational or irrational.

4. Isolated and embedded solutions of the combined system

Consider now eigenvalue equation (3a). In order to approximate system $\mathcal{S}_\infty^b$ with a finite-dimensional system $\mathcal{S}_n^b$ containing n eigenvalues, we partition the interval $[k_a, k_b]$ into n equal subintervals. In a midpoint of each of these subintervals we take a value of the function $\lambda(k)$. In this way a continuous function $\lambda(k)$ is replaced by n eigenvalues λ_i. Similarly, matrix elements $\langle\Theta|\mathbf{V}|\Phi(k)\rangle$ that depend on the continuous parameter k are replaced by n matrix elements $\langle\Theta|\mathbf{V}|\Phi_i\rangle$. This corresponds to the replacement of the infinite-dimensional system that contains eigenvalue band with a finite-dimensional system that can be solved by relations (7) and (8). As n increases solution (7) and (8) of the approximate finite-dimensional system improves, and in a limit $n \to \infty$ it converges to the solution of (3a).

As a consequence of the interlacing rule, in a limit $n \to \infty$ one obtains two qualitatively different solutions to the combined system $\mathcal{S}_\infty$. According to the above construction, $\lambda_a < \lambda_1$ and $\lambda_n < \lambda_b$. As n increases λ_1 approaches to λ_a while λ_n approaches to λ_b. In a limit $n \to \infty$ unperturbed eigenvalues λ_i are dense in the interval $[\lambda_a, \lambda_b]$. Due to the interlacing rule perturbed eigenvalues $\varepsilon_2, \ldots, \varepsilon_n$ are also dense in this interval. Thus in a limit $n \to \infty$ each $\varepsilon \in [\lambda_a, \lambda_b]$ is a perturbed eigenvalue. In addition, there are two perturbed eigenvalues that may escape interval $[\lambda_a, \lambda_b]$. Those are perturbed eigenvalue ε_1 that may satisfy $\varepsilon_1 < \lambda_a$, and perturbed eigenvalue ε_{n+1} that may satisfy $\varepsilon_{n+1} > \lambda_b$. (See figure 2).

In conclusion, the combined system $\mathcal{S}_\infty$ may in general contain two kinds of perturbed eigenvalues and eigenstates. An eigenvalue ε of a perturbed system satisfies either $\varepsilon \notin [\lambda_a, \lambda_b]$ or $\varepsilon \in [\lambda_a, \lambda_b]$. We call the perturbed eigenvalue $\varepsilon_I \notin [\lambda_a, \lambda_b]$ an *isolated* eigenvalue. Since this eigenvalue is outside the band $[\lambda_a, \lambda_b]$, it is discrete. The corresponding eigenstate $|\Psi_I\rangle$ can be hence normalized to unity. In this respect isolated eigenstate $|\Psi_I\rangle$ is similar to the local state $|\Theta\rangle \in X_1^a$ that is also normalized to unity. There are at most two isolated eigenvalues (and eigenstates), one left $\varepsilon_L < \lambda_a$ and one right $\varepsilon_R > \lambda_b$. We call the perturbed eigenvalue $\varepsilon \in [\lambda_a, \lambda_b]$ 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 this respect embedded eigenstates of the combined system are similar to the eigenstates $|\Phi(k)\rangle$ of the system $\mathcal{S}_\infty^b$ that are also normalized to a δ-function.

4.1. Isolated eigenvalues and eigenstates

In order to find isolated eigenvalues we look for roots ε_I of relation (7a) that in a limit $n \to \infty$ satisfy $\varepsilon_I \notin [\lambda_a, \lambda_b]$. In this limit the sum in (7b) becomes an integral, and the equation (7a) is replaced with

$$h(\varepsilon_I) \equiv \beta^2 \omega(\varepsilon_I) + E - \varepsilon_I = 0, \quad \varepsilon_I \notin [\lambda_a, \lambda_b], \tag{10a}$$
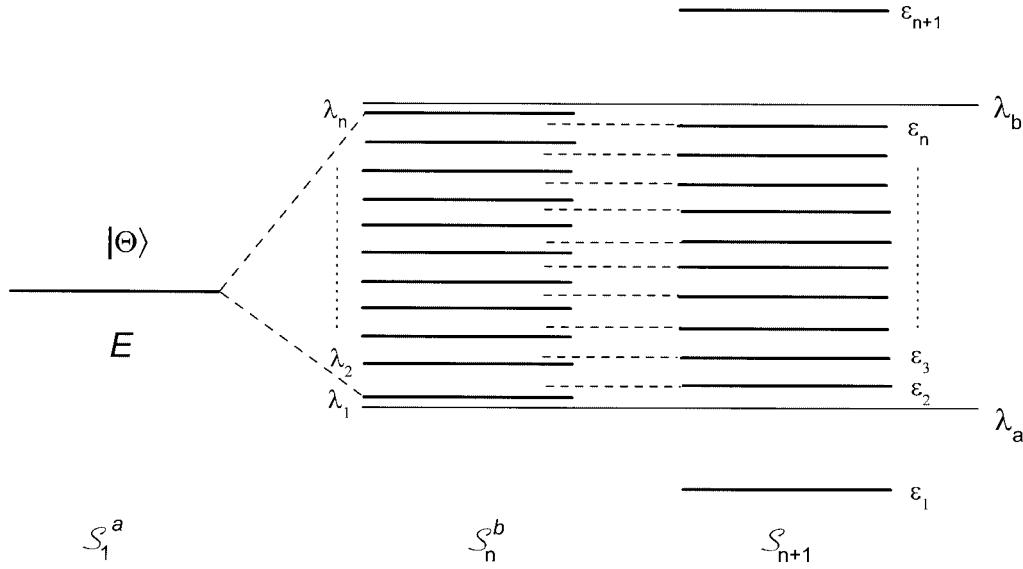
Figure 2. Interaction of the one-dimensional system $\mathcal{S}_1^a$ with the finite-dimensional system $\mathcal{S}_n^b$ containing n eigenstates. Eigenvalues ε_r of the combined system $\mathcal{S}_{n+1}$ are interlaced with eigenvalues λ_i of the system $\mathcal{S}_n^b$ according to (9). In the limit $n \to \infty$ eigenvalues ε_r form a continuous band in the interval $[\lambda_a, \lambda_b]$. In addition, eigenvalue ε_1 may converge to isolated eigenvalue $\varepsilon_L < \lambda_a$, while eigenvalue ε_{n+1} may converge to isolated eigenvalue $\varepsilon_R > \lambda_b$.

where in the case $\mathbf{P} = 0$

$$\omega(\varepsilon) = \int_{k_a}^{k_b} \frac{\langle \Theta | \mathbf{V} | \Phi(k) \rangle \langle \Phi(k) | \mathbf{V} | \Theta \rangle}{\varepsilon - \lambda(k)} \, \mathrm{d}k, \quad \varepsilon \notin [\lambda_a, \lambda_b]. \tag{10b}$$

Function $\omega(\varepsilon)$ can be written in the equivalent form

$$\omega(\varepsilon) = \int_{\lambda_a}^{\lambda_b} \frac{f(\lambda)}{\varepsilon - \lambda} \, \mathrm{d}\lambda, \quad \varepsilon \notin [\lambda_a, \lambda_b], \tag{10c}$$

where

$$f(\lambda) = \frac{\langle \Theta | \mathbf{V} | \Phi(k) \rangle \langle \Phi(k) | \mathbf{V} | \Theta \rangle}{\mathrm{d}\lambda(k)/\mathrm{d}k} \bigg|_{\lambda = \lambda(k)}, \quad \lambda \in [\lambda_a, \lambda_b]. \tag{11}$$

Right-hand side of (11) is evaluated in the point k that satisfies $\lambda = \lambda(k)$. Since $\lambda(k)$ is nondecreasing function of k, $f(\lambda)$ is nonnegative. Also, derivative $\mathrm{d}k/\mathrm{d}\lambda = \rho(\lambda)$ is a density of states [2,7], and hence one can write

$$f(\lambda) = \rho(\lambda) \langle \Theta | \mathbf{V} | \Phi(k) \rangle \langle \Phi(k) | \mathbf{V} | \Theta \rangle \big|_{\lambda = \lambda(k)}, \quad \lambda \in [\lambda_a, \lambda_b]. \tag{11'}$$

Let us now investigate conditions for the existence of the isolated eigenvalues ε_I. From (10c) one finds

$$\omega(\pm\infty) = 0, \qquad \frac{d\omega(\varepsilon)}{d\varepsilon} = -\int_{\lambda_a}^{\lambda_b} \frac{f(\lambda)}{(\varepsilon - \lambda)^2}\, d\lambda < 0, \quad \varepsilon \notin [\lambda_a, \lambda_b]. \qquad (12a)$$

Since $f(\lambda) \geqslant 0$, function $\omega(\varepsilon)$ is monotonically decreasing function in the intervals $(-\infty, \lambda_a)$ and (λ_b, ∞), while in a limit $\varepsilon \to \pm\infty$ this function converges asymptotically to zero. We also consider the value of $\omega(\varepsilon)$ in the points λ_a and λ_b on the edge of the band $[\lambda_a, \lambda_b]$. It is convenient to define those values as left and right limits, respectively

$$\omega_a^- \equiv \omega(\lambda_a) = \lim_{\varepsilon \to \lambda_a-} \omega(\varepsilon) < 0, \qquad \omega_b^+ \equiv \omega(\lambda_b) = \lim_{\varepsilon \to \lambda_b+} \omega(\varepsilon) > 0. \qquad (12b)$$

Function $\omega(\varepsilon)$ may diverge in the point λ_a (λ_b) in which case one has $\omega_a^- = -\infty$ ($\omega_b^+ = \infty$). For example, if $f(\lambda_a) \neq 0$ function $\omega(\varepsilon)$ diverges in the point $\varepsilon = \lambda_a$ and one has $\omega_a^- = -\infty$. One has $f(\lambda_a) \neq 0$ whenever $\langle\Theta|\mathbf{V}|\Phi(k_a)\rangle \neq 0$ and $\rho(k_a) \neq 0$. Similar conclusion applies to the point $\varepsilon = \lambda_b$. Note that in the case of one-dimensional solids density of states $\rho(k)$ usually becomes infinite at the edges of the band [2,7]. However, in the case of higher dimensional solids $\rho(k)$ is usually highest towards the center of the band, and is least at the edges [2,7].

Interlacing rule implies that there is at most one left-isolated eigenvalue $\varepsilon_L < \lambda_a$ and at most one right-isolated eigenvalue $\varepsilon_R > \lambda_b$. The same conclusion follows from the above relations. Since $\omega(\varepsilon)$ is monotonically decreasing in the intervals $(-\infty, \lambda_a)$ and (λ_b, ∞), $h(\varepsilon) \equiv \beta^2\omega(\varepsilon) + E - \varepsilon$ is also monotonically decreasing in those intervals. Hence $h(\varepsilon) = 0$ can have at most one root in the interval $(-\infty, \lambda_a)$ and at most one root in the interval (λ_b, ∞).

Relation (10a) also implies conditions for the existence of isolated solutions. One finds that in the (E, β)-plane right-isolated eigenvalue ε_R exist in the region on the right side of the parabola $E = \lambda_b - \beta^2\omega_b^+$, while on the left side of this parabola it does not exist. Similarly, left-isolated eigenvalue ε_L exist in the region on the left side of the parabola $E = \lambda_a - \beta^2\omega_a^-$, while it does not exist on the right side of this parabola. Considered as a function of a parameter E, right-isolated eigenvalue ε_R exist if and only if $E > E_R$, while left-isolated eigenvalue ε_L exist if and only if $E < E_L$ where E_R and E_L are right and left critical points, respectively

$$E_R = \lambda_b - \beta^2\omega_b^+, \qquad E_L = \lambda_a - \beta^2\omega_a^-. \qquad (13a)$$

In a similar way one can define critical points β_L and β_R relative to the coupling β:

$$\beta_L = \left(\frac{E - \lambda_a}{|\omega_a^-|}\right)^{1/2} \text{ if } E > \lambda_a, \qquad \beta_R = \left(\frac{\lambda_b - E}{|\omega_b^+|}\right)^{1/2} \text{ if } E < \lambda_b. \qquad (13b)$$

Critical point β_L applies to the case $E > \lambda_a$, while critical point β_R applies to the case $E < \lambda_b$. If namely $E < \lambda_a$ left-isolated eigenvalue ε_L exist for each value of β, while if $E > \lambda_b$ right-isolated eigenvalue ε_R exists for each value of β. However, if

$E > \lambda_a$ left-isolated eigenvalue ε_L exists if and only if β satisfies $\beta > \beta_L$, while if $E < \lambda_b$ right-isolated eigenvalue ε_R exists if and only if β satisfies $\beta > \beta_R$.

Using relations (10) one can estimate the interval where isolated eigenvalue ε_I should be confined. In the case of the right-isolated eigenvalue one finds (see appendix):

- if $E \in (E_R, \lambda_b)$ then

$$\lambda_b < \varepsilon_R < \lambda_b + \beta^2 \frac{\langle \Theta | \mathbf{V}^2 | \Theta \rangle}{|E - \lambda_b|}; \tag{14a}$$

- if $E \in (\lambda_b, \infty)$ then

$$E < \varepsilon_R < E + \beta^2 \frac{\langle \Theta | \mathbf{V}^2 | \Theta \rangle}{|E - \lambda_b|}. \tag{14b}$$

Thus if $E < \lambda_b$ right-isolated eigenvalue is at most at the distance $\beta^2 \langle \Theta | \mathbf{V}^2 | \Theta \rangle / (\lambda_b - E)$ from the band $[\lambda_a, \lambda_b]$, i.e., it is relatively close to this band. If, however, $E > \lambda_b$, this eigenvalue is at least at the distance $E - \lambda_b$ from $[\lambda_a, \lambda_b]$, i.e., it is relatively far from this band. If β is small, the distinction between those two cases is sharp. With the increase of the coupling β this distinction is increasingly more blurred. For example, if $\omega(\varepsilon)$ diverges in the point $\varepsilon = \lambda_b$, eigenvalue ε_R exists for each value of E and for each $\beta \neq 0$. However, if $E < \lambda_b$ and if the coupling β is relatively small, this eigenvalue is very close to λ_b. For small β this eigenvalue can appreciable drift away from the band $[\lambda_a, \lambda_b]$ only if $E > \lambda_b$.

Isolated eigenvalue ε_I is a function of the local eigenvalue E and of the coupling β. This dependence can be derived from the relation (10a). One has $0 = \mathrm{d}(\beta^2 \omega(\varepsilon_I) + E - \varepsilon_I) = (\beta^2 \mathrm{d}\omega/\mathrm{d}\varepsilon_I - 1)\, \mathrm{d}\varepsilon_I + 2\beta\omega\, \mathrm{d}\beta + \mathrm{d}E$ and hence

$$\frac{\partial \varepsilon_I}{\partial E} = \frac{1}{1 - \beta^2 \mathrm{d}\omega(\varepsilon_I)/\mathrm{d}\varepsilon_I}, \qquad \frac{\partial \varepsilon_I}{\partial \beta} = \frac{2\beta\omega(\varepsilon_I)}{1 - \beta^2 \mathrm{d}\omega(\varepsilon_I)/\mathrm{d}\varepsilon_I}. \tag{15}$$

Above relations give the rate of change of the eigenvalue ε_I with a change of the local eigenvalue E, and with a change of the coupling β. According to the first relation and since $\mathrm{d}\omega/\mathrm{d}\varepsilon < 0$, one has $0 \leqslant \partial \varepsilon_I / \partial E < 1$ except in a trivial case $\beta = 0$ when $\partial \varepsilon_I / \partial E = 1$. Thus if the local eigenvalue E increases (decreases), isolated eigenvalue ε_I also increases (decreases), i.e., it moves in the same direction. However, the change of this isolated eigenvalue is in the absolute value smaller than the change of the local eigenvalue E. According to the second relation and since $\omega(\varepsilon_R) > 0$ while $\omega(\varepsilon_L) < 0$, if the coupling β increases, isolated eigenvalue ε_I moves further away from the band $[\lambda_a, \lambda_b]$. The effect of the coupling β is thus to repeal isolated eigenvalues ε_I from this eigenvalue band and from each other: eigenvalue ε_R increases while eigenvalue ε_L decreases. This effect is analogous to the mutual repulsion of the perturbed eigenvalues in the case of the two level system subject to the interaction $\mathbf{V}$ [7].

Once ε_I is known, one can find the corresponding eigenstate $|\Psi_I\rangle$. In a limit $n \to \infty$ and in the case $\mathbf{P} = 0$ relations (8a) and (8b) are replaced with

$$|\Psi_I\rangle = \frac{1}{Q_I^{1/2}} \left[|\Theta\rangle + \beta \int_{k_a}^{k_b} \frac{\langle\Phi(k)|\mathbf{V}|\Theta\rangle}{\varepsilon_I - \lambda(k)} |\Phi(k)\rangle \, \mathrm{d}k \right], \quad \varepsilon_I \notin [\lambda_a, \lambda_b], \tag{16a}$$

where

$$Q_I = 1 + \beta^2 \int_{k_a}^{k_b} \frac{\langle\Theta|\mathbf{V}|\Phi(k)\rangle\langle\Phi(k)|\mathbf{V}|\Theta\rangle}{(\varepsilon_I - \lambda(k))^2} \, \mathrm{d}k. \tag{16b}$$

Quantity Q_I can be written in the equivalent form

$$Q_I = 1 + \beta^2 \int_{\lambda_a}^{\lambda_b} \frac{f(\lambda)}{(\varepsilon_I - \lambda)^2} \, \mathrm{d}\lambda = 1 - \beta^2 \frac{\mathrm{d}\omega(\varepsilon_I)}{\mathrm{d}\varepsilon_I}. \tag{16b'}$$

Above relations complete the solution of the combined eigenvalue equation (3a) as far as isolated eigenvalues and eigenstates are concerned. In order to find those eigenvalues and eigenstates one has first to solve equation (10a). If this equation has no solution, isolated eigenstates do not exist. If there is a solution ε_I, it is an isolated eigenvalue of the combined system, and the corresponding normalized eigenstate $|\Psi_I\rangle$ is given by (16).

All properties of the isolated eigenstate $|\Psi_I\rangle$ can be now easily obtained. For example, the probability w_I^a to find this eigenstate in the local state $|\Theta\rangle \in X_1^a$ and the probability density $\rho_I^b(k)$ to find this eigenstate in the unperturbed states $|\Phi(k)\rangle \in X_\infty^b$ are

$$w_I^a = \left| \langle\Theta|\Psi_I\rangle \right|^2, \qquad \rho_I^b(k) = \left| \langle\Phi(k)|\Psi_I\rangle \right|^2. \tag{17a}$$

From (16) one obtains required amplitudes $\langle\Theta|\Psi_I\rangle$ and $\langle\Phi(k)|\Psi_I\rangle$

$$\langle\Theta|\Psi_I\rangle = \frac{1}{Q_I^{1/2}}, \qquad \langle\Phi(k)|\Psi_I\rangle = \frac{\beta}{Q_I^{1/2}} \frac{\langle\Phi(k)|\mathbf{V}|\Theta\rangle}{(\varepsilon_I - \lambda(k))}. \tag{17b}$$

In particular, (15) and (16b') imply

$$w_I^a = \frac{\partial \varepsilon_I}{\partial E} = \frac{1}{1 - \beta^2 \, \mathrm{d}\omega(\varepsilon_I)/\mathrm{d}\varepsilon_I}. \tag{15'}$$

Above probabilities satisfy completeness relation

$$w_I^a + w_I^b = 1, \quad \text{where } w_I^b = \int \rho_I^b(k) \, \mathrm{d}k. \tag{17c}$$

Probability to find isolated eigenstate $|\Psi_I\rangle$ in a system $\mathcal{S}_\infty^b$, i.e., probability to find this eigenstate in any of the states $|\Phi(k)\rangle \in X_\infty^b$ is w_I^b. Completeness relation (17c) expresses the fact that total probability to find eigenstate $|\Psi_I\rangle$ either in a system $\mathcal{S}_1^a$ or in a system $\mathcal{S}_\infty^b$ equals one. If $w_I^a > 0.5$ isolated eigenstate $|\Psi_I\rangle$ is $\mathcal{S}_1^a$-dominant, while if $w_I^a < 0.5$ it is $\mathcal{S}_\infty^b$-dominant. In the former case one can consider $|\Psi_I\rangle$ to be the eigenstate $|\Theta\rangle$ of a system $\mathcal{S}_1^a$ perturbed by the interaction with the system $\mathcal{S}_\infty^b$. In the

latter case it is more appropriate to consider $|\Psi_I\rangle$ as an eigenstate of the system $\mathcal{S}_\infty^b$ perturbed by the interaction with the system $\mathcal{S}_1^a$.

Let us now investigate in more detail probability w_I^a to find isolated eigenstate $|\Psi_I\rangle$ in a local state $|\Theta\rangle$. One has $\lim_{\varepsilon_I \to \pm\infty} w_I^a = 1$. One also finds that w_I^a monotonically decreases as ε_I approaches band $[\lambda_a, \lambda_b]$ from either side. Thus w_I^a assumes a minimum value at the band boundary. According to (16b′) and (15′), one has $\lim_{\varepsilon_L \to \lambda_a-} w_L^a = 0$, unless in a limit $\lambda \to \lambda_a$ the function $f(\lambda)$ approaches to zero at least quadraticaly. Similar conclusion applies to $\lim_{\varepsilon_R \to \lambda_b+} w_R^a = 0$. The probability w_I^a is hence close to one for large ε_I, and it is usually close to zero for ε_I near the band $[\lambda_a, \lambda_b]$. Trivial case is $\beta = 0$. In this case there is no interaction between systems $\mathcal{S}_1^a$ and $\mathcal{S}_\infty^b$. The state $|\Theta\rangle$ is hence an eigenstate of the combined system with the eigenvalue E. If $E \notin [\lambda_a, \lambda_b]$ this eigenstate is isolated, and hence $w_I^a = 1$. If $E \in [\lambda_a, \lambda_b]$ this eigenstate is not isolated, and hence $w_I^a = 0$. Thus if $\beta = 0$ there is a sharp distinction between two extreme cases, $E \notin [\lambda_a, \lambda_b]$ and $E \in [\lambda_a, \lambda_b]$. The same conclusion follows from the above relations. If there is no interaction between systems $\mathcal{S}_1^a$ and $\mathcal{S}_\infty^b$ relation (10a) reduces to $\varepsilon_I = E$, and if $E \notin [\lambda_a, \lambda_b]$ relation (16) reduces to $|\Psi_I\rangle = |\Theta\rangle$.

This behavior slightly changes when the coupling is small but nonzero, $\beta \neq 0$. According to (16b) and (17), probability w_I^a is very sensitive on the distance of the isolated eigenvalue ε_I from the band $[\lambda_a, \lambda_b]$. If ε_I is close to $[\lambda_a, \lambda_b]$ this probability tends to be small. In view of the estimates (14) this means that w_I^a will be small if $E \in [\lambda_a, \lambda_b]$. On the other hand, if $E \notin [\lambda_a, \lambda_b]$ probability w_I^a tends to be large. Qualitatively this is the same behavior as in the case $\beta = 0$, though not with such a sharp distinction between those two cases. If $\beta \neq 0$ there is some intermediate region where either $E \approx \lambda_a$ or $E \approx \lambda_b$ and where w_I^a is intermediate. With the increase of the coupling this distinction between the region $E \notin [\lambda_a, \lambda_b]$ where w_I^a is relatively large and the region $E \in [\lambda_a, \lambda_b]$ where w_I^a is relatively small is increasingly more blurred.

To complete our discussion, note that in the case of the weak coupling and provided $E \notin [\lambda_a, \lambda_b]$, one can approximate root ε_I of (10a) as

$$\varepsilon_I \approx E + \beta^2 \omega(E), \quad E \notin [\lambda_a, \lambda_b]. \tag{18}$$

According to (10b) the quantity $\beta^2 \omega(E)$ has a formal structure of the second order perturbative correction to the eigenvalue E. Since $\langle \Theta | \mathbf{V} | \Theta \rangle = 0$ there is no first order eigenvalue correction. The above approximation is hence identical with a result one would obtain in a standard perturbation expansion that includes second order eigenvalue correction.

4.2. Embedded eigenvalues and eigenstates

Consider now the case when the perturbed eigenvalue ε is embedded in the eigenvalue band $[\lambda_a, \lambda_b]$. We again approximate relations (2) with relations (4) and we look for a limit $n \to \infty$ of the expression (7). As n increases, intervals $\Delta\lambda_i = \lambda_i - \lambda_{i-1}$ between successive unperturbed eigenvalues λ_i decrease and $\Delta\lambda_i \to 0$. Due to the interlacing rule intervals $\Delta\varepsilon_r = \varepsilon_r - \varepsilon_{r-1}$ between successive perturbed eigenvalues ε_r also

decrease, and those eigenvalues become more and more dense in the band $[\lambda_a, \lambda_b]$. In a limit $n \to \infty$ each ε in this band is an eigenvalue of the perturbed equation. Moreover, since for each finite n one has $\lambda_i \leqslant \varepsilon_{i+1} \leqslant \lambda_{i+1}$, in this limit functional dependence of the continuous perturbed eigenvalue ε on parameter k is the same as functional dependence of unperturbed eigenvalue λ on k, i.e., $\varepsilon(k) \equiv \lambda(k)$. It remains to find the structure of the corresponding perturbed eigenstates $|\Psi(\varepsilon)\rangle$.

In the appendix we show that in the case of the embedded eigenvalues relation (7a) should be replaced with

$$\pi \beta^2 f(\varepsilon) \cot\big(\pi x(\varepsilon)\big) + \beta^2 \omega(\varepsilon) + E - \varepsilon = 0, \quad \varepsilon \in [\lambda_a, \lambda_b], \tag{19a}$$

where $f(\varepsilon)$ is given by relation (11) and where

$$\omega(\varepsilon) = P \int_{k_a}^{k_b} \frac{\langle\Theta|\mathbf{V}|\Phi(k)\rangle\langle\Phi(k)|\mathbf{V}|\Theta\rangle}{\varepsilon - \lambda(k)} \, dk, \quad \varepsilon \in [\lambda_a, \lambda_b]. \tag{19b}$$

In analogy to (10c) function $\omega(\varepsilon)$ ($\varepsilon \in [\lambda_a, \lambda_b]$) can be expressed in terms of the function $f(\varepsilon)$:

$$\omega(\varepsilon) = P \int_{\lambda_a}^{\lambda_b} \frac{f(\lambda)}{\varepsilon - \lambda} \, d\lambda, \quad \varepsilon \in [\lambda_a, \lambda_b]. \tag{19c}$$

In relations (19b) and (19c) symbol P denotes principal Cauchy integral value. Those relations extend the definition of the function $\omega(\varepsilon)$ to the interval $\varepsilon \in [\lambda_a, \lambda_b]$. If $\varepsilon \notin [\lambda_a, \lambda_b]$ this function is defined according to (10b) or (10c), while if $\varepsilon \in [\lambda_a, \lambda_b]$ it is defined according to (19b) or (19c). In the former case there is no need to take principal Cauchy value. Consider, for example, expression (10b). Subintegral function in this expression is either uniformly nonnegative or uniformly nonpositive in the entire integration range $k \in [k_a, k_b]$, and hence there is no cancellation of infinite positive and infinite negative integral contributions characteristic of the principal Cauchy value. The function $\omega(\varepsilon)$ is hence well defined for each $\varepsilon \notin [\lambda_a, \lambda_b]$. However, in the interval $[\lambda_a, \lambda_b]$ this function may diverge for some isolated values of ε. Most important such points are edges $\varepsilon = \lambda_a$ and $\varepsilon = \lambda_b$ of this interval. For example, if $f(\lambda_a) \neq 0$ function $\omega(\varepsilon)$ diverges in a point $\varepsilon = \lambda_a$.

