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Interaction of an isolated state with an infinite quantum system containing several one-parameter eigenvalue bands: I. Time-independent case

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A new method for the exact solution of the interaction of an isolated state $|\Theta\rangle$ with an infinite dimensional quantum system $\boldsymbol{S}_\infty^b$ containing several one-parameter eigenvalue bands $\lambda_\nu(k) \in I_\nu \equiv [a_\nu, b_\nu]$ is developed. Unlike standard perturbation expansion approach, this method produces correct results however strong the interaction between the state $|\Theta\rangle$ and the system $\boldsymbol{S}_\infty^b$. It is shown that in the case of the weak interaction this method correctly reproduces standard results obtained within the formalism of the perturbation expansion method. In particular, due to the interaction with the system $\boldsymbol{S}_\infty^b$, eigenvalue E of the state $|\Theta\rangle$ shifts to a new position. In addition, if this eigenvalue is embedded inside the range $D = \bigcup_\nu I_\nu$ of the unperturbed eigenvalues, this shifted eigenvalue broadens and spectral distribution of the state $|\Theta\rangle$ has the shape of the universal resonance curve. However, if the interaction is strong, one finds much more complex and much more complicated behavior.

KEY WORDS: interaction of quantum systems, time independent perturbation, transition probabilities

1. Introduction

In a previous paper [1] the interaction of a state $|\Theta\rangle$ with a known infinite quantum system $\boldsymbol{S}_\infty^b$ that contains a single one-parameter eigenvalue band was considered. The state $|\Theta\rangle$ with associated eigenvalue E represents one-dimensional system $\boldsymbol{S}_1^a$. The union of systems $\boldsymbol{S}_1^a$ and $\boldsymbol{S}_\infty^b$ represents a combined system $\boldsymbol{S}_\infty = \boldsymbol{S}_1^a \oplus \boldsymbol{S}_\infty^b$. The solution to this system was obtained by a new mathematical method [1]. Unlike standard perturbation expansion approach [2,3], this method provides exact expressions for the eigenvalues and eigenstates of $\boldsymbol{S}_\infty$. No power series expansion in terms of the coupling parameter is involved, and the results obtained are valid, however strong the interaction between the systems $\boldsymbol{S}_1^a$ and $\boldsymbol{S}_\infty^b$. This is particularly important if the coupling between those systems is so strong that the standard perturbation expansion series diverges. Also, if highly precise solution to the system $\boldsymbol{S}_\infty$ is required, perturbation expansion series may

converge unacceptably slow. In addition to those computational benefits, it is usually advantageous to find new solutions to old problems. This may provide some previously unknown way of looking at those problems, thus suggesting novel conceptual insight that could not be obtained otherwise.

There are numerous problems in physics and chemistry of the interaction of a single state with a known infinite system. For example, one can consider the interaction of a molecule with the electromagnetic field. To a very good approximation the interaction of an isolated eigenstate $|\Theta\rangle$ of this molecule with the electromagnetic field can be represented as the interaction of the one-dimensional system (the state $|\Theta\rangle$ with the eigenvalue E) with the known infinite system $\mathcal{S}_\infty^b$ (free electromagnetic field) [2]. Due to this interaction, eigenvalue E of $|\Theta\rangle$ is slightly shifted to a new position. In addition, this eigenvalue is not sharp and it has the shape of the universal resonance curve with finite uncertainty [2]. If $|\Theta\rangle$ is an excited molecular state, it is not stable and there is a finite probability for the transition of this state to other molecular states. All those properties are important experimental quantities. Investigation and theoretical prediction of those properties is a main subject of spectroscopy. As another example consider the interaction of the molecule situated on the surface of some solid with this solid. One can again consider the interaction of the particular molecular eigenstate $|\Theta\rangle$ with this solid. System $\mathcal{S}_\infty^b$ represents a solid with a surface. The solution to this system usually consists of multiple eigenvalue bands $\lambda_s(\mathbf{k})$ $(s=1, 2, \dots)$ [4]. In addition, system $\mathcal{S}_\infty^b$ may contain some discrete eigenvalues that correspond to the surface states [5]. One can obtain the solution to the system $\mathcal{S}_\infty^b$ alone by various other methods [4,5]. Usually one knows only an approximate solution of this system [4]. Assuming this approximate solution to be good enough, the problem is to find a solution of the combined system $\mathcal{S}_\infty = \mathcal{S}_1^a \oplus \mathcal{S}_\infty^b$ with emphasize on the properties of the subsystem $\mathcal{S}_1^a$. Investigation of this problem is one of the main subjects of the surface state physics [5].

The mathematical formalism developed in the original paper [1] is not general enough to include the treatment of the above and similar problems. In this original formulation it was assumed that the system $\mathcal{S}_\infty^b$ contains a single one-parameter eigenvalue band [1]. This is rather restrictive, since all eigenstates $|\Phi(k)\rangle$ of such a system are nondegenerate. There are few infinite systems with this property. For example, electromagnetic field forms a degenerate eigenvalue band since photons in various quantum states may have the same energy. The same applies to eigenvalues and eigenstates of a three-dimensional solid [4].

In the present and in the following paper [6] original mathematical formalism is generalized to the case when the system $\mathcal{S}_\infty^b$ contains a finite number of one-parameter eigenvalue bands. Those bands may overlap, thus describing degenerate eigenvalue bands. An arbitrary (multiparameter) eigenvalue band can be approximated to any desired degree of accuracy with a finite number of overlapping one-parameter eigenvalue bands. Hence the results obtained in those papers can be generalized in a rather straightforward way to the case when the

system $\mathcal{S}_\infty^b$ contains any number of arbitrary eigenvalue bands [7]. If the system $\mathcal{S}_\infty^b$ contains some discrete eigenvalues and eigenstates, this can be also easily incorporated in the suggested formalism. In this way the interaction of an isolated state $|\Theta\rangle$ with an arbitrary infinite dimensional quantum system $\mathcal{S}_\infty^b$ can be described [7].

In the present and in the following paper are considered, respectivelly, time-independent and time-dependent properties of the combined system $\mathcal{S}_\infty$.

2. Mathematical formulation of a problem

Let us formulate in more mathematical terms the problem to be treated in a present paper.

The state $|\Theta\rangle$ with the eigenvalue E represents one-dimensional system $\mathcal{S}_1^a$. With this system is associated one-dimensional space X_1^a spanned by $|\Theta\rangle$. The corresponding eigenvalue equation is

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

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

System $\mathcal{S}_\infty^b$ contains κ one-parameter eigenvalue bands with eigenvalue functions $\lambda_\nu(k)$ ($k \in [k_{a\nu}, k_{b\nu}]$, $\nu = 1, \ldots, \kappa$). Each $\lambda_\nu(k)$ is continuous and monotonic function of a parameter k in the interval $[k_{a\nu}, k_{b\nu}]$. We will assume that each $\lambda_\nu(k)$ is monotonic increasing function. With minor and essentially unimportant adjustments all conclusions to be derived apply also to the case when some or all $\lambda_\nu(k)$ are monotonic decreasing functions.

Formally, system $\mathcal{S}_\infty^b$ consists of κ subsystems $\mathcal{S}_\infty^{b\nu}$, i.e., $\mathcal{S}_\infty^b = \cup_\nu \mathcal{S}_\infty^{b\nu}$. With the system $\mathcal{S}_\infty^b$ is associated an infinite-dimensional space X_∞^b, while with each subsystem $\mathcal{S}_\infty^{b\nu}$ is associated an infinite-dimensional space $X_\infty^{b\nu}$, subspace of X_∞^b. Further, in each eigenvalue band ν, to the eigenvalue $\lambda_\nu(k)$ ($k \in [k_{a\nu}, k_{b\nu}]$) corresponds one and only one eigenstate $|\Phi_\nu(k)\rangle \in X_\infty^{b\nu}$. Eigenvalue equation describing system $\mathcal{S}_\infty^b$ is hence

$$\mathrm{B}\,|\Phi_\nu(k)\rangle = \lambda_\nu(k)\,|\Phi_\nu(k)\rangle\,, \quad k \in [k_{a\nu}, k_{b\nu}], \quad \nu = 1, \ldots, \kappa, \tag{2a}$$

where **B** is a Hermitian operator.

Eigenstates $|\Phi_\nu(k)\rangle$ of **B** can be orthonormalized according to

$$\left\langle \Phi_\nu(k) \,\middle|\, \Phi_{\nu'}(k') \right\rangle = \delta_{\nu\nu'}\delta(k-k'), \quad k \in [k_{a\nu}, k_{b\nu}]\,. \tag{2b}$$

Relations (1) and (2) describe systems $\mathcal{S}_1^a$ and $\mathcal{S}_\infty^b$ without mutual interaction. An arbitrary interaction can be written in the form $\beta\,\mathbf{V}$ where $\mathbf{V} \neq 0$ is a Hermitian operator and where $\beta \geqslant 0$ is a coupling parameter. Operator **V** has nonvanishing matrix elements between the state $|\Theta\rangle \in X_1^a$ and the states $|\Phi_\nu(k)\rangle \in$

X_∞^b. Eigenvalue equation describing combined system $\mathcal{S}_\infty = \mathcal{S}_1^a \oplus \mathcal{S}_\infty^b$ subject to this interaction is

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

where

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

Without loss of generality operator $\mathbf{V}$ can be normalized according to

$$\langle\Theta\,|\,\mathbf{V}^2\,|\Theta\rangle = 1. \tag{3c}$$

Combined system $\mathcal{S}_\infty$ is schematically shown in figure 1. We formally consider $\mathcal{S}_\infty^b$ as the unperturbed system. Since each $\lambda_\nu(k)$ is an increasing function of k, all eigenvalues of the eigenvalue band ν are confined to the eigenvalue interval $I_\nu = [a_\nu, b_\nu]$ where $a_\nu = \lambda_\nu(k_{a\nu})$ and $b_\nu = \lambda_\nu(k_{b\nu})$ are the smallest and the largest possible eigenvalue, respectively. Those eigenvalue intervals may overlap, in which case the corresponding eigenvalues of $\mathbf{B}$ are degenerate. Union of all eigenvalue intervals I_ν forms a range D of the unperturbed eigenvalues, $D = \cup_\nu I_\nu$. This range may contain one or several nonoverlaping intervals D_μ, where each D_μ is a union of one or several eigenvalue intervals I_ν. We also define a point set $\bar{D}$ to be a complement of D. Accordingly, $D \cup \bar{D} = R$ is the entire real axis.

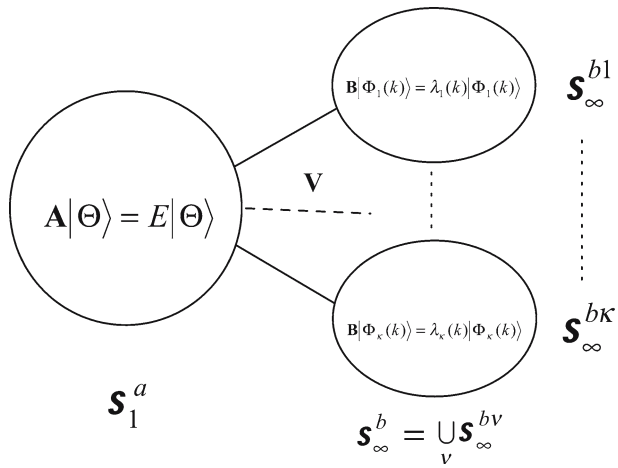

Figure 1. Interaction of the one-dimensional system $\mathcal{S}_1^a$ with the infinite-dimensional system $\mathcal{S}_\infty^b$. System $\mathcal{S}_1^a$ is described by a single state $|\Theta\rangle$ with the eigenvalue E. System $\mathcal{S}_\infty^b$ is a union of κ infinite-dimensional subsystems $\mathcal{S}_\infty^{b\nu}$. Each subsystem $\mathcal{S}_\infty^{b\nu}$ contains a single one-parameter eigenvalue band. Systems $\mathcal{S}_1^a$ and $\mathcal{S}_\infty^b$ are described by eigenvalue equations (1) and (2), respectively. Combined system $\mathcal{S}_\infty$ is described by the eigenvalue equation (3).

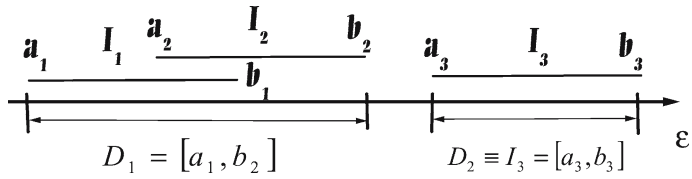

Figure 2. An example of a system $\mathcal{S}_\infty^b$ containing three subsystems $\mathcal{S}_\infty^{b\nu}$ and three one-parameter eigenvalue bands. For explanation see text.

An example is shown in figure 2. System $\mathcal{S}_\infty^b$ contains three one-parameter eigenvalue bands: eigenvalue band $\nu = 1$ (eigenvalue interval $I_1 = [a_1, b_1]$), eigenvalue band $\nu = 2$ (eigenvalue interval $I_2 = [a_2, b_2]$), and eigenvalue band $\nu = 3$ (eigenvalue interval $I_3 = [a_3, b_3]$). Eigenvalue range $D = \cup_\nu I_\nu$ contains two nonoverlaping intervals, interval $D_1 = I_1 \cup I_2 = [a_1, b_2]$ and interval $D_2 \equiv I_3$. Unperturbed eigenvalues $\lambda \in I_1 \cap I_2 \equiv [a_2, b_1]$ are doubly degenerate, while all other eigenvalues $\lambda \in D$ are nondegenerate.