The solution to the equation (19a) is a function $x(\varepsilon)$. This function is a "fractional shift" of ε in the intervals $(\lambda_{r-1}, \lambda_r)$ and in a limit $n \to \infty$. More precisely, for each finite n one can define $(n-1)$ quantities

$$x(\varepsilon_r) = \frac{\varepsilon_r - \lambda_{r-1}}{\lambda_r - \lambda_{r-1}}, \quad r = 2, \ldots, n. \tag{20a}$$

As n increases, perturbed eigenvalues ε_r become more and more dense in the interval $[\lambda_a, \lambda_b]$. In the limit $n \to \infty$ quantities $x(\varepsilon_r)$ converge to a function $x(\varepsilon)$ of a continuous parameter ε. Due to the interlacing rule one has $0 \leqslant x(\varepsilon_r) \leqslant 1$. Since $\cot(0) = \cot(\pi) = \pm\infty$, the points $x(\varepsilon) = 0$ and $x(\varepsilon) = 1$ are in the relation (19a)

equivalent. Hence one can identify $x(\varepsilon) = 1$ with $x(\varepsilon) = 0$ and one can restrict fractional shift $x(\varepsilon)$ to the interval $[0, 1)$:

$$0 \leqslant x(\varepsilon) < 1. \tag{20b}$$

According to (20a), for each finite n fractional shift $x(\varepsilon_r) = 0$ (and $x(\varepsilon_r) = 1$) corresponds to singular solutions, while all other values of $x(\varepsilon_r)$ correspond to cardinal solutions. We use this property in order to extend the notion of cardinal and singular solutions in a natural way to the limit $n \to \infty$. Accordingly, if $x(\varepsilon) = 0$ the solution is singular, while if $x(\varepsilon) \neq 0$ it is cardinal.

If $x(\varepsilon) = 0$ one has $\cot(\pi x(\varepsilon)) = \pm\infty$. Strictly, this value is not a solution of (19a). However, if one takes a limit $\cot(\pi x(\varepsilon)) \to \pm\infty$ this relation in this limit describes singular solutions as well. If $f(\varepsilon) \neq 0$ and $\omega(\varepsilon) \neq \infty$ one obtains a finite value for $\cot(\pi x(\varepsilon))$, and the solution is cardinal. Hence only the case $f(\varepsilon) = 0$ and/or $\omega(\varepsilon) = \infty$ needs some special treatment and only in this case one may have singular solution.

For each finite n the solutions of (7a) are discrete eigenvalues ε_r. In the limit $n \to \infty$ and in the band $[\lambda_a, \lambda_b]$ the notion of discrete eigenvalues looses any meaning since each $\varepsilon \in [\lambda_a, \lambda_b]$ becomes an eigenvalue of the combined system. The information provided by the eigenvalues ε_r in (7a) is in (19a) replaced by the information provided by the fractional shift $x(\varepsilon)$. This shows an important difference between treatments of the cases $\varepsilon \notin [\lambda_a, \lambda_b]$ and $\varepsilon \in [\lambda_a, \lambda_b]$. In the former case relation (10a) is obtained from the relation (7a) by the formal replacement $\Omega(\varepsilon) \to \omega(\varepsilon)$ and the solutions of (10a) are isolated eigenvalues ε_I. In the latter case relation (19a) is obtained from the relation (7a) by the formal replacement $\Omega(\varepsilon) \to \pi f(\varepsilon) \cot(\pi x(\varepsilon)) + \omega(\varepsilon)$ and the solution to (19a) is a fractional shift $x(\varepsilon)$. The appearance of the additional term $\pi f(\varepsilon) \cot(\pi x(\varepsilon))$ is due to the fact that perturbed eigenvalues ε are now embedded in the continuum, and those eigenvalues can assume any value in the eigenvalue band $[\lambda_a, \lambda_b]$. This additional term is crucial since it alone contains unknown fractional shift $x(\varepsilon)$.

The solution of (19a) is trivial:

$$x(\varepsilon) = \frac{1}{\pi} \cot^{-1}\left(\frac{\varepsilon - E - \beta^2\omega(\varepsilon)}{\pi\beta^2 f(\varepsilon)}\right), \quad \varepsilon \in [\lambda_a, \lambda_b]. \tag{21}$$

This relation expresses fractional shift $x(\varepsilon)$ in terms of the local eigenvalue E, in terms of the coupling β, and in terms of functions $\omega(\varepsilon)$ and $f(\varepsilon)$. If $f(\varepsilon) = 0$ and $h(\varepsilon) \equiv \beta^2\omega(\varepsilon) + E - \varepsilon \neq 0$ one has $x(\varepsilon) = 0$. Fractional shift is zero and the perturbed eigenvalue coincides with the unperturbed eigenvalue. By definition, this corresponds to a singular solution. One can justify this conclusion by the following heuristic argument: One may have $f(\varepsilon) = 0$ only if $\langle\Theta|\mathbf{V}|\Phi(k)\rangle_{\varepsilon=\lambda(k)} = 0$. However, in this case the state $|\Phi(k)\rangle_{\varepsilon=\lambda(k)}$ and the eigenvalue $\varepsilon = \lambda(k)$ corresponding to this state are not perturbed by the interaction $\beta\mathbf{V}$. This state is hence an eigenstate of the combined system, i.e., it is singular.

Once fractional shift is known, one can proceed to calculate perturbed eigenstates $|\Psi(\varepsilon)\rangle$. An important quantity is the amplitude $\langle\Theta|\Psi(\varepsilon)\rangle$ that determines probability

density $\rho^a(\varepsilon) = |\langle\Theta|\Psi(\varepsilon)\rangle|^2$ to find the state $|\Theta\rangle$ in the eigenstate $|\Psi(\varepsilon)\rangle$. In the appendix we show that this amplitude can be expressed in terms of the fractional shift $x(\varepsilon)$ as

$$\langle\Theta|\Psi(\varepsilon)\rangle = \frac{\sin(\pi x(\varepsilon))}{\pi\beta\sqrt{f(\varepsilon)}}, \quad \varepsilon \in [\lambda_a, \lambda_b]. \tag{22}$$

Since fractional shift satisfies $0 \leqslant x(\varepsilon) < 1$ one has $\langle\Theta|\Psi(\varepsilon)\rangle \geqslant 0$.
Relations (21) and (22) imply

$$\langle\Theta|\Psi(\varepsilon)\rangle = \begin{cases} \left[\dfrac{\beta^2 f(\varepsilon)}{\pi^2\beta^4 f^2(\varepsilon) + (\beta^2\omega(\varepsilon) + E - \varepsilon)^2}\right]^{1/2}, & \text{if } \varepsilon \in [\lambda_a, \lambda_b], \\ 0, & \text{otherwise,} \end{cases} \tag{23a}$$

$$\rho^a(\varepsilon) \equiv |\langle\Theta|\Psi(\varepsilon)\rangle|^2 = \frac{\beta^2 f(\varepsilon)}{\pi^2\beta^4 f^2(\varepsilon) + (\beta^2\omega(\varepsilon) + E - \varepsilon)^2}, \quad \varepsilon \in [\lambda_a, \lambda_b]. \tag{23b}$$

Relations (23) are valid whenever fractional shift $x(\varepsilon)$ as given by expression (21) is well defined. An exception is the point $\varepsilon = \varepsilon_c$ that satisfies $f(\varepsilon_c) = 0$ and at the same time $h(\varepsilon_c) = 0$ (see appendix). We refer to such a point as a point of "anomal resonance" [4]. In this point expression (21) contains undefined ratio $0/0$ and fractional shift $x(\varepsilon_c)$ is not well defined. If the system contains any such point, a correction to the above expressions is required. In particular, in each point $\varepsilon = \varepsilon_c$ expression (23b) for the density $\rho^a(\varepsilon)$ is corrected by an additional term proportional to $\delta(\varepsilon - \varepsilon_c)$ [4]. In what follows we will assume that the system contains no such points, or that such points can be neglected.

Since $|\Psi(\varepsilon)\rangle$ is an eigenstate of the combined system with the eigenvalue ε, density $\rho^a(\varepsilon)$ is a probability density to find the state $|\Theta\rangle$ with the eigenvalue $\varepsilon \in [\lambda_a, \lambda_b]$. If there is no coupling ($\beta = 0$), the state $|\Theta\rangle$ is an eigenstate of the combined system with the eigenvalue E. In this case and if $E \in [\lambda_a, \lambda_b]$ density $\rho^a(\varepsilon)$ collapses to a δ-function $\rho^a(\varepsilon) = \delta(\varepsilon - E)$, while if $E \notin [\lambda_a, \lambda_b]$ one has $\langle\Theta|\Psi(\varepsilon)\rangle = \langle\Theta|\Phi(k)\rangle = 0$ and hence $\rho^a(\varepsilon) \equiv 0$. The same result is obtained from (23b) in a limit $\beta \to 0$. If one includes the coupling, the state $|\Theta\rangle$ has no more well-defined eigenvalue. If the coupling β is relatively weak, two things usually happen. First, due to the interaction of the system $\mathcal{S}_1^a$ with the system $\mathcal{S}_\infty^b$, the eigenvalue E of the system $\mathcal{S}_1^a$ is shifted to a new eigenvalue ε_0. Second, shifted eigenvalue is usually broadened, and it obtains some width $\Delta\varepsilon_0$. With increase of the coupling, the distinction between the systems $\mathcal{S}_1^a$ and $\mathcal{S}_\infty^b$ is increasingly less sharp, and the eigenvalue of the state $|\Theta\rangle \in X_1^a$ becomes increasingly more diffuse. Eigenvalue distribution of this state in the interval $[\lambda_a, \lambda_b]$ is described in precise terms by the density function $\rho^a(\varepsilon)$. In addition to this density, eigenvalue distribution of the state $|\Theta\rangle$ may also include isolated eigenvalues ε_I. If, namely, the combined system has an isolated eigenstate $|\Psi_I\rangle$ with the eigenvalue ε_I, there is some probability $w_I^a = |\langle\Theta|\Psi_I\rangle|^2$ to find the state $|\Theta\rangle$ with this eigenvalue.

Total probability should be one, and hence

$$\sum_I w_I^a + w_C^a = 1, \tag{24a}$$

where

$$w_C^a = \int \rho^a(\varepsilon)\,\mathrm{d}\varepsilon \tag{24b}$$

is the probability to find local state $|\Theta\rangle$ in any of the embedded eigenstates $|\Psi(\varepsilon)\rangle$. In the expression (24b) one formally integrates over the entire interval $(-\infty, \infty)$. However, since $\rho^a(\varepsilon) = 0$ outside the band $[\lambda_a, \lambda_b]$, this integration is restricted to this band.

Relation (24a) is a completeness relation that expresses the fact that total probability to find the state $|\Theta\rangle$ in any of the eigenstates of the combined system must be one. This relation can be derived in a more formal way. Since isolated eigenstates $|\Psi_I\rangle$ and embedded eigenstates $|\Psi(\varepsilon)\rangle$ of the combined system form a complete set in the combined space X_∞, each state $|\Xi\rangle \in X_\infty$ can be expressed as a linear combination of those eigenstates. In particular, using relations (17) and (23) one finds

$$|\Theta\rangle = \sum_I \sqrt{w_I^a}|\Psi_I\rangle + \int_{\lambda_a}^{\lambda_b} \sqrt{\rho^a(\varepsilon)}\big|\Psi(\varepsilon)\big\rangle\mathrm{d}\varepsilon. \tag{25}$$

The summation is performed over existing isolated eigenstates $|\Psi_I\rangle$, i.e., it can contain zero, one or two terms. For example, if isolated eigenstates do not exist (equation (10a) has no solution), there is no summation term in the above expression. Normalization condition $\langle\Theta|\Theta\rangle = 1$ now implies (24).

In order to analyze the shape of the probability density $\rho^a(\varepsilon)$, define quantity $\varepsilon_0 \in [\lambda_a, \lambda_b]$ as a root of

$$\beta^2\omega(\varepsilon_0) + E - \varepsilon_0 = 0, \quad \varepsilon_0 \in [\lambda_a, \lambda_b]. \tag{26}$$

In general, this equation may have zero, one or multiple roots in the interval $[\lambda_a, \lambda_b]$. According to (23b), if (26) has a root $\varepsilon_0 \in [\lambda_a, \lambda_b]$ probability density $\rho^a(\varepsilon_0)$ tends to be large.

Equation (26) is formally identical to the equation (10a). However, in the case of equation (10a) one has the condition $\varepsilon_I \notin [\lambda_a, \lambda_b]$, and the roots of this equation, if any, are isolated eigenvalues ε_I. In the above equation one has the condition $\varepsilon_0 \in [\lambda_a, \lambda_b]$, and the roots of (26) are not isolated eigenvalues. One finds that in a limit of weak coupling and provided $\omega(\varepsilon)$ is bounded in the interval $[\lambda_a, \lambda_b]$, relation (26) may have at most one root. We will show that this root should be identified with the eigenvalue E shifted to the position ε_0 as a result of the interaction of the system $\mathcal{S}_1^a$ with a system $\mathcal{S}_\infty^b$.

If $f(\varepsilon_0) \neq 0$ the root ε_0 of (26) has a simple interpretation. According to (21), if ε_0 satisfies (26) and if, in addition, $f(\varepsilon_0) \neq 0$, then $x(\varepsilon_0) = 0.5$. The point $\varepsilon = \varepsilon_0$ hence corresponds to the perturbed eigenvalue that is in the middle between two successive unperturbed eigenvalues. This interpretation is strictly valid as long as n is finite (however large), since only in this case one can say that a perturbed eigenvalue ε_0 is in the

middle between two unperturbed eigenvalues λ_{r-1} and λ_r. As n increases and intervals $\Delta\lambda_r$ decrease, more and more perturbed eigenvalues close to the eigenvalue ε_0 are to a very good approximation in the middle between two successive unperturbed eigenvalues. Therefore one can loosely say that in the point $\varepsilon = \varepsilon_0$, and in some infinitesimal neighborhood of this point, perturbed eigenvalue is in a middle between two successive unperturbed eigenvalues.

If $f(\varepsilon_0) = 0$, the point $\varepsilon_0 = \varepsilon_c$ is a point of anomal resonance. In this case fractional shift $x(\varepsilon_0)$ is undefined. In general, fractional shift $x(\varepsilon)$ is a continuous function of ε except in the points of anomal resonance where it is usually discontinuous [4].

4.3. Eigenvalue distribution of a local state in the weak coupling limit

Eigenvalue distribution of the local state $|\Theta\rangle$ is completely determined by the isolated eigenvalues ε_I (if any), corresponding probabilities w_I^a, and by the probability density $\rho^a(\varepsilon)$. We will now consider this distribution in the case when coupling β is relatively weak.

If β is small, there are two qualitatively different cases, the case $E \in [\lambda_a, \lambda_b]$ and the case $E \notin [\lambda_a, \lambda_b]$. There are also two small transition regions where either $E \approx \lambda_a$ or $E \approx \lambda_b$.

For small enough β and provided $\omega(\varepsilon)$ is bounded, equation (26) has a root $\varepsilon_0 \in [\lambda_a, \lambda_b]$ if and only if $E \in [\lambda_a, \lambda_b]$. If β is sufficiently small, this root is unique. According to (23b) and (26), density $\rho^a(\varepsilon)$ tends to have a maximum close to the point $\varepsilon = \varepsilon_0$, and at this point one has $\rho^a(\varepsilon_0) = 1/(\pi^2\beta^2 f(\varepsilon_0))$. Expanding quantities $\beta^2\omega(\varepsilon) + E - \varepsilon$ and $f(\varepsilon)$ in this point one finds:

$$\beta^2\omega(\varepsilon) + E - \varepsilon = \left[\beta^2\left(\frac{d\omega}{d\varepsilon}\right)_0 - 1\right](\varepsilon - \varepsilon_0) + \beta^2 O\big((\varepsilon - \varepsilon_0)^2\big), \qquad (27a)$$

$$f(\varepsilon) = f(\varepsilon_0) + \left(\frac{df}{d\varepsilon}\right)_0 (\varepsilon - \varepsilon_0) + O\big((\varepsilon - \varepsilon_0)^2\big). \qquad (27b)$$

According to (23b), main contribution to the density $\rho^a(\varepsilon)$ comes from those values of ε that approximately satisfy $(\varepsilon - \varepsilon_0)^2 < \beta^4 f^2(\varepsilon) \approx \beta^4 f^2(\varepsilon_0)$. The quantity $(\varepsilon - \varepsilon_0)$ is hence effectively of the order $O(\beta^2)$ and one has $f(\varepsilon) = f(\varepsilon_0) + O(\beta^2)$ and $\varepsilon - E - \beta^2\omega(\varepsilon) = (\varepsilon - \varepsilon_0) + O(\beta^4)$. Those approximations improve if $\varepsilon - \varepsilon_0$ decreases, and in the point $\varepsilon = \varepsilon_0$ they are exact. If $f(\varepsilon_0) \neq 0$ this implies

$$\rho^a(\varepsilon) \approx \rho^{a0}(\varepsilon) = \begin{cases} \dfrac{\beta^2 f(\varepsilon_0)}{\pi^2\beta^4 f^2(\varepsilon_0) + (\varepsilon - \varepsilon_0)^2}, & \text{if } \varepsilon \in [\lambda_a, \lambda_b], \\ 0, & \text{otherwise.} \end{cases} \qquad (28)$$

The position of the point ε_0 can be estimated as

$$\varepsilon_0 \approx E + \beta^2\omega(E), \quad E \in [\lambda_a, \lambda_b]. \qquad (29a)$$

Function $\rho^{a0}(\varepsilon)$ is a typical approximation of the exact density distribution $\rho^a(\varepsilon)$ in the case of the weak coupling and provided $f(\varepsilon_0) \neq 0$ and $E \in [\lambda_a, \lambda_b]$. If $E \notin [\lambda_a, \lambda_b]$ one finds $\rho^a(\varepsilon) \approx 0$.

In the derivation of the expression (28) we have assumed that $\omega(\varepsilon)$ is bounded in the interval $[\lambda_a, \lambda_b]$. This guaranties that for small enough β relation (26) has at most one root $\varepsilon_0 \in [\lambda_a, \lambda_b]$. However, if $\omega(\varepsilon)$ is not bounded in this interval, there is usually another root of (26) close to the point where $\omega(\varepsilon)$ diverges. For example, $\omega(\varepsilon)$ may diverge in the point $\varepsilon = \lambda_b$ on the edge of the band $[\lambda_a, \lambda_b]$. In this case (26) may have two roots, ε_0 and $\varepsilon_0' \approx \lambda_b$. This situation is more complicated. However, density $\rho^a(\varepsilon)$ is again relatively well approximated with $\rho^{a0}(\varepsilon)$ where the root ε_0' is ignored and where only the root ε_0 is taken onto account.

Inside the band $[\lambda_a, \lambda_b]$ function $\rho^{a0}(\varepsilon)$ is identical to the universal resonance curve [8]. However, outside this band function $\rho^{a0}(\varepsilon)$ is zero, while the universal resonance curve is nonzero in the entire interval $(-\infty, \infty)$. Thus $\rho^{a0}(\varepsilon)$ equals universal resonance curve truncated on both edges of the band $[\lambda_a, \lambda_b]$.

If the point $\varepsilon_0 \in [\lambda_a, \lambda_b]$ is relatively far from the edges of the band $[\lambda_a, \lambda_b]$, function $\rho^{a0}(\varepsilon)$ is a bell-shaped curve centered at this point and with a width

$$\Delta\varepsilon_0 = 2\pi\beta^2 f(\varepsilon_0). \tag{29b}$$

Integrating density $\rho^{a0}(\varepsilon)$ one finds

$$\int_{\lambda_a}^{\lambda_b} \rho^{a0}(\varepsilon)\,d\varepsilon \approx \int_{-\infty}^{\infty} \frac{\beta^2 f(\varepsilon_0)\,d\varepsilon}{\pi^2\beta^4 f^2(\varepsilon_0) + (\varepsilon - \varepsilon_0)^2} = 1. \tag{30}$$

The approximation ($\approx$) is due to the extension of the integration over finite band $[\lambda_a, \lambda_b]$ to the integration from $-\infty$ to $+\infty$. This extension is justified if the point $\varepsilon = \varepsilon_0$ is relatively far from both edges of this band, that is if $|\varepsilon_0 - \lambda_a| > \Delta\varepsilon_0$ and $|\varepsilon_0 - \lambda_b| > \Delta\varepsilon_0$. Due to the completeness relation (24), if this is the case one has $w_I^a \approx 0$. We refer to the approximation (28), where $\varepsilon_0 \in [\lambda_a, \lambda_b]$ is relatively far from the edges of the band $[\lambda_a, \lambda_b]$ as a *resonance approximation*.

Close to the edge of the band $[\lambda_a, \lambda_b]$ integral (30) decreases and accordingly one of the probabilities w_I^a increases. In particular, if the point $\varepsilon = \varepsilon_0$ is exactly on the edge of this band, i.e., if either $\varepsilon_0 = \lambda_a$ or $\varepsilon_0 = \lambda_b$, one has $\int \rho^a(\varepsilon)\,d\varepsilon \approx \int \rho^{a0}(\varepsilon)\,d\varepsilon = 0.5$. Such points correspond to the intermediate region where one has either $E \approx \lambda_a$ or $E \approx \lambda_b$. As eigenvalue E drifts way from the band $[\lambda_a, \lambda_b]$ one obtains $\int \rho^a(\varepsilon)\,d\varepsilon \approx 0$.

Consider now in more details relative position of the maximum of the approximate and exact density curves. Approximate density $\rho^{a0}(\varepsilon)$ has maximum in the point $\varepsilon = \varepsilon_0$ while exact density $\rho^a(\varepsilon)$ has maximum in some point $\varepsilon_{\max}$. In the point $\varepsilon = \varepsilon_0$ approximate and exact densities coincide, i.e., $\rho^a(\varepsilon_0) = \rho^{a0}(\varepsilon_0)$. Let us now estimate the difference $\varepsilon_{\max} - \varepsilon_0$. The condition $d\rho^a/d\varepsilon = 0$ implies

$$\beta^2\omega(\varepsilon) + E - \varepsilon = \beta^4 \frac{\pi^2 f(\varepsilon)^2 df(\varepsilon)/d\varepsilon}{(\beta^2\omega(\varepsilon) + E - \varepsilon)\,df(\varepsilon)/d\varepsilon + 2(1 - \beta^2\,d\omega(\varepsilon)/d\varepsilon)f(\varepsilon)}. \tag{31}$$

The point $\varepsilon_{\max}$ is a root of this equation. Expanding this equation in the point $\varepsilon = \varepsilon_0$ in terms of a small quantity β one finds

$$\varepsilon_{\max} - \varepsilon_0 = -\beta^4 \frac{\pi^2 f(\varepsilon_0)(\mathrm{d}f/\mathrm{d}\varepsilon)_0}{2[1 - \beta^2(\mathrm{d}\omega/\mathrm{d}\varepsilon)_0]^2} + O(\beta^6). \tag{32}$$

Thus ε_0 approximates $\varepsilon_{\max}$ up to the order $O(\beta^4)$ in β. In addition, if the function $f(\varepsilon)$ is sufficiently small and/or sufficiently flat close to the point ε_0 (that is if $(f \cdot \mathrm{d}f/\mathrm{d}\varepsilon)_0 \approx 0$) then the first term on the right-hand side of (32) can be neglected, and ε_0 approximates $\varepsilon_{\max}$ essentially up to the order $O(\beta^6)$ in β.

In conclusion, in the resonance approximation (β small and $E \in [\lambda_a, \lambda_b]$), relation (26) has a root $\varepsilon_0 \approx E + \beta^2\omega(E) \in [\lambda_a, \lambda_b]$. In this case probability density $\rho^a(\varepsilon)$ has the shape of the truncated universal resonance curve with maximum at the point $\varepsilon = \varepsilon_0$ and with width $\Delta\varepsilon_0 = 2\pi\beta^2 f(\varepsilon_0)$. In addition $\int \rho^a(\varepsilon)\,\mathrm{d}\varepsilon \approx 1$. If, however, $E \notin [\lambda_a, \lambda_b]$ and if the eigenvalue E is not too close to the band edges, then $\rho^a(\varepsilon) \approx 0$. In this case there exists either right- or left-isolated eigenstate and the corresponding probability equals $w_I^a \approx 1$. There is also a small intermediate region where either $E \approx \lambda_a$ or $E \approx \lambda_b$ and where $\rho^a(\varepsilon)$ and w_I^a are intermediate. This has a simple and straightforward interpretation. If $E \in [\lambda_a, \lambda_b]$ the interaction $\beta\mathbf{V}$ of the system $\mathcal{S}_1^a$ with the system $\mathcal{S}_\infty^b$ shifts eigenvalue E of $\mathcal{S}_1^a$ to the eigenvalue $\varepsilon_0 \in [\lambda_a, \lambda_b]$. This shifted eigenvalue is broadened and it obtains a width $\Delta\varepsilon_0$. Both effects are of the order $O(\beta^2)$. Hence in the case of the weak coupling the root $\varepsilon_0 \in [\lambda_a, \lambda_b]$ of (26) should be interpreted as the eigenvalue of the system $\mathcal{S}_1^a$ in the interaction with the system $\mathcal{S}_\infty^b$. If, however, $E \notin [\lambda_a, \lambda_b]$, the interaction $\beta\mathbf{V}$ shifts this eigenvalue to the isolated eigenvalue $\varepsilon_I \approx E + \beta^2\omega(E)$. In this case there is no eigenvalue broadening, and shifted eigenvalue ε_I is isolated and sharp.

If the coupling β increases, density $\rho^a(\varepsilon)$ deviates from the bell-shaped curve $\rho^{a0}(\varepsilon)$ and maximum $\varepsilon_{\max}$ of $\rho^a(\varepsilon)$ deviates from the maximum $\varepsilon = \varepsilon_0$ of $\rho^{a0}(\varepsilon)$. Depending on the coupling β and on the position of the eigenvalue E, approximation $\rho^{a0}(\varepsilon)$ may fail and equation (26) may have multiple roots $\varepsilon = \varepsilon_0$. In this case density $\rho^a(\varepsilon)$ usually has multiple maxima in the interval $[\lambda_a, \lambda_b]$.

5. Time evolution of a local state

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

$$i\hbar\frac{\partial}{\partial t}\big|\Psi(t)\big\rangle = \mathbf{H}\big|\Psi(t)\big\rangle. \tag{33}$$

Each solution of this equation can be expressed as a linear combination:

$$\big|\Psi(t)\big\rangle = \sum_I c_I|\Psi_I\rangle \exp\left(-\frac{i\varepsilon_I t}{\hbar}\right) + \int_{\lambda_a}^{\lambda_b} c(\varepsilon)\big|\Psi(\varepsilon)\big\rangle \exp\left(-\frac{i\varepsilon t}{\hbar}\right)\mathrm{d}\varepsilon, \tag{34}$$

where $|\Psi_I\rangle$ and $|\Psi(\varepsilon)\rangle$ are eigenstates of the time-independent eigenvalue equation (3a), while c_I and $c(\varepsilon)$ are unknown coefficients and unknown function to be determined from the initial conditions.

One usually considers time evolution of a system that is at time $t = 0$ prepared in the local state $|\Theta\rangle \in X_1^a$. If the system is at time $t = 0$ prepared in this state, at some latter time t it will evolve in the state $|\Theta(t)\rangle \notin X_1^a$.

From (25) and (34) one obtains

$$|\Theta(t)\rangle = \sum_I \sqrt{w_I^a}|\Psi_I\rangle \exp\left(-\frac{i\varepsilon_I t}{\hbar}\right) + \int_{\lambda_a}^{\lambda_b} \sqrt{\rho^a(\varepsilon)}|\Psi(\varepsilon)\rangle \exp\left(-\frac{i\varepsilon t}{\hbar}\right) d\varepsilon. \quad (35)$$

One is usually interested in the probability $w^a(t) = |\langle\Theta|\Theta(t)\rangle|^2$ to find the state $|\Theta(t)\rangle$ at time t in the original state $|\Theta\rangle$. This probability describes decay of the system $\mathcal{S}_1^a$ to the system $\mathcal{S}_\infty^b$. One is also interested in the probability density $\rho(k, t) = |\langle\Phi(k)|\Theta(t)\rangle|^2$ to find the state $|\Theta(t)\rangle$ at time t in the state $|\Phi(k)\rangle \in X_\infty^b$. This density describes probability of a transition of a state $|\Theta(t)\rangle$ at time t in a state $|\Phi(k)\rangle \in X_\infty^b$.

Consider, first, probability $w^a(t)$. According to (23) and (35) one has

$$w^a(t) = |\langle\Theta|\Theta(t)\rangle|^2, \quad (36a)$$

where the amplitude $\langle\Theta|\Theta(t)\rangle$ is

$$\langle\Theta|\Theta(t)\rangle = \int \rho^a(\varepsilon) \exp\left(-\frac{i\varepsilon t}{\hbar}\right) d\varepsilon + \sum_I w_I^a \exp\left(-\frac{i\varepsilon_I t}{\hbar}\right). \quad (36b)$$

The quantity

$$\widetilde{\rho}^a(t) = \int \rho^a(\varepsilon) \exp\left(-\frac{i\varepsilon t}{\hbar}\right) d\varepsilon \quad (36c)$$

is a Fourier transform of the probability density $\rho^a(\varepsilon)$. Note that $\widetilde{\rho}^a(0) = w_C^a$ is total probability to find the state $|\Theta\rangle$ with an eigenvalue in the band $[\lambda_a, \lambda_b]$.

Let us now investigate general properties of the probability $w^a(t)$.

At time $t = 0$ one has $|\Theta(0)\rangle \equiv |\Theta\rangle$, and hence $w^a(0) = 1$. As required, this follows from (36b), since for $t = 0$ this relation reduces to the completeness relation (24). Consider now probability $w^a(t)$ in the limit $t \to \infty$. According to the general properties of a Fourier transform $\lim_{t\to\infty} \widetilde{\rho}^a(t) = 0$. Hence

$$\lim_{t\to\infty} \langle\Theta|\Theta(t)\rangle = \sum_I w_I^a \exp\left(-\frac{i\varepsilon_I t}{\hbar}\right). \quad (37)$$

There are various possibilities depending on the coupling β and depending on the existence or nonexistence of isolated eigenstate(s).

If there are no isolated eigenstates or if the corresponding probabilities w_I^a are negligible, one has $\lim_{t\to\infty} \langle\Theta|\Theta(t)\rangle \approx 0$. In this case in a limit $t \to \infty$ the state $|\Theta(t)\rangle$ contains no component of the local state $|\Theta\rangle$. Therefore after long enough time the state

$|\Theta(t)\rangle$ is entirely represented as a linear combination of states $|\Phi(k)\rangle$ that belong to the system $\mathcal{S}_\infty^b$. In other words, time evaluation of a state $|\Theta(t)\rangle$ describes a complete decay of a system $\mathcal{S}_1^a$ to the system $\mathcal{S}_\infty^b$. This decay is due to the interaction between those two systems and due to the fact that system $\mathcal{S}_\infty^b$ is infinite. One usually has $w_I^a \approx 0$ if the coupling is weak and if in addition local eigenvalue E is inside the band $[\lambda_a, \lambda_b]$.

Another possibility is that the combined system contains one isolated eigenstate $|\Psi_I^a\rangle$ with a nonvasnishing probability $w_I^a \neq 0$. In this case qualitative behavior of the eigenstate $|\Theta(t)\rangle$ is different, and one has $\lim_{t\to\infty}\langle\Theta|\Theta(t)\rangle = w_I^a \exp(-i\varepsilon_I t/\hbar)$. Hence $w^a(\infty) = (w_I^a)^2$. Therefore, after long enough time the state $|\Theta(t)\rangle$ will be found in the local state $|\Theta\rangle$ with a finite probability $(w_I^a)^2$. Depending on the probability w_I^a, decay of a system $\mathcal{S}_1^a$ to a system $\mathcal{S}_\infty^b$ will be partial or negligible. For example, if $w_I^a \approx 1$ one has $\rho^a(\varepsilon) \approx 0$ and hence $w^a(t) \approx 1$. There is no decay, and the state $|\Theta(t)\rangle \approx |\Theta\rangle$ is essentially an isolated eigenstate of the combined system that is only slightly perturbed by the interaction of $\mathcal{S}_1^a$ with $\mathcal{S}_\infty^b$. However, if $w_I^a < 1$ the system $\mathcal{S}_1^a$ will decay to a system $\mathcal{S}_\infty^b$, but only partially.

Finally, one may have significant values for both probabilities w_L^a and w_R^a. For this to happen coupling β should be sufficiently strong. In this case (37) implies

$$\lim_{t\to\infty} w^a(t) = \left(w_L^a\right)^2 + \left(w_R^a\right)^2 + 2w_L^a w_R^a \cos\left(\frac{(\varepsilon_R - \varepsilon_L)t}{\hbar}\right).$$

Accordingly, after long enough time system $\mathcal{S}_1^a$ will only partially decay, and in the limit $t \to \infty$ there will be an oscillatory probability to find the state $|\Theta(t)\rangle$ in the local state $|\Theta\rangle$. In particular, if $w_L^a = w_R^a$ this probability will oscillate between zero and maximum value $4(w_L^a)^2$. Unless the eigenvalue band $[\lambda_a, \lambda_b]$ is very narrow and since $|\varepsilon_R - \varepsilon_L| > \lambda_b - \lambda_a$, this oscillation will be extremely fast. It is usually quite difficult to detect such a fast oscillation experimentally. Hence experimentally one should detect a time-average, i.e., the value $\overline{w}^a(\infty) = (w_L^a)^2 + (w_R^a)^2$.

In addition to the probability $w^a(t)$, another quantity of interest is the probability density $\rho(k, t) = |\langle\Phi(k)|\Theta(t)\rangle|^2$. By definition, product $\rho(k, t)\, dk$ is a probability to find the state $|\Theta(t)\rangle$ at time t in the state $|\Phi(k)\rangle$ and in the interval dk. One can express density $\rho(k, t)$ as

$$\rho(k, t) = \left|u(k, t)\right|^2, \tag{38a}$$

where

$$u(k, t) = \left\langle\Phi(k)\middle|\Theta(t)\right\rangle e^{i\lambda(k)t/\hbar}. \tag{38b}$$

In the appendix we show that the amplitude $u(k, t)$ satisfies

$$\frac{du(k, t)}{dt} = -i\beta\frac{\langle\Phi(k)|\mathbf{V}|\Theta\rangle}{\hbar}\left[\int_{\lambda_a}^{\lambda_b} \rho^a(\varepsilon)e^{-i(\varepsilon-\lambda(k))t/\hbar}\, d\varepsilon + \sum_I w_I^a e^{-i(\varepsilon_I-\lambda(k))t/\hbar}\right]. \tag{38c}$$

According to (38b) initial condition is $u(k, 0) = 0$. One can now integrate (38c) to obtain density $\rho(k, t)$. However, it is more convenient to express above probability

density as a function of the eigenvalue λ instead of as a function of a parameter k. This can be done by a simple transformation of above expressions.

Let $\rho^b(\lambda, t)\,\mathrm{d}\lambda$ be probability to find the state $|\Theta(t)\rangle$ at time t in a state $|\Phi(k)\rangle$ with the eigenvalue $\lambda = \lambda(k)$ and in the eigenvalue interval $\mathrm{d}\lambda$. Probability densities $\rho(k, t)$ and $\rho^b(\lambda, t)$ satisfy $\rho(k, t)\,\mathrm{d}k = \rho^b(\lambda, t)\,\mathrm{d}\lambda$. Hence

$$\rho^b(\lambda, t) = \left|u^b(\lambda, t)\right|^2, \tag{39a}$$

where the amplitude $u^b(\lambda, t)$ satisfies

$$\frac{\mathrm{d}u^b(\lambda, t)}{\mathrm{d}t} = -\mathrm{i}\beta\frac{\sqrt{f(\lambda)}}{\hbar}\left[\int_{\lambda_a}^{\lambda_b}\rho^a(\varepsilon)\mathrm{e}^{-\mathrm{i}(\varepsilon-\lambda)t/\hbar}\,\mathrm{d}\varepsilon + \sum_I w_I^a\mathrm{e}^{-\mathrm{i}(\varepsilon_I-\lambda)t/\hbar}\right] \tag{39b}$$

and where $u^b(\lambda, 0) = 0$.

Relation (39b) can be integrated to obtain

$$u^b(\lambda, t) = \beta\sqrt{f(\lambda)}\left[\int_{\lambda_a}^{\lambda_b}\frac{\rho^a(\varepsilon)[\mathrm{e}^{-\mathrm{i}(\varepsilon-\lambda)t/\hbar} - 1]}{\varepsilon - \lambda}\,\mathrm{d}\varepsilon + \sum_I w_I^a\frac{[\mathrm{e}^{-\mathrm{i}(\varepsilon_I-\lambda)t/\hbar} - 1]}{\varepsilon_I - \lambda}\right]. \tag{40a}$$

It is easy to solve (40a) by performing the required integration in this expression. Note in this respect that the subintegral function in (40a) has no singularity in the point $\varepsilon = \lambda$, since the apparent singularity in this point is removable.

One can also expand the subintegral function in (40a) in the power series in t

$$\int_{\lambda_a}^{\lambda_b}\frac{\rho^a(\varepsilon)[\mathrm{e}^{-\mathrm{i}(\varepsilon-\lambda)t/\hbar} - 1]}{\varepsilon - \lambda}\,\mathrm{d}\varepsilon = \sum_{n=1}^{\infty}\frac{(-\mathrm{i})^n}{n!}\left(\frac{t}{\hbar}\right)^n I_{n-1}(\lambda), \tag{41a}$$

where

$$I_n(\lambda) = \int_{\lambda_a}^{\lambda_b}\rho^a(\varepsilon)(\varepsilon - \lambda)^n\,\mathrm{d}\varepsilon, \quad n = 0, 1, 2, \ldots. \tag{41b}$$

For very small times one can approximate $\exp(-\mathrm{i}(\varepsilon - \lambda)t/\hbar) \approx 1 - \mathrm{i}(\varepsilon - \lambda)t/\hbar$. With this approximation and using completeness relation (24) one finds

$$u^b(\lambda, t) \approx -\mathrm{i}\frac{t}{\hbar}\beta\sqrt{f(\lambda)}, \tag{42a}$$

$$\rho^b(\lambda, t) \approx \frac{t^2}{\hbar^2}\beta^2 f(\lambda), \qquad t < \frac{\hbar}{\lambda_b - \lambda_a}. \tag{42b}$$

The solution to (39b) can be expressed in yet another form

$$u^b(\lambda, t) = \beta\sqrt{f(\lambda)}\left[-\mathrm{i}\int_0^t \widetilde{\rho}^a(t)\mathrm{e}^{\mathrm{i}\lambda t/\hbar}\,\mathrm{d}t + \sum_I w_I^a\frac{[\mathrm{e}^{-\mathrm{i}(\varepsilon_I-\lambda)t/\hbar} - 1]}{\varepsilon_I - \lambda}\right], \tag{40b}$$

where $\widetilde{\rho}^a(t)$ is a Fourier transform (36c) of a density distribution $\rho^a(\varepsilon)$. Using (36) amplitude $u^b(\lambda, t)$ can be also expressed in terms of the amplitude $\langle\Theta|\Theta(t)\rangle$

$$u^b(\lambda, t) = -\mathrm{i}\beta\sqrt{f(\lambda)} \int_0^t \langle\Theta|\Theta(t)\rangle \mathrm{e}^{\mathrm{i}\lambda t/\hbar} \, \mathrm{d}t. \tag{40c}$$

This expression provides an interesting connection between the amplitude $\langle\Theta|\Theta(t)\rangle$ that determines probability $w^a(t)$ and the amplitude $u^b(\lambda, t)$ that determines probability density $\rho^b(\lambda, t)$. Note that, unlike expressions (40a) and (40b), expression (40c) contains no reference to the isolated eigenvalues ε_I and corresponding probabilities w_I^a.

As required, for $t = 0$ all above expressions give $u^b(\lambda, 0) = 0$ and hence $\rho^b(\lambda, 0) = 0$. As t increases, one obtains nonvanishing probability density $\rho^b(\lambda, t)$ to find the state $|\Theta(t)\rangle$ in the state $|\Phi(k)\rangle$ that has eigenvalue $\lambda = \lambda(k)$. If there are no isolated eigenstates ($w_I^a = 0$) there is a well-defined limit $\rho^b(\lambda, \infty) = \lim_{t\to\infty} \rho^b(\lambda, t)$ to find local state $|\Theta\rangle$ after long enough time in the state $|\Phi(k)\rangle$. Otherwise for big times probability density $\rho^b(\lambda, t)$ exhibits an oscillatory behavior. Probability to find the state $|\Theta(t)\rangle$ at time t in the system $\mathcal{S}_\infty^b$, that is to find it in any of the states $|\Phi(k)\rangle \in X_\infty^b$, equals

$$w^b(t) = \int_{\lambda_a}^{\lambda_b} \rho^b(\lambda, t) \, \mathrm{d}\lambda. \tag{43a}$$

Relations of completeness require

$$w^a(t) + w^b(t) = 1. \tag{43b}$$

This relation should be satisfied for each time t.

5.1. *Decay of a local state in the weak coupling limit*

In the weak coupling limit above probabilities and probability densities simplify. If relation (26) has a root $\varepsilon_0 \in [\lambda_a, \lambda_b]$ and if β is relatively small, one has $\rho^a(\varepsilon) \approx \rho^{a0}(\varepsilon)$. If, in addition, $|\varepsilon_0 - \lambda_a| > \Delta\varepsilon_0$ and $|\varepsilon_0 - \lambda_b| > \Delta\varepsilon_0$ (resonance approximation) one has $\sum_I w_I^a \approx 0$. Amplitude (36b) can hence be approximated as

$$\langle\Theta|\Theta(t)\rangle \approx \int_{\lambda_a}^{\lambda_b} \rho^{a0}(\varepsilon) \exp\left(-\frac{\mathrm{i}\varepsilon t}{\hbar}\right) \mathrm{d}\varepsilon \approx \int_{-\infty}^{\infty} \rho^{a0}(\varepsilon) \exp\left(-\frac{\mathrm{i}\varepsilon t}{\hbar}\right) \mathrm{d}\varepsilon.$$

This integral has an exact solution

$$\langle\Theta|\Theta(t)\rangle \approx \mathrm{e}^{-\mathrm{i}\varepsilon_0 t/\hbar} \mathrm{e}^{-\pi\beta^2 f(\varepsilon_0)t/\hbar}. \tag{44a}$$

Hence

$$w^a(t) \approx w^{a0}(t) = \mathrm{e}^{-2\pi\beta^2 f(\varepsilon_0)t/\hbar}. \tag{44b}$$

This expression describes exponential decay of the state $|\Theta\rangle$. The mean life Δt of this state is

$$\Delta t = \frac{\hbar}{2\pi\beta^2 f(\varepsilon_0)}. \tag{44c}$$

This is consistent with the width $\Delta\varepsilon_0 = 2\pi\beta^2 f(\varepsilon_0)$ of the shifted eigenvalue ε_0:

$$\Delta\varepsilon_0 \Delta t = \hbar.$$

In the same approximation amplitude $u^b(\lambda, t)$ is found to be (see appendix)

$$u^b(\lambda, t) \approx u^{b0}(\lambda, t) = i\beta\sqrt{f(\lambda)}\frac{e^{-\pi\beta^2 f(\varepsilon_0)t/\hbar}e^{-i(\varepsilon_0-\lambda)t/\hbar} - 1}{\pi\beta^2 f(\varepsilon_0) + i(\varepsilon_0 - \lambda)}. \tag{45}$$

Probability density $\rho^b(\lambda, t)$ is hence

$$\rho^b(\lambda, t) \approx \rho^{b0}(\lambda, t)$$
$$= \frac{\beta^2 f(\lambda)}{\pi^2\beta^4 f^2(\varepsilon_0) + (\varepsilon_0 - \lambda)^2}$$
$$\times \left[e^{-2\pi\beta^2 f(\varepsilon_0)t/\hbar} - 2e^{-\pi\beta^2 f(\varepsilon_0)t/\hbar}\cos\left(\frac{(\varepsilon_0 - \lambda)t}{\hbar}\right) + 1 \right]. \tag{46a}$$

In particular, if $t = 0$ one obtains as required $\rho^{b0}(\lambda, 0) = 0$, while in a limit $t \to \infty$ one has

$$\rho^{b0}(\lambda, \infty) = \frac{\beta^2 f(\lambda)}{\pi^2\beta^4 f^2(\varepsilon_0) + (\varepsilon_0 - \lambda)^2} = \frac{f(\lambda)}{f(\varepsilon_0)}\rho^{a0}(\lambda) \approx \rho^{a0}(\lambda). \tag{46b}$$

More precisely, (46a) reduces to (46b) if $2\pi\beta^2 f(\varepsilon_0)t/\hbar \gg 1$. This condition reads

$$t \gg \frac{\hbar}{2\pi\beta^2 f(\varepsilon_0)} = \Delta t.$$

Thus approximation (46b) applies to such times t that are bigger than the mean life Δt of the state $|\Theta\rangle$. According to this expression, in a resonance approximation and in a limit $t \to \infty$ transition probability $\rho^b(\lambda, \infty)$ approximately equals resonance curve $\rho^{a0}(\lambda)$. Since $\rho^{a0}(\lambda)$ has maximum at the point ε_0, transition probability $\rho^b(\lambda, \infty)$ has maximum at the point $\lambda_{\max} \approx \varepsilon_0$.

If one integrates probability density $\rho^{b0}(\lambda, t)$ over all $\lambda \in [\lambda_a, \lambda_b]$ one obtains (see appendix)

$$w^b(t) \approx \int_{\lambda_a}^{\lambda_b} \rho^{b0}(\lambda, t)\,dk = 1 - e^{-2\pi\beta^2 f(\varepsilon_0)t/\hbar}. \tag{47}$$

Relations (44b) and (47) are in accord with the completeness requirement (43).

If $E \notin [\lambda_a, \lambda_b]$ is not too close to the band edges and if β is small, one has $\int \rho^a(\varepsilon)\,d\varepsilon \approx 0$. In this case $|\Theta(t)\rangle \approx |\Theta\rangle$ and there is no decay. Hence $w^a(t) \approx 1$ and $\rho^b(\lambda, t) \approx 0$.

6.   Generalized eigenvalue equation

In some cases one has to consider more general problems where instead of the eigenvalue equation (2a) one has generalized eigenvalue equation

$$\mathbf{B}\big|\Phi(k)\big\rangle = \lambda(k)\mathbf{S}^b\big|\Phi(k)\big\rangle, \quad k \in [k_a, k_b], \tag{2a'}$$

where $\mathbf{B}$ and $\mathbf{S}^b$ are Hermitian operators while $\mathbf{S}^b$ is, in addition, positive definite. Eigenstates $|\Phi(k)$ can be now orthonormalized according to

$$\big\langle\Phi(k)\big|\mathbf{S}^b\big|\Phi(k')\big\rangle = \delta\big(k - k'\big). \tag{2b'}$$

In addition, instead of the eigenvalue equation (3a) one has a more general eigenvalue equation

$$\mathbf{H}|\Psi\rangle = \varepsilon\mathbf{S}|\Psi\rangle, \tag{3a'}$$

where

$$\mathbf{H} = \mathbf{A} + \mathbf{B} + \beta\mathbf{V}, \qquad \mathbf{S} = |\Theta\rangle\langle\Theta| + \mathbf{S}^b + \beta\mathbf{P} \tag{3b'}$$

and where $\mathbf{S}$ is a positive definite Hermitian operator.

It is easy to modify all obtained results in order to find corresponding relations for the above generalized problem. In particular, and as suggested by the relations (7) and (8), operator $\mathbf{V}$ should be everywhere replaced with $\mathbf{V} - \varepsilon\mathbf{P}$. For example, functions $f(\lambda)$ and $\omega(\varepsilon)$ generalize to

$$f(\lambda) = \frac{\langle\Theta|\mathbf{V} - \varepsilon\mathbf{P}|\Phi(k)\rangle\langle\Phi(k)|\mathbf{V} - \varepsilon\mathbf{P}|\Theta\rangle}{\mathrm{d}\lambda(k)/\mathrm{d}k}\bigg|_{\lambda=\lambda(k)}, \qquad \lambda \in [\lambda_a, \lambda_b],$$

$$\omega(\varepsilon) = P\int_{k_a}^{k_b} \frac{\langle\Theta|\mathbf{V} - \varepsilon\mathbf{P}|\Phi(k)\rangle\langle\Phi(k)|\mathbf{V} - \varepsilon\mathbf{P}|\Theta\rangle}{\varepsilon - \lambda(k)}\,\mathrm{d}k, \quad \varepsilon \in (-\infty, \infty).$$

One can again express $\omega(\varepsilon)$ in terms of $f(\lambda)$ according to (10c) and (19c), and relations (10a) and (19a) that refer to the eigenvalues of the combined system are still valid. In the case of isolated eigenstates relations (16) are modified to

$$|\Psi_I\rangle = \frac{1}{Q_I^{1/2}}\left[|\Theta\rangle + \beta\int_{k_a}^{k_b} \frac{\langle\Phi(k)|\mathbf{V} - \varepsilon_I\mathbf{P}|\Theta\rangle}{\varepsilon_I - \lambda(k)}\big|\Phi(k)\big\rangle\mathrm{d}k\right], \quad \varepsilon_I \notin [\lambda_a, \lambda_b],$$

where

$$Q_I = 1 + \beta^2\int_{k_a}^{k_b} \frac{\langle\Theta|\mathbf{V} - \lambda(k)\mathbf{P}|\Phi(k)\rangle\langle\Phi(k)|\mathbf{V} - \lambda(k)\mathbf{P}|\Theta\rangle}{(\varepsilon_I - \lambda(k))^2}\,\mathrm{d}k$$

$$- \beta^2\int_{k_a}^{k_b}\langle\Theta|\mathbf{P}\big|\Phi(k)\big\rangle\big\langle\Phi(k)\big|\mathbf{P}|\Theta\rangle\,\mathrm{d}k.$$

In a similar way can be modified all other expressions.

7. Example: interaction of a single state with one-dimensional solid in the nearest-neighbor tight-binding approximation

In order to illustrate suggested method, consider the following simple model. As a system $\mathcal{S}_\infty^b$ take one-dimensional solid in the nearest-neighbor tight-binding approximation [2,7]. With each site of this solid is associated a single state $|j\rangle$ ($j = 1, 2, \ldots$). In this approximation one assumes matrix elements $\langle i|\mathbf{H}|i\rangle$ between states on the same atomic site to equal α, and matrix elements $\langle i|\mathbf{H}|j\rangle$ between states on the adjacent atomic sites to equal γ. All remaining matrix elements are zero. This model is widely used in chemistry where it is known as a Hückel approximation [7]. Without loss of generality one can assume $\alpha = 0$ and $\gamma = 1$. The only effect of this assumption is the redefinition of zero eigenvalue and of eigenvalue rescaling. Eigenvalues λ_i and eigenstates $|\Phi_i\rangle$ of such one-dimensional solid containing n atoms are [7]:

$$\lambda_i = 2\cos\left(\frac{\pi}{n+1}i\right), \quad |\Phi_i\rangle = \sqrt{\frac{2}{n+1}} \sum_{j=1}^n \sin\left(\frac{\pi}{n+1}ij\right)|j\rangle, \qquad i = 1, \ldots, n.$$

(48)

We refer to such a solid as a Hückel chain. System $\mathcal{S}_\infty^b$ is an infinite Hückel chain, which is obtained in the limit $n \to \infty$. In this limit eigenvalues λ_i are replaced with a continuous function $\lambda(k) = 2\cos(k)$ of a parameter k ($0 < k < \pi$), and discrete eigenstates $|\Phi_i\rangle$ are replaced with continuous eigenstates $|\Phi(k)\rangle$:

$$\lambda(k) = 2\cos(k), \quad |\Phi(k)\rangle = \sqrt{\frac{2}{\pi}} \sum_{j=1}^\infty \sin(jk)|j\rangle, \qquad 0 < k < \pi. \tag{49}$$

Relations (49) give all necessary information for the system $\mathcal{S}_\infty^b$. This system contains a single continuous eigenvalue band $\lambda(k)$ in the interval $[\lambda_a, \lambda_b] \equiv [-2, 2]$. The system $\mathcal{S}_1^a$ contains a single state $|\Theta\rangle$ with the eigenvalue E. An arbitrary interaction between $\mathcal{S}_1^a$ and $\mathcal{S}_\infty^b$ can be written in the form $\beta\mathbf{V}$ ($\beta \geqslant 0$) where matrix element of the Hermitian operator $\mathbf{V}$ between the state $|\Theta\rangle$ and jth state of the Hückel chain is $\langle\Theta|\mathbf{V}|j\rangle = \beta_j$, and where this operator is normalized according to $\langle\Theta|\mathbf{V}^2|\Theta\rangle = 1$. This normalization is equivalent to the condition $\sum_j \beta_j^2 = 1$. Hence and from (49) one obtains

$$\langle\Theta|\mathbf{V}|\Phi(k)\rangle = \sqrt{\frac{2}{\pi}} \sum_{j=1}^\infty \beta_j \sin(kj), \tag{50a}$$

$$\sum_j \beta_j^2 = 1. \tag{50b}$$

Relations (50) describe an arbitrary interaction of the local state $|\Theta\rangle$ with the infinite Hückel chain. In this general form the state $|\Theta\rangle$ is allowed to interact with each state $|j\rangle$ of the Hückel chain. Usually this interaction is confined to few initial states close
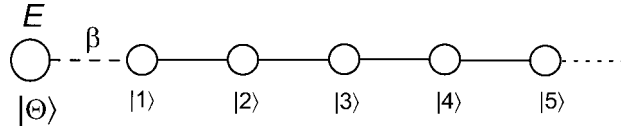
Figure 3. Interaction of a local state $|\Theta\rangle$ (system $\mathcal{S}_1^a$) with the infinite one-dimensional solid (Hückel chain) in the nearest-neighbor tight-binding approximation (system $\mathcal{S}_\infty^b$). State $|\Theta\rangle$ has eigenvalue E and it interacts with a first atom of the one-dimensional solid. Coupling parameter is β.

to the surface of a solid. For the sake of simplicity we will assume that local state $|\Theta\rangle$ interacts only with the first state $|1\rangle$. In this case (50) reduces to

$$\langle\Theta|\mathbf{V}|\Phi(k)\rangle = \sqrt{\frac{2}{\pi}} \sin(k), \tag{51}$$

where $\langle\Theta|\mathbf{V}|1\rangle = \beta_1 = 1$. This situation is shown in figure 3.