3. Eigenvalues and eigenstates of the combined system

Following the original approach [1], one finds that eigenvalue equation (3a) may contain two qualitatively different types of solutions (see Appendix A). This equation may have *embedded* and *isolated* eigenvalues and eigenstates [1]. Each $\varepsilon \in D$ contained in the range D of the unperturbed eigenvalues is also an eigenvalue of the perturbed eigenvalue equation (3a). One can denote the corresponding eigenstates as $|\Psi_\nu(\varepsilon)\rangle$ where index ν is reserved to label possible degeneracy. Eigenvalues $\varepsilon \in D$ and eigenstates $|\Psi_\nu(\varepsilon)\rangle$ are *embedded* eigenvalues and eigenstates. Since parameter ε assumes continuous values, with respect to this parameter embedded eigenstates are normalized to a δ-function. This is similar to the normalization (2b) of the unperturbed eigenstates $|\Phi_\nu(k)\rangle$. In addition to the embedded eigenvalues, eigenvalue equation (3a) may have some discrete eigenvalues $\varepsilon_I \in \overline{D}$ with the corresponding eigenstates $|\Psi_I\rangle$. Those are *isolated* eigenvalues and eigenstates. Eigenstates $|\Psi_I\rangle$ can be normalized to unity and in this respect those eigenstates are similar to the local state $|\Theta\rangle$ that is also normalized to unity.

3.1. Characteristic and derived functions of the combined system

As shown in the Appendix A, properties of the combined system $\mathcal{S}_\infty$ can be expressed in terms of the characteristic functions $f_\nu(\varepsilon)$ and in terms of the derived functions $\omega_\nu(\varepsilon)$, $(\nu = 1, \ldots, \kappa)$. With each eigenvalue band ν is associated characteristic function $f_\nu(\varepsilon)$. This function is defined in terms of the matrix elements $\langle \Theta | \mathbf{V} | \Phi_\nu(k) \rangle$ and in terms of the derivatives $\mathrm{d}\lambda_\nu/\mathrm{d}k$ according to

$$f_\nu(\varepsilon)=\frac{\langle\Theta|\mathbf{V}|\Phi_\nu(k)\rangle\langle\Phi_\nu(k)|\mathbf{V}|\Theta\rangle}{|\mathrm{d}\lambda_\nu(k)/\mathrm{d}k|}\Big|_{\varepsilon=\lambda_\nu(k)}\cdot\begin{cases}1 & \text{if} \quad \varepsilon\in I_\nu,\\ 0 & \text{if} \quad \varepsilon\notin I_\nu.\end{cases}, \tag{4a}$$

If $\lambda_\nu(k)$ is monotonic increasing function one has $\mathrm{d}\lambda_\nu/\mathrm{d}k\geqslant 0$ while if $\lambda_\nu(k)$ is monotonic decreasing function one has $\mathrm{d}\lambda_\nu/\mathrm{d}k\leqslant 0$. In both cases in the expression (4a) one has to take absolute value $\left|\mathrm{d}\lambda_\nu/\mathrm{d}k\right|$ of this derivative.

Characteristic functions $f_\nu(\varepsilon)$ form a global characteristic function $f(\varepsilon)$

$$f(\varepsilon)=\sum_\nu^\kappa f_\nu(\varepsilon). \tag{4b}$$

This function incorporates essential features of the unperturbed system $\mathcal{S}_\infty^b$ and of the interaction of this system with the local state $|\Theta\rangle$. Definition (4b) is a natural generalization of the original definition [1] of this function. Each function $f_\nu(\varepsilon)$ is nonnegative. In particular, $f_\nu(\varepsilon)$ is positive almost everywhere in the interval I_ν and it is zero outside this interval. Function $f(\varepsilon)$ is hence positive almost everywhere in the range D and it is zero outside this range. One also finds that the integral $\int f(\varepsilon)\mathrm{d}\varepsilon$ is finite. Characteristic function $f(\varepsilon)$ thus satisfies:

$$f(\varepsilon)\geqslant 0, \quad \varepsilon\in\bar{D} \quad \Rightarrow \quad f(\varepsilon)=0, \quad \int f(\varepsilon)\mathrm{d}\varepsilon<\infty. \tag{4c}$$

Each derived function $\omega_\nu(\varepsilon)$ is expressed in terms of the corresponding characteristic function $f_\nu(\varepsilon)$ according to

$$\omega_\nu(\varepsilon)=P\int\frac{f_\nu(\lambda)}{\varepsilon-\lambda}\mathrm{d}\lambda. \tag{5a}$$

In this expression P denotes principal Cauchy integral value. If $\varepsilon\notin I_\nu$, integration in (5a) reduces to a standard integral. If however $\varepsilon\in I_\nu$, subintegral function in (5a) diverges in the point $\lambda=\varepsilon$ and one has to calculate principal Cauchy integral value from this expression. If $f_\nu(\lambda)$ is polynomial in the interval I_ν, integral (5a) can be obtained in a closed analytic form [8].

Functions $\omega_\nu(\varepsilon)$ can be expressed explicitly in terms of matrix elements $\langle\Theta\,|\,\mathbf{V}\,|\Phi_\nu(k)\rangle$ and in terms of the eigenvalue functions $\lambda_\nu(k)$ as

$$\omega_\nu(\varepsilon)=P\int\frac{\langle\Theta|\mathbf{V}|\Phi_\nu(k)\rangle\,\langle\Phi_\nu(k)|\mathbf{V}|\Theta\rangle}{\varepsilon-\lambda_\nu(k)}\mathrm{d}k. \tag{5b}$$

In analogy to (4b), functions $\omega_\nu(\varepsilon)$ form a global function $\omega(\varepsilon)$

$$\omega(\varepsilon)=\sum_\nu^\kappa\omega_\nu(\varepsilon). \tag{5c}$$

One also finds

$$\omega(\varepsilon)=P\int\frac{f(\lambda)}{\varepsilon-\lambda}\mathrm{d}\lambda. \tag{5d}$$

Since $f(\varepsilon)$ is nonnegative one has

$$\omega'(\varepsilon) = -\int \frac{f(\lambda)}{(\varepsilon-\lambda)^2}\, \mathrm{d}\lambda < 0, \quad \varepsilon \in \bar{D}, \tag{6}$$

where $\omega'(\varepsilon) \equiv \mathrm{d}\omega(\varepsilon)/\mathrm{d}\varepsilon$ is a derivative of $\omega(\varepsilon)$. Function $\omega(\varepsilon)$ is hence monotonic decreasing outside the range D. However, inside this range expression (6) is not valid and derivative $\omega'(\varepsilon)$ may have any value. In addition, function $\omega(\varepsilon)$ may diverge in some singular points inside D. Such points are usually boundary points of D [1,8].

In addition to functions $f(\varepsilon)$ and $\omega(\varepsilon)$, it is convenient to define auxiliary function $h(\varepsilon)$

$$h(\varepsilon) \equiv \beta^2 \omega(\varepsilon) + E - \varepsilon. \tag{7}$$

Above functions provide all necessary information for the derivation of various properties of isolated and embedded solutions of the combined system.

3.2. *Isolated eigenvalues and eigenstates*

As shown in the Appendix A, each isolated eigenvalue $\varepsilon_I \in \overline{D}$ of $\mathcal{S}_\infty$ is a root of the auxiliary function $h(\varepsilon)$

$$h(\varepsilon_I) \equiv \beta^2 \omega(\varepsilon_I) + E - \varepsilon_I = 0, \quad \varepsilon_I \in \overline{D}. \tag{8}$$

Since $\omega(\varepsilon)$ is monotonic decreasing in the point set $\overline{D}$, function $h(\varepsilon)$ is also monotonic decreasing in this point set. Hence (8) may have at most one root ε_I in each open interval $\bar{I} \equiv (L, R) \subseteq \overline{D}$. As shown in the Appendix A, this property can be also derived from the interlacing rule (A4). As a result, if the point set $\overline{D}$ is a union of τ nonoverlaping intervals, combined system $\mathcal{S}_\infty$ may contain at most τ isolated solutions. In addition, if $\bar{I}$ is such an interval, relation (8) has a root $\varepsilon_I \in \bar{I}$ if and only if

$$h(L+0) \equiv \beta^2 \omega(L+0) + E - L > 0, \tag{9a}$$

and

$$h(R-0) \equiv \beta^2 \omega(R-0) + E - R < 0. \tag{9b}$$

In those expressions $\omega(L+0)$ and $\omega(R-0)$ denotes right and left limits, respectively

$$\omega(L+0) = \lim_{\varepsilon \to L+0} \omega(\varepsilon), \quad \omega(R-0) = \lim_{\varepsilon \to R-0} \omega(\varepsilon). \tag{9c}$$

One can consider isolated eigenvalue $\varepsilon_I \in \bar{I}$ as a function of parameters E and β. Considered as a function of a local eigenvalue E, isolated eigenvalue $\varepsilon_I \in \bar{I}$ exists if and only if $E \in (E_L, E_R)$ where $E_L < E_R$ and where

$$E_L = L - \beta^2 \omega(L+0), \quad E_R = R - \beta^2 \omega(R-0)$$

are left and right "critical points", respectively. Considered as a function of a coupling parameter β, eigenvalue $\varepsilon_I \in \bar{I}$ exists if and only if

$$\beta \begin{cases} > \beta_L & \text{if} \quad \omega(L+0) > 0, \\ < \beta_L & \text{if} \quad \omega(L+0) < 0, \end{cases} \tag{10a}$$

and

$$\beta \begin{cases} > \beta_R & \text{if} \quad \omega(R-0) < 0, \\ < \beta_R & \text{if} \quad \omega(R-0) > 0, \end{cases} \tag{10b}$$

where "critical points" β_L and β_R are

$$\beta_L^{=} \sqrt{\frac{L-E}{\omega(L+0)}}, \quad \beta_R^{=} \sqrt{\frac{R-E}{\omega(R-0)}}. \tag{10c}$$

If either β_L or β_R is complex, the corresponding condition (10) does not apply. In particular, if both critical points are complex, isolated eigenvalue $\varepsilon_I \in \bar{I}$ exists for each value of the coupling parameter β.

Of particular interest is the case when $L \equiv b_\nu$ is right edge of some interval $I_\nu = [a_\nu, b_\nu] \subseteq D$ while $R \equiv a_\mu > L$ is a left edge of another interval $I_\mu = [a_\mu, b_\mu] \subseteq D$. In addition, one may have $L = -\infty$ as well as $R = \infty$. Since $\omega(-\infty) = 0$, in the interval $\bar{I}_L = (-\infty, a_1) \subset \overline{D}$ on the extreme left the condition $h(-\infty) > 0$ is always satisfied. Hence one has to verify only the condition $h(a_1 - 0) < 0$. Similarly, in the interval $\bar{I}_R = (b_\kappa, \infty) \subset \overline{D}$ on the extreme right the condition $h(\infty) < 0$ is always satisfied and one has to verify only the condition $h(b_\kappa + 0) > 0$. In the remaining intermediate intervals $\bar{I}_M \subset \overline{D}$ (if any) one has usually two conditions (9a) and (9b) to satisfy. Further simplification may arise if the function $\omega(\varepsilon)$ diverges in some boundary point ε_0 of the interval under consideration. In this case the corresponding condition (9) is automatically satisfied [1]. In most cases, however, function $\omega(\varepsilon)$ is finite and continuous in those boundary points and one has $\omega(\varepsilon_0 \pm 0) = \omega(\varepsilon_0)$.

One also finds [1]

$$\frac{\partial \varepsilon_I}{\partial E} = \frac{1}{1 - \beta^2 \omega'(\varepsilon_I)}, \quad \frac{\partial \varepsilon_I}{\partial \beta} = \frac{2\beta\omega(\varepsilon_I)}{1 - \beta^2 \omega'(\varepsilon_I)}. \tag{11}$$

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. In particular and since $\omega'(\varepsilon_I) < 0$, one has $0 < \partial \varepsilon_I / \partial E < 1$. As E increases (decreases) each isolated eigenvalue ε_I also increases (decreases), but with slower pace.

Once ε_I is obtained as a root of (8), the corresponding normalized eigenstate $|\Psi_I\rangle$ can be easily derived. This eigenstate is nondegenerate, and it is given by

$$|\Psi_I\rangle = \frac{1}{Q_I^{1/2}}\left[|\Theta\rangle + \beta\sum_\nu \int \frac{\langle\Phi_\nu(k)|\mathbf{V}|\Theta\rangle}{\varepsilon_I - \lambda_\nu(k)}\,|\Phi_\nu(k)\rangle \mathrm{d}k\right], \quad \varepsilon_I \in \bar{D}, \tag{12a}$$

where

$$Q_I = 1 + \beta^2 \int \frac{f(\lambda)}{(\varepsilon_I - \lambda)^2}\,\mathrm{d}\lambda. \tag{12b}$$

Normalization constant Q_I can be expressed in terms of a derivative $\omega'(\varepsilon)$ of a function $\omega(\varepsilon)$ as

$$Q_I = 1 - \beta^2\omega'(\varepsilon_I). \tag{12c}$$

Above relations provide complete solution for all the properties of the isolated eigenstates of the combined system. In particular, probability $w_I^a = |\langle\Theta\,|\,\Psi_I\rangle|^2$ to find local state $|\Theta\rangle$ in the isolated eigenstate $|\Psi_I\rangle$, i.e. probability for the state $|\Theta\rangle$ to have eigenvalue ε_I is

$$w_I^a \equiv \frac{\partial\varepsilon_I}{\partial E} = \frac{1}{1 - \beta^2\omega'(\varepsilon_I)}. \tag{13}$$

Similarly, probability density $\rho_I^\nu(k) = |\langle\Phi_\nu(k)\,|\,\Psi_I\rangle|^2$ to find eigenstate $|\Psi_I\rangle$ in the state $|\Phi_\nu(k)\rangle$ is

$$\rho_I^\nu(k) = \frac{\beta^2}{Q_I}\frac{|\langle\Phi_\nu(k)\,|\,\mathbf{V}\,|\Theta\rangle|^2}{(\varepsilon_I - \lambda_\nu(k))^2}. \tag{14a}$$

Total probability w_I^b to find isolated eigenstate $|\Psi_I\rangle$ in a system $\boldsymbol{S}_\infty^b$ hence equals

$$w_I^b = \sum_\nu^\kappa w_I^\nu, \tag{14b}$$

where

$$w_I^\nu = \int \rho_I^\nu(k)\mathrm{d}k \tag{14c}$$

is the probability to find this eigenstate in the subsystem $\boldsymbol{S}_\infty^{b\nu}$ of a system $\boldsymbol{S}_\infty^b$. Since one must find each isolated eigenstate $|\Psi_I\rangle$ with certainty either in the local state $|\Theta\rangle$ or in some eigenstate $|\Phi_\nu(k)\rangle$ of a system $\boldsymbol{S}_\infty^b$, one has

$$w_I^a + w_I^b \equiv \frac{1}{1 - \beta^2\omega'(\varepsilon_I)} + \sum_\nu^\kappa \int \rho_I^\nu(k)\mathrm{d}k = 1. \tag{15}$$

This is a completeness relation that in a natural way generalizes corresponding expression for the case when the system $\mathcal{S}_\infty^b$ contains a single one-parameter eigenvalue band [1] to the case when this system contains a finite number of one-parameter eigenvalue bands. This result can be formally derived from the normalization condition $\langle \Psi_I \,|\, \Psi_I \rangle = 1$.