Function $\lambda(k)$ as defined in (49) is nonincreasing in the interval $[\lambda_a, \lambda_b]$, while we have assumed in the theoretical considerations that $\lambda(k)$ is nondecreasing. This can be easily corrected by a formal replacement of a parameter k with a parameter $k' = \pi - k$. However, we prefer not to change the expression (49) for this function. Instead, in the definition (11) of the function $f(\varepsilon)$ one should take the absolute value of the derivative $d\lambda/dk$ in order to ensure the nonnegativity of $f(\varepsilon)$.

Relations (11), (49) and (51) imply

$$f(\lambda) = \left.\frac{\sin(k)}{\pi}\right|_{\lambda = 2\cos(k)} = \frac{1}{\pi}\sqrt{1 - \frac{\lambda^2}{4}}, \quad \lambda \in [-2, 2]. \tag{52}$$

Hence and from (10c) and (19c)

$$\omega(\varepsilon) = \frac{1}{\pi} P \int_{-2}^{2} \frac{\sqrt{1 - \lambda^2/4}}{\varepsilon - \lambda} d\lambda, \quad \varepsilon \in (-\infty, \infty). \tag{53}$$

One can integrate this expression to obtain

$$\omega(\varepsilon) = \frac{1}{2} \begin{cases} \left(\varepsilon + \sqrt{\varepsilon^2 - 4}\right), & \text{if } \varepsilon < -2, \\ \varepsilon, & \text{if } \varepsilon \in [-2, 2], \\ \left(\varepsilon - \sqrt{\varepsilon^2 - 4}\right), & \text{if } \varepsilon > 2. \end{cases} \tag{54}$$

We have now all necessary information for the description of the combined system $\mathcal{S}_\infty \equiv \mathcal{S}_1^a \oplus \mathcal{S}_\infty^b$.

In the following discussion we will make frequent reference to the "weak" and "strong" coupling between subsystems $\mathcal{S}_1^a$ and $\mathcal{S}_\infty^b$ of a system $\mathcal{S}_\infty$. Since the interaction between adjacent sites of the Hückel chain is normalized to $\gamma = 1$, coupling β is weak if $\beta \ll 1$ and it is strong if $\beta \geqslant 1$ or if $\beta \approx 1$. Only if $\beta \ll 1$ one can consider the state $|\Theta\rangle \in X_1^a$ to be loosely bound to the Hückel chain. If, however, $\beta \approx 1$ or $\beta > 1$ interaction between two adjacent sites of the Hückel chain is smaller or at best

approximately equal to the interaction of the local state $|\Theta\rangle$ and this chain. This is strong coupling.

7.1. Isolated eigenstates

Let us first consider isolated eigenstates of the combined system $\mathcal{S}_\infty$. Function $\omega(\varepsilon)$ given by the relation (54) is continuous on the entire real axis. In particular, in the points $\lambda_a = -2$ and $\lambda_b = 2$ this function is finite: $\omega_a \equiv \omega(\lambda_a) = -1$ and $\omega_b \equiv \omega(\lambda_b) = 1$. There are hence finite critical points that determine existence and nonexistence of the isolated eigenstates. According to (13) one has

$$E_L = -2 + \beta^2, \qquad\qquad E_R = 2 - \beta^2, \qquad\qquad (55a)$$

$$\beta_L = (2 + E)^{1/2} \quad \text{if } E > -2, \qquad \beta_R = (2 - E)^{1/2} \quad \text{if } E < 2. \qquad (55b)$$

Considered as a function of E, necessary and sufficient condition for the existence of the left-isolated eigenstate is $E < E_L$, while necessary and sufficient condition for the existence of the right-isolated eigenstate is $E > E_R$. In particular, if $\beta < \sqrt{2}$ then $E_L < E_R$. In this case and if $E \in [E_L, E_R]$ no isolated eigenstate exists. However, if the coupling is as strong as $\beta > \sqrt{2}$ then $E_L > E_R$. In this case for each E at least one isolated eigenstate exists. In addition, if $E \in [E_R, E_L]$ both isolated eigenstates exist. Considered as a function of β, if $E > 2$ right-isolated eigenstate exists for each value of β. If, however, $E < 2$, necessary and sufficient condition for the existence of this eigenstate is $\beta > \beta_R$. Similar conclusion applies to the left-isolated eigenstate.

Inserting (54) into basic relation (10a), right- ($\varepsilon_R > 2$) and left- ($\varepsilon_L < -2$) isolated eigenvalues are found to satisfy

$$\frac{\beta^2}{2}\left(\varepsilon_R - \sqrt{\varepsilon_R^2 - 4}\right) + E - \varepsilon_R = 0, \quad \varepsilon_R > 2, \qquad (56a)$$

$$\frac{\beta^2}{2}\left(\varepsilon_L + \sqrt{\varepsilon_L^2 - 4}\right) + E - \varepsilon_L = 0, \quad \varepsilon_L < -2. \qquad (56b)$$

Those equations have a solution

$$\varepsilon_R = \frac{E(\beta^2 - 2) + \beta^2\sqrt{E^2 + 4(\beta^2 - 1)}}{2(\beta^2 - 1)}, \quad \text{if } E > 2 - \beta^2, \qquad (57a)$$

$$\varepsilon_L = \frac{E(\beta^2 - 2) - \beta^2\sqrt{E^2 + 4(\beta^2 - 1)}}{2(\beta^2 - 1)}, \quad \text{if } E < \beta^2 - 2. \qquad (57b)$$

Isolated eigenvalues ε_R and ε_L are eigenvalues of the infinite system $\mathcal{S}_\infty$. One can compare those eigenvalues with corresponding eigenvalues of a finite system $\mathcal{S}_{n+1}$. Isolated eigenvalues of $\mathcal{S}_{n+1}$ can be defined in the following way: All eigenvalues of a finite noninteracting Hückel chain satisfy $-2 < \lambda_i < 2$. Interlacing rule implies that, once the interaction $\beta \neq 0$ is included, perturbed eigenvalues ε_r also satisfy $-2 < \varepsilon_r < 2$, except possibly the smallest eigenvalue $\varepsilon_{\min}(n) \equiv \varepsilon_1$ and the largest eigenvalue $\varepsilon_{\max}(n) \equiv \varepsilon_{n+1}$ (see figure 2). Since in the limit $n \to \infty$ eigenvalues of an infinite noninteracting Hückel

chain assume all values in the interval $[-2, 2]$, one should identify $\varepsilon_{\max}(n)$ with right-isolated eigenvalue $\varepsilon_R(n)$ if and only if $\varepsilon_{\max}(n) > 2$. Otherwise right-isolated eigenstate does not exist. Similarly one should identify $\varepsilon_{\min}(n)$ with left-isolated eigenvalue $\varepsilon_L(n)$ if and only if $\varepsilon_{\min}(n) < -2$. Otherwise left-isolated eigenstate does not exists. Accordingly, $E_R(n)$ is a right-critical point of $\mathcal{S}_{n+1}$ if $E \leqslant E_R(n)$ implies $\varepsilon_{\max}(n) \leqslant 2$, and if, in addition, $E > E_R(n)$ implies $\varepsilon_{\max}(n) > 2$. Thus if $E = E_R(n)$ one should have $\varepsilon_{\max}(n) = 2$. Similarly is defined left-critical point $E_L(n)$. Since $\mathcal{S}_{n+1}$ is a finite-dimensional system, this system can be solved by a standard diagonalization method. In this way one can find isolated eigenvalues $\varepsilon_L(n)$ and $\varepsilon_R(n)$. Those eigenvalues can be compared with eigenvalues ε_L and ε_R given by expressions (57). If those expressions are correct, as n increases $\varepsilon_L(n)$ should converge to ε_L while $\varepsilon_R(n)$ should converge to ε_R.

The comparison of ε_R and $\varepsilon_R(n)$ is shown in figure 4. In figure 4(a) are compared right-isolated eigenvalues ε_R of an infinite system $\mathcal{S}_\infty$ (solid lines) with right-isolated eigenvalues $\varepsilon_R(10)$ of the corresponding finite system $\mathcal{S}_{10+1}$ that contains Hückel chain with $n = 10$ atoms (dashed lines). Quantities ε_R and $\varepsilon_R(n)$ are plotted as functions of the local eigenvalue E for four selected values of the coupling β. If the eigenvalue ε_R does not exist ($E \leqslant E_R$) we set $\varepsilon_R = 0$, and similarly if the eigenvalue $\varepsilon_R(10)$ does not exist ($E \leqslant E_R(10)$ i.e., $\varepsilon_{\max}(10) \leqslant 2$) we set $\varepsilon_R(10) = 0$. If there is no interaction ($\beta = 0$) right-isolated eigenvalue equals local eigenvalue ($\varepsilon_R = E$), and critical point of $\mathcal{S}_\infty$ is $E_R = 2$. As the interaction β increases, eigenvalue ε_R also increases, and the onset of a critical point $E_R = 2 - \beta^2$ moves to the lower values of the eigenvalue E. Note that $E_R(n) \geqslant E_R$ and if $E \leqslant E_R$ neither ε_R nor $\varepsilon_R(n)$ exists. Hence one should compare ε_R and $\varepsilon_R(n)$ only for those values of E that satisfy $E > E_R$.

The curves ε_R and $\varepsilon_R(10)$ in figure 4(a) are very close to each other and they differ to any significan amount only in the vicinity of the critical point. In particular, in the interval between critical points E_R and $E_R(10)$, right-isolated eigenvalue ε_R exists, while right-isolated eigenvalue $\varepsilon_R(10)$ does not exists. With the increase of n eigenvalues $\varepsilon_R(n)$ converge to the eigenvalue ε_R. This convergence is shown in figure 4(b). In this figure differences $\Delta\varepsilon_R(n) = \varepsilon_R(n) - \varepsilon_R$ for the curve $\beta = 0.8$ from figure 4(a) are given. In order to emphasize the convergence of $\varepsilon_R(n)$ to ε_R, vertical scale in figure 4(b) is amplified by the factor 10^5 relative to the vertical scale in figure 4(a). As n increases, eigenvalues $\varepsilon_R(n)$ converge very fast to the eigenvalue ε_R. The only significant discrepancy is in a region close to the critical point $E_R = 2 - \beta^2 = 1.36$ and on the right-hand side of this point. However, this region also decreases with the increase of n. Thus one finds $\Delta\varepsilon_R(20) < 10^{-15}$ if $(E - E_R) > 1$, $\Delta\varepsilon_R(80) < 10^{-15}$ if $(E - E_R) > 0.2$ and $\Delta\varepsilon_R(320) < 10^{-15}$ if $(E - E_R) > 0.03$. The dimension of the region where ε_R differs from $\varepsilon_R(n)$ by more than 10^{-15} uniformly decreases with the increase of n. One can also consider the convergence of the critical points $E_R(n)$ to the limit critical point E_R. One finds: $E_R(10) = 1.4181818, \ldots, E_R(80) = 1.3679022$, $E_R(160) = 1.3639752$, $E_R(320) = 1.3619937$. Those numbers converge to $E_R = 1.36$. Moreover, a linear extrapolation of last two values against $1/n$ produces estimate $E_R(\infty) = 1.3600123$. This agrees up to five significant figures with E_R. Quadratic extrapolation of last three values gives $E_R(\infty) = 1.3600000$. This agrees
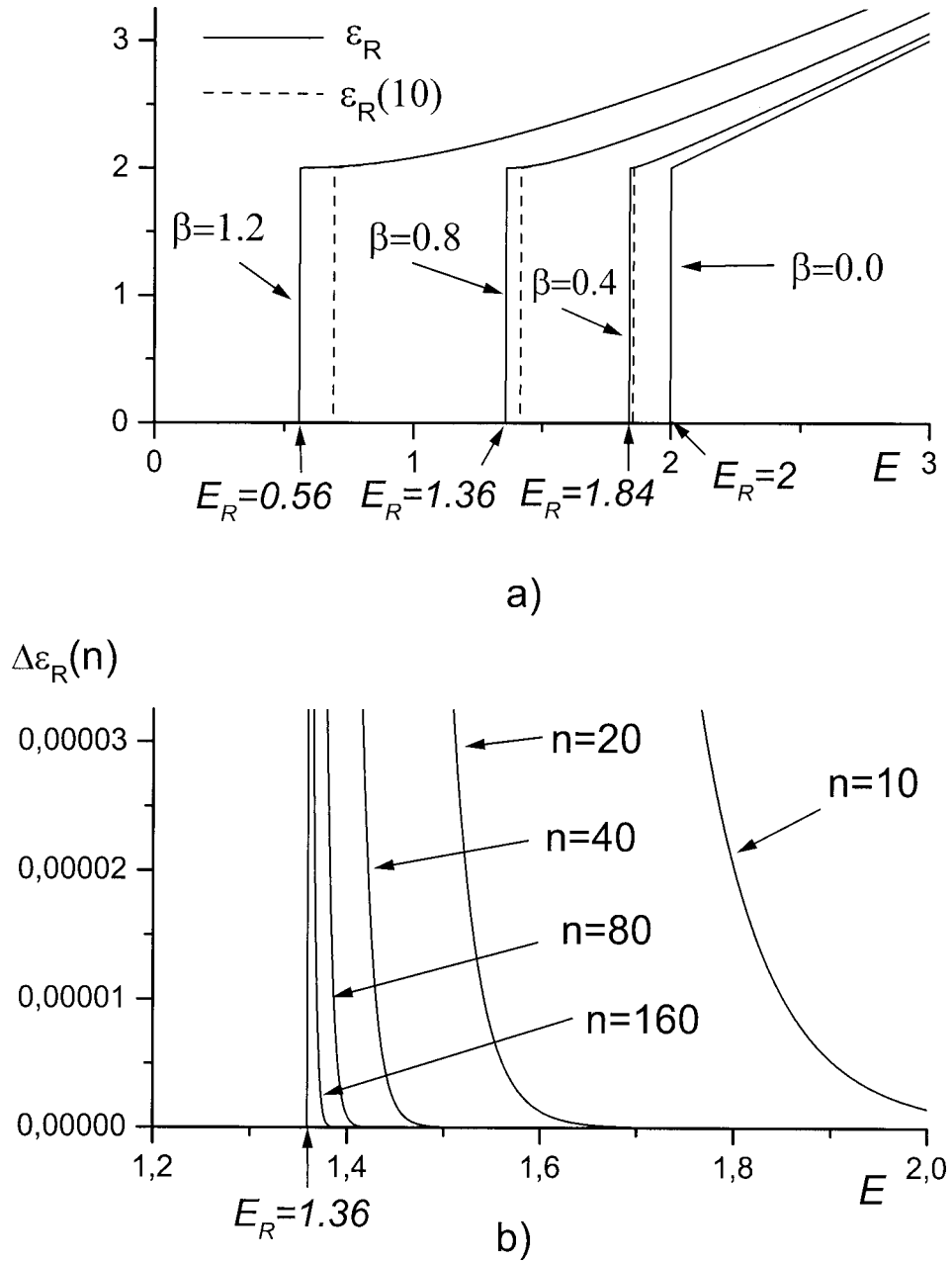
Figure 4. Isolated eigenvalues ε_R of an infinite system $\mathcal{S}_\infty$ and eigenvalues $\varepsilon_R(n)$ of the corresponding finite systems $\mathcal{S}_{n+1}$ given as functions of the local eigenvalue E. (a) Eigenvalues ε_R (solid lines) and corresponding eigenvalues $\varepsilon_R(10)$ (dashed lines) for few selected values of β. (b) Differencies $\Delta\varepsilon_R(n) = \varepsilon_R - \varepsilon_R(n)$ for few selected values of n. Coupling is $\beta = 0.8$ from figure (a). Point $E_R = 2 - \beta^2 = 1.36$ is a critical point for a system $\mathcal{S}_\infty$.

with E_R up to eight significant figures. Those extrapolations demonstrate convergence $\lim_{n\to\infty} E_R(n) = E_R$.

Once the eigenvalue ε_I is known, one can find the corresponding isolated eigenstate $|\Psi_I\rangle$. According to (16) one has

$$|\Psi_I\rangle = \frac{1}{\sqrt{Q_I}}\left[|\Theta\rangle + \beta\sqrt{\frac{2}{\pi}}\int_0^\pi \frac{\sin(k)}{\varepsilon_I - 2\cos(k)}|\Phi(k)\rangle\,dk\right], \tag{58a}$$

where

$$Q_I = 1 - \beta^2\frac{d\omega(\varepsilon_I)}{d\varepsilon_I} = 1 + \frac{\beta^2}{2\sqrt{\varepsilon_I^2 - 4}}\begin{cases} \varepsilon_I + \sqrt{\varepsilon_I^2 - 4}, & \text{if } \varepsilon_I = \varepsilon_L < -2, \\ \varepsilon_I - \sqrt{\varepsilon_I^2 - 4}, & \text{if } \varepsilon_I = \varepsilon_R > 2 \end{cases} \tag{58b}$$

and where ε_I is given by (57).

In particular, the probability $w_R^a = |\langle\Theta|\Psi_R\rangle|^2$ to find the right-isolated eigenstate $|\Psi_R\rangle$ in a local state $|\Theta\rangle$ and the probability density $\rho_R^b(k) = |\langle\Phi(k)|\Psi_R\rangle|^2$ to find this eigenstate in the state $|\Phi(k)\rangle$ are

$$w_R^a = \frac{1}{1 + (\beta^2/2)((\varepsilon_R - \sqrt{\varepsilon_R^2 - 4})/\sqrt{\varepsilon_R^2 - 4})}, \qquad \varepsilon_R > 2, \tag{59a}$$

$$\rho_R^b(k) = \frac{2\beta^2}{\pi[\varepsilon_R - 2\cos(k)]^2}$$

$$\times \frac{\sin^2(k)}{1 + (\beta^2/2)((\varepsilon_R - \sqrt{\varepsilon_R^2 - 4})/\sqrt{\varepsilon_R^2 - 4})}, \qquad k \in [-2, 2]. \tag{59b}$$

Similar expressions are obtained for the probability $w_L^a = |\langle\Theta|\Psi_L\rangle|^2$ and probability density $\rho_L^b(k) = |\langle\Phi(k)|\Psi_L\rangle|^2$.

One can compare above quantities with results for a finite system $\mathcal{S}_{n+1}$. In particular, one can compare probabilities w_R^a with corresponding probabilities $w_{max}^a(n)$ for the systems $\mathcal{S}_{n+1}$. Note that $w_{max}^a(n) = |\langle\Theta|\Psi_{n+1}\rangle|^2$ is a probability to find eigenstate $|\Psi_{max}\rangle \equiv |\Psi_{n+1}\rangle$ with the maximum eigenvalue $\varepsilon_{max} \equiv \varepsilon_{n+1}$ in the local state $|\Theta\rangle$. This probability equals probability $w_R^a(n)$ whenever $\varepsilon_{max} > \lambda_b = 2$. However, if $\varepsilon_{max} \leqslant 2$ probability $w_R^a(n)$ drops to zero, while probability $w_{max}^a(n)$ is still different from zero. For the purpose of comparison with probabilities w_R^a, it is more instructive to use probabilities $w_{max}^a(n)$ instead of probabilities $w_R^a(n)$, since those former probabilities differ from w_R^a to any significant amount in much larger range. In particular, if $E \leqslant E_R$ probabilities w_R^a and $w_R^a(n)$ are both zero, while probability $w_{max}^a(n)$ differs from zero.

In figure 5 are compared in this way probabilities w_R^a (solid lines) with probabilities $w_{max}^a(n)$ (dashed lines). Those probabilities are given as functions of a coupling β. In figure 5(a) probabilities w_R^a are plotted for few selected values of E. Those probabilities are compared with corresponding probabilities $w_{max}^a(10)$ for the finite systems $\mathcal{S}_{10+1}$ containing Hückel chain with 10 atoms. If $E > 2$ right-isolated eigenstate exists for each value of β (curve $E = 2.5$). If $E < 2$ there is a critical point $\beta_R = \sqrt{2 - E}$ such
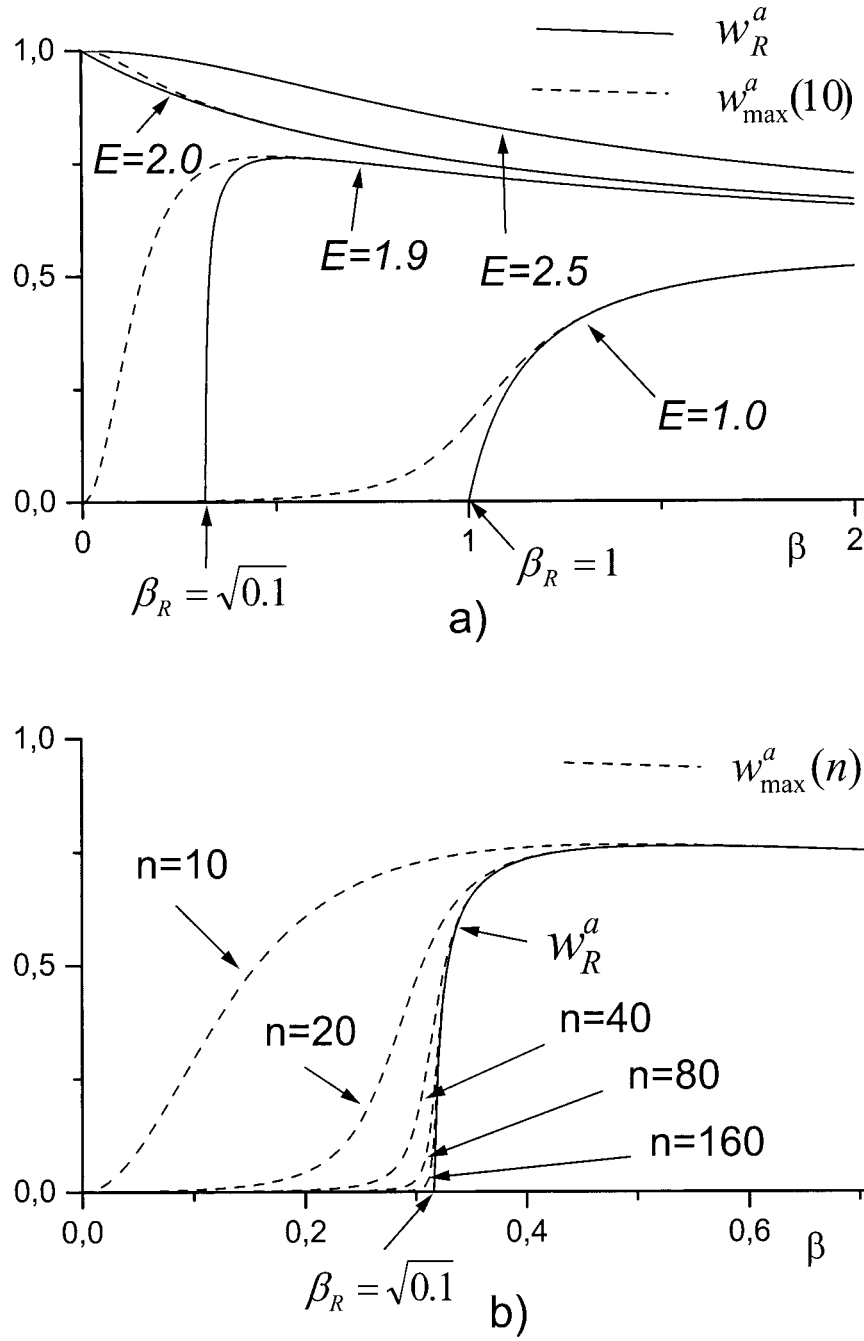
Figure 5. Probabilities w_R^a (solid lines) and $w_{max}^a(n)$ (dashed lines) as functions of the coupling β. (a) Probabilities w_R^a and $w_{max}^a(10)$ as functions of β for few selected values of the local eigenvalue E. (b) Convergence of the probabilities $w_{max}^a(n)$ to the probability w_R^a as n increases. Probability w_R^a is line $E = 1.9$ from figure (a) and critical point for the corresponding infinite system $\mathcal{S}_\infty$ is $\beta_R = \sqrt{\lambda_b - E} = 0.3162$.

that for $\beta < \beta_R$ no isolated eigenstate exists (curve $E = 1.9$ with a critical point $\beta_R = \sqrt{0.1} = 0.3162$ and curve $E = 1$ with a critical point $\beta_R = 1$). Case $E = 2$ is a border case when isolated eigenstate exists for each $\beta \neq 0$. The convergence of the probabilities $w^a_{\max}(n)$ to the probability w^a_R as n increases is illustrated in figure 5(b). Probability w^a_R (solid line) is line $E = 1.9$ from figure 5(a). Dashed lines are probabilities $w^a_{\max}(n)$ for various values of n. Since each probability $w^a_R(n)$ equals probability $w^a_{\max}(n)$ truncated below the critical point $\beta_R(n)$, and since $\lim_{n \to \infty} \beta_R(n) = \beta_R$, this also demonstrates the convergence $w^a_R(n) \to w^a_R$ with the increase of n.