3.3. Embedded eigenvalues and eigenstates

Each $\varepsilon \in D$ is an embedded eigenvalue of the combined system. In order to derive properties of the corresponding eigenstates $|\Psi_\nu(\varepsilon)\rangle$, we first introduce the notion of a *fractional shift* $x(\varepsilon)$. This quantity was originally defined for the case when the system $\mathcal{S}_\infty^b$ contains a single one-parameter eigenvalue band [1]. In the present paper fractional shift is generalized to the case when this system contains a finite number of one-parameter eigenvalue bands.

One arrives at the notion of the fractional shift in the following way: Infinite dimensional combined system $\mathcal{S}_\infty = \mathbf{S}_1^a \oplus \mathbf{S}_\infty^b$ can be approximated to any desired degree of accuracy with a finite-dimensional combined system $\mathcal{S}_{n+1} = \mathbf{S}_1^a \oplus \mathbf{S}_n^b$. This finite system contains $n+1$ eigenvalues ε_k and $n+1$ corresponding eigenstates $|\Psi_k\rangle$ where n is some huge number. System $\mathcal{S}_{n+1}$ can be constructed in such a way that all eigenvalues λ_i of the corresponding unperturbed system $\mathcal{S}_n^b$ are nondegenerate and that in each sufficiently small interval $I \subset D$ successive unperturbed eigenvalues λ_i are approximately equidistant (with possible exception of few isolated points). In addition, corresponding eigenstates $|\Phi_i\rangle$ can be chosen in such a way that matrix elements $\langle \Theta \,|\, \mathbf{V} \,|\, \Phi_i \rangle$ are approximately constant within this interval (see Appendix A). In other words, in each interval $D_\mu \subset D$ the distances $\Delta\lambda_i = \lambda_i - \lambda_{i-1}$ between adjacent unperturbed eigenvalues of $\mathcal{S}_n^b$ as well as corresponding matrix elements $\langle \Theta \,|\, \mathbf{V} \,|\, \Phi_i \rangle$ smoothly change with the change of i. As n increases this smooth change improves, and in a limit $n \to \infty$ it is exact. Given a finite combined system $\mathcal{S}_{n+1}$ with such properties, one can in each interval $D_\mu \subset D$ define quantities

$$x(\varepsilon_k) = \frac{\varepsilon_k - \lambda_{k-1}}{\lambda_k - \lambda_{k-1}}, \quad \lambda_k, \lambda_{k-1} \in D_\mu. \tag{16}$$

Quantity $x(\varepsilon_k)$ is a *fractional shift* of the perturbed eigenvalue ε_k relative to the unperturbed eigenvalue λ_{k-1}. Due to the interlacing rule (A4), ε_k is contained in the interval $I_k = [\lambda_{k-1}, \lambda_k] \subset D_\mu$ and hence $0 \leqslant x(\varepsilon_k) \leqslant 1$. In the limit $n \to \infty$ quantities $x(\varepsilon_k)$ converge to a function $x(\varepsilon)$ of a continuous parameter ε. As shown in the Appendix A, this function equals

$$x(\varepsilon) = \frac{1}{\pi} \cot^{-1}\left(\frac{\varepsilon - E - \beta^2 \omega(\varepsilon)}{\pi \beta^2 f(\varepsilon)}\right), \quad \varepsilon \in D. \tag{17a}$$

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

$$0 \leqslant x(\varepsilon) < 1. \tag{17b}$$

In conclusion, fractional shift $x(\varepsilon)$ is defined via auxiliary finite systems $\boldsymbol{S}_{n+1}$ as a limit of the process $n \to \infty$. It is hence a property of the infinite system $\boldsymbol{S}_{\infty}$, which is the $n \to \infty$ limit of those finite systems. One can visualize fractional shift as the ratio of two infinitesimal quantities. It is the ratio of the infinitesimal shift $(\varepsilon_k - \lambda_{k-1})$ of the perturbed eigenvalue ε_k relative to the unperturbed eigenvalue λ_{k-1} and of the infinitesimal interval $d_k = \lambda_k - \lambda_{k-1}$ between two adjacent unperturbed eigenvalues. The notion of a fractional shift is explained in more details in the Appendix A.

According to (17a), fractional shift is well defined almost everywhere in the range D where the functions $f(\varepsilon)$ and $\omega(\varepsilon)$ are well defined. Exceptions are the points $\varepsilon = \varepsilon_a \in D$ (provided such points exist) that satisfy conditions $f(\varepsilon_a)=0$ and $h(\varepsilon_a)=0$. In each point $\varepsilon=\varepsilon_a$ expression (17a) formally contains undefined ratio $0/0$ and fractional shift can assume any value in the interval [0, 1). We call each such point a point of *anomal resonance* [1]. We also call each point $\varepsilon=\varepsilon_c$ that satisfies $f(\varepsilon_c)=0$ a *critical* point. For the reasons to be explained in the following section, we call each point $\varepsilon=\varepsilon_r$ that satisfies $h(\varepsilon_r)=0$ a *resonant* point. According to those definitions, point $\varepsilon=\varepsilon_a$ is an anomal point if it is simultaneously a critical point and a resonant point. Unless otherwise specified, we will assume that the system $\boldsymbol{S}_{\infty}$ contains no anomal points.

Fractional shift is a key quantity for the derivation of various properties of embedded eigenstates. Of special importance is the probability density $\rho^a(\varepsilon)$ to find the state $|\Theta\rangle$ with the eigenvalue $\varepsilon \in D$. This probability density is a sum

$$\rho^a(\varepsilon) = \sum_{\nu} |\langle \Theta \,|\, \Psi_\nu(\varepsilon)\rangle|^2, \tag{18}$$

where $|\Psi_\nu(\varepsilon)\rangle$ is an eigenstate of the combined system with the eigenvalue ε and where the summation is performed over all such eigenstates.

In the Appendix A we show that $\rho^a(\varepsilon)$ can be expressed in terms of the fractional shift $x(\varepsilon)$ according to

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

Hence and from (17a) one derives

$$\rho^a(\varepsilon) = \frac{\beta^2 f(\varepsilon)}{\pi^2 \beta^4 f^2(\varepsilon) + \big(\beta^2 \omega(\varepsilon) + E - \varepsilon\big)^2}. \tag{20}$$

Since $f(\varepsilon) = 0$ if $\varepsilon \in \bar{D}$, density $\rho^a(\varepsilon)$ vanishes in the point-set $\bar{D}$. As expected, probability to find local state $|\Theta\rangle$ in some embedded eigenstate $|\Psi_\nu(\varepsilon)\rangle$ with $\varepsilon \in \bar{D}$ is zero, since no such eigenstate exists.

Density $\rho^a(\varepsilon)$ can be written as a sum

$$\rho^a(\varepsilon) = \sum_{\nu=1}^{\kappa} \rho_\nu^a(\varepsilon), \tag{21a}$$

where

$$\rho_\nu^a(\varepsilon) = \frac{\beta^2 f_\nu(\varepsilon)}{\pi^2 \beta^4 f^2(\varepsilon) + \left(\beta^2 \omega(\varepsilon) + E - \varepsilon\right)^2}. \tag{21b}$$

In analogy to (20) one has $\rho_\nu^a(\varepsilon) = 0$ if $\varepsilon \notin I_\nu$. Density $\rho_\nu^a(\varepsilon)$ can be nonzero only inside the interval I_ν. In addition, one finds that there exists an orthonormalized set $\{|\Psi_\nu(\varepsilon)\rangle\}$ that satisfies (see Appendix A)

$$\langle \Theta \,|\, \Psi_\nu(\varepsilon)\rangle = \sqrt{\rho_\nu^a(\varepsilon)}, \quad \nu = 1, \ldots, \kappa. \tag{21c}$$

With this choice one has $\rho_\nu^a(\varepsilon) = |\langle \Theta \,|\, \Psi_\nu(\varepsilon)\rangle|^2$. Accordingly, $\rho_\nu^a(\varepsilon)$ is a probability density to find the state $|\Theta\rangle$ in the eigenstate $|\Psi_\nu(\varepsilon)\rangle$ of the combined system.

Since $\rho_\nu^a(\varepsilon)$ vanishes outside the interval I_ν, one has $\langle \Theta \,|\, \Psi_\nu(\varepsilon)\rangle = 0$ if $\varepsilon \notin I_\nu$. This suggests that embedded eigenstates $|\Psi_\nu(\varepsilon)\rangle$ are defined only for those values of ε that satisfy $\varepsilon \in I_\nu$. One finds that this is indeed the case. However, unperturbed eigenstates $|\Phi_\nu(k)\rangle$ are also defined only for those values of k that satisfy $\lambda_\nu(k) = \varepsilon \in I_\nu$. There is hence one-to-one correspondence between unperturbed eigenstates $|\Phi_\nu(k)\rangle$ and embedded eigenstates $|\Psi_\nu(\varepsilon)\rangle$. In particular, if $|\Phi_\nu(k)\rangle$ is m-degenerate, embedded eigenstate $|\Psi_\nu(\varepsilon)\rangle$ where $\varepsilon = \lambda_\nu(k)$ is also m-degenerate. Hence in analogy to (2b)

$$\left\langle \Psi_\nu(\varepsilon) \,\middle|\, \Psi_{\nu'}(\varepsilon') \right\rangle = \delta_{\nu\nu'}(\varepsilon - \varepsilon'), \quad \varepsilon \in I_\nu. \tag{21d}$$

Density $\rho^a(\varepsilon)$ can be conveniently analyzed in terms of the root or roots $\varepsilon_r \in D$ of the auxiliary function $h(\varepsilon)$, provided such root or roots exist:

$$h(\varepsilon_r) \equiv \beta^2 \omega(\varepsilon_r) + E - \varepsilon_r = 0, \quad \varepsilon_r \in D. \tag{22}$$

By definition, each such root is a resonant point. According to (17a), if $f(\varepsilon_r) \neq 0$ then $x(\varepsilon_r) = 0.5$. Resonant point $\varepsilon = \varepsilon_r$ hence corresponds to the perturbed eigenvalue that is exactly in the middle between two adjacent infinitesimally close unperturbed eigenvalues [1]. If however $f(\varepsilon_r) = 0$, the point $\varepsilon_r \equiv \varepsilon_a$

is the point of anomal resonance, and in this case fractional shift $x(\varepsilon_r)$ is undefined. According to (20) close to the resonant point $\varepsilon = \varepsilon_r$, density $\rho^a(\varepsilon)$ tends to have a maximum. In particular, density $\rho^a(\varepsilon_r)$ in a resonant point equals

$$\rho^a(\varepsilon_r) = \frac{1}{\pi^2 \beta^2 f(\varepsilon_r)}.$$

This density is especially large if the coupling β is relatively small. Note that this density diverges if ε_r is an anomal point, that is if $f(\varepsilon_r) = 0$.

Relations (8), (13) and (20) determine eigenvalue or spectral distribution of the local state $|\Theta\rangle$. If one performs a measurement of the eigenvalue on this state, one obtains the result $\varepsilon_I \notin D$ with the probability w_I^a (expression (13)) and the result $\varepsilon \in D$ with a probability density $\rho^a(\varepsilon)$ (expression (20)). Hence those relations completely determine spectrum of the state $|\Theta\rangle$ that interacts with the infinite system $\boldsymbol{S}_\infty$. This spectral (eigenvalue) distribution can be written in a more compact form

$$\rho(\varepsilon) \equiv \rho^a(\varepsilon) + \sum_I w_I^a \delta(\varepsilon - \varepsilon_I). \tag{23}$$

Total probability for the state $|\Theta\rangle$ to have either some isolated eigenvalue $\varepsilon_I \in \bar{D}$ or some embedded eigenvalue $\varepsilon \in D$ must be one. Hence

$$\int \rho(\varepsilon) \mathrm{d}\varepsilon \equiv \int \rho^a(\varepsilon) \mathrm{d}\varepsilon + \sum_I w_I^a = 1, \tag{24a}$$

where

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

is the probability to find the state $|\Theta\rangle$ in any of the embedded eigenstates $|\Psi_\nu(\varepsilon)\rangle$, i.e. to find it with any of the eigenvalues $\varepsilon \in D$.

Relation (24a) is a key completeness relation. It can be used as an efficient test for the validity of the suggested approach. This relation can be derived in a more formal way from the definition $w_I^a = |\langle \Theta \,|\, \Psi_I \rangle|^2$ and from the expression (21c). Since the eigenstates $|\Psi_I\rangle$ and $|\Psi_\nu(\varepsilon)\rangle$ form a complete set in a space corresponding to the combined system $\boldsymbol{S}_\infty$, those expressions imply

$$|\Theta\rangle = \sum_I \sqrt{w_I^a}\, |\Psi_I\rangle + \sum_\nu \int \sqrt{\rho_\nu^a(\varepsilon)}\, |\Psi_\nu(\varepsilon)\rangle \, \mathrm{d}\varepsilon. \tag{25}$$

Normalization condition $\langle \Theta \,|\, \Theta \rangle = 1$ now implies (24a).

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

In the case of the weak coupling (small β), eigenvalue distribution $\rho(\varepsilon)$ of the state $|\Theta\rangle$ simplifies. If β is small there are two qualitatively different cases, the case $E \in \bar{D}$ and the case $E \in D$. There are also small transition regions close to the boundaries between D and $\bar{D}$.

If $E \in \bar{D}$ is an interior point in $\bar{D}$ and if β is sufficiently small, relation (8) has a root $\varepsilon_I \in \bar{D}$ that is close to E. This root is an isolated eigenvalue. Neglecting terms of the order $O(\beta^4)$, it can be approximated as

$$\varepsilon_I \approx E + \beta^2 \omega(E), \quad \varepsilon_I \in \bar{D}. \tag{26}$$

In addition, if β is small relation (13) implies $w_I^a \approx 1$. Corresponding isolated eigenstate $|\Psi_I\rangle$ is hence essentially local state $|\Theta\rangle$ that is slightly perturbed. In conclusion, the effect of the weak interaction of the local state $|\Theta\rangle$ that has the eigenvalue $E \in \bar{D}$ with the system $\boldsymbol{S}_\infty^b$ is that this eigenvalue is shifted to a new position $\varepsilon_I \in \bar{D}$. The corresponding perturbed eigenstate $|\Psi_I\rangle$ is essentially identical to the unperturbed eigenstate $|\Theta\rangle$. Eigenvalue distribution $\rho(\varepsilon)$ of a state $|\Theta\rangle$ is hence $\rho(\varepsilon) \approx \delta(\varepsilon - \varepsilon_I)$.

Another possibility is $E \in D$ where E is an interior point in D. In this case and if β is sufficiently small (resonance approximation [1]), relation (22) has a root $\varepsilon_r \in D$ that is close to E. If $f(\varepsilon_r) \neq 0$, density $\rho^a(\varepsilon)$ can be approximated as [1]

$$\rho^a(\varepsilon) \approx \rho^{a0}(\varepsilon) = \frac{\beta^2 f(\varepsilon_r)}{\pi^2 \beta^4 f^2(\varepsilon_r) + (\varepsilon - \varepsilon_r)^2} \cdot \begin{cases} 1 & \text{if } \varepsilon \in D, \\ 0 & \text{if } \varepsilon \notin D. \end{cases} \tag{27}$$

Inside range D function $\rho^{a0}(\varepsilon)$ is identical to the universal resonance curve [9], while outside this range it is zero. This function is a bell shaped curve truncated at the boundary points of the interval $D_\mu \subseteq D$ that contains resonant point $\varepsilon = \varepsilon_r$. It has maximum $\rho_{\max}^{a0}$ in the point $\varepsilon_r \in D$. One finds

$$\rho_{\max}^{a0} = \rho^a(\varepsilon_r) = \frac{1}{\pi^2 \beta^2 f(\varepsilon_r)}. \tag{28a}$$

For small β this maximum is very large. At the position where $\rho^{a0}(\varepsilon)$ has half of its maximum value, it has the width

$$\Delta\varepsilon_r = 2\pi\beta^2 f(\varepsilon_r). \tag{28b}$$

In a resonance approximation the distance between the resonant point $\varepsilon = \varepsilon_r$ and the nearest boundary point of D is much larger than the width $\Delta\varepsilon_r$. Hence

$$\int \rho^{a0}(\varepsilon) \mathrm{d}\varepsilon \approx 1. \tag{29}$$

Completeness relation (24a) implies $w_I^a \approx 0$. Eigenvalue distribution $\rho(\varepsilon)$ of a state $|\Theta\rangle$ is hence $\rho(\varepsilon) \approx \rho^{a0}(\varepsilon)$.

Neglecting terms of the order $O(\beta^4)$, resonant point can be approximated as

$$\varepsilon_r \approx E + \beta^2 \omega(E), \quad \varepsilon_r \in D. \tag{28c}$$

This expression is formally identical to the expression (26). However, $\varepsilon_r \in D$ is now a resonant eigenvalue that is embedded in the range D. Unlike isolated eigenvalues $\varepsilon_I \in \bar{D}$ that are sharp and have no width, each resonant eigenvalue $\varepsilon_r \in D$ that satisfies $f(\varepsilon_r) \neq 0$ generates a universal resonance curve with maximum at this eigenvalue and with a finite width $\Delta\varepsilon_r \neq 0$.

In conclusion, in the resonance approximation local eigenvalue $E \in D$ is shifted to a resonant point $\varepsilon_r \in D$. In addition, due to the interaction with the infinite system $\mathcal{S}_\infty^b$, this shifted eigenvalue is broadened and it has the shape of a resonance curve with the width $\Delta\varepsilon_r$. The area of this curve equals one. This reproduces well-known results obtained within the formalism of the perturbation expansion approach [2]. It also justifies the name "resonant point" for each root $\varepsilon_r \in D$ of $h(\varepsilon)$. Strictly, this name is justifies only in the case of the weak coupling. It is however natural to generalize this notion to the case of an arbitrary strong interaction.

There is finally a third possibility that the unperturbed eigenvalue E is either a boundary point of a range D or very close to some boundary point of this range. In this case the result is intermediate between the above two cases. For example, if E is a boundary point of D and if the coupling β is small, instead of the expression (29) one obtains

$$\int \rho^{a0}(\varepsilon) \mathrm{d}\varepsilon \approx 0.5.$$

Due to the completeness relation (24a) the missing probability is contained in the isolated eigenstate $|\Psi_I\rangle$ and the probability to find the state $|\Theta\rangle$ in this eigenstate equals $w_I^a \approx 0.5$.

In the above discussion we have tacitly assumed that for sufficiently small β either relation (8) or relation (22) has one and only one solution. If $\omega(\varepsilon)$ is bounded everywhere, this is indeed the case. However, in boundary points of the range D function $\omega(\varepsilon)$ may diverge [1,7,8]. If this is the case, than relation (8) and/or relation (22) has an additional root close to this boundary point. Due to the completeness relation (24a), in the case of sufficiently small β the importance of those additional points is negligible. Only if the interaction is not small the contribution of those additional points to probabilities w_I^a and other quantities of interest can be significant.

4. Example: interaction of a state $|\Theta\rangle$ with several one-dimensional solids in the nearest neighbor tight-binding approximation

We will illustrate the method described in previous sections with a following simple example. Let the system $\mathcal{S}_\infty^b$ be the set of κ one-dimensional solids in the nearest-neighbor tight-binding approximation [3,4]. Each such solid is a subsystem $\mathcal{S}_\infty^{b\nu}$ ($\nu = 1, \ldots, \kappa$) of the system $\mathcal{S}_\infty^b$. With each site of the subsystem $\mathcal{S}_\infty^{b\nu}$ is associated a single state $|\nu, j\rangle$ ($j = 1, 2, \ldots$). In the nearest neighbor tight-binding approximation all matrix elements $\langle \nu, i \,|\, \mathbf{H} \,|\, \nu, i \rangle$ of the Hamiltonian $\mathbf{H}$ between states on the same atomic site equal α_ν, while all matrix elements $\langle \nu, i \,|\, \mathbf{H} \,|\, \nu, j \rangle$ between states on the adjacent atomic sites equal γ_ν. All remaining matrix elements are zero. In chemistry this model is known as a Hückel approximation [3]. Eigenvalues $\lambda_{\nu,i}$ and eigenstates $|\Phi_{\nu,i}\rangle$ of such one-dimensional solid containing n atoms are [3]

$$\lambda_{\nu,i} = \alpha_\nu + 2\gamma_\nu \cos\left(\frac{\pi}{n+1} i\right), \quad |\Phi_{\nu,i}\rangle = \sqrt{\frac{2}{n+1}} \sum_{j=1}^{n} \sin\left(\frac{\pi}{n+1} ij\right) |\nu, j\rangle, \quad i = 1, \ldots, n. \tag{30}$$

This solid represents a finite Hückel chain. System $\mathcal{S}_\infty^{b\nu}$ is an infinite Hückel chain obtained in a limit $n \to \infty$. In this limit discrete eigenvalues and eigenstates are replaced with continuous eigenvalues and eigenstates, respectively [1]

$$\lambda_\nu(k) = \alpha_\nu + 2\gamma_\nu \cos(k), \quad |\Phi_\nu(k)\rangle = \sqrt{\frac{2}{\pi}} \sum_{j=1}^{\infty} \sin(kj)\, |\nu, j\rangle, \qquad 0 < k < \pi. \tag{31a}$$

According to (31a), each subsystem $\mathcal{S}_\infty^{b\nu}$ of $\mathcal{S}_\infty^b$ contains a single one-parameter eigenvalue band with the eigenvalue function $\lambda_\nu(k)$ in the interval I_ν [10].

$$I_\nu = [a_\nu, b_\nu] \equiv [\alpha_\nu - 2\gamma_\nu, \lambda_\nu + 2\gamma_\nu], \quad \nu = 1, \ldots, \kappa. \tag{31b}$$

System $\mathcal{S}_\infty^b$ is a union of κ such subsystems and range $D = \bigcup_\nu I_\nu$ is a union of κ intervals I_ν.

An arbitrary interaction of a local state $|\Theta\rangle$ with a system $\mathcal{S}_\infty^b$ 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 νth Hückel chain is $\langle \Theta \,|\, \mathbf{V} \,|\, \nu, j \rangle = \beta_{\nu,j}$. Hence and from (31a)

$$\langle \Theta \,|\, \mathbf{V} \,|\, \Phi_\nu(k) \rangle = \sqrt{\frac{2}{\pi}} \sum_{j=1}^{\infty} \beta_{\nu,j} \sin(kj), \tag{32a}$$

while normalization (3c) implies

$$\sum_{j,\nu} \beta_{\nu,j}^2 = 1. \tag{32b}$$

Above relations describe most general interaction between a local state $|\Theta\rangle$ and a set of κ infinite Hückel chains. For the sake of simplicity assume that local state $|\Theta\rangle$ interacts only with first state $|\nu, 1\rangle$ of each Hückel chain. In this case (32) reduces to

$$\langle \Theta \,|\, \mathbf{V} \,|\, \Phi_\nu(k) \rangle = \beta_\nu \sqrt{\frac{2}{\pi}} \sin(k), \quad \sum_{\nu}^{\kappa} \beta_\nu^2 = 1, \tag{33}$$

where $\beta_\nu \equiv \beta_{\nu,1}$.This situation is shown in figure 3.

We will solve combined system $\boldsymbol{S}_\infty$ shown in figure 3 with the method described in previous sections. First step in this method is to derive characteristic functions of the system $\boldsymbol{S}_\infty$. According to the definition (4a) and using (31)–(33) one finds

$$f_\nu(\varepsilon) = \frac{\beta_\nu^2}{2\pi\gamma_\nu} \sqrt{4 - g_\nu(\varepsilon)^2} \cdot \begin{cases} 1 & \text{if } \varepsilon \in I_\nu, \\ 0 & \text{if } \varepsilon \notin I_\nu, \end{cases} \tag{34a}$$

where

$$g_\nu(\varepsilon) = \frac{\varepsilon - \alpha_\nu}{\gamma_\nu}. \tag{34b}$$

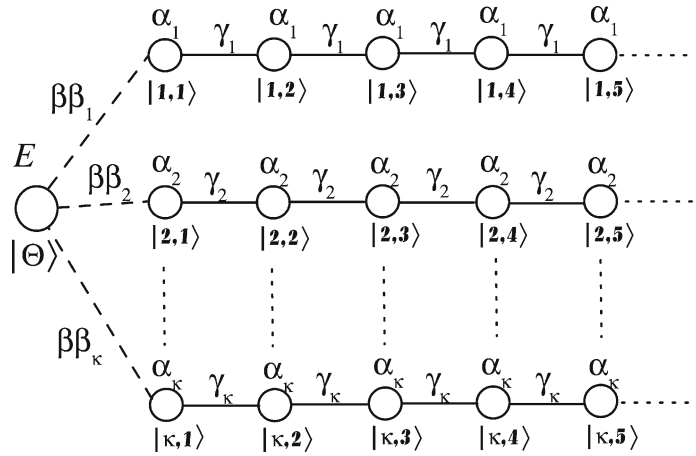

Figure 3. Interaction of a local state $|\Theta\rangle$(system $\boldsymbol{S}_1^a$) with κ infinite one-dimensional solids (Hückel chains) in the nearest-neighbor tight-binding approximation (system $\boldsymbol{S}_\infty^b$). Each solid (subsystem $\boldsymbol{S}_\infty^{b\nu}$) is characterized by two parameters: α_ν (Hückel parameter α) and γ_ν (Hückel parameter β). The state $|\Theta\rangle$ has eigenvalue E and it interacts only with the first atom of each one-dimensional solid. This interaction is fully defined by matrix elements $\langle \Theta | \beta \mathbf{V} | \nu, 1 \rangle = \beta\beta_\nu$.

Note that if $\varepsilon \in I_\nu$ one has $g_\nu(\varepsilon) \in [-2, 2]$ while if $\varepsilon \notin I_\nu$ one has $g_\nu(\varepsilon) \notin [-2, 2]$.

Expression (34) generalizes corresponding expression derived in [1] and it can be obtained along the same lines.

Once characteristic functions $f_\nu(\varepsilon)$ are known, one derives functions $\omega_\nu(\varepsilon)$ according to (5a). One finds

$$\omega_\nu(\varepsilon) \equiv P\int \frac{f_\nu(\lambda)}{\varepsilon-\lambda}\mathrm{d}\lambda = \frac{\beta_\nu^2}{2\gamma_\nu}\begin{cases} \left(g_\nu(\varepsilon)+\sqrt{g_\nu(\varepsilon)^2-4}\right) & \text{if } \varepsilon < a_\nu, \\ g_\nu(\varepsilon) & \text{if } \varepsilon \in I_\nu = [a_\nu, b_\nu], \\ \left(g_\nu(\varepsilon)-\sqrt{g_\nu(\varepsilon)^2-4}\right) & \text{if } \varepsilon > b_\nu. \end{cases} \tag{35a}$$

Each $\omega_\nu(\varepsilon)$ is a continuous function of ω on the entire real axes. In particular, in the boundary points of the interval $I_\nu = [a_\nu, b_\nu]$ one has

$$\omega_\nu(a_\nu \pm 0) \equiv \omega_\nu(a_\nu) = -\frac{\beta_\nu^2}{\gamma_\nu}, \quad \omega_\nu(b_\nu \pm 0) \equiv \omega_\nu(b_\nu) = \frac{\beta_\nu^2}{\gamma_\nu}. \tag{35b}$$

Global functions $f(\varepsilon)$ and $\omega(\varepsilon)$ are sums (4b) and (5c), respectively. Since each $\omega_\nu(\varepsilon)$ is continuous on the real axis, global function $\omega(\varepsilon)$ is also continuous on the real axis. This has nontrivial consequences on the solutions of the combined system.