7.2. Embedded eigenstates

Consider now embedded eigenstates of the combined system $\mathcal{S}_\infty$. Inserting (52) and (54) into (21) fractional shift $x(\varepsilon)$ is found to be

$$x(\varepsilon) = \frac{1}{\pi} \cot^{-1}\left(\frac{\varepsilon(1 - \beta^2/2) - E}{\beta^2 \sqrt{1 - \varepsilon^2/4}}\right), \quad \varepsilon \in [-2, 2]. \tag{60}$$

According to (23) probability density $\rho^a(\varepsilon) = |\langle \Theta | \Psi(\varepsilon) \rangle|^2$ to find local state $|\Theta\rangle$ in the perturbed eigenstate $|\Psi(\varepsilon)\rangle$ is

$$\rho^a(\varepsilon) = \frac{\beta^2 \sqrt{1 - \varepsilon^2/4}}{\pi \beta^4 (1 - \varepsilon^2/4) + \pi(\beta^2 \varepsilon/2 + E - \varepsilon)^2}, \quad \varepsilon \in [-2, 2]. \tag{61}$$

One can compare this probability density with probabilities $w^a_r = |\langle \Theta | \Psi_r \rangle|^2$ that are obtained in the case of the finite combined system $\mathcal{S}_{n+1}$. Since in the limit $n \to \infty$ probabilities w^a_r are replaced with $\rho^a(\varepsilon)d\varepsilon$, one should compare density $\rho^a(\varepsilon_r)$ with discrete probability w^a_r normalized per unit interval, i.e., one should compare $\rho^a(\varepsilon_r)$ with the ratio $w^a_r/\Delta\varepsilon_r$ where $\Delta\varepsilon_r = \varepsilon_r - \varepsilon_{r-1}$. Slightly better choice is to use the average of the intervals $\Delta\varepsilon_{r+1}$ and $\Delta\varepsilon_r$ on both sides of the eigenvalue ε_r instead of the interval $\Delta\varepsilon_r$ alone. From this comparison isolated eigenstates, if any, should be excluded. In addition, the smallest and the largest eigenvalue that in a limit $n \to \infty$ converge to some point inside the band $[\lambda_a, \lambda_b]$ should be separately normalized, since for the purpose of normalization only the intervals $\Delta\varepsilon_r$ that are inside the band $[\lambda_a, \lambda_b]$ can be utilized. Hence if $\mathcal{S}_\infty$ contains no isolated eigenvalue, extreme eigenvalues ε_1 and ε_{n+1} of $\mathcal{S}_{n+1}$ should be normalized according to $W^a_1 = w^a_1/\Delta\varepsilon_2$ and $W^a_{n+1} = w^a_{n+1}/\Delta\varepsilon_{n+1}$, respectively. Accordingly, in the absence of isolated eigenstates we make the following comparison

$$\rho^a(\varepsilon_r) \leftrightarrow W^a_r = \begin{cases} \dfrac{w^a_1}{\Delta\varepsilon_2}, & \text{if } r = 1, \\[2mm] \dfrac{w^a_r}{(\Delta\varepsilon_r + \Delta\varepsilon_{r+1})/2}, & \text{if } r = 2, \ldots, n, \\[2mm] \dfrac{w^a_{n+1}}{\Delta\varepsilon_{n+1}}, & \text{if } r = n + 1. \end{cases} \tag{62}$$

If the system $\mathcal{S}_\infty$ contains left-isolated eigenstate one should in the above expression replace $w_1^a/\Delta\varepsilon_2$ with $w_2^a/\Delta\varepsilon_3$, while if this system contains right-isolated eigenstate one should replace $w_{n+1}^a/\Delta\varepsilon_{n+1}$ with $w_n^a/\Delta\varepsilon_n$.

In figure 6 is compared in this way continuous probability density $\rho^a(\varepsilon)$ (dashed lines) with normalized discrete probabilities W_r^a (vertical columns) for the case $E = 0.5$ and $\beta = 0.9$. In order to emphasize the convergence of probabilities W_r^a to $\rho^a(\varepsilon)$ as n increases, density $\rho^a(\varepsilon)$ is compared with probabilities W_r^a for the system $\mathcal{S}_{5+1}$ (figure 6(a)) and with probabilities W_r^a for the system $\mathcal{S}_{100+1}$ (figure 6(b)). Even in the case when the system $\mathcal{S}_{n+1}$ is as small as $n = 5$, the agreement of probabilities W_r^a with the continuous density distribution $\rho^a(\varepsilon)$ is quite good. Standard deviation of normalized probabilities W_r^a from the corresponding densities $\rho^a(\varepsilon_r)$ ($r = 1, \ldots, 6$) is $\Delta \approx 0.029$. In the case $n = 100$ the agreement between probabilities W_r^a and corresponding densities $\rho^a(\varepsilon_r)$ ($r = 1, \ldots, 101$) substantially improves, and one finds $\Delta \approx 0.00056$. If one excludes points W_1^a and W_{101}^a that are least reliable and that are close to the edge of the interval $[-2, 2]$, standard deviation drops to $\Delta \approx 0.00004$. In general, with the increase of n results for a finite system $\mathcal{S}_{n+1}$ rapidly converge to the theoretical value $\rho^a(\varepsilon)$. In figure 6 system $\mathcal{S}_\infty$ without isolated eigenstates is considered. However, the agreement is equally good in those cases when $\mathcal{S}_\infty$ contains isolated eigenstates.

If the coupling is weak and if the relation (26) has a root $\varepsilon_0 \in [-2, 2]$, one can approximate $\rho^a(\varepsilon)$ with resonant curve $\rho^{a0}(\varepsilon)$. One finds

$$\varepsilon_0 = \frac{2E}{2 - \beta^2} \in [-2, 2] \quad \text{if} \quad |E| \leqslant |2 - \beta^2|. \tag{63a}$$

If $\beta^2 < 2$ and since $E_R = 2 - \beta^2$ and $E_L = \beta^2 - 2$, above condition is equivalent to the requirement that there are no isolated eigenstates. Hence in the case of the weak coupling and if $|E| \leqslant |2 - \beta^2|$ completeness relation (25) implies $\int \rho^a(\varepsilon)\,d\varepsilon = 1$.

According to (28) approximate density $\rho^{a0}(\varepsilon)$ is

$$\rho^{a0}(\varepsilon) = \frac{\beta^2\sqrt{1 - \varepsilon_0^2/4}}{\pi\beta^4(1 - \varepsilon_0^2/4) + \pi(\varepsilon - \varepsilon_0)^2}, \quad \varepsilon \in [-2, 2]. \tag{64}$$

This is a universal resonance curve centered at $\varepsilon = \varepsilon_0$ and with a width

$$\Delta\varepsilon_0 = 2\beta^2\sqrt{1 - \frac{\varepsilon_0^2}{4}}. \tag{63b}$$

If $|E| > |2 - \beta^2|$ relation (26) has no root in the interval $[\lambda_a, \lambda_b]$, and hence $\rho^{a0}(\varepsilon) = 0$. If the coupling is weak, this implies $\rho^a(\varepsilon) \approx 0$. Also the condition $|E| > |2 - \beta^2|$ guaranties the existence of at least one isolated eigenstate. However, if the coupling is strong, the approximation (64) fails, and one should use exact expression (61).

In conclusion, in the case of weak interaction and provided $|E| < |2 - \beta^2|$ the effect of the interaction is that local eigenvalue E shifts to the eigenvalue ε_0, and this shifted eigenvalue broadens to $\Delta\varepsilon_0$. There are no isolated eigenstates and hence $\int \rho^a(\varepsilon)\,d\varepsilon = 1$.
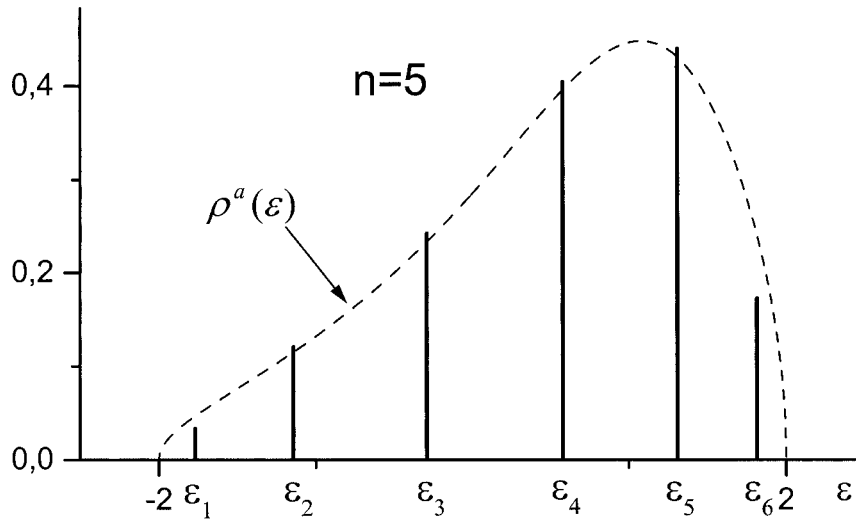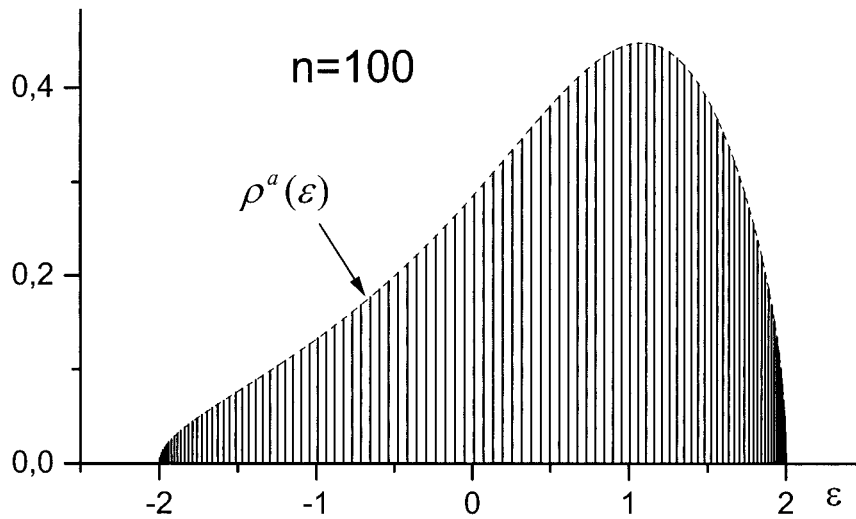
Figure 6. Density distribution $\rho^a(\varepsilon)$ of a system $\mathcal{S}_\infty$ (dashed lines) and normalized probabilities W_r^a of the corresponding system $\mathcal{S}_{n+1}$ (vertical columns) in the case $E = 0.5$ and $\beta = 0.9$. Each vertical column is situated at the positions ε_k of the corresponding perturbed eigenvalue and the height of this column is normalized probability W_r^a. (a) Quantities W_r^a refer to a system $\mathcal{S}_{5+1}$. (b) Quantities W_r^a refer to a system $\mathcal{S}_{100+1}$.

If, however, $|E| > |2 - \beta^2|$ there exist at least one isolated eigenstate, and hence $\int \rho^a(\varepsilon) \, d\varepsilon < 1$. In this case the approximation (64) fails.

We compare $\rho^a(\varepsilon)$ with resonant curve approximation $\rho^{a0}(\varepsilon)$ in figure 7. In this figure case $E = 1.7$ for two qualitatively different values of the coupling β is considered. In figure 7(a) exact density $\rho^a(\varepsilon)$ (solid line) is compared with approximate density $\rho^{a0}(\varepsilon)$ (dashed line) for the coupling $\beta = 0.3$. In this case there is no isolated eigenstate and hence $w_C^a \equiv \int \rho^a(\varepsilon) \, d\varepsilon = 1$. Though interaction is relatively strong, density $\rho^{a0}(\varepsilon)$ is quite good approximation of the exact density $\rho^a(\varepsilon)$. Due to the interaction eigenvalue $E = 1.7$ shifts to the new position $\varepsilon_0 = 1.7801$ and it broadens to the width $\Delta\varepsilon_0 = 0.082$. Note that maximum of the exact density $\rho^a(\varepsilon)$ is $\varepsilon_{\max} = 1.7821$, while approximation (29a) yields $\varepsilon_0 \approx 1.7765$. In general, the root ε_0 of (26) is much better approximation of the true maximum $\varepsilon_{\max}$ of $\rho^a(\varepsilon)$ than the approximation (26). In figure 7(b) coupling is quite strong ($\beta = 1.1$). The density $\rho^a(\varepsilon)$ is now very different from a resonant curve and approximation $\rho^{a0}(\varepsilon)$ fails. In particular, relation (26) has no root $\varepsilon_0 \in [\lambda_a, \lambda_b]$. In addition, one finds $w_C^a \equiv \int \rho^a(\varepsilon) \, d\varepsilon = 0.34506 < 1$. Eigenvalue distribution of a state $|\Theta\rangle$ hence includes contribution of a right-isolated eigenstate $|\Psi_R\rangle$ in addition to the density $\rho^a(\varepsilon)$. Using (57a) one finds isolated eigenvalue $\varepsilon_R = 2.36642$. Probability to find local state $|\Theta\rangle$ in the eigenstate $|\Psi_R\rangle$ is given by (59a) and one finds $w_R^a = 0.65494$. Hence $w_R^a + w_C^a = 1$ in accord with completeness relation (24). Note also that in this case approximation (18) fails, and hence it is not possible to obtain ε_R within the standard perturbation expansion.

Completeness relation (24) is verified in more details in figure 8. In this figure probabilities w_L^a, w_R^a and $w_C^a = \int \rho^a(\varepsilon) \, d\varepsilon$ as well as their sum $w_C^a + w_L^a + w_R^a$ are plotted as functions of a coupling β. This is done for two qualitatively different values of the local eigenvalue E. In figure 8(a) one has $E = 1.5 \in [\lambda_a, \lambda_b]$. There are hence two critical points, a critical point $\beta_R = \sqrt{2 - E} = 0.70711$ for the right-isolated eigenstate, and a critical point $\beta_L = \sqrt{2 + E} = 1.87083$ for the left-isolated eigenstate. If $\beta < \beta_R$ there is no right-isolated eigenstate, while if $\beta < \beta_L$ there is no left-isolated eigenstate. If the coupling is as small as $\beta \in [0, \beta_R]$ no isolated eigenstate exist. One has $w_C^a = 1$ and the state $|\Theta\rangle$ is a linear combination of the embedded eigenstates $|\Psi(\varepsilon)\rangle$ alone. If $\beta \in [\beta_R, \beta_L]$ only right-isolated eigenstate $|\Psi_R\rangle$ exists. The state $|\Theta\rangle$ is hence a linear combination of this eigenstate and embedded eigenstates $|\Psi(\varepsilon)\rangle$. In this case $w_C^a + w_R^a = 1$. Finally if $\beta > \beta_L$ both isolated eigenstates exist and they both contribute to the local state $|\Theta\rangle$. In this case $w_C^a + w_R^a + w_L^a = 1$ in accord with completeness requirement (24). In figure 8(b) one has $E = 2.1 > \lambda_b$. In this case right-isolated eigenstate exists for each value of β. However, left-isolated eigenstate exist if and only if $\beta > \beta_L = 2.02485$. One again finds $w_C^a + w_R^a + w_L^a = 1$ in complete agreement with the relation (24).

In the entire interval $\beta \in [0, 3]$ shown in figure 8 theoretical probabilities w_C^a, w_L^a and w_R^a are in perfect agreement with completeness relation (24). This demonstrates that, unlike standard perturbation expansion, the suggested approach does not suffer from any convergence problem, and the obtained relations are equally efficient for each coupling, however strong. The only case when a caution is required is when the system
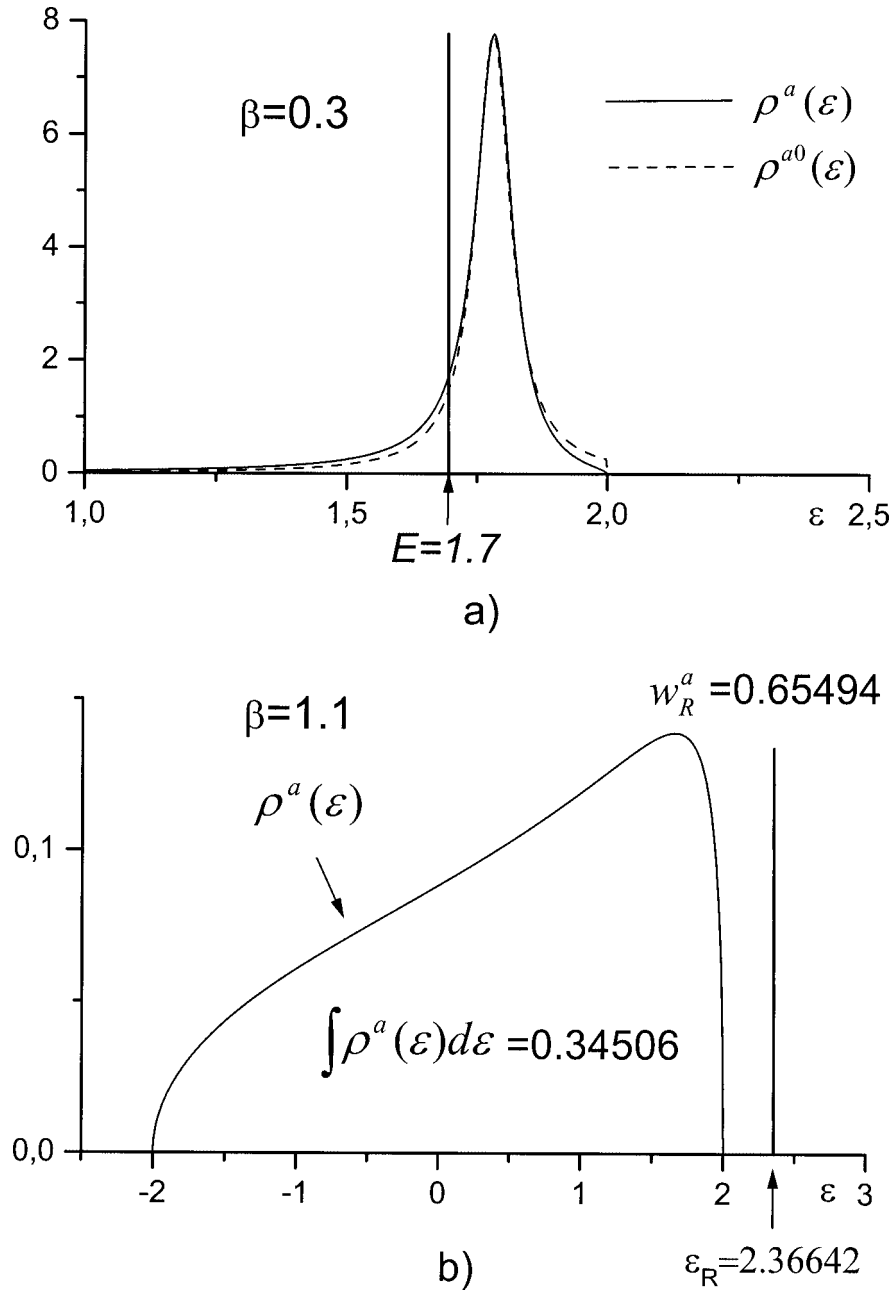
Figure 7. Eigenvalue distributions of the local state $|\Theta\rangle$ in the case $E = 1.7$. (a) $\beta = 0.3$. Density distribution $\rho^a(\varepsilon)$ is relatively well approximated with truncated universal resonance curve $\rho^{a0}(\varepsilon)$. No isolated eigenstate exist. Typical for such weak coupling is eigenvalue shift and eigenvalue spread. (b) $\beta = 1.1$. Approximation $\rho^{a0}(\varepsilon)$ fails and density distribution is distorted. In addition, eigenvalue distribution of the state $|\Theta\rangle$ contains isolated eigenvalue ε_R.
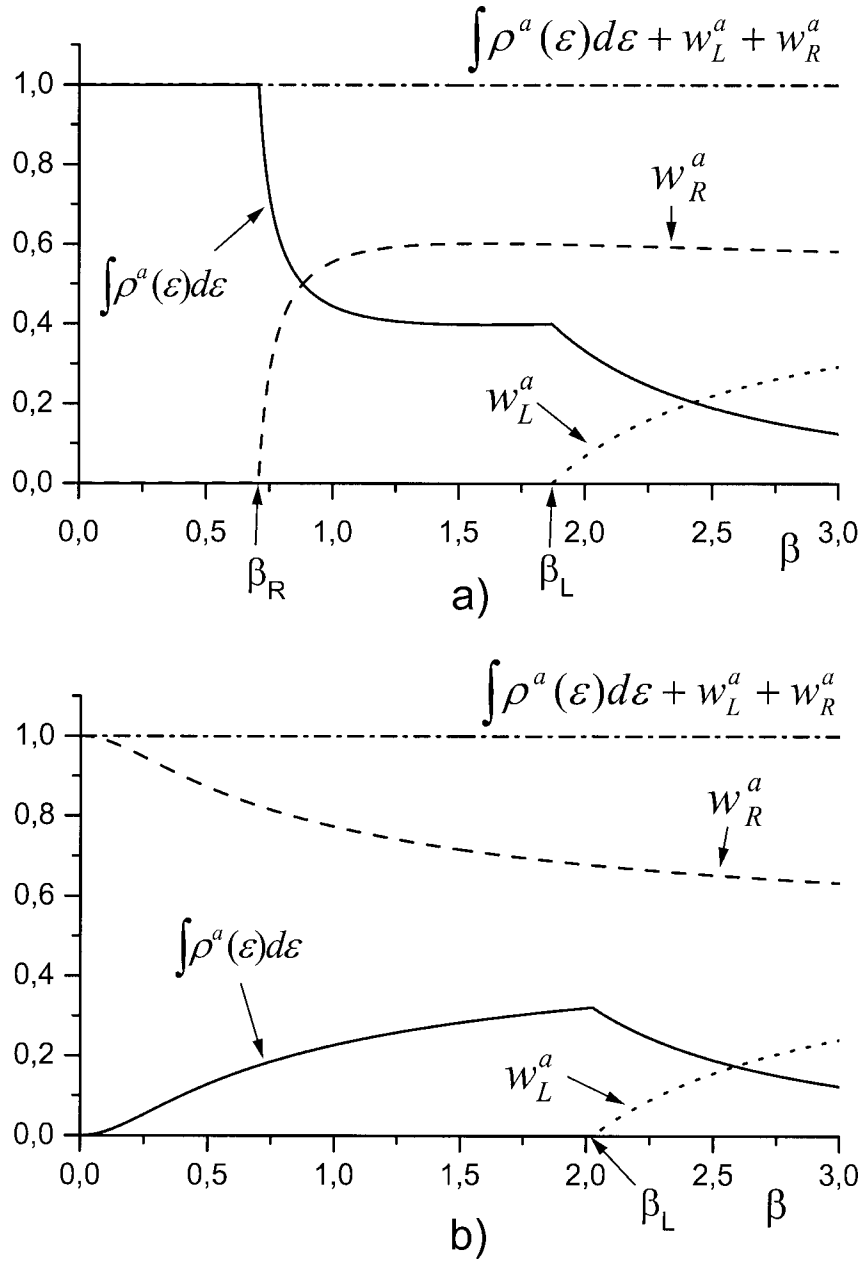
Figure 8. Probabilities w_L^a, w_R^a and $w_C^a = \int \rho^a(\varepsilon)\,d\varepsilon$ as functions of a coupling β for two qualitatively different values of the local eigenvalue E. (a) $E = 1.5$. (b) $E = 2.1$.

contains some anomal point $\varepsilon = \varepsilon_c$ [4]. In this case one may have $w_C^a + w_R^a + w_L^a < 1$. Missing probability is due to anomal point contributions. Those contributions can be also expressed in a closed form, which restores validity of the completeness relation (24) [4].

7.3. Time evolution of a local state

If the combined system $\mathcal{S}_\infty$ is at time $t = 0$ prepared in a local state $|\Theta\rangle \in X_1^a$, at some later time t it will evolve in the state $|\Theta(t)\rangle$. Probability $w^a(t)$ to find the state $|\Theta(t)\rangle$ at time t in the initial state $|\Theta(0)\rangle \equiv |\Theta\rangle$ is a square of the amplitude $\langle\Theta|\Theta(t)\rangle$. This amplitude is given by basic relation (36b). In our case $\rho^a(\varepsilon)$ in this relation is density (61), isolated eigenvalues ε_I are given by (57), while the corresponding probabilities w_I^a are given by (59a) for the probability w_R^a and by an analogous expression for the probability w_L^a. Similarly, probability density $\rho^b(\lambda, t)$ for the transition of the state $|\Theta(t)\rangle$ at time t in any particular state $|\Phi(k)\rangle \in X_\infty^b$ is a square of the amplitude $u^b(\lambda, t)$. This amplitude is given by basic relation (40a) where quantities $f(\lambda)$ and $\rho^a(\varepsilon)$ are expressed by (52) and (61), respectively. In order to verify relations (36b) and (40) one can compare probability $w^a(t)$ and probability density $\rho^b(\lambda, t)$ obtained by those relations with corresponding probabilities for a finite combined system $\mathcal{S}_{n+1}$.

In figure 9 combined system $\mathcal{S}_\infty$ with local eigenvalue $E = 1.5$ and with two qualitatively different values of the coupling β is considered. In this figure probabilities $w^a(t)$ (solid lines) are compared with corresponding probabilities $w_n^a(t)$ for selected finite combined systems $\mathcal{S}_{n+1}$ (other lines). Those probabilities are given as functions of time t. Time is expressed in units $\hbar/\gamma$ where γ is a resonance interaction between adjacent atoms of a Hückel chain. This is a natural time unit for a model considered. In the case $\beta = 0.6$ (figure 9(a)) system $\mathcal{S}_\infty$ contains no isolated eigenstate, and hence after long enough time the state $|\Theta(t)\rangle$ makes a complete decay to the system $\mathcal{S}_\infty^b$, i.e., $\lim_{t\to\infty} w^a(t) = 0$. In order to illustrate the convergence of $w_n^a(t)$ to $w^a(t)$ as n increases, probability $w^a(t)$ is compared with successive probabilities $w_5^a(t)$, $w_{10}^a(t)$ and $w_{20}^a(t)$. For small times t probabilities $w_n^a(t)$ follow theoretical curve $w^a(t)$. However, each curve $w_n^a(t)$ at some large enough time t' separates from $w^a(t)$. As n increases t' also increases. In the case $\beta = 1.5$ (figure 9(b)) system $\mathcal{S}_\infty$ contains right-isolated eigenstate $|\Psi_R\rangle$ and the state $|\Theta(t)\rangle$ only partially decays to the system $\mathcal{S}_\infty^b$. This decay exhibits damped oscillations, and for large times probability $w^a(t)$ converges to $(w_R^a)^2 = 0.36165$. This probability is compared with probabilities $w_{10}^a(t)$ and $w_{20}^a(t)$. For small times probabilities $w_n^a(t)$ again follow theoretical curve $w^a(t)$, while at some large enough time t' each curve $w_n^a(t)$ separates from $w^a(t)$. As n increases this point of separation again shifts towards higher values of t.

Above property is quite general. Each probability $w_n^a(t)$ of a finite system $\mathcal{S}_{n+1}$ reproduces theoretical probability $w^a(t)$ of the corresponding infinite system $\mathcal{S}_\infty$ up to some point $t = t'$. If $t < t'$ probability $w_n^a(t)$ is virtually identical to the theoretical limit probability $w^a(t)$. However, if $t > t'$ probability $w_n^a(t)$ deviates significantly from $w_n^a(t)$. As n increases the point $t = t'$ increases approximately linearly with n. In addition, the agreement between $w_n^a(t)$ and $w_n^a(t)$ for small values of t also improves. Accordingly, probabilities $w_n^a(t)$ converge to the probability $w^a(t)$ for an infinite system $\mathcal{S}_\infty$, i.e., $\lim_{n\to\infty} w_n^a(t) = w^a(t)$.