Expressions (34) and (35) provide all necessary information for the description of isolated and embedded solutions of the combined system.

4.1. Isolated and embedded solutions

Each isolated eigenvalue $\varepsilon_I \in \bar{D}$ is a root of the equation (8) where function $\omega(\varepsilon)$ is given by (5c) and (35a). According to (35b), all $\omega(a_\nu)$ and $\omega(b_\nu)$ are finite. Hence, in order for an isolated eigenstate ε_I to exist in the interval $(b_\nu, a_\mu) \subset \bar{D}$, two nontrivial conditions (9) should be satisfied. Once an isolated eigenvalue ε_I is found as a root of (8), the corresponding normalized eigenstate $|\Psi_I\rangle$ is given by (12). Using (31a) and (33) one finds

$$|\Psi_I\rangle = \frac{1}{Q_I^{1/2}}\left[|\Theta\rangle + \beta\sqrt{\frac{2}{\pi}}\sum_\nu \int_0^\pi \frac{\sin(k)}{\varepsilon_I - \alpha_\nu - 2\gamma_\nu\cos(k)}|\Phi_\nu(k)\rangle \mathrm{d}k\right], \quad \varepsilon_I \in \bar{D}, \tag{36a}$$

where $Q_I = 1 - \beta^2 \omega'(\varepsilon_I)$ and where $\omega'(\varepsilon_I) = \sum_\nu^\kappa \omega'_\nu(\varepsilon_I)$. From (35a) and in the case $\varepsilon \notin I_\nu$ one finds [1,11]

$$\omega'_\nu(\varepsilon) = \frac{\beta_\nu^2}{2\gamma_\nu^2 \sqrt{g_\nu^2(\varepsilon) - 4}} \begin{cases} \sqrt{g_\nu^2(\varepsilon) - 4} + g_\nu(\varepsilon) & \text{if} \quad \varepsilon < a_\nu, \\ \sqrt{g_\nu^2(\varepsilon) - 4} - g_\nu(\varepsilon) & \text{if} \quad \varepsilon > b_\nu, \end{cases} . \tag{36b}$$

Since $g_\nu(\varepsilon) < -2$ if $\varepsilon < a_\nu$ while $g_\nu(\varepsilon) > 2$ if $\varepsilon > b_\nu$, one has $\omega'_\nu(\varepsilon) < 0$ whenever $\varepsilon \notin I_\nu$. Hence $\omega'(\varepsilon) < 0$ if $\varepsilon \in \bar{D}$, in accord with (6).

For completeness note that inside the interval I_ν one has

$$\omega'_\nu(\varepsilon) = \frac{\beta_\nu^2}{2\gamma_\nu^2} \quad \text{if} \quad \varepsilon \in \left[a_\nu^{\cdot}, b_\nu\right]. \tag{36c}$$

From above relations one finds amplitudes $\langle \Theta \mid \Psi_I \rangle = Q_I^{-1/2}$ and $\langle \nu, i \mid \Psi_I \rangle$. In particular one has

$$\langle \nu, i \mid \Psi_I \rangle = \frac{2\beta}{\pi \sqrt{Q_I}} \int_0^\pi \frac{\sin(k) \sin(ik)}{\varepsilon_I - \alpha_\nu - 2\gamma_\nu \cos(k)} \, \mathrm{d}k. \tag{37}$$

Each eigenstate of the combined system can be expressed as a linear combination of a local state $|\Theta\rangle$ and of all states $|\nu, i\rangle$ situated on κ Hückel chains. According to (37), only those states $|\nu, i\rangle$ that are close to the beginning of Hückel chains may have significant contribution to an isolated eigenstate $|\Psi_I\rangle$ of the combined system. As one penetrates inside those chains, amplitudes $\langle \nu, i \mid \Psi_I \rangle$ generally decrease. This is a property that characterizes surface states. It follows from the fact that as i increases $\sin(ik)$ becomes strongly oscillatory function of k. Hence for large i amplitudes $\langle \nu, i \mid \Psi_I \rangle$ tend to be small. In particular one has $\lim_{i \to \infty} \langle \nu, i \mid \Psi_I \rangle = 0$.

Using above relations one can find all isolated eigenvalues and eigenstates of the combined system. First one has to verify conditions (9) in order to find out whether a particular interval $\bar{I} = (L, R) \subseteq \bar{D}$ contains an isolated eigenvalue $\varepsilon_I \in \bar{I}$. If this is the case, ε_I is obtained as a root of the auxiliary function $h(\varepsilon)$. Once ε_I is known, the corresponding normalized eigenstate $|\Psi_I\rangle$ is given by (36). In particular, probability $w_I^a = |\langle \Theta \mid \Psi_I \rangle|^2$ to find the state $|\Theta\rangle$ with the eigenvalue ε_I is given by (13) where derivative $\omega'(\varepsilon_I)$ is obtained using expression (36b). Concerning embedded eigenstates, probability density $\rho^a(\varepsilon)$ to find the state $|\Theta\rangle$ with the eigenvalue $\varepsilon \in D$ is given by relation (20) where functions $f(\varepsilon)$ and $\omega(\varepsilon)$ are obtained using (34) and (35a). Those probabilities and probability density determine eigenvalue distribution $\rho(\varepsilon)$ of the local state $|\Theta\rangle$. One way to verify this distribution and therefore to verify the suggested method is to verify if this distribution satisfies completeness relation (24a).

4.2. Calculated examples

In order to illustrate key features of the interaction of the state $|\Theta\rangle$ with several infinite Hückel chains, it is sufficient to consider the interaction of this state with only two such chains. Accordingly, we consider system $\boldsymbol{S}_\infty^b$ that contains two infinite Hückel chains which represent subsystems $\boldsymbol{S}_\infty^{b1}$ and $\boldsymbol{S}_\infty^{b2}$, respectively. Each of those subsystems generates one-parameter eigenvalue band. Two qualitatively different cases are possible. Either those eigenvalue bands partially or completely overlap, or those eigenvalue bands are distinct and they do not overlap.

As a first example consider the unperturbed system $\boldsymbol{S}_\infty^b$ characterized by the parameters $\alpha_1 = -2$, $\alpha_2 = 2$, $\gamma_1 = 1$ and $\gamma_2 = 0.5$. Assume also that the relative couplings of subsystems $\boldsymbol{S}_\infty^{b1}$ and $\boldsymbol{S}_\infty^{b2}$ with the local state $|\Theta\rangle$ are $\beta_1 = 0.9$ and $\beta_2 = \sqrt{1-\beta_1^2} = 0.43589$, respectively. This last expression follows from the normalization condition (33). We shell refer to this choice of parameters as choice A. According to (31b), with such a choice one has $I_1 = [-4, 0]$ and $I_2 = [1, 3]$. Intervals I_1 and I_2 do not overlap and point set $\bar{D}$ is a union of three intervals, left interval $\bar{I}_L = (-\infty, -4)$, intermediate interval $\bar{I}_M = (0, 1)$ and right interval $\bar{I}_R = (3, \infty)$. Hence the combined system $\boldsymbol{S}_\infty$ may contain at most three isolated eigenstates. Using expression (35a) one finds values of the function $\omega(\varepsilon)$ in the boundary points of the range D: $\omega(-4) = -0.84189 < 0$, $\omega(0) = 0.70818 > 0$, $\omega(1) = -0.07061 < 0$ and $\omega(3) = 0.54906 > 0$. Hence and according to conditions (9), left isolated eigenvalue $\varepsilon_L < -4$ exists if and only if

$$\beta^2\omega(-4) + E + 4 \equiv -0.84189\beta^2 + E + 4 < 0. \tag{38a}$$

Right isolated eigenvalue $\varepsilon_R > 3$ exists if and only if

$$0.54906\beta^2 + E - 3 > 0, \tag{38b}$$

while intermediate isolated eigenvalue $\varepsilon_M \in \bar{I}_M$ exists if and only if

$$0.70818\beta^2 + E > 0 \text{ and } -0.07061\beta^2 + E - 1 < 0. \tag{38c}$$

Once ε_I is known to exist, it is obtained as a root of the expression (8) and the corresponding probability w_I^a is obtained according to (13) where derivative $\omega'(\varepsilon_I)$ is obtained using (5c) and (36b). Concerning probability density $\rho^a(\varepsilon)$ to find the state $|\Theta\rangle$ with the eigenvalue $\varepsilon \in D$, this density is given by general relation (20) where functions $f(\varepsilon)$ and $\omega(\varepsilon)$ can be obtained using relations (34) and (35a), respectively.

Some examples of eigenvalue distributions corresponding to the parameter choice **A** are shown in figures 4 and 5. In figure 4 the case $E = -1 \in D$ and $\beta = 0.2$ is considered. In this case coupling β is relatively weak and eigenvalue E is an interior point of the range D. Those are conditions of the resonance

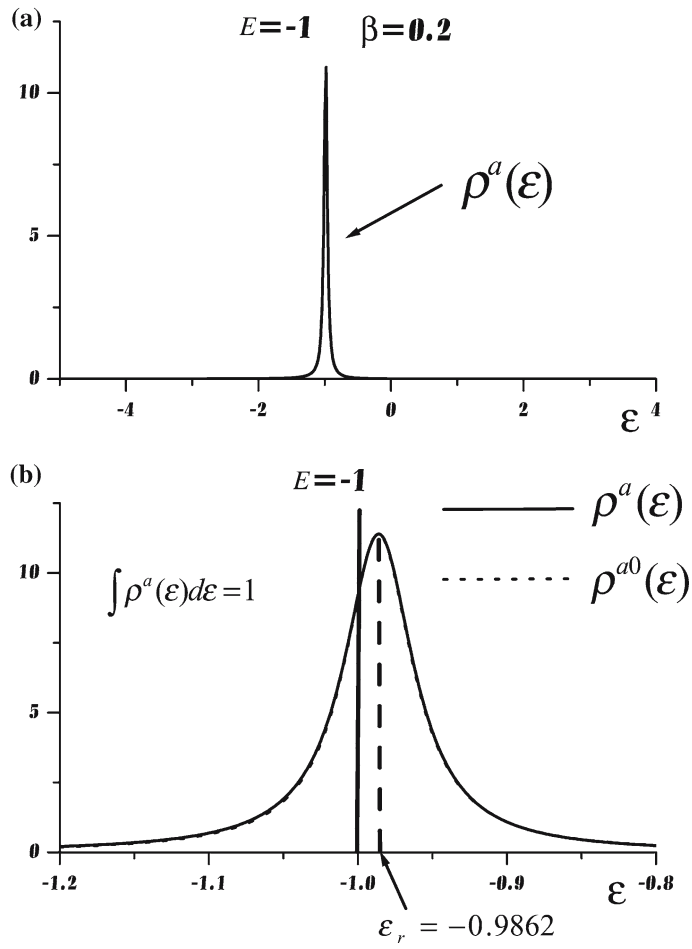

Figure 4. Density distribution $\rho^a(\varepsilon)$ of a local state $|\Theta\rangle$ for a parameter choice **A** and in the case $E=-1$ and $\beta=0.2$. (a) Density distribution $\rho^a(\varepsilon)$. (b) Figure (a) amplified. Density $\rho^a(\varepsilon)$ (solid line) is almost identical to the truncated universal resonance curve $\rho^{a0}(\varepsilon)$ (dashed line).

approximation and eigenvalue distribution of the state $|\Theta\rangle$ has approximately the shape of the universal resonance curve. This is emphasized in figure 4(b) which is figure 4(a) amplified. As shown in this figure, there is almost no difference between exact density $\rho^a(\varepsilon)$ and truncated universal resonance curve $\rho^{a0}(\varepsilon)$. Density $\rho^{a0}(\varepsilon)$ has maximum in the resonant point $\varepsilon=\varepsilon_r$ and it has the width $\Delta\varepsilon_r=2\pi\beta^2 f(\varepsilon_r)$. Solving (22) and using (28b) one finds $\varepsilon_r=-0.9862$ and $\Delta\varepsilon_r=0.0558$. Approximation (28c) produces $\varepsilon_r\approx-0.9864$ which differs only slightly from the exact value for ε_r. One also finds $\int\rho^a(\varepsilon)\mathrm{d}\varepsilon=1$ in accord with the resonance approximation. Completeness requirement (24a) hence implies that there are no isolated eigenvalues. This also follows from the conditions (38).

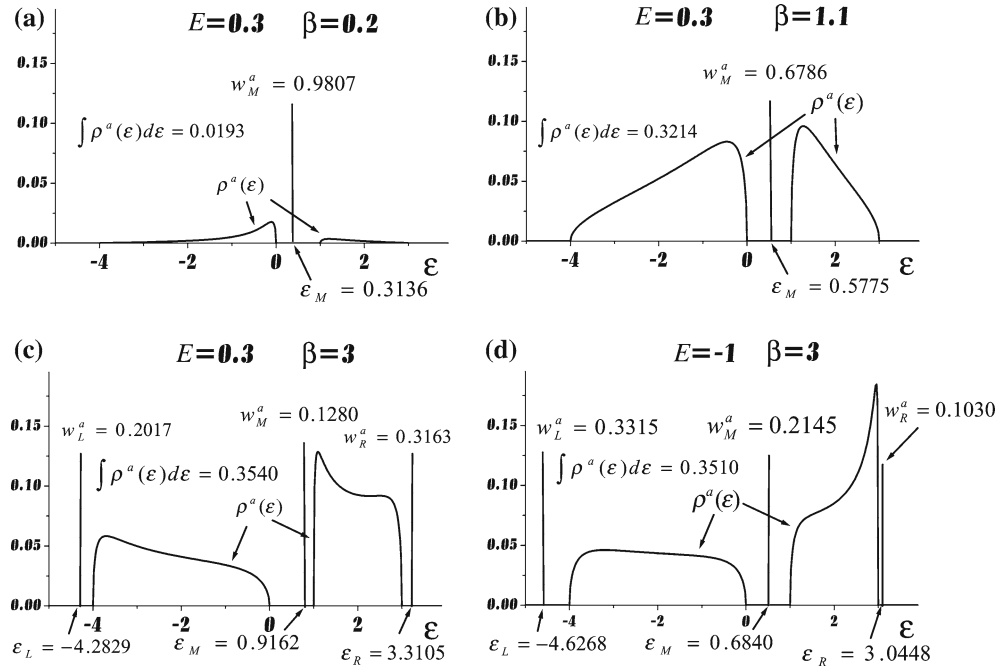

Figure 5. Eigenvalue distribution of a local state $|\Theta\rangle$ for a parameter choice **A** and with few selected values of parameters E and β. (a) $E = 0.3 \notin D, \beta = 0.2$, (b) $E = 0.3, \beta = 1.1$, (c) $E = 0.3 \notin D$, $\beta = 3$, (d) $E = -1 \in D, \beta = 3$.

Few other examples are shown in figure 5. In figure 5(a) the case $E = 0.3 \in \bar{D}$ and $\beta = 0.2$ is considered. Coupling is again relatively weak, but this time eigenvalue E is an interior point of the point set $\bar{D}$. Conditions (38) now imply that combined system contains an isolated eigenvalue ε_M in the interval $\bar{I}_M = (0, 1)$ and no other isolated eigenvalues. Exact expression (8) gives $\varepsilon_M = 0.3136$, while approximate expression (26) yields $\varepsilon_M \approx 0.3139$ which is quite close to the exact value. The interaction of the local state $|\Theta\rangle$ with the infinite system $\mathcal{S}_\infty$ shifts original eigenvalue $E = 0.3$ to a new position $\varepsilon_M = 0.3136$. The corresponding isolated eigenstate $|\Psi_I\rangle$ is given by expression (36a). In particular, the probability w_M^a to find local state $|\Theta\rangle$ in this eigenstate is given by relation (13). Using (36b) one finds $w_M^a = 0.9807 \approx 1$. Isolated eigenstate $|\Psi_M\rangle$ is thus essentially initial eigenstate $|\Theta\rangle$ slightly perturbed. In addition to the isolated eigenvalue ε_M, eigenvalue distribution of the state $|\Theta\rangle$ contains a small contribution from embedded eigenvalues $\varepsilon \in D$. Using (20) one derives density distribution $\rho^a(\varepsilon)$. In particular, one finds $w_D^a = \int \rho^a(\varepsilon)\mathrm{d}\varepsilon = 0.0193$. Hence $w_M^a + w_D^a = 1$ in accord with the completeness requirement (24a).

In figures 4 and 5(a) coupling β is relatively weak and local state $|\Theta\rangle$ is only slightly perturbed by the interaction with the system $\mathcal{S}_\infty^b$. The effect of

this interaction can be well described within the formalism of the perturbation expansion method. The case with relatively strong coupling is shown in figure 5(b) where one has $E = 0.3 \in \bar{D}$ and $\beta = 1.1$. Conditions (38) again imply that combined system contains a single isolated eigenvalue ε_M in the interval $\bar{I}_M = (0, 1)$. This time one finds $\varepsilon_M = 0.5775$, $w_M^a = 0.6786$ and $w_D^a = \int \rho^a(\varepsilon)\mathrm{d}\varepsilon = 0.3214$. The contribution w_D^a of embedded eigenstates to the local state $|\Theta\rangle$ is now significant. As required by the completeness relation, one finds $w_M^a + w_D^a = 1$. In figure 5(c) the case $E = 0.3 \in \bar{D}$ and $\beta = 3$ is considered. Coupling is extremely strong and the system $\boldsymbol{S}_\infty$ contains three isolated eigenstates. One finds $\varepsilon_L = -4.2829$, $\varepsilon_M = 0.9162$ and $\varepsilon_R = 3.3105$ with corresponding probabilities $w_L^a = 0.2017$, $w_M^a = 0.1280$ and $w_R^a = 0.3163$, respectively. One also finds $w_D^a \equiv \int \rho^a(\varepsilon)\mathrm{d}\varepsilon = 0.3540$. Hence $w_D^a + w_L^a + w_R^a + w_M^a = 1$ in complete agreement with the completeness requirement. In figure 6(d) the case $E = -1 \in D$ and $\beta = 3$ is considered. Local eigenvalue E is now embedded in the continuum of the unperturbed eigenvalues and the coupling β is also extremely strong. The system again contains three isolated eigenstates and one finds eigenvalues $\varepsilon_L = -4.6268$, $\varepsilon_M = 0.6840$ and $\varepsilon_R = 3.0448$ with probabilities $w_L^a = 0.3315$, $w_M^a = 0.2145$ and $w_R^a = 0.1030$, respectively. One also finds $w_D^a \equiv \int \rho^a(\varepsilon)\mathrm{d}\varepsilon = 0.3510$ and hence $w_D^a + w_L^a + w_R^a + w_M^a = 1$.

In the case of strong couplings resonance approximation breaks and eigenvalue distribution of a local state $|\Theta\rangle$ has no resemblance to the universal resonance curve, neither in the case $E \in D$ nor in the case $E \notin D$ (see figure 5(b,c,d)). However and as required by the completeness relation, in all cases one has $w_D^a + w_L^a + w_R^a + w_I^a = 1$.

4.2.1. Verification of the completeness relation (24a)

Verification of the completeness relation provides a strong support for the correctness of the suggested method. In the above examples this relation is verified for few selected values of the coupling β. In figure 6 this relation is verified more systematically. In this figure probabilities w_L^a, w_M^a, w_R^a and $w_D^a = \int \rho^a(\varepsilon)\mathrm{d}\varepsilon$ as well as their sum are plotted as functions of a coupling β. This is done for the parameter choice **A** considered above and for two qualitatively different values of a local eigenvalue E. In figure 6(a) one has $E = 0.3 \in \bar{D}$ which is an interior point of the point set $\bar{D}$. The points $(*)$, $(\circ)$ and $(\bullet)$ in this figure correspond to the spectral distributions shown in figures 5(a–c), respectively. In the case $E = 0.3$ conditions (38c) are satisfied for each value of β. Hence intermediate isolated eigenvalue $\varepsilon_M \in (0, 1)$ exists for each β. Concerning left isolated eigenvalue $\varepsilon_L < -4$, condition (38a) implies that this eigenvalue exists if and only if $\beta > \beta_L$ where $\beta_L = \sqrt{-4.3/\omega(-4)} = 2.2600$. Similarly, condition (38b) implies that right isolated eigenvalues $\varepsilon_R > 3$ exists if and only if $\beta > \beta_R$ where $\beta_R = \sqrt{2.7/\omega(3)} = 2.2176$. If the coupling is as small as $\beta \in [0, \beta_R]$ combined system contains only intermediate isolated eigenstate $|\Psi_M\rangle$. The state $|\Theta\rangle$ is hence a linear combination of

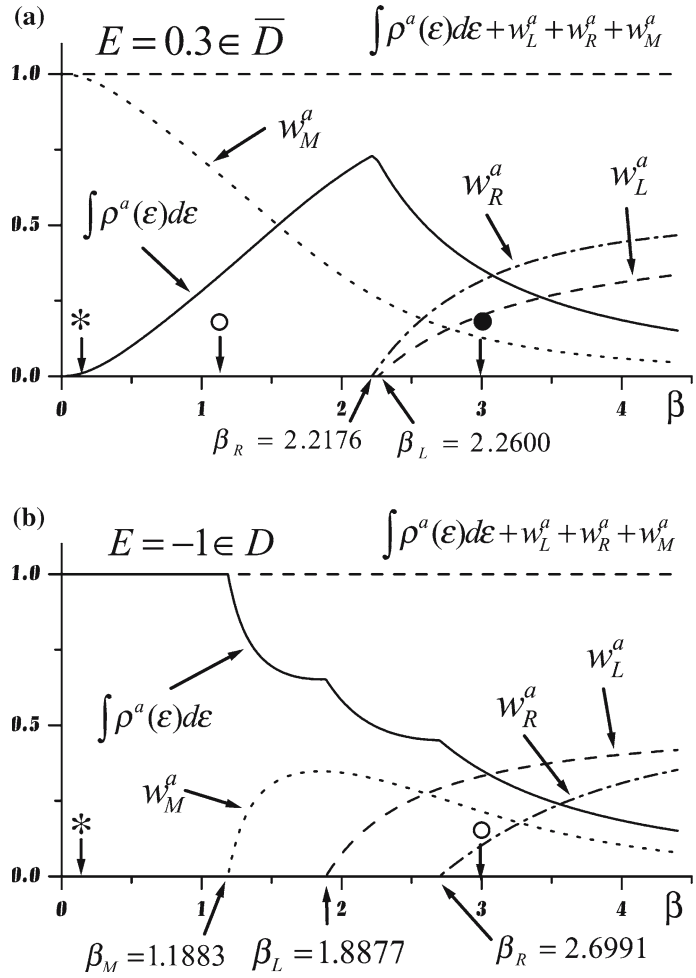

Figure 6. Probabilities w_L^a, w_R^a, w_M^a and $w_D^a = \int \rho^a(\varepsilon)\mathrm{d}\varepsilon$ as functions of a coupling β for a parameter choice **A** and for two qualitatively different values of the local eigenvalue E. (a) $E = 0.3 \in \overline{D}$. Eigenvalue distributions corresponding to points (∗), (○) and (●) are shown in figures 5(a–c), respectively. (b) $E = -1 \in D$. Eigenvalue distributions corresponding to points (∗) and (○) are shown in figures (4) and 5(d), respectively.

this eigenstate and of the embedded eigenstates $|\Psi_\nu(\varepsilon)\rangle$. If $\beta \in (\beta_R, \beta_L]$ combined system contains intermediate eigenstate $|\Psi_M\rangle$ as well as right isolated eigenstate $|\Psi_R\rangle$. In this case the state $|\Theta\rangle$ is a linear combination of those two isolated eigenstates and of the embedded eigenstates $|\Psi_\nu(\varepsilon)\rangle$. Finally if the coupling is as strong as $\beta > \beta_L$, combined system contains all three isolated eigenstates. In this case the state $|\Theta\rangle$ is a linear combination of all those isolated eigenstates and of the embedded eigenstates $|\Psi_\nu(\varepsilon)\rangle$. In all cases one finds $w_D^a + w_L^a + w_M^a + w_R^a = 1$.

In figure 6(b) the case $E=-1\in D$ is considered. The points (∗) and (○) in this figure correspond to spectral distributions shown in figures (4) and 5(d), respectively. Local eigenvalue $E=-1$ is embedded in the range D of unperturbed eigenvalues. Therefore, if the coupling is small enough the system $\boldsymbol{S}_\infty$ contains no isolated eigenstate. One finds that the intermediate eigenvalue $\varepsilon_M\in(0,1)$ exists if and only if $\beta>\beta_M=1.1883$, left isolated eigenvalue $\varepsilon_L<-4$ exists if and only if $\beta>\beta_L=1.8877$, while right isolated eigenvalue $\varepsilon_R>3$ exists if and only if $\beta>\beta_R=2.6991$. One again finds $w_D^a+w_L^a+w_M^a+w_R^a=1$ in complete agreement with the completeness requirement.

In figure 6 is considered a parameter choice **A** when intervals I_1 and I_2 do not overlap. Completeness relation for the case when those intervals overlap is verified in figure 7. In this figure parameter choice $\alpha_1=0$, $\alpha_2=0.5$, $\gamma_1=1$, $\gamma_2=0.5$, $\beta_1=0.7$, and $\beta_2=\sqrt{1-\beta_1^2}=0.71414$ is considered (choice **B**). According to (31b) those parameters imply $I_1=[-2,\,2]$ and $I_2=[-0.5,\,1.5]$. Since $I_2\subset I_1$ the range D coincides with the interval I_1 ($D\equiv I_1$). In addition, in the interval I_2 the unperturbed system $\boldsymbol{S}_\infty^b$ as well as the combined system $\boldsymbol{S}_\infty$ is degenerate. Since D contains a single finite interval I_1, point-set $\bar{D}$ is a union of two intervals, left interval $\bar{I}_L=(-\infty,-2)$ and right interval $\bar{I}_R=(2,\infty)$. Hence the combined system $\boldsymbol{S}_\infty$ may contain at most two isolated eigenstates, left isolated eigenstate $|\Psi_L\rangle$ with the eigenvalue $\varepsilon_L<-2$ and right isolated eigenstate $|\Psi_R\rangle$ with the eigenvalue $\varepsilon_R>2$. In the boundary points –2 and 2 of the range D function $\omega(\varepsilon)$ has values $\omega(-2)=-0.70289$ and $\omega(2)=0.87961$, respectively. Hence left isolated eigenvalue ε_L exists if and only if

$$-0.70289\beta^2+E+2<0, \tag{39a}$$

while right isolated eigenvalue ε_R exists if and only if

$$0.87961\beta^2+E-2>0. \tag{39b}$$

Considered as a function of β, left isolated eigenvalue ε_L exists if and only if $\beta>\beta_L$, where

$$\beta_L=\sqrt{\frac{E+2}{-\omega(-2)}},$$

while right isolated eigenvalue ε_R exists if and only if $\beta>\beta_R$, where

$$\beta_R=\sqrt{\frac{2-E}{\omega(2)}}.$$

If $E=1\in D$ local eigenvalue is embedded in the range D and one finds two critical points, $\beta_L=2.0659$ and $\beta_R=1.0662$. This situation is shown in figure 7(a). If however $E=2.5\in\bar{D}$ there is only one critical point $\beta_L=2.5303$, while

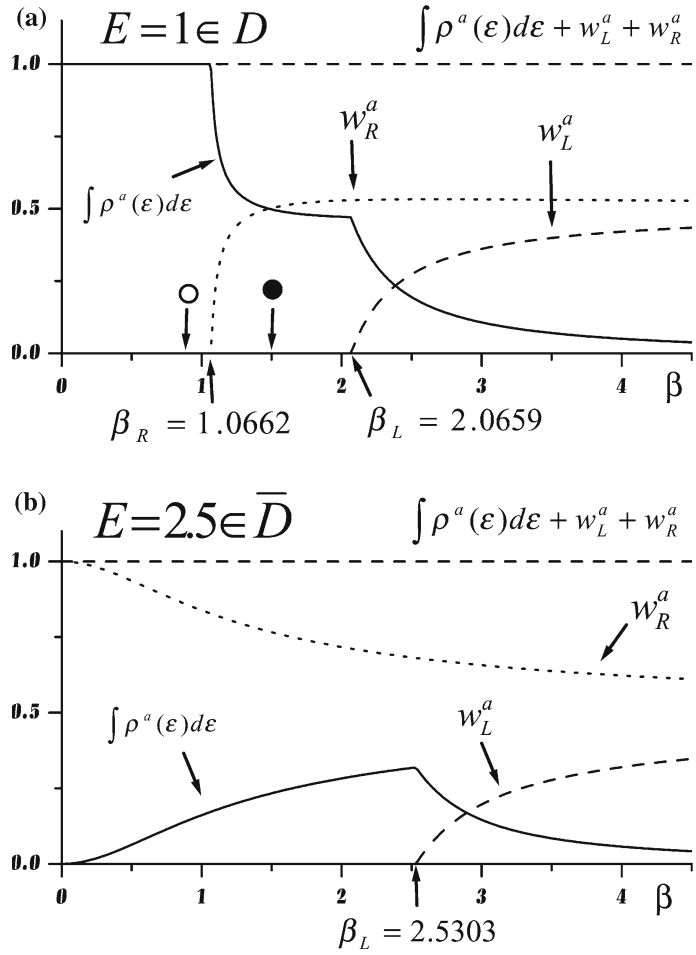

Figure 7. Probabilities w_L^a, w_R^a, and $w_D^a = \int \rho^a(\varepsilon)\mathrm{d}\varepsilon$ as functions of a coupling β for a parameter choice **B** and for two qualitatively different values of the local eigenvalue E. (a) $E = 1 \in D$, (b) $E = 2.5 \in \overline{D}$.