In figure 10 are compared exact probabilities $w^a(t)$ (solid lines) with approximate exponential decay probabilities $w^{a0}(t)$ (equation (44b)) for the case $E = 1.0$ and for
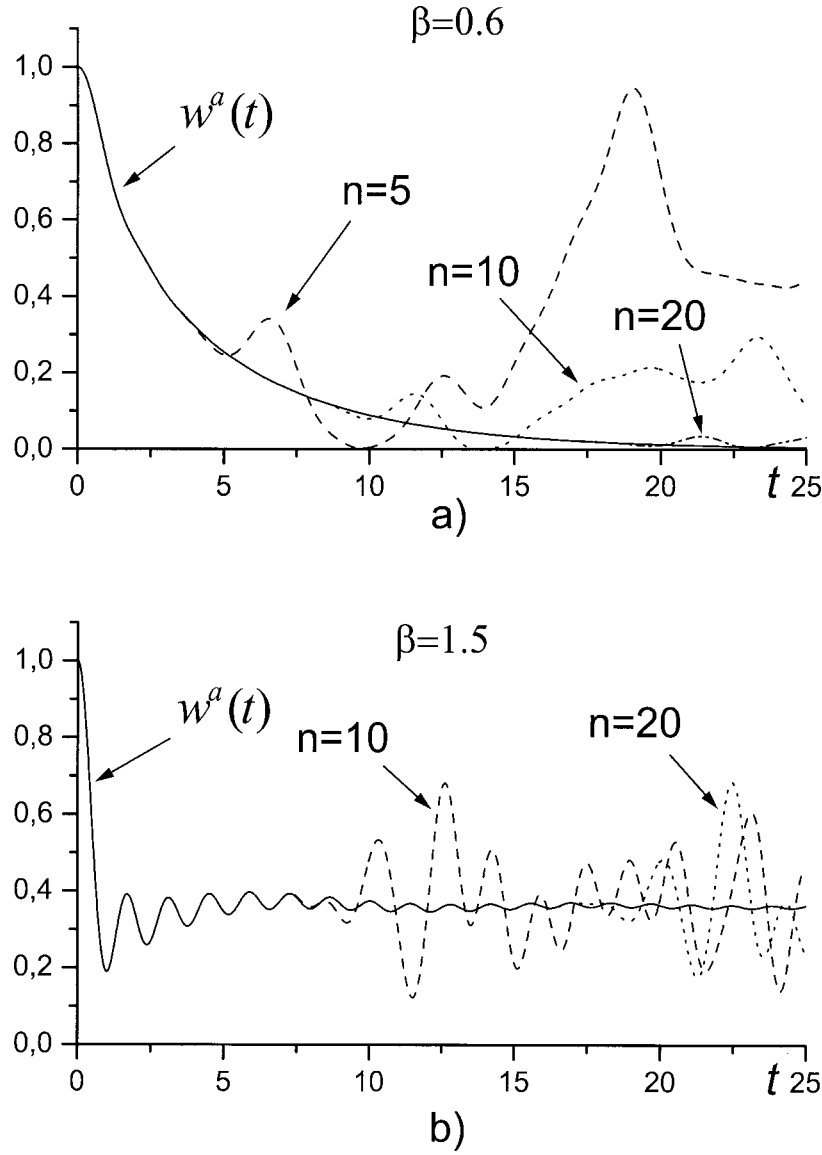
Figure 9. Probabilities $w^a(t)$ (solid lines) and probabilities $w_n^a(t)$ (other lines) in the case $E = 1.5$ and for two qualitatively different values of β (times in units of $\hbar/\gamma$). (a) $\beta = 0.6$. There is no isolated eigenstate and the state $|\Theta\rangle$ completely decays in the system $\mathcal{S}_\infty^b$. Probability $w^a(t)$ is compared with corresponding probabilities for finite combined systems $\mathcal{S}_{5+1}$, $\mathcal{S}_{10+1}$ and $\mathcal{S}_{20+1}$. (b) $\beta = 1.5$. Right isolated eigenstate exists and the decay of the state $|\Theta\rangle$ in the system $\mathcal{S}_\infty^b$ is oscillatory and only partial. Probability $w^a(t)$ is compared with corresponding probabilities for finite combined systems $\mathcal{S}_{10+1}$ and $\mathcal{S}_{20+1}$.

four qualitatively different values of a coupling β. In figure 10(a) coupling $\beta = 0.1$ is relatively weak and the probability $w^{a0}(t)$ is a good approximation of $w^a(t)$. In this case one has a standard exponential decay of a state $|\Theta(t)\rangle$. In figure 10(b) coupling
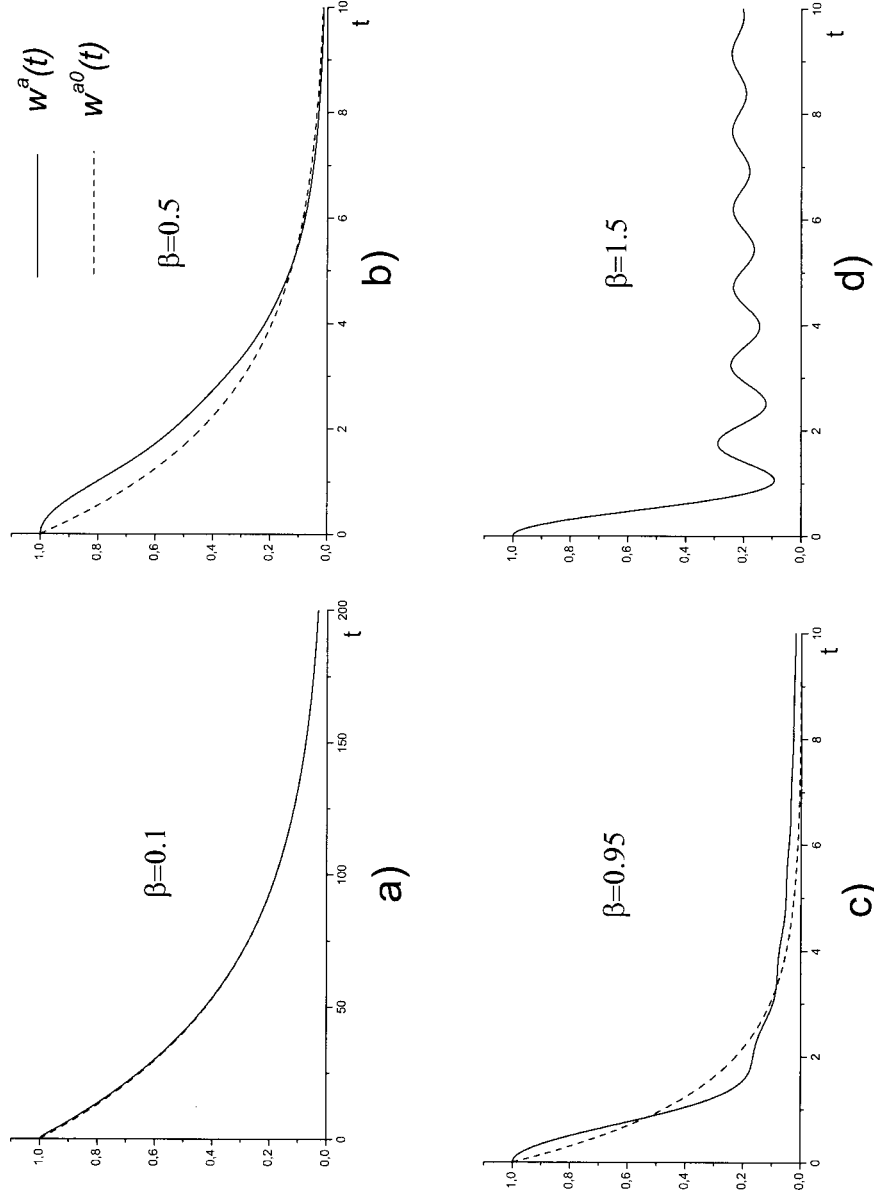
Figure 10. Exact probabilities $w^a(t)$ (solid lines) and approximate exponential decay probabilities $w^{a0}(t)$ (dashed lines) in the case $E = 1.0$ and for few selected values of the coupling β. (a) $\beta = 0.1$. $w^{a0}(t)$ is a good approximation of $w^a(t)$ and decay is exponential. (b) $\beta = 0.5$ and (c) $\beta = 0.95$. Exact decay $w^a(t)$ deviates from the approximate exponential decay $w^{a0}(t)$. (d) $\beta = 1.5$. Equation (26) has no root $\varepsilon_0 \in [-2, 2]$ and approximation $w^{a0}(t)$ fails.

$\beta = 0.5$ is much stronger and $w^{a0}(t)$ is not such a good approximation of $w^a(t)$. The same applies to the case $\beta = 0.95$ (figure 10(c)). Finally, in figure 10(d) coupling $\beta = 1.5$ is very strong, the system $\mathcal{S}_\infty$ contains right-isolated eigenstate, and resonant approximation $w^{a0}(t)$ fails.

Figures 9 and 10 illustrate global decay of a state $|\Theta(t)\rangle$. One can analyze this decay in more details by analyzing probability densities $\rho^b(\lambda, t)$ for the transition of the state $|\Theta(t)\rangle$ at time t in any particular state $|\Phi(k)\rangle \in X_\infty^b$. One can compare those probability densities with discrete probabilities $w_i^b(t) = |\langle\Phi_i|\Theta(t)\rangle|^2$ ($|\Phi_i\rangle \in X_n^b$) that apply to the corresponding finite system $\mathcal{S}_{n+1}$. In order to emphasize that λ_i is ith eigenvalue of the finite Hückel chain containing n atoms (system $\mathcal{S}_n^b$), we will denote this eigenvalue more explicitly as $\lambda_i^{(n)}$. Since $\rho^b(\lambda, t)\mathrm{d}\lambda$ is a probability to find a state $|\Theta(t)\rangle$ at time t in the state $|\Phi(k)\rangle$ ($\lambda = \lambda(k)$) and in the eigenvalue interval $\mathrm{d}\lambda$, one has to compare density $\rho^b(\lambda_i^{(n)}, t)$ with discrete probability $w_i^b(t)$ normalized per unit interval $\Delta\lambda_i$. In analogy to (62), one finds that continuous probability density $\rho^b(\lambda, t)$ should be compared with discrete normalized probabilities $W_i^b(t)$ according to

$$\rho^b\big(\lambda_i^{(n)}, t\big) \leftrightarrow W_i^b(t) = \begin{cases} \dfrac{w_1^b(t)}{\Delta\lambda_2}, & \text{if } i = 1, \\[2mm] \dfrac{w_i^b(t)}{(\Delta\lambda_i + \Delta\lambda_{i+1})/2}, & \text{if } i = 2, \ldots, n-1, \\[2mm] \dfrac{w_n^b(t)}{\Delta\lambda_n}, & \text{if } i = n. \end{cases} \quad (65)$$

Note that $\Delta\lambda_i \approx \Delta\varepsilon_i$ and in the limit $n \to \infty$ one has $\mathrm{d}\varepsilon = \mathrm{d}\lambda$ (see appendix). Hence in the case of large n there is no substantial difference between normalizations (62) and (65).

In figure 11 are compared in this way probability densities $\rho^b(\lambda, t)$ (dashed lines) with corresponding normalized probabilities $W_i^b(t)$ $i = 1, \ldots, n$ (vertical columns) for the case $E = 1.5$ and $\beta = 0.6$. Those parameters describe the same combined system $\mathcal{S}_\infty$ as in figure 9(a). Densities $\rho^b(\lambda, t)$ are shown as continuous functions of the unperturbed eigenvalue λ, while each normalized probability $W_i^b(t)$ is represented as a column situated at the position of the corresponding eigenvalue $\lambda_i^{(n)}$. This is done for three selected values of the time t (expressed in units of $\hbar/\gamma$). In figures 11(a), (b) one has $t = t_1 = 1$, in figures 11(c), (d) one has $t = t_2 = 5$, while in figures 11(e) and (f) one has $t = t_3 = 20$. Those values cover three characteristic moments in the time evolution of a state $|\Theta(t)\rangle$. One namely finds $w^a(t_1) = 0.75063$, $w^a(t_2) = 0.25422$ and $w^a(t_3) = 0.01264$ (compare with figure 9(a)). Thus at time $t = t_1$ the decay of the state $|\Theta(t)\rangle$ into the system $\mathcal{S}_\infty^b$ is on its beginning, at time $t = t_2$ this decay has already advanced, while at time $t = t_3$ it is almost completed. One finds that probabilities $w^a(t)$ are in accord with probability densities $\rho^b(\lambda, t)$. In particular, if one integrates probability densities $\rho^b(\lambda, t)$ over λ to obtain total probability $w^b(t)$ for the transition of the state $|\Theta(t)\rangle$ at time t into the system $\mathcal{S}_\infty^b$, one obtains: $w^b(t_1) = \int \rho^b(\lambda, t_1)\,\mathrm{d}\lambda = 0.24937$,
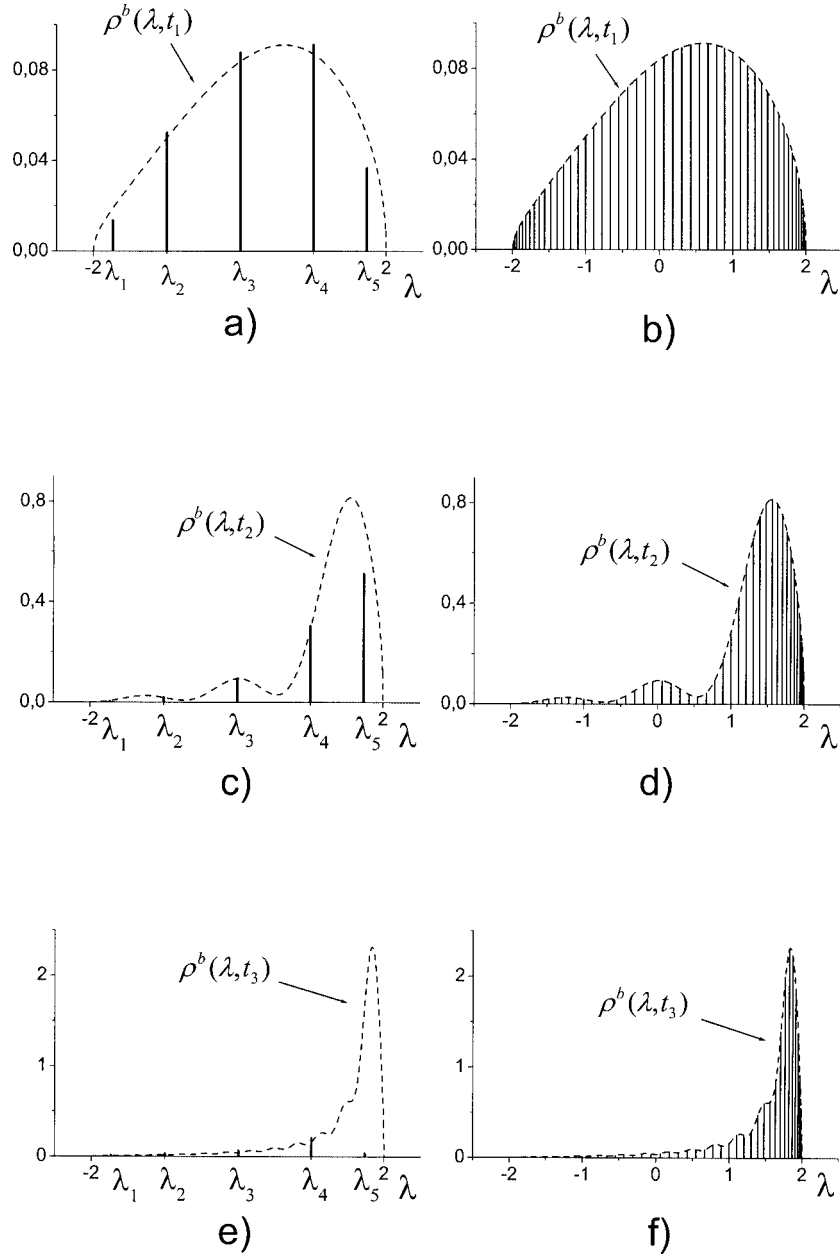
Figure 11. Probability densities $\rho^b(\lambda, t)$ (dashed lines) and normalized probabilities $W_i^b(t)$ for the corresponding finite systems S_{n+1} (vertical columns) in the case $E = 1.5$ and $\beta = 0.6$. Those quantities are shown as functions of the unperturbed eigenvalue λ for three selected values of time t: $t_1 = 1$, $t_2 = 5$ and $t_3 = 20$ (times in units of $\hbar/\gamma$). In (a), (c) and (e) system S_{5+1} is considered, while in (b), (d) and (f) system S_{50+1} is considered.

$w^b(t_2) = 0.74578$ and $w^b(t_3) = 0.98736$. Hence $w^a(t_i) + w^b(t_i) = 1$ ($i = 1, 2, 3$) in complete agreement with completeness requirement (43).

In order to illustrate convergence of normalized probabilities $W_i^b(t)$ to $\rho^b(\lambda, t)$ with the increase of n, probability densities $\rho^b(\lambda, t)$ are compared with normalized probabilities $W_i^b(t)$ for a finite system $\mathcal{S}_{5+1}$ (figures 11(a), (c) and (e)) and with normalized probabilities $W_i^b(t)$ for a finite system $\mathcal{S}_{50+1}$ (figures 11(b), (d) and (f)). Thus at time $t = t_1$ and in the case when the system $\mathcal{S}_{n+1}$ is as small as $n = 5$, standard deviation of five normalized probabilities $W_i^b(t_1)$ from the corresponding densities $\rho^b(\lambda_i^{(5)}, t_1)$ ($i = 1, \ldots, 5$) is $\Delta \approx 0.0075$ (figure 11(a)). In the case $n = 50$ the agreement between probabilities $W_i^b(t_1)$ and corresponding densities $\rho^b(\lambda_i^{(50)}, t_1)$ ($i = 1, \ldots, 50$) substantially improves and standard deviation drops to $\Delta \approx 0.0003$ (figure 11(b)). One finds similar improvements in the cases $t = t_2$ and $t = t_3$. In general, as n increases normalized probabilities $W_i^b(t)$ rapidly converge to the theoretical probability density $\rho^b(\lambda, t)$ for an infinite system. One can also compare exact density $\rho^b(\lambda, t)$ with approximate density $\rho^{b0}(\lambda, t)$ (equation (46a)). Though coupling $\beta = 0.6$ is quite strong, density $\rho^{b0}(\lambda, t)$ is relatively good approximation of $\rho^a(\lambda, t)$. We omit the details of this comparison here. Note only that in a resonance approximation and in a limit $t \to \infty$ one has $\rho^{b0}(\lambda, \infty) \approx \rho^{a0}(\lambda)$ (see equation (46b)). In this case maximum λ_{max} of the density $\rho^b(\lambda, \infty)$ is approximately $\lambda_{max} \approx \varepsilon_0$. In particular, in the case $E = 1.5$ and $\beta = 0.6$ one has $\varepsilon_0 = 1.82927$. Thus for large enough times density $\rho^b(\lambda, t)$ should have its maximum approximately at the point $\lambda_{max} \approx 1.82927$. One finds that density $\rho^b(\lambda, t_3)$ taken at relatively large time $t = t_3$ when the transition of the state $|\Theta(t)\rangle$ to the system $\mathcal{S}_\infty^b$ is mainly completed has maximum quite close to this point (see figures 11(e) and (f)).

Consider now the dependence of probabilities $W_i^b(t)$ and densities $\rho^b(\lambda, t)$ on time t. If one compares figures 11(a), (c) and (e) one can see that as time t increases, the agreement between discrete probabilities $W_i^b(t)$ and probability densities $\rho^b(\lambda_i^{(5)}, t)$ deteriorates. Thus, in the case $t = t_1$ standard deviation of normalized probabilities $W_i^b(t_1)$ from the corresponding densities $\rho^b(\lambda_i^{(5)}, t_1)$ is $\Delta \approx 0.0075$ (figure 11(a)), in the case $t = t_2$ this standard deviation increases to $\Delta \approx 0.0934$ (figure 11(c)), while in the case $t = t_3$ it increases to $\Delta \approx 0.7683$ (figure 11(e)). In this last case similarity between densities $\rho^b(\lambda_i^{(5)}, t_3)$ and probabilities $W_i^b(t_3)$ is completely lost. However, if n increases the agreement between probabilities $W_i^b(t_3)$ and densities $\rho^b(\lambda_i^{(n)}, t)$ is regained. Thus in the case $t = t_3$ and $n = 50$ one finds $\Delta \approx 0.0122$ (figure 11(f)), while if n increases to $n = 100$ standard deviation drops to $\Delta \approx 0.0043$.

Time dependence of densities $\rho^b(\lambda, t)$ is analyzed in more details in figure 12. In this figure the case $E = 1.0$ and $\beta = 0.5$ is considered. Those are the same parameters as in figure 10(b). Probability densities $\rho^b(\lambda, t)$ (solid lines) and corresponding normalized probabilities $W_i^b(t)$ (dashed lines) are plotted as functions of t for few selected unperturbed eigenvalues $\lambda_i^{(n)}$. In figures 12(a) and (c) system $\mathcal{S}_\infty$ is compared with finite system $\mathcal{S}_{10+1}$, while in figures 12(b) and (d) system $\mathcal{S}_\infty$ is compared with finite system $\mathcal{S}_{20+1}$. In particular, in figure 12(a) probability density $\rho^b(\lambda_5^{(10)}, t)$ ($\lambda_5^{(10)} = -0.28463$) is compared with the corresponding normalized probability $W_5^b(t)$ for a combined system
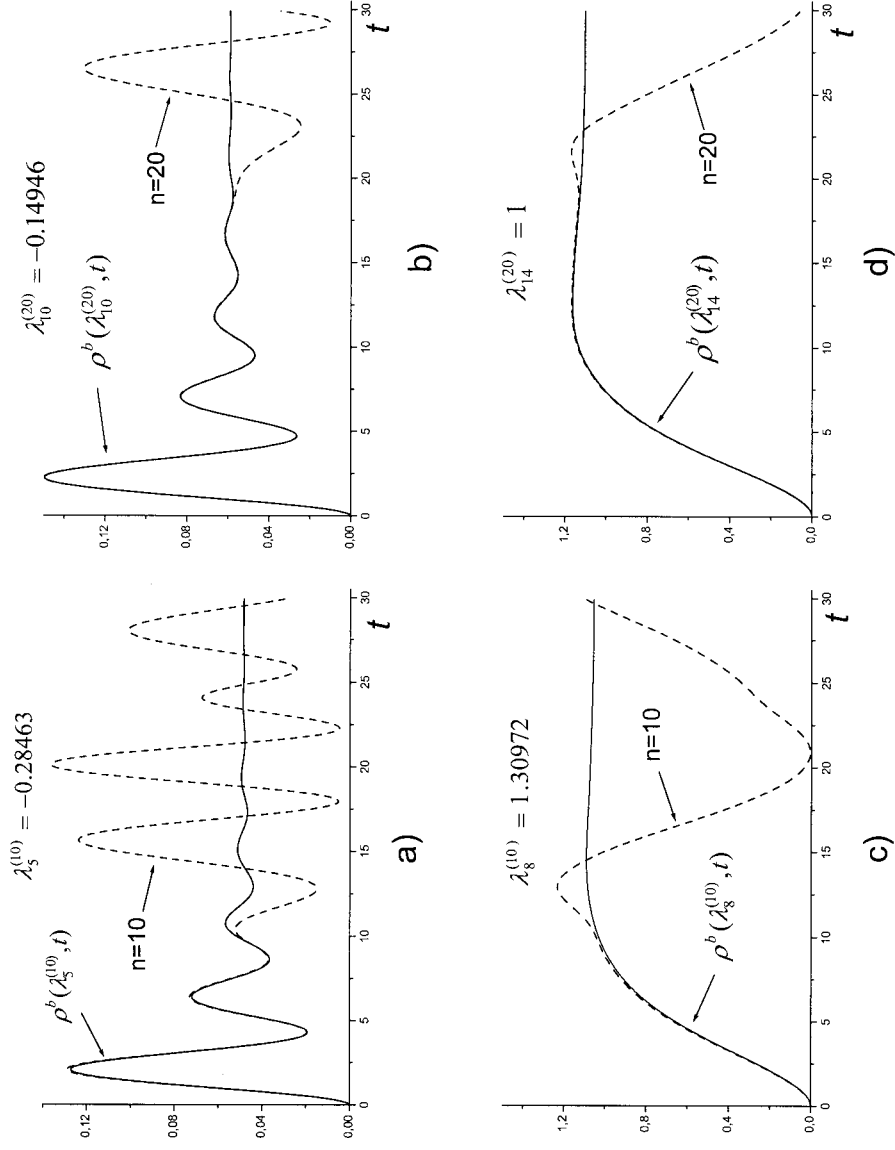
Figure 12. Probability densities $\rho^b(\lambda_i^{(n)}, t)$ (solid lines) and normalized probabilities $W_i^b(t)$ (dashed lines) in the corresponding finite systems $\mathcal{S}_{n+1}$ (dashed lines) in the case $E = 1$ and $\beta = 0.5$. Those quantities are shown as functions of time t for four selected unperturbed eigenvalues $\lambda_i^{(n)}$. (a) $\lambda_5^{(10)} = -0.28463$. (b) $\lambda_{10}^{(20)} = -0.14946$. (c) $\lambda_8^{(10)} = 1.30972$. (d) $\lambda_{14}^{(20)} = 1$.