β_R is complex. In this case left isolated eigenvalue $\varepsilon_L < -2$ exists if and only if $\beta > \beta_L$, while right isolated eigenvalue ε_R exists for each value of the coupling β. This situation is shown in figure 7(b).

In the entire interval $\beta \in [0, 4.5]$ considered in figures 6 and 7 theoretical probabilities w_D^a and w_I^a are in complete agreement with the completeness requirement (24a). This agreement is a strong though indirect verification of the expression (20) for the density $\rho^a(\varepsilon)$ (since this density determines probability $w_D^a = \int \rho^a(\varepsilon)\mathrm{d}\varepsilon$) and of the expressions (8) and (13) (since those expressions determine probabilities w_I^a). Suggested approach produces correct results for each coupling, however strong. This is not the case with standard perturba-

tion expansion method. No power series expansion can produce correct result beyond the critical points in figures 6 and 7. For example, in the point $\beta = \beta_R$ in figure 7(a) probability w_D^a considered as a function of coupling β is not analytic. Hence standard perturbation expansion approach can not produce correct results for $\beta \geqslant \beta_R$.

4.2.2. Eigenvalue distribution of the isolated state $|\Theta\rangle$

As shown in a previous section, completeness relation (24a) is correctly reproduced by the suggested approach. However, this relation expresses only a global property of the eigenvalue distribution $\rho(\varepsilon)$ of a state $|\Theta\rangle$. We will now verify in more details this distribution. In order to do this one has to verify probability density $\rho^a(\varepsilon)$ as well as eigenvalues ε_I and corresponding probabilities w_I^a. This will be done by comparing those quantities with the results obtained in a standard way from finite-dimensional combined systems $\boldsymbol{S}_{n+1}$ containing finite Hückel chains. Each such finite system is described by an $(n+1) \times (n+1)$ eigenvalue equation that can be solved by standard diagonalization methods. In the limit $n \to \infty$ the results obtained in a standard way from those finite systems should converge to the theoretical results for the infinite system $\boldsymbol{S}_\infty$. In order to emphasize that various quantities refer to a finite combined system $\boldsymbol{S}_{n+1}$, we will denote those quantities with explicit dependence on n. Accordingly, $\varepsilon_k(n)$ are eigenvalues of $\boldsymbol{S}_{n+1}$, $w_k^a(n)$ are corresponding probabilities, etc.

Concerning isolated eigenvalues ε_I and the corresponding probabilities w_I^a, this comparison is simple. One has to compare each isolated eigenvalue $\varepsilon_I \in \bar{D}$ of $\boldsymbol{S}_\infty$ with the corresponding eigenvalue $\varepsilon_k(n) \in \bar{D}$ of $\boldsymbol{S}_{n+1}$. Since in each open interval $\bar{I} \subset \bar{D}$ can exist at most one eigenvalue ε_I of $\boldsymbol{S}_\infty$ and at most one eigenvalue $\varepsilon_k(n)$ of $\boldsymbol{S}_{n+1}$, it is easy to identify eigenvalue $\varepsilon_k(n)$ that corresponds to the isolated eigenvalue ε_I. Once those eigenvalues are known, one has to compare probability $w_I^a = |\langle\Theta \,|\, \Psi_I\rangle|^2$ with the probability $w_k^a(n) = |\langle\Theta \,|\, \Psi_k\rangle|^2$ where $|\Psi_k\rangle$ is eigenstate of $\boldsymbol{S}_{n+1}$ with the eigenvalue $\varepsilon_k(n)$. Concerning probability density $\rho^a(\varepsilon)$, it should be compared with probabilities $w_k^a(n)$ that correspond to the eigenvalues $\varepsilon_k(n) \in D$ of $\boldsymbol{S}_{n+1}$. This comparison requires more subtle approach. If probabilities $w_k^a(n)$ and eigenvalues $\varepsilon_k(n) \in D$ change relatively smoothly with index k, in a limit $n \to \infty$ those probabilities can be replaced with $\rho^a(\varepsilon)\mathrm{d}\varepsilon$. Hence a rather simple approach is to compare discrete probability $w_k^a(n)$ with $\rho^a(\varepsilon_k(n))\Delta\varepsilon_k(n)$ where $\Delta\varepsilon_k(n) = \varepsilon_k(n) - \varepsilon_{k-1}(n)$ is the interval between two adjacent eigenvalues $\varepsilon_k(n)$ and $\varepsilon_{k-1}(n)$. Slightly better choice is to use the average of the intervals $\Delta\varepsilon_{k+1}(n)$ and $\Delta\varepsilon_k(n)$ on both sides of the eigenvalue $\varepsilon_k(n)$ instead of the interval $\Delta\varepsilon_k(n)$ alone. Accordingly, if $\varepsilon_k(n)$ is contained inside the interval $D_\mu \subseteq D$ and if in addition adjacent eigenvalues $\varepsilon_{k-1}(n)$ and $\varepsilon_{k+1}(n)$ are contained in the same interval, we make the following comparison

$$\rho^a(\varepsilon_k(n)) \leftrightarrow W_k^a(n) = \frac{w_k^a(n)}{(\Delta\varepsilon_k(n) + \Delta\varepsilon_{k+1}(n))/2}, \quad \varepsilon_{k-1}(n), \varepsilon_k(n), \varepsilon_{k+1}(n) \in D_\mu. \tag{40}$$

A special care is required for the eigenvalue $\varepsilon_k(n) \in D_\mu$ that is adjacent either to the left or to the right edge of the interval $D_\mu \subseteq D$. If $\varepsilon_k(n)$ is adjacent to the left edge of this interval, we calculate $W_k^a(n)$ according to $W_k^a(n) = w_k^a(n)/\Delta\varepsilon_k(n)$ where the interval $\Delta\varepsilon_k(n)$ is defined as the distance between the left edge of the interval D_μ and a mean point $(\varepsilon_k(n) + \varepsilon_{k+1}(n))/2$. Similarly is calculated $W_k^a(n)$ in the case when $\varepsilon_k(n)$ is adjacent to the right edge of D_μ [12]. We refer to the quantities $W_k^a(n)$ as *normalized probabilities*.

As a first example consider eigenvalue distribution of the state $|\Theta\rangle$ shown in figure 5(b). This distribution is due to the parameter choice **A** and to the values $E = 0.3$ and $\beta = 1.1$. It corresponds to the point ($\circ$) in figure 6(a). In figure 8(a) is this distribution shown once more and in figures 8(b–d) it is compared with results obtained from three finite systems $\boldsymbol{S}_{n+1}$. Each system $\boldsymbol{S}_{n+1}$ contains two finite Hückel chains and it is assumed that those chains contain an equal number of states. For example, in the case $n = 10$ each Hückel chain contains 5 states. Cases $n = 10$ (figure 8(b)), $n = 40$ (figure 8(c)) and $n = 160$ (figure 8(d)) are considered. Since intervals $I_1 = [-4, 0]$ and $I_2 = [1, 3]$ do not overlap, discrete probabilities $w_k^a(n)$ and intervals $\Delta\varepsilon_k(n)$ smoothly change with the index k. Comparison (40) is hence appropriate. In figures 8(b–d) probability density $\rho^a(\varepsilon)$ (solid lines) is compared with normalized probabilities $W_k^a(n)$ (vertical columns). Each normalized probability $W_k^a(n)$ is situated at the position of the corresponding eigenvalue $\varepsilon_k(n)$. As a quantitative measure of the agreement between normalized probabilities $W_k^a(n)$ and theoretical density $\rho^a(\varepsilon)$ one can use a standard deviation $\Delta(n)$

$$\Delta(n) = \left[\frac{\sum_{\varepsilon_k(n) \in D} \left(\rho^a(\varepsilon_k(n)) - W_k^a(n) \right)^2}{n} \right]^{\frac{1}{2}}. \tag{41}$$

This quantity measures average deviation of normalized probabilities $W_k^a(n)$ from a theoretical density $\rho^a(\varepsilon)$ at the points where $\varepsilon = \varepsilon_k(n)$. One finds $\Delta(10) = 0.0051$, $\Delta(40) = 0.0016$ and $\Delta(160) = 0.0002$. As n increases the agreement between finite chain result and theoretical density $\rho^a(\varepsilon)$ rapidly improves and in a limit $n \to \infty$ it is exact. The same applies to the isolated eigenvalue $\varepsilon_M \in [0, 1]$ and the corresponding probability w_M^a. Using relations (8), (13) and (36b) one finds $\varepsilon_M = 0.5775$ and $w_M^a = 0.6786$. In a finite system $\boldsymbol{S}_{n+1}$ to the isolated eigenvalue ε_M corresponds the eigenvalue $\varepsilon_{n/2+1}(n) \in [0, 1]$. If $n = 10$ one finds $\varepsilon_6(10) = 0.5773$ and $w_6^a(10) = 0.6794$. With further increase of n those values rapidly converge to the theoretical values ε_I and w_I^a of an infinite system. Thus already for $n = 20$ one finds $\varepsilon_{11}(20) = 0.5775$ and $w_{11}^a(20) = 0.6786$. This agrees up to four significant figures with ε_I and w_I^a, respectively.

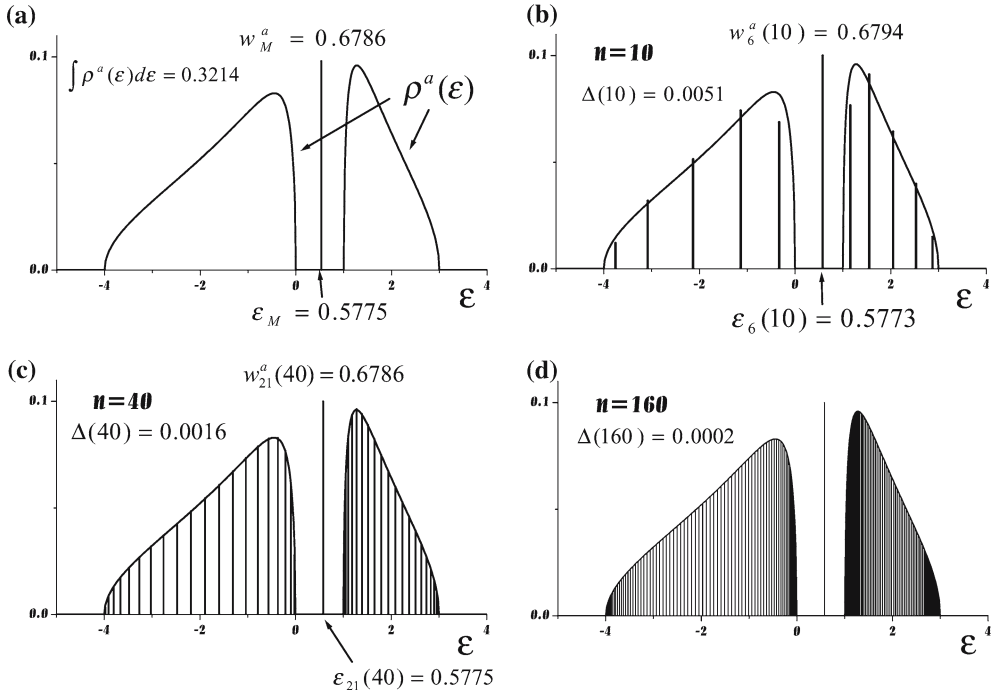

Figure 8. Eigenvalue distribution of a local state $|\Theta\rangle$ for a parameter choice **A** and for the case $E = 0.3$ and $\beta = 1.1$. This distribution corresponds to the point (○) in figure 6(a). It is compared with the results obtained from three selected finite systems $\boldsymbol{S}_{n+1}$. Comparison is done using normalized probabilities W_k^a (vertical columns). Each vertical column is situated at the position of the corresponding perturbed eigenvalue $\varepsilon_k(n) \in D$. In addition, isolated eigenvalue ε_M and probability w_M^a are compared with corresponding quantities of a finite system $\boldsymbol{S}_{n+1}$. (a) Eigenvalue distribution $\rho(\varepsilon)$, (b) comparison for $n = 10$, (c) comparison for $n = 40$, (d) comparison for $n = 160$.