$\mathcal{S}_{10+1}$. Note that in the case $E = 1.0$ and $\beta = 0.5$ one has $\varepsilon_0 = 1.14286$. Maximum $\lambda_{\max}$ of the probability density $\rho^b(\lambda, \infty)$ is hence $\lambda_{\max} \approx 1.14286$. Eigenvalue $\lambda_5^{(10)}$ is relatively far from this maximum, and the curve $\rho^b(\lambda_5^{(10)}, t)$ is oscillatory with an asymptotic value in a limit $t \to \infty$. This oscillatory behavior is in accord with the resonance approximation (46a). Normalized probability $W_5^b(t)$ initially follows the curve $\rho^b(\lambda_5^{(10)}, t)$, but for $t > t' \approx 10$ it starts to deviate from it. In figure 12(b) probability density $\rho^b(\lambda_{10}^{(20)}, t)$ $(\lambda_{10}^{(20)} = -0.14946)$ is compared with the corresponding normalized probability $W_{10}^b(t)$ for a combined system $\mathcal{S}_{20+1}$. Eigenvalue $\lambda_{10}^{(20)}$ is also relatively far from $\lambda_{\max}$. However, it is relatively close to the eigenvalue $\lambda_5^{(10)}$ and hence the corresponding theoretical curve $\rho^b(\lambda_{10}^{(20)}, t)$ is similar to the curve $\rho^b(\lambda_5^{(10)}, t)$. Since normalized probability $W_{10}^b(t)$ in figure 12(b) refers to the system $\mathcal{S}_{20+1}$, the agreement between $\rho^b(\lambda_{10}^{(20)}, t)$ and $W_{10}^b(t)$ is much better. In particular, the curve $W_{10}^b(t)$ deviates significantly from $\rho^b(\lambda_{10}^{(20)}, t)$ only for $t > t' \approx 20$. Similar comparisons are shown in figure 12(c) $(\lambda_8^{(10)} = 1.30972)$ and in figure 12(d) $(\lambda_{14}^{(20)} = 1)$. In those last two examples eigenvalues $\lambda_8^{(10)}$ and $\lambda_{14}^{(20)}$ are relatively close to the point $\lambda_{\max} \approx \varepsilon_0$, and the corresponding probability densities $\rho^b(\lambda_8^{(10)}, t)$ and $\rho^b(\lambda_{14}^{(20)}, t)$ are not oscillatory. This absence of oscillations close to the point ε_0 is suggested by the resonance approximation (46a). In addition, due to the vicinity of $\lambda_8^{(10)}$ and $\lambda_{14}^{(20)}$ to $\lambda_{\max}$, those densities are much larger that densities $\rho^b(\lambda_5^{(10)}, t)$ and $\rho^b(\lambda_{10}^{(20)}, t)$. Again, the increase of n from $n = 10$ to $n = 20$ significantly improves the agreement between theoretical densities for a system $\mathcal{S}_\infty$ and the corresponding normalized probabilities for a finite system $\mathcal{S}_{n+1}$. Note also that for $t > 10$ one has $w^a(t) \approx 0$ (see figure 10(b)) and for such times the decay of a state $|\Theta(t)\rangle$ to the system $\mathcal{S}_\infty^b$ is mainly completed. This is qualitatively in accord with figure 12 where probabilities $\rho^b(\lambda_i^{(n)}, t)$ change quite substantially for $t < 10$, while for $t > 10$ those probabilities approach to an asymptotic value.

Above behavior of densities $\rho^b(\lambda_i^{(n)}, t)$ and corresponding normalized probabilities $W_i^b(t)$ is analogous to the behavior of the probabilities $w^a(t)$ and $w_n^a(t)$ illustrated in figure 9. In general, each normalized probability $W_i^b(t)$ of a finite system $\mathcal{S}_{n+1}$ reproduces theoretical probability $\rho^b(\lambda_i^{(n)}, t)$ of the corresponding infinite system $\mathcal{S}_\infty$ up to some point $t = t'$. If $t < t'$ curve $W_i^b(t)$ is virtually identical to the theoretical curve $\rho^b(\lambda_i^{(n)}, t)$. However, if $t > t'$ curve $W_i^b(t)$ starts to deviate significantly from $\rho^b(\lambda_i^{(n)}, t)$. As n increases the point $t = t'$ increases approximately linearly with n. One finds that in all cases probabilities $W_i^b(t)$ converge to the probability $\rho^b(\lambda_i^{(n)}, t)$ of an infinite system $\mathcal{S}_\infty$.

7.4. General interaction of the state $|\Theta\rangle$ with the one-dimensional solid

In the above model we have considered a state $|\Theta\rangle$ that interacts with the first atom of the infinite one-dimensional solid (Hückel chain). This interaction is described by relation (51). In a more realistic model the state $|\Theta\rangle$ interacts with several atoms of

a Hückel chain, and in this case instead of the relation (51) one should use relation (50). Generalization to this case is straightforward. In particular, one finds

$$f(\varepsilon) = \left[\sum_j \beta_j a_j(\varepsilon) \right]^2, \qquad \omega(\varepsilon) = \sum_{ij} \beta_i \beta_j \omega_{ij}(\varepsilon), \qquad (66a)$$

where coefficients β_j satisfy $\sum_j \beta_j^2 = 1$ and where

$$a_j(\varepsilon) = \left. \frac{\sin(kj)}{\sqrt{\pi \sin(k)}} \right|_{\varepsilon = 2\cos(k)}, \qquad\qquad\qquad \varepsilon \in [-2, 2],$$

$$\omega_{ij}(\varepsilon) = P \frac{2}{\pi} \int_0^\pi \frac{\sin(ki)\sin(kj)}{\varepsilon - 2\cos(k)} dk = P \int_{-2}^2 \frac{a_i(x)a_j(x)}{\varepsilon - x} dx, \quad \varepsilon \in (-\infty, \infty).$$

$$(66b)$$

One can obtain all functions $\omega_{ij}(\varepsilon)$ and $a_j(\varepsilon)$ in a closed form [4]. One thus finds that each function $\omega_{ij}(\varepsilon)$ is continuous on the entire real axis. Accordingly, if the local state $|\Theta\rangle$ interacts with a finite number of the states $|j\rangle \in X_\infty^b$ of an infinite Hückel chain, characteristic function $\omega(\varepsilon)$ is continuous for each $\varepsilon \in (-\infty, \infty)$. Critical points E_L and E_R are hence finite, and in the (E, β)-plane there is well defined separation between the regions where particular isolated eigenstate exist and where it does not exist.

For reference, we report functions $\omega_{ij}(\varepsilon)$ and $a_j(\varepsilon)$ for the case $i, j = 1, 2, 3$. This is sufficient for the description of an arbitrary interaction of the state $|\Theta\rangle$ with first three atoms of an infinite Hückel chain. After some algebra one finds

$$a_1(\varepsilon) = \frac{1}{\sqrt{\pi}} \left(1 - \frac{\varepsilon^2}{4}\right)^{1/4}, \qquad a_2(\varepsilon) = \frac{\varepsilon}{\sqrt{\pi}} \left(1 - \frac{\varepsilon^2}{4}\right)^{1/4},$$

$$a_3(\varepsilon) = \frac{\varepsilon^2 - 1}{\sqrt{\pi}} \left(1 - \frac{\varepsilon^2}{4}\right)^{1/4}, \qquad \varepsilon \in [-2, 2].$$

$$(67)$$

This implies

$$\omega_{11}(\varepsilon) = \frac{1}{2} \begin{cases} \varepsilon + \sqrt{\varepsilon^2 - 4}, \\ \varepsilon, \\ \varepsilon - \sqrt{\varepsilon^2 - 4}, \end{cases}$$

$$\omega_{12}(\varepsilon) = \frac{1}{2} \begin{cases} \varepsilon^2 - 2 + \varepsilon\sqrt{\varepsilon^2 - 4}, \\ \varepsilon^2 - 2, \\ \varepsilon^2 - 2 - \varepsilon\sqrt{\varepsilon^2 - 4}, \end{cases}$$

$$\omega_{13}(\varepsilon) = \frac{1}{2} \begin{cases} \varepsilon^3 - 3\varepsilon + (\varepsilon^2 - 1)\sqrt{\varepsilon^2 - 4}, \\ \varepsilon^3 - 3\varepsilon, \\ \varepsilon^3 - 3\varepsilon - (\varepsilon^2 - 1)\sqrt{\varepsilon^2 - 4}, \end{cases}$$

$$(68)$$

$$\omega_{22}(\varepsilon) = \frac{\varepsilon}{2} \begin{cases} \varepsilon^2 - 2 + \varepsilon\sqrt{\varepsilon^2 - 4}, \\ \varepsilon^2 - 2, \\ \varepsilon^2 - 2 - \varepsilon\sqrt{\varepsilon^2 - 4}, \end{cases}$$

$$\omega_{23}(\varepsilon) = \frac{\varepsilon}{2} \begin{cases} \varepsilon^3 - 3\varepsilon + (\varepsilon^2 - 1)\sqrt{\varepsilon^2 - 4}, \\ \varepsilon^3 - 3\varepsilon, \\ \varepsilon^3 - 3\varepsilon - (\varepsilon^2 - 1)\sqrt{\varepsilon^2 - 4}, \end{cases}$$

$$\omega_{33}(\varepsilon) = \frac{1}{2} \begin{cases} \varepsilon^5 - 4\varepsilon^3 + 3\varepsilon + (\varepsilon^2 - 1)^2\sqrt{\varepsilon^2 - 4}, \\ \varepsilon^5 - 4\varepsilon^3 + 3\varepsilon, \\ \varepsilon^5 - 4\varepsilon^3 + 3\varepsilon - (\varepsilon^2 - 1)^2\sqrt{\varepsilon^2 - 4}. \end{cases}$$

In each of the above relations the top expression refers to the case $\varepsilon \leqslant -2$, middle expression refers to the case $\varepsilon \in [-2, 2]$, while bottom expression refers to the case $\varepsilon \geqslant 2$.

Relations (66a) with explicit expressions (67) and (68) provide all necessary information for the complete description of isolated and embedded eigenstates of the corresponding combined system $\mathcal{S}_\infty$. In this way one can analyze and describe more complex interactions of the state $|\Theta\rangle$ with the infinite system $\mathcal{S}_\infty^b$. An example is shown in figure 13. In this figure few eigenvalue distributions of the state $|\Theta\rangle$ that interacts with the third site $|3\rangle \in X_\infty^b$ of the infinite Hückel chain are shown. In this case one has $\beta_1 = \beta_2 = 0$ and $\beta_3 = 1$. Hence $f(\varepsilon) = (a_3(\varepsilon))^2$ and $\omega(\varepsilon) = \omega_{33}(\varepsilon)$. Eigenvalue distributions are given for the case $E = 1.5$ and for few selected values of the coupling β. If the coupling is weak ($\beta = 0.1$ and $\beta = 0.3$) no isolated eigenstate exists and one finds $w_C^a = \int \rho^a(\varepsilon)\,d\varepsilon = 1$. With the increase of the coupling ($\beta = 0.5$, $\beta = 0.7$ and $\beta = 0.9$) in addition to the density distribution $\rho^a(\varepsilon)$ one has also the contribution w_R^a of the right-isolated eigenstate. As required, one finds $w_C^a + w_R^a = 1$. Finally, if the coupling is as strong as $\beta = 1.1$ both isolated eigenstates exist. In this case one has $w_C^a + w_R^a + w_L^a = 1$ in complete agreement with completeness relation (24). Note also that only in the case of relatively weak coupling $\beta = 0.1$ and $\beta = 0.3$ density $\rho^a(\varepsilon)$ has an approximate shape of the resonance curve $\rho^{a0}(\varepsilon)$. In all other cases this density has multiple maxima indicating that relation (26) has multiple roots in the interval $[\lambda_a, \lambda_b]$. The breakdown of the resonance approximation implies sever difficulties for a standard perturbation method. It is highly doubtful that this method could reproduce densities $\rho^a(\varepsilon)$ shown in figure 13, even with the inclusion of many expansion terms. The appearance of isolated eigenstates for $\beta \geqslant 0.5$ indicated possible breakdown of the perturbation expansion and very likely divergence of the perturbation series.

8. Conclusion

Interaction of the one-dimensional quantum system $\mathcal{S}_1^a$ with the known infinite-dimensional quantum system $\mathcal{S}_\infty^b$ is considered. System $\mathcal{S}_1^a$ contains a single state
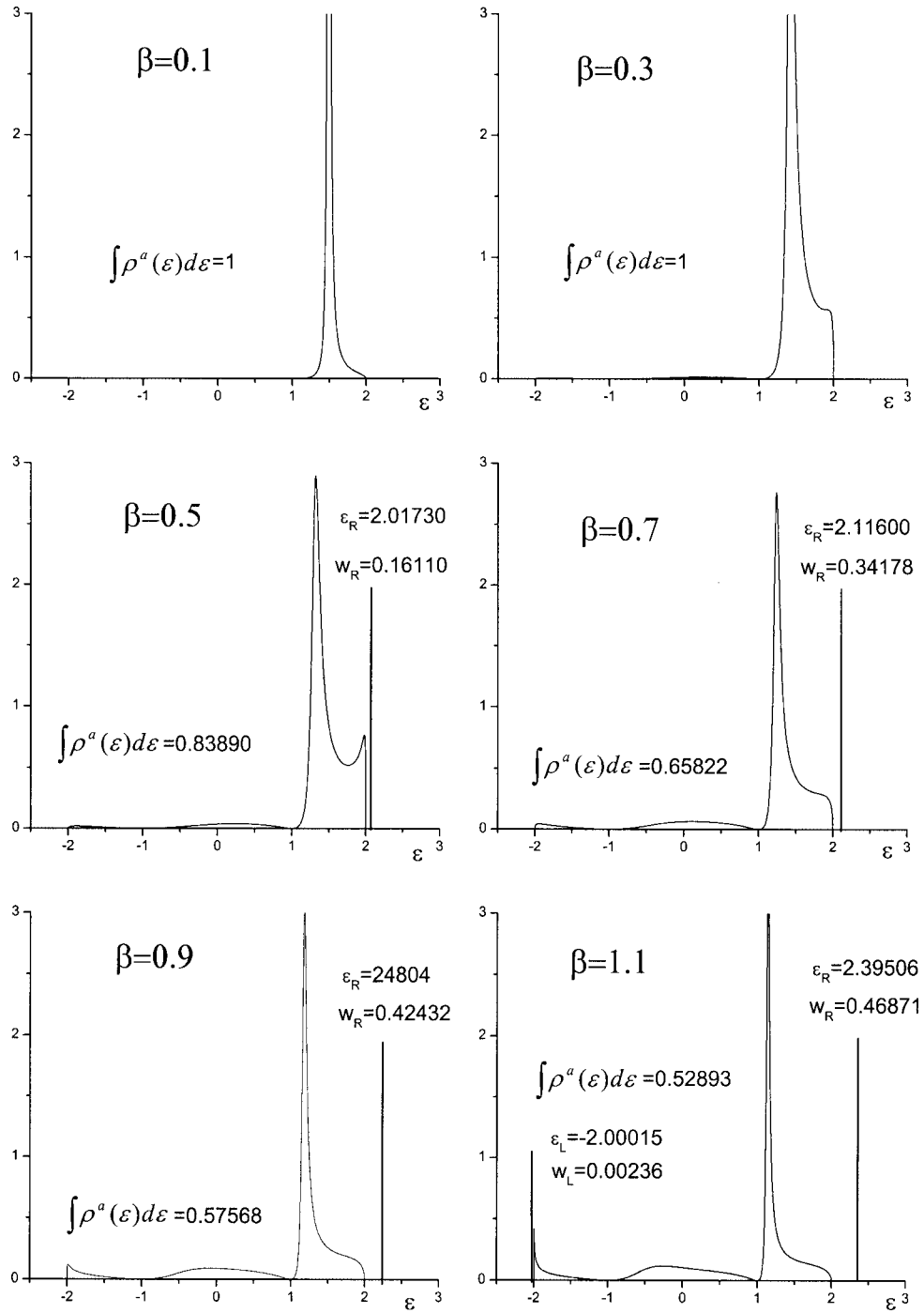
Figure 13. Eigenvalue distributions of a state $|\Theta\rangle$ for a combined system $\mathcal{S}_\infty$ characterized by parameters $\beta_1 = \beta_2 = 0$ and $\beta_3 = 1$. The case $E = 1.5$ with few selected values for the coupling β is considered.

$|\Theta\rangle$ with the eigenvalue E, while system $\mathcal{S}_\infty^b$ contains one-parameter eigenvalue band $\lambda(k)$ ($\lambda \in [\lambda_a, \lambda_b]$). An exact approach for the treatment of the combined system $\mathcal{S}_\infty = \mathcal{S}_1^a \oplus \mathcal{S}_\infty^b$ is developed. It is shown that $\mathcal{S}_\infty$ contains embedded eigenstates $|\Psi(\varepsilon)\rangle$ with continuous eigenvalues $\varepsilon \in [\lambda_a, \lambda_b]$, and, in addition, it may contain isolated eigenstates $|\Psi_I\rangle$ with discrete eigenvalues $\varepsilon_I \notin [\lambda_a, \lambda_b]$.

Closed expressions for the embedded and isolated solutions of the combined system are derived. In the limit of the weak coupling those expressions reproduce well-known results for the behavior of the system $\mathcal{S}_1^a$ in the weak interaction with a system $\mathcal{S}_\infty^b$. In particular, due to the interaction with the system $\mathcal{S}_\infty^b$, eigenvalue E of the state $|\Theta\rangle$ shifts and, in addition, if $E \in [\lambda_a, \lambda_b]$ this eigenvalue broadens [1]. Those results are usually obtained within the formalism of the time-independent perturbation theory in the weak coupling limit. In particular, eigenvalue shift and eigenvalue uncertainty of the initial eigenvalue E are in most cases obtained using only first term of the perturbation expansion, since the calculation of higher terms is quite complex and tedious [1,7]. In the present paper closed expressions for this eigenvalue shift and for the eigenvalue distribution of the state $|\Theta\rangle$ are derived. Those expressions involve no approximation, and they apply to each coupling of the system $\mathcal{S}_1^a$ with the system $\mathcal{S}_\infty^b$, however strong.

The above approach is generalized to the time-dependent eigenvalue equation. Here again it is well known that if a system is initially prepared in a state $|\Theta\rangle$ with $E \in [\lambda_a, \lambda_b]$, and if this state is in the weak interaction with a system $\mathcal{S}_\infty^b$, than the state $|\Theta(t)\rangle$ ($|\Theta(0)\rangle \equiv |\Theta\rangle$) will decay in an exponential way to the system $\mathcal{S}_\infty^b$. This exponential decay law is usually obtained as a result of a first order time-dependent perturbation expansion [1]. Here again closed expressions for the time evolution of the state $|\Theta(t)\rangle$ are derived. In particular, an exact expression for the amplitude $\langle\Theta|\Theta(t)\rangle$ and hence for the probability $\rho^a(t) = |\langle\Theta|\Theta(t)\rangle|^2$ to find the state $|\Theta(t)\rangle$ at time t in the initial state $|\Theta(0)\rangle \equiv |\Theta\rangle$ is derived. In the limit of weak coupling probability $\rho^a(t)$ reduces to the well-known exponential decay of the state $|\Theta(t)\rangle$. However, if the coupling is not small, a more complex decay pattern is obtained. In addition, exact expressions for the amplitudes $\langle\Phi(k)|\Theta(t)\rangle$ that determine probability of a transition of the state $|\Theta(t)\rangle$ at time t in a state $|\Phi(k)\rangle \in X_\infty^b$ are also obtained. In conclusion, the suggested method provides exact and closed expressions for the solution of the combined system $\mathcal{S}_\infty$, both in the time-independent as well as in the time-dependent version. There is no power series expansion, no convergence problem, and this method applies to an arbitrary coupling between the subsystems $\mathcal{S}_1^a$ and $\mathcal{S}_\infty^b$ of $\mathcal{S}_\infty$.

The application of the suggested method is illustrated with a simple model for the interaction of a single state $|\Theta\rangle$ (system $\mathcal{S}_1^a$) with an infinite one-dimensional solid in the nearest-neighbor tight-binding approximation (system $\mathcal{S}_\infty^b$). Though this model is not very realistic, it is sufficiently complex in order to illustrate applicability of all derived expressions. In addition, this model provides a good test for the correctness of those expressions. To this effect we have also considered the interaction of the system $\mathcal{S}_1^a$ with a finite one-dimensional solid that contains n atoms (system $\mathcal{S}_n^b$). Since the combined system $\mathcal{S}_{n+1} = \mathcal{S}_1^a \oplus \mathcal{S}_n^b$ is finite-dimensional, it can be solved by standard diagonalisa-

tion methods. In this way one can compare all results that apply to an infinite system $\mathcal{S}_\infty$ (obtained using expressions derived in this paper) with corresponding results for finite system $\mathcal{S}_{n+1}$ (obtained independently in the standard way). As n increases, the results for the system $\mathcal{S}_{n+1}$ should converge to the corresponding results for the system $\mathcal{S}_\infty$. This is shown to be true in all cases considered.

Obtained results are not restricted to the above simple model. Those results and their generalization [4] apply to all cases where one considers a finite quantum system $\mathcal{S}_\rho^a$ in the interaction with an infinite quantum system $\mathcal{S}_\infty^b$ where the solution to the system $\mathcal{S}_\infty^b$ is either known, or where one can model this solution in an appropriate way. In particular, this includes a general problem of the interaction of a molecule with a radiation, of the interaction of a molecule with a surface of a solid, and also of the interaction of a molecule in solution with this solution. In the present paper we make in this respect two important restrictions: the system $\mathcal{S}_1^a$ is assumed to be one-dimensional and, in addition, the system $\mathcal{S}_\infty^b$ is assumed to contain a single one-parameter eigenvalue band. Both restrictions can be relaxed, and one can generalize results presented here to the case of the interaction of an arbitrary finite dimensional system $\mathcal{S}_\rho^a$ with an arbitrary infinite dimensional system $\mathcal{S}_\infty^b$ [4].

Appendix

A.1. Derivation of estimates (14)

If $\varepsilon > \lambda_b$ then $\omega(\varepsilon) > 0$. From the relation (10b) and representation

$$\mathbf{I} = |\Theta\rangle\langle\Theta| + \int_{k_a}^{k_b} \big|\Phi(k)\big\rangle\big\langle\Phi(k)\big| \, \mathrm{d}k$$

of a unit operator $\mathbf{I}$ in the space X_∞ one derives

$$\frac{\langle\Theta|\mathbf{V}^2|\Theta\rangle}{\varepsilon - \lambda_a} < \omega(\varepsilon) < \frac{\langle\Theta|\mathbf{V}^2|\Theta\rangle}{\varepsilon - \lambda_b}, \quad \varepsilon > \lambda_b.$$

Hence and from (10a)

$$\beta^2 \frac{\langle\Theta|\mathbf{V}^2|\Theta\rangle}{\varepsilon - \lambda_a} + E - \varepsilon < h(\varepsilon) < \beta^2 \frac{\langle\Theta|\mathbf{V}^2|\Theta\rangle}{\varepsilon - \lambda_b} + E - \varepsilon, \quad \varepsilon > \lambda_b, \tag{A.1}$$

where $h(\varepsilon)$ is a monotonically decreasing function of ε and where $h(\varepsilon_R) = 0$. Thus $h(\varepsilon) > 0$ implies that ε_R exists and, in addition, $\varepsilon_R > \varepsilon$. If, however, $h(\varepsilon) < 0$ this implies that, provided ε_R exists (i.e., $\varepsilon_R > \lambda_b$), it satisfies $\varepsilon_R < \varepsilon$. Hence, and from (A.1), one finds that if ε_R exists it satisfies

$$\frac{E + \lambda_a + \sqrt{(E - \lambda_a)^2 + 4\beta^2\langle\Theta|\mathbf{V}^2|\Theta\rangle}}{2}$$
$$< \varepsilon_R < \frac{E + \lambda_b + \sqrt{(E - \lambda_b)^2 + 4\beta^2\langle\Theta|\mathbf{V}^2|\Theta\rangle}}{2}. \tag{A.2}$$

Inequality $\sqrt{1 + x} \leqslant 1 + x/2$ $(x \geqslant 0)$ now implies estimates (14).

A.2. Embedded eigenvalues and eigenstates

Let $\lambda(k)$ and $\langle\Theta|\mathbf{V}|\Phi(k)\rangle$ be continuous functions of k in the interval (k_a, k_b). Let further $\lambda(k)$ be nondecreasing function. Partition the interval $[k_a, k_b]$ into n subintervals of equal length $\Delta k = D/n$ $(D = k_b - k_a)$ and let $k_i = k_a + (i-1/2)\Delta k$ $(i = 1, \ldots, n)$ be the midpoint of ith subinterval. Replace function $\lambda(k)$ with n values $\lambda_i \equiv \lambda(k_i)$ in those midpoints. Similarly, replace function $\langle\Theta|\mathbf{V}|\Phi(k)\rangle$ with n values $\langle\Theta|\mathbf{V}|\Phi_i\rangle$ according to

$$\langle\Theta|\mathbf{V}|\Phi_i\rangle = \langle\Theta|\mathbf{V}|\Phi(k_i)\rangle\sqrt{\Delta k}. \tag{A.3}$$

Normalization in (A.3) follows from the requirement that in a limit $n \to \infty$ one should have $\sum_i \langle\Theta|\mathbf{V}|\Phi_i\rangle\langle\Phi_i|\mathbf{V}|\Theta\rangle \to \int \langle\Theta|\mathbf{V}|\Phi(k)\rangle\langle\Phi(k)|\mathbf{V}|\Theta\rangle \, dk$.

Expand $\lambda(k)$ in the point $k = k_0 \in [k_a, k_b]$:

$$\lambda(k_0 + h) = \lambda(k_0) + \left(\frac{d\lambda}{dk}\right)_0 h + O(h^2), \tag{A.4}$$

where $(d\lambda/dk)_0$ is a derivative of $\lambda(k)$ in the point $k = k_0$ and where $O(h^2)$ is a small quantity of the order h^2. Inserting $k_0 = k_r$ and $k_0 + h = k_{r+j}$ into (A.4) one obtains

$$\lambda_{r+j} = \lambda_r + \left(\frac{d\lambda}{dk}\right)_r D\frac{j}{n} + O\left(\frac{j^2}{n^2}\right). \tag{A.5}$$

In particular one has

$$\Delta\lambda_r = \lambda_r - \lambda_{r-1} = \left(\frac{d\lambda}{dk}\right)_r \Delta k + O(n^{-2}), \quad r = 2, \ldots, n. \tag{A.6}$$

In a similar way one finds

$$\langle\Theta|\mathbf{V}|\Phi_{r+j}\rangle = \begin{cases} \langle\Theta|\mathbf{V}|\Phi_r\rangle\left(1 + O\left(\frac{j}{n}\right)\right), & \text{if } \langle\Theta|\mathbf{V}|\Phi(k_r)\rangle \neq 0, \\[2mm] O\left(\dfrac{j}{n}\right), & \text{if } \langle\Theta|\mathbf{V}|\Phi(k_r)\rangle = 0. \end{cases} \tag{A.7}$$

A.2.1. Calculation of the fractional shift (equations (19) and (21))

Let ε_r be cardinal. In this case $\lambda_{r-1} < \varepsilon_r < \lambda_r$ and ε_r satisfies (7a) where $\Omega(\varepsilon_r)$ is given by (7b). Consider the case $\mathbf{P} = 0$ and write $\Omega(\varepsilon_r)$ as a sum of two terms

$$\Omega(\varepsilon_r) = \Omega^{(0)}(\varepsilon_r) + \Omega^{(1)}(\varepsilon_r),$$

where

$$\Omega^{(0)}(\varepsilon_r) = \sum_{j=-N(n)}^{N(n)} \frac{\langle\Theta|\mathbf{V}|\Phi_{r+j}\rangle\langle\Phi_{r+j}|\mathbf{V}|\Theta\rangle}{\varepsilon_r - \lambda_{r+j}},$$

$$\Omega^{(1)}(\varepsilon_r) = \sum_{j<-N(n)} \frac{\langle\Theta|\mathbf{V}|\Phi_{r+j}\rangle\langle\Phi_{r+j}|\mathbf{V}|\Theta\rangle}{\varepsilon_r - \lambda_{r+j}} + \sum_{j>N(n)} \frac{\langle\Theta|\mathbf{V}|\Phi_{r+j}\rangle\langle\Phi_{r+j}|\mathbf{V}|\Theta\rangle}{\varepsilon_r - \lambda_{r+j}}. \tag{A.8}$$

Choose $N(n) = \lfloor n^{1/3} \rfloor$ to be the largest integer smaller than $n^{1/3}$. Expression $\Omega^{(0)}(\varepsilon_r)$ contains contributions to $\Omega(\varepsilon_r)$ from approximately $2n^{1/3}$ terms that involve unperturbed eigenvalues λ_i that are close to ε_r. Expression $\Omega^{(1)}(\varepsilon_r)$ contains approximately $n - 2n^{1/3} \approx n$ remaining terms. Above relations apply to those ε_r that satisfy $n^{1/3} < r < n - n^{1/3}$. As n increases, eigenvalues ε_r become more and more dense in the interval $[\lambda_a, \lambda_b]$ and in the limit $n \to \infty$ discrete eigenvalues ε_r are replaced with continuous eigenvalues ε. In this limit $n^{1/3}$ is negligible relative to n. We are hence justified to apply relations (A.8) to each $\varepsilon_r = \varepsilon \in [\lambda_a, \lambda_b]$, except the points $\varepsilon = \lambda_a$ and $\varepsilon = \lambda_b$.

We shell now estimate expressions $\Omega^{(0)}(\varepsilon_r)$ and $\Omega^{(1)}(\varepsilon_r)$ in a limit $n \to \infty$.

Consider first $\Omega^{(0)}(\varepsilon_r)$. Using (A.5) and (A.7) one obtains

$$\Omega^{(0)}(\varepsilon_r) = \frac{\langle \Theta | \mathbf{V} | \Phi_r \rangle \langle \Phi_r | \mathbf{V} | \Theta \rangle}{\Delta \lambda_r} I(\varepsilon_r),$$

where

$$I(\varepsilon_r) = \sum_{j=-N(n)}^{N(n)} \frac{1 + O(j/n)}{x(\varepsilon_r) - j - O(j^2/n)}$$

and where

$$x(\varepsilon_r) = \frac{\varepsilon_r - \lambda_{r-1}}{\lambda_r - \lambda_{r-1}}.$$

The quantity $x(\varepsilon_r)$ is a fractional shift of ε_r in the interval $[\lambda_{r-1}, \lambda_r]$. Since ε_r is cardinal, one has $\lambda_{r-1} < \varepsilon_r < \lambda_r$ and hence $0 < x(\varepsilon_r) < 1$.

The quantity $I(\varepsilon_r)$ can be written as a sum of three terms:

$$I(\varepsilon_r) = I_0(\varepsilon_r) + R_1(\varepsilon_r) + R_2(\varepsilon_r),$$

where

$$I_0(\varepsilon_r) = \sum_{j=-N(n)}^{N(n)} \frac{1}{x(\varepsilon_r) - j}, \qquad R_1(\varepsilon_r) = \sum_{j=-N(n)}^{N(n)} \frac{O(j/n)}{x(\varepsilon_r) - j - O(j^2/n)},$$

$$R_2(\varepsilon_r) = \sum_{j=-N(n)}^{N(n)} \frac{O(j^2/n)}{(x(\varepsilon_r) - j)(x(\varepsilon_r) - j - O(j^2/n))}.$$

We shell now show that in a limit $n \to \infty$ only the sum $I_0(\varepsilon_r)$ is nonzero, while sums $R_1(\varepsilon_r)$ and $R_2(\varepsilon_r)$ are in this limit negligible.

Using identity [9]

$$\frac{1}{x} + \sum_{j=1}^{\infty} \left(\frac{1}{x - j} + \frac{1}{x + j} \right) = \pi \cot(\pi x) \tag{A.9}$$

one finds:

$$\lim_{n\to\infty} I_0(\varepsilon_r) = \pi \cot(\pi x(\varepsilon_r)).$$

Consider now $R_1(\varepsilon_r)$. Since $|j| < n^{1/3}$ there is some large positive number K such that $|O(j/n)| < K|j|/n \leqslant Kn^{-2/3}$. Further, for sufficiently big n there is some positive number L such that

$$\frac{1}{|x(\varepsilon_r) - j - O(j^2/n)|} < L.$$

Hence

$$|R_1| < KLn^{-2/3} \sum_{i=-N(n)}^{N(n)} 1 \approx 2KLn^{-1/3} = O(n^{-1/3}).$$

One similarly finds $|R_2| < O(n^{-2/3})$. In a limit $n \to \infty$ both terms are zero. Hence

$$\lim_{n\to\infty} I(\varepsilon_r) = \lim_{n\to\infty} I_0(\varepsilon_r) = \pi \cot(\pi x(\varepsilon_r)).$$

Using (A.3) and (A.6) one now finds

$$\Omega^{(0)}(\varepsilon_r) \approx \pi \frac{\langle\Theta|\mathbf{V}|\Phi(k_r)\rangle\langle\Phi(k_r)|\mathbf{V}|\Theta\rangle}{(d\lambda/dk)_r} \cot(\pi x(\varepsilon_r)). \tag{A.10}$$

Relation (A.10) is valid as long as $n \neq \infty$, and as n increases, it is more and more exact. In the limit $n \to \infty$ eigenvalues ε_r are dense in the interval $[k_a, k_b]$, and in this limit one has to replace discrete quantities ε_r, k_r and $(d\lambda/dk)_r$ with continuous quantities. Thus one obtains

$$\Omega^0(\varepsilon_r) \to \pi f(\varepsilon) \cot(\pi x(\varepsilon)), \quad \varepsilon \in [\lambda_a, \lambda_b], \tag{A.11}$$

where the function $f(\varepsilon)$ is given by (11).

Consider now the expression $\Omega^{(1)}(\varepsilon)$. Using (A.3) one finds

$$\Omega^{(1)}(\varepsilon_r) = \sum_{j<-N(n)} \frac{\langle\Theta\mathbf{V}|\Phi(k_{r+j})\rangle\langle\Phi(k_{r+j})|\mathbf{V}|\Theta\rangle}{\varepsilon_r - \lambda(k_{r+j})} \Delta k$$

$$+ \sum_{j>N(n)} \frac{\langle\Theta|\mathbf{V}|\Phi(k_{r+j})\rangle\langle\Phi(k_{r+j})|\mathbf{V}|\Theta\rangle}{\varepsilon_r - \lambda(k_{r+j})} \Delta k. \tag{A.8$'$}$$

Each sum exclude $\approx n^{1/3}$ terms close to the point $\varepsilon_r \approx \lambda(k_r)$. Successive terms in those sums are hence slowly varying functions of k_{r+j}, and those sums can be approximated with corresponding integrals. As n increases this approximation improves and in a limit $n \to \infty$ it is exact. According to (A.5) one has

$$\lambda(k_{r-N(n)}) \equiv \lambda_{r-N(n)} \approx \varepsilon_r - \delta, \qquad \lambda_{r+N(n)} \approx \varepsilon_r + \delta,$$

where $\delta = (\varepsilon_r - \lambda_r) + (d\lambda/dk)_r Dn^{-2/3} \approx (d\lambda/dk)_r Dn^{-2/3}$. Since $\lim_{n\to\infty} \delta = 0$ one has

$$
\begin{aligned}
\Omega^{(1)}(\varepsilon_r) \to \omega(\varepsilon) = \lim_{\delta \to 0} \Bigg[&\int_{k_a}^{k_\varepsilon - \delta} \frac{\langle\Theta|\mathbf{V}|\Phi(k)\rangle\langle\Phi(k)|\mathbf{V}|\Theta\rangle}{\varepsilon - \lambda(k)} \, dk \\
&+ \int_{k_\varepsilon + \delta}^{k_b} \frac{\langle\Theta|\mathbf{V}|\Phi(k)\rangle\langle\Phi(k)|\mathbf{V}|\Theta\rangle}{\varepsilon - \lambda(k)} dk \Bigg] \\
= P &\int_{k_a}^{k_b} \frac{\langle\Theta|\mathbf{V}|\Phi(k)\rangle\langle\Phi(k)|\mathbf{V}|\Theta\rangle}{\varepsilon - \lambda(k)} \, dk, \quad \varepsilon \in [\lambda_a, \lambda_b],
\end{aligned}
$$

where $\lambda(k_\varepsilon) = \varepsilon$ and where P denotes principal Cauchy integral value. Hence, and from (A.11),

$$
\Omega(\varepsilon_r) \to \pi f(\varepsilon) \cot\big(\pi x(\varepsilon)\big) + \omega(\varepsilon). \tag{A.12}
$$

This proves relations (19).

A.2.2. Calculation of the amplitude $\langle\Theta|\Psi(\varepsilon)\rangle$

Eigenstate (8a) can be written as a sum of three terms

$$
|\Psi_r\rangle = \frac{1}{\sqrt{Q_r}} \big[|\Theta\rangle + \beta\big|\Psi_r^{(0)}\big\rangle + \beta\big|\Psi_r^{(1)}\big\rangle\big],
$$

where in the case $\mathbf{P} = 0$

$$
\big|\Psi_r^{(0)}\big\rangle = \sum_{j=-M(n)}^{M(n)} \frac{\langle\Phi_{r+j}|\mathbf{V}|\Theta\rangle}{\varepsilon_r - \lambda_{r+j}} |\Phi_{r+j}\rangle,
$$

$$
\big|\Psi_r^{(1)}\big\rangle = \sum_{j<-M(n)} \frac{\langle\Phi_{r+j}|\mathbf{V}|\Theta\rangle}{\varepsilon_r - \lambda_{r+j}} |\Phi_{r+j}\rangle + \sum_{j>M(n)} \frac{\langle\Phi_{r+j}|\mathbf{V}|\Theta\rangle}{\varepsilon_r - \lambda_{r+j}} |\Phi_{r+j}\rangle
$$

and where

$$
Q_r = 1 + \beta^2\big\langle\Psi_r^{(0)}\big|\Psi_r^{(0)}\big\rangle + \beta^2\big\langle\Psi_r^{(1)}\big|\Psi_r^{(1)}\big\rangle.
$$

In the above expressions we choose $M(n) = \lfloor n^{2/3} \rfloor$ to be the largest integer smaller than $n^{2/3}$.

Function $\big|\Psi_r^{(0)}\big\rangle$ contains contributions to the perturbed eigenstate $|\Psi_r\rangle$ from approximately $2n^{2/3}$ unperturbed states $|\Phi_i\rangle \in X_n^b$ whose eigenvalues λ_{r+j} are close to ε_r. Function $\big|\Psi_r^{(1)}\big\rangle$ contains contributions from approximately $n - 2n^{2/3} \approx n$ remaining states $|\Phi_{r+j}\rangle \in X_n^b$.

Let us first estimate quantity Q_r that determines normalization of the eigenstate $|\Psi_r\rangle$. One has

$$
\big\langle\Psi_r^{(0)}\big|\Psi_r^{(0)}\big\rangle = \sum_{j=-M(n)}^{M(n)} \frac{\langle\Theta|\mathbf{V}|\Phi_{r+j}\rangle\langle\Phi_{r+j}|\mathbf{V}|\Theta\rangle}{(\varepsilon_r - \lambda_{r+j})^2}, \tag{A.13}
$$

$$\langle\Psi_r^{(1)}|\Psi_r^{(1)}\rangle = \sum_{j<-M(n)} \frac{\langle\Theta|\mathbf{V}|\Phi_{r+j}\rangle\langle\Phi_{r+j}|\mathbf{V}|\Theta\rangle}{(\varepsilon_r - \lambda_{r+j})^2}$$
$$+ \sum_{j>M(n)} \frac{\langle\Theta|\mathbf{V}|\Phi_{r+j}\rangle\langle\Phi_{r+j}|\mathbf{V}|\Theta\rangle}{(\varepsilon_r - \lambda_{r+j})^2}. \tag{A.14}$$

Consider $\langle\Psi_r^{(0)}|\Psi_r^{(0)}\rangle$. All terms in the expression (A.13) are nonnegative and hence there is no possibility of a subtle cancellation of terms with opposite sign. Using (A.4), (A.6) and (A.7) one finds

$$\langle\Psi_r^{(0)}|\Psi_r^{(0)}\rangle \approx \frac{\langle\Theta|\mathbf{V}|\Phi_r\rangle\langle\Phi_r|\mathbf{V}|\Theta\rangle}{(\Delta\lambda_r)^2} \sum_{j=-M(n)}^{M(n)} \frac{1}{(x(\varepsilon_r) - j)^2}.$$

As n increases this expression is more and more exact. Since $M(n) \approx n^{2/3}$ one can in a limit $n \to \infty$ extend summation over $j \in [-M(n), M(n)]$ to the interval $j \in [-\infty, \infty]$. Further, if one takes derivation of (A.9) with respect to x one finds

$$\sum_{j=-\infty}^{\infty} \frac{1}{(x - j)^2} = \frac{\pi^2}{\sin^2(\pi x)}. \tag{A.15}$$

Hence and from (A.3) and (A.6) for sufficiently big n one has

$$\langle\Psi_r^{(0)}|\Psi_r^{(0)}\rangle = \frac{1}{\Delta\lambda_r} \frac{\langle\Theta|\mathbf{V}|\Phi(k_r)\rangle\langle\Phi(k_r)|\mathbf{V}|\Theta\rangle}{(\mathrm{d}\lambda/\mathrm{d}k)_r} \frac{\pi^2}{\sin^2(\pi x(\varepsilon_r))}. \tag{A.16}$$

Intervals $\Delta\lambda_r$ scale as $O(n^{-1})$. Hence with the increase of n and if $\langle\Theta|\mathbf{V}|\Phi(k_r)\rangle \neq 0$ and $(\mathrm{d}\lambda/\mathrm{d}k)_r \neq 0$, the quantity $\langle\Psi_r^{(0)}|\Psi_r^{(0)}\rangle$ scales as $O(n)$.

Consider now $\langle\Psi_r^{(1)}|\Psi_r^{(1)}\rangle$. Since $|j| \geqslant M(n) \approx n^{2/3}$ one has $|\lambda_{r+j} - \varepsilon_r| \geqslant n^{2/3}\Delta\lambda_r$. Hence

$$\langle\Psi_r^{(1)}|\Psi_r^{(1)}\rangle \leqslant \frac{1}{n^{4/3}(\Delta\lambda_r)^2}\Bigg[\sum_{j<-M(n)} \langle\Theta|\mathbf{V}|\Phi_{r+j}\rangle\langle\Phi_{r+j}|\mathbf{V}|\Theta\rangle$$
$$+ \sum_{j>M(n)} \langle\Theta|\mathbf{V}|\Phi_{r+j}\rangle\langle\Phi_{r+j}|\mathbf{V}|\Theta\rangle\Bigg]$$
$$< \frac{1}{n^{4/3}(\Delta\lambda_r)^2} \sum_i \langle\Theta|\mathbf{V}|\Phi_i\rangle\langle\Phi_i|\mathbf{V}|\Theta\rangle = \frac{\langle\Theta|\mathbf{V}^2|\Theta\rangle}{n^{4/3}(\Delta\lambda_r)^2}.$$

Since intervals $\Delta\lambda_r$ scale as $O(n^{-1})$ one has $\langle\Psi_r^{(1)}|\Psi_r^{(1)}\rangle < O(n^{2/3})$. In conclusion, as n increases quantity $\langle\Psi_r^{(0)}|\Psi_r^{(0)}\rangle$ scales as $O(n)$ while $\langle\Psi_r^{(1)}|\Psi_r^{(1)}\rangle < O(n^{2/3})$. Therefore in a limit $n \to \infty$ one can neglect $\langle\Psi_r^{(1)}|\Psi_r^{(1)}\rangle$ relative to $\langle\Psi_r^{(0)}|\Psi_r^{(0)}\rangle$. Hence for a very big n and provided $\langle\Theta|\mathbf{V}|\Phi(k_r)\rangle \neq 0$ and $(\mathrm{d}\lambda/\mathrm{d}k)_r \neq 0$ one obtains

$$Q_r = \frac{\beta^2}{\Delta\lambda_r} \frac{\langle\Theta|\mathbf{V}|\Phi(k_r)\rangle\langle\Phi(k_r)|\mathbf{V}|\Theta\rangle}{(\mathrm{d}\lambda/\mathrm{d}k)_r} \frac{\pi^2}{\sin^2(\pi x(\varepsilon_r))}. \tag{A.17}$$

Probability w_r^a to find the state $|\Psi_r\rangle$ in the state $|\Theta\rangle$ is $w_r^a = |\langle\Theta|\Psi_r\rangle|^2$. Hence and from (8a) $w_r^a = 1/Q_r$:

$$w_r^a = \Delta\lambda_r \frac{(\mathrm{d}\lambda/\mathrm{d}k)_r}{\beta^2\langle\Theta|\mathbf{V}|\Phi(k_r)\rangle\langle\Phi(k_r)|\mathbf{V}|\Theta\rangle} \frac{\sin^2(\pi x(\varepsilon_r))}{\pi^2}. \tag{A.18}$$

In the limit $n \to \infty$ eigenstates $|\Psi_r\rangle$ normalized to unity are replaced with the eigenstates $|\Psi(\varepsilon)\rangle$ normalized to a δ-function. Consider now system $\mathcal{S}_\infty$. Let $\rho^a(\varepsilon) = |\langle\Theta|\Psi(\varepsilon)\rangle|^2$ be probability density to find a state $|\Theta\rangle$ in the eigenstate $|\Psi(\varepsilon)\rangle$. In the limit $n \to \infty$ discrete probability w_r^a is replaced with the probability $\rho^a(\varepsilon)\,\mathrm{d}\varepsilon$ to find the state $|\Theta\rangle$ in any of the eigenstates $|\Psi(\varepsilon)\rangle$ that are contained in the eigenvalue interval $\mathrm{d}\varepsilon$. Further, according to (21) fractional shift $x(\varepsilon)$ is continuous function of ε for each ε where $f(\varepsilon)$ and $h(\varepsilon) \equiv \beta^2\omega(\varepsilon) + E - \varepsilon$ are continuous, with the possible exception of the points $x = x_c$ that satisfy $f(\varepsilon_c) = 0$ and at the same time $h(\varepsilon_c) = 0$. Hence and from (20a) one finds $\Delta\varepsilon_k \approx \Delta\lambda_k$ and in the limit $n \to \infty$ one has $\mathrm{d}\varepsilon = \mathrm{d}\lambda$. Thus relation (A.18) implies

$$\rho^a(\varepsilon) = \frac{\sin^2(\pi x(\varepsilon))}{\beta^2\pi^2 f(\varepsilon)}, \tag{A.19}$$

where $f(\varepsilon)$ is given by (17b). Hence one derives probability amplitude (22).

There are few assumptions involved in the derivation of expressions (A.12) and (A.19). The conditions for the validity of those expressions should be clarified. We assume $\lambda(k)$ and $\langle\Theta|\mathbf{V}|\Phi(k)\rangle$ to be continuous functions of a parameter λ. Moreover, in order to use expansion (A.4), derivative $\mathrm{d}\lambda/\mathrm{d}k$ should be well defined. Those are reasonable assumptions. In particular, in the case of solids the quantity $\rho(\lambda) = \mathrm{d}k/\mathrm{d}\lambda$ is a density of levels, and this quantity is continuous function of λ, except in those points where $\mathrm{d}\lambda/\mathrm{d}k = 0$ and where $\rho(\lambda)$ diverges. Even the derivative $\mathrm{d}\rho(\lambda)/\mathrm{d}\lambda$ is continuous, with the possible exception of few isolated points known as van Hove singularities [2]. In those points $\mathrm{d}\rho(\lambda)/\mathrm{d}\lambda$ diverges. Thus $\lambda(k)$ behaves correctly almost everywhere. The same applies to the function $\langle\Theta|\mathbf{V}|\Phi(k)\rangle$. Another type of problems present those points where $\mathrm{d}\lambda(k)/\mathrm{d}k = 0$ and/or $\langle\Theta|\mathbf{V}|\Phi(k)\rangle = 0$. For example, in a point $\mathrm{d}\lambda(k)/\mathrm{d}k = 0$ estimate (A.6) for the small quantity $\Delta\lambda_r$ gives only $\Delta\lambda_r = O(n^{-2})$. This presents some difficulties for the correct estimation of quantities $\Omega^{(0)}(\varepsilon_r)$ and $\Omega^{(1)}(\varepsilon_r)$. However, all such points are isolated and usually very few in number. In conclusion, derived expressions should be valid everywhere, except possibly in the case of few isolated points. More detailed analyze shows that majority of such points can be neglected. One finds that the key expressions (21) and (23) are valid whenever those expressions are well defined. In particular, those expressions apply also to the case $f(\varepsilon) = 0$ provided $h(\varepsilon) \neq 0$, as well as to the case $h(\varepsilon) = 0$ provided $f(\varepsilon) \neq 0$. The only points that require some special treatment and where derived expressions may fail are the points ε_c of anomal resonance [4]. Each such point satisfies both conditions $f(\varepsilon_c) = 0$ and also $h(\varepsilon_c) = 0$.

A.3. Time-dependent eigenstates

A.3.1. Derivation of the expressions (38)

Consider the interaction of the system $\mathcal{S}_1^a$ with the n-dimensional system $\mathcal{S}_n^b$ in the case $\mathbf{P} = 0$ and $\mathbf{S}^b = \mathbf{I}^b$. Let $|\Psi_r\rangle$ be eigenstates of the combined system $\mathcal{S}_{n+1}$ orthonormalized according to (5c). The sum $\sum_r |\Psi_r\rangle\langle\Psi_r| = \mathbf{I}$ is a unit operator in X_{n+1}, and hence $|\Theta\rangle = \sum_r \langle\Psi_r|\Theta\rangle|\Psi_r\rangle$. Since $|\Psi_r\rangle$ are eigenstates of the combined system $\mathcal{S}_{n+1}$ with the eigenvalues ε_r, this implies

$$|\Theta(t)\rangle = \sum_r \langle\Psi_r|\Theta\rangle|\Psi_r\rangle e^{-i\varepsilon_r t/\hbar}, \tag{A.20}$$

where $|\Theta(t)\rangle$ is a time-dependent eigenstate of $\mathcal{S}_{n+1}$ that is at time $t = 0$ prepared in a state $|\Theta(0)\rangle \equiv |\Theta\rangle$. Let the combined system $\mathcal{S}_{n+1}$ contain no singular eigenstate. In this case expression (A.20) contains only cardinal eigenstates of $\mathcal{S}_{n+1}$. Define amplitudes

$$u_j(t) = \langle\Phi(k_j)|\Theta(t)\rangle e^{i\lambda_j t/\hbar} = \frac{1}{\sqrt{\Delta k}}\langle\Phi_j|\Theta(t)\rangle e^{i\lambda_j t/\hbar}. \tag{A.21}$$

Since $\langle\Phi_j|\Theta(0)\rangle \equiv \langle\Phi_j|\Theta\rangle = 0$ one has $u_j(0) = 0$.
Relation (A.20) implies

$$u_j(t) = \sum_r \langle\Psi_r|\Theta\rangle\langle\Phi(k_j)|\Psi_r\rangle e^{-i(\varepsilon_r - \lambda_j)t/\hbar}.$$

Using (8a) with $\mathbf{P} = 0$ one finds that amplitudes $u_j(t)$ satisfy

$$\frac{du_j(t)}{dt} = -i\beta\frac{\langle\Phi(k_j)|\mathbf{V}|\Theta\rangle}{\hbar}\sum_r w_r^a e^{-i(\varepsilon_r - \lambda_j)t/\hbar}, \tag{A.22}$$

where $w_r^a = |\langle\Theta|\Psi_r\rangle|^2$ is the probability to find the state $|\Theta\rangle$ in the (cardinal) eigenstate $|\Psi_r\rangle$ of the combined system $\mathcal{S}_{n+1}$.

In the limit $n \to \infty$ one has $\lambda_j \to \lambda(k)$ and hence $u_j(t) \to u(k, t)$ where the function $u(k, t)$ is given by (38b). Also in this limit $w_r^a \to \rho^a(\varepsilon)d\varepsilon$ except for probabilities w_I^a for isolated eigenstates which should be treated separately. One thus finds that in a limit $n \to \infty$ expression (A.22) is replaced with (38c).

In order to derive relation (A.22) we did assume that cardinal eigenstates of the combined system form a complete set, i.e., there are no singular eigenstates. As explained in the main text, this assumption is justified since with an infinitesimal variation of the operators $\mathbf{B}$ and $\mathbf{V}$ one can always transform eigenvalue equation (5a) containing singular solutions into another eigenvalue equation containing no singular solution.

A.3.2. Derivation of the expressions (45) and (47)

In the case of a resonance approximation one has $\rho^a(\varepsilon) \approx \rho^{a0}(\varepsilon)$ and $w_I^a \approx 0$. Hence

$$\int_{\lambda_a}^{\lambda_b} \rho^a(\varepsilon)e^{-i(\varepsilon-\lambda)t/\hbar}\,d\varepsilon \approx \int_{-\infty}^{\infty} \rho^{a0}(\varepsilon)e^{-i(\varepsilon-\lambda)t/\hbar}\,d\varepsilon = e^{-\pi\beta^2 f(\varepsilon_0)t/\hbar}e^{-i(\varepsilon_0-\lambda)t/\hbar}.$$

This implies

$$\frac{\mathrm{d}u^b(\lambda, t)}{\mathrm{d}t} \approx \frac{\mathrm{d}u^{b0}(\lambda, t)}{\mathrm{d}t} = -\mathrm{i}\beta \frac{\sqrt{f(\lambda)}}{\hbar} \mathrm{e}^{-(\pi\beta^2 f(\varepsilon_0) - \mathrm{i}(\lambda - \varepsilon_0))t/\hbar}$$

which has a solution (45).

Concerning relation (47), consider first the integral $\int \rho^{b0}(\lambda, \infty) \, \mathrm{d}\lambda$:

$$\int_{\lambda_a}^{\lambda_b} \rho^{b0}(\lambda, \infty) \, \mathrm{d}\lambda = \int_{\lambda_a}^{\lambda_b} \frac{\beta^2 f(\lambda) \, \mathrm{d}\lambda}{\pi^2 \beta^4 f^2(\varepsilon_0) + (\varepsilon_0 - \lambda)^2} \approx \int \rho^{a0}(\lambda) \, \mathrm{d}\lambda \approx 1.$$

In a similar way one finds

$$\int_{\lambda_a}^{\lambda_b} \frac{\beta^2 f(\lambda) \cos[(\varepsilon_0 - \lambda)t/\hbar] \, \mathrm{d}\lambda}{\pi^2 \beta^4 f^2(\varepsilon_0) + (\varepsilon_0 - \lambda)^2} \approx \int_{-\infty}^{\infty} \frac{\beta^2 f(\varepsilon_0) \cos[(\varepsilon_0 - \lambda)t/\hbar] \, \mathrm{d}\lambda}{\pi^2 \beta^4 f^2(\varepsilon_0) + (\varepsilon_0 - \lambda)^2} = \mathrm{e}^{-\pi\beta^2 f(\varepsilon_0)t/\hbar}.$$

In combination with (46) and (A.22) this proves (47).

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