4.2.3. The method of the moving Gaussian window

As another example consider parameter choice **B** and assume $E = 1$ and $\beta = 0.9$. This example corresponds to the point (○) in figure 7(a). Since intervals $I_1 = [-2, 2]$ and $I_2 = [-0.5, 1.5]$ partialy overlap and since $I_2 \subset I_1$, unperturbed eigenvalues $\lambda_\nu(k) \in I_2$ as well as perturbed eigenvalues $\varepsilon \in I_2$ are degenerate. In figure 9(a) is shown corresponding eigenvalue distribution $\rho(\varepsilon)$ of a local state $|\Theta\rangle$. System $\boldsymbol{S}_\infty$ contains no isolated eigenstates and hence $\rho(\varepsilon) = \rho^a(\varepsilon)$ and $\int \rho^a(\varepsilon)\mathrm{d}\varepsilon = 1$. Distribution $\rho(\varepsilon)$ is in figure 9(b–d) compared with the normalized probabilities $W_k^a(n)$ for three selected finite systems $\boldsymbol{S}_{n+1}$. In the intervals $[-2, -0.5]$ and $[1.5, 2]$ where unperturbed eigenvalues $\lambda_\nu(k)$ are nondegenerate, the agreement between probability density $\rho^a(\varepsilon)$ and normalized probabilities $W_k^a(n)$ improves with the increase of n. However, in the interval $I_2 = [-0.5, 1.5]$ normalized probabilities $W_k^a(n)$ considered as a function of k are strongly irregular and the agreement of those probabilities with density $\rho^a(\varepsilon)$ is not so good.

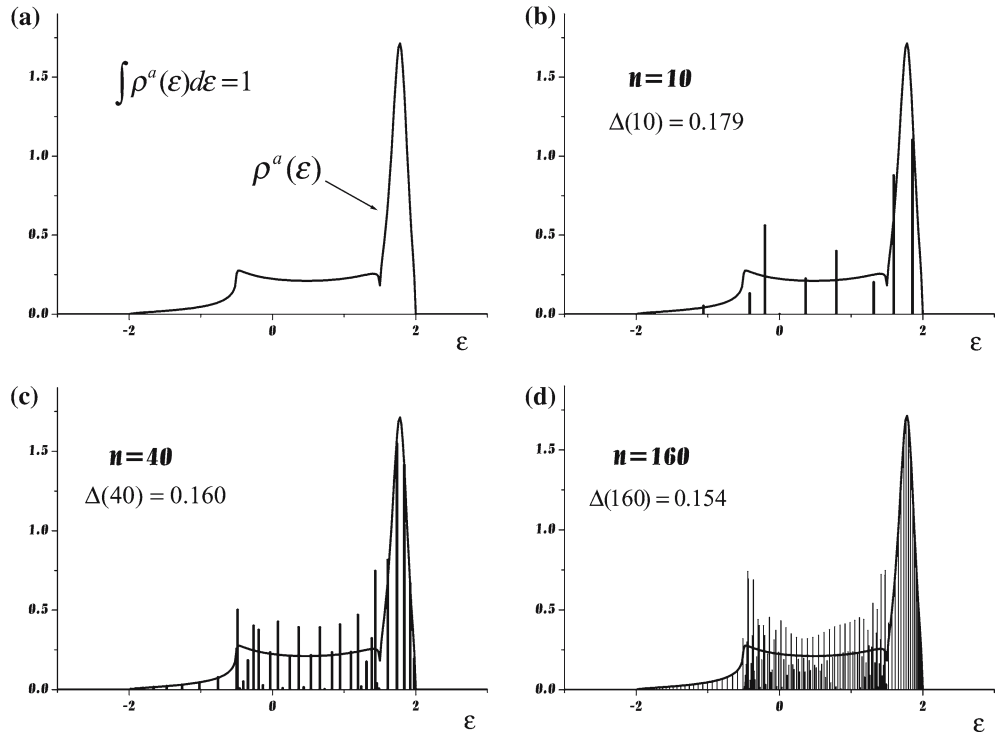

Figure 9. Eigenvalue distribution of a local state $|\Theta\rangle$ for a parameter choice **B** and for the case $E = 1$ and $\beta = 0.9$. This distribution corresponds to the point (○) in figure 7(a). It is compared with the results obtained from three selected finite systems $\boldsymbol{S}_{n+1}$. Comparison is done using normalized probabilities W_k^a (vertical columns). Each vertical column is situated at the position of the corresponding perturbed eigenvalue $\varepsilon_k(n) \in D$. (a) Eigenvalue distribution $\rho(\varepsilon)$, (b) comparison for $n = 10$, (c) comparison for $n = 40$, (d) comparison for $n = 160$.

In particular, one finds $\Delta(10) = 0.179$, $\Delta(40) = 0.160$ and $\Delta(160) = 0.154$. Those standard deviations do not converge to zero as $n \to \infty$. This is due to the fact that in the interval I_2 neither eigenvalues $\varepsilon_k(n)$ nor probabilities $w_k^a(n)$ change smoothly with index k. As a consequence expression (40) fails. The failure of this expression under such conditions is understandable. Consider for example extreme possibility $\varepsilon_{k-1}(n) = \varepsilon_k(n) = \varepsilon_{k+1}(n)$. In this case expression (40) produces absurd value $W_k^a(n) = \infty$. A more subtle method is required in this and similar cases in order to compare eigenvalues $\varepsilon_k(n) \in D$ and corresponding probabilities $w_k^a(n)$ with density $\rho^a(\varepsilon)$. We will now describe the method of a moving Gaussian window. This method works in all cases.

An ideal measurement (performed with an infinite precision) of an eigenvalue $\varepsilon_k(n)$ with the probability $w_k^a(n)$ is represented by the function $w_k^a(n)\delta(\varepsilon - \varepsilon_k(n))$. This is a δ-like function situated at the position $\varepsilon = \varepsilon_k(n)$ and with an area $w_k^a(n)$. However, each real measurement of an eigenvalue can be performed

only with a finite precision $\Delta > 0$. This finite precision represents a finite resolution of the measurement process. In order to represent such a measurement one has to replace δ-function $\delta(\varepsilon - \varepsilon_k(n))$ with some function $g(\varepsilon - \varepsilon_k(n), \Delta)$ that has a finite width Δ. Function $g(\varepsilon, \Delta)$ should be centered at $\varepsilon = 0$, it should be relatively smooth with a finite width Δ, and it should be normalized to unity, $\int g(\varepsilon, \Delta)\mathrm{d}\varepsilon = 1$. For the intended purpose exact form of this function is not essential, and it is convenient to choose a Gaussian

$$g(\varepsilon, \Delta) = \frac{1}{\Delta\sqrt{\pi}} e^{-\left(\frac{\varepsilon}{\Delta}\right)^2}, \quad \int g(\varepsilon, \Delta)\mathrm{d}\varepsilon = 1. \tag{42a}$$

We will refer to this function as a *Gaussian window*. Function $w_k^a(n)g(\varepsilon - \varepsilon_k(n), \Delta)$ represents a measurement of the eigenvalue $\varepsilon_k(n)$ with the finite resolution Δ. If instead of a single eigenvalue one considers a finite system $\boldsymbol{S}_{n+1}$ with several discrete eigenvalues $\varepsilon_k(n) \in D$ and the corresponding probabilities $w_k^a(n)$, such a measurement will produce the value ε with the probability density

$$\rho_n^a(\varepsilon, \Delta) = \sum_{\varepsilon_k(n) \in D} w_k^a(n) g\,(\varepsilon - \varepsilon_k(n), \Delta). \tag{42b}$$

From the summation in (42b) eigenvalues $\varepsilon_k(n) \in \bar{D}$ are excluded. Those eigenvalues correspond to isolated eigenvalues ε_I of $\boldsymbol{S}_\infty$ and they should be treated separately. Note that due to (42a) one has

$$\int \rho_n^a(\varepsilon, \Delta)\mathrm{d}\varepsilon = \sum_{\varepsilon_k(n) \in D} w_k^a(n). \tag{42c}$$

In particular, if the finite system $\boldsymbol{S}_{n+1}$ contains no eigenvalues outside the range D, one has $\int \rho_n^a(\varepsilon, \Delta)\mathrm{d}\varepsilon = 1$.

Probability density $\rho_n^a(\varepsilon, \Delta)$ represents a finite-precision measurement performed with the resolution Δ on a finite system $\boldsymbol{S}_{n+1}$. This density should be compared with probability density $\rho^a(\varepsilon)$ of the infinite system $\boldsymbol{S}_\infty$. In analogy to (41) the agreement between $\rho_n^a(\varepsilon, \Delta)$ and $\rho^a(\varepsilon)$ can be estimated with a standard deviation

$$\Delta\rho_n^a(\Delta) = \sqrt{\int \left(\rho_n^a(\varepsilon, \Delta) - \rho^a(\varepsilon)\right)^2 \mathrm{d}\varepsilon}. \tag{43}$$

In a limit $n \to \infty$ densities $\rho_n^a(\varepsilon, \Delta)$ should converge to $\rho^a(\varepsilon)$ and standard deviation $\Delta\rho_n^a(\Delta)$ should converge to zero. Since each density $\rho_n^a(\varepsilon, \Delta)$ depends on the resolution Δ, this limit should be performed in a particular way. If Δ is bigger than the average separation $\overline{\Delta\varepsilon_k(n)}$ between adjacent eigenvalues $\varepsilon_k(n) \in D$ of a finite system $\boldsymbol{S}_{n+1}$, density $\rho_n^a(\varepsilon, \Delta)$ will be relatively smooth function of ε. However, large Δ means small resolution of the measurement process and hence if $\Delta \gg \overline{\Delta\varepsilon_r(n)}$ density $\rho_n^a(\varepsilon, \Delta)$ will not be a very good approximation of $\rho^a(\varepsilon)$.

This can be improved by decreasing Δ which should increase resolution and decrease standard deviation $\Delta\rho_n^a(\Delta)$. However, if the width Δ is much smaller than maximum separation between adjacent eigenvalues $\varepsilon_k(n) \in D$ and especially if it is much smaller than average separation $\overline{\Delta\varepsilon_k(n)}$ between those eigenvalues, there is another problem. In this case discrete character of separate eigenvalues $\varepsilon_k(n)$ becomes manifest, and density $\rho_n^a(\varepsilon, \Delta)$ considered as a function of ε varies quite strongly from one eigenvalue $\varepsilon_k(n)$ to another. As a consequence, standard deviation $\Delta\rho_n^a(\Delta)$ is again large. Between those two extremes there is an optimum resolution $\Delta \equiv \Delta_0(n)$ which minimizes $\Delta\rho_n^a(\Delta)$. This minimum value equals $\Delta\rho_n^{a0} \equiv \Delta\rho_n^a(\Delta_0(n))$. We will denote the corresponding density distribution as $\rho_n^{a0}(\varepsilon) \equiv \rho_n^a(\varepsilon, \Delta_0(n))$.

According to the above analyze, optimum resolution $\Delta_0(n)$ is of the order of the average separation $\overline{\Delta\varepsilon_k(n)}$ between two adjacent eigenvalues $\varepsilon_k(n) \in D$ of $\mathcal{S}_{n+1}$, but it is also quite sensitive on the maximum separation between those adjacent eigenvalues. With the increase of n average separation $\overline{\Delta\varepsilon_k(n)}$ as well as maximum separation between adjacent eigenvalues decreases. Hence $\Delta_0(n)$ decreases with the increase of n, and in a limit $n \to \infty$ it converges to zero. Experimentally, this final goal ($\Delta_0 = 0$) can never be achieved.

In figures 10 and 11 eigenvalue distribution shown in figure 9 is reconsidered using above Gaussian window method. In figure 10 are shown standard deviations $\Delta\rho_n^a(\Delta)$ as functions of Δ for five selected values of n. For each n there is an optimum resolution $\Delta = \Delta_0(n)$ such that this standard deviation has a minimum $\Delta\rho_n^{a0}$. One finds $\Delta_0(10) = 0.193$, $\Delta_0(20) = 0.121$, $\Delta_0(40) = 0.087$, $\Delta_0(80) = 0.062$ and $\Delta_0(160) = 0.038$. As required, those values decrease with the increase of n and in a limit $n \to \infty$ they converge to zero. Corresponding standard deviations $\Delta\rho_n^{a0}$ are $\Delta\rho_{10}^{a0} = 0.351$, $\Delta\rho_{20}^{a0} = 0.200$, $\Delta\rho_{40}^{a0} = 0.111$, $\Delta\rho_{80}^{a0} = 0.059$ and $\Delta\rho_{160}^{a0} = 0.025$. As n increases, those values also converge to zero.

In figure 11 is compared exact density $\rho^a(\varepsilon)$ (solid lines) with optimum finite chain densities $\rho_n^{a0}(\varepsilon)$ (dashed lines) for three selected values of n. If n is as low as $n = 10$, optimum width $\Delta_0(10) = 0.193$ of the Gaussian window is relatively large. Standard deviation $\Delta\rho_{10}^{a0} = 0.351$ is hence also relatively large, and density $\rho_{10}^{a0}(\varepsilon)$ is relatively pure approximation of $\rho^a(\varepsilon)$ (figure 11(b)). If n increases to $n = 40$, optimum width of the Gaussian window decreases to $\Delta_0(40) = 0.087$. In this case resolution is much better, one finds $\Delta\rho_{40}^{a0} = 0.111$ and the agreement between $\rho_{40}^{a0}(\varepsilon)$ and $\rho^a(\varepsilon)$ substantially improves (figure 11(c)). Finally if n increases to $n = 160$, optimum width of the Gaussian window decreases to $\Delta_0(160) = 0.038$, one finds $\Delta\rho_{160}^{a0} = 0.025$ and finite chains density $\rho_{160}^{a0}(\varepsilon)$ is almost identical to the exact density $\rho^a(\varepsilon)$ (figure 11(d)).

Another example treating parameter choice **B** with the value $E = 1$ is shown in figure 12. In this example the coupling β is as strong as $\beta = 1.5$. This choice of parameters corresponds to the point (•) in figure 7(a). Eigenvalue distribution of the state $|\Theta\rangle$ for this case is shown in figure 12(a). This eigenvalue distribution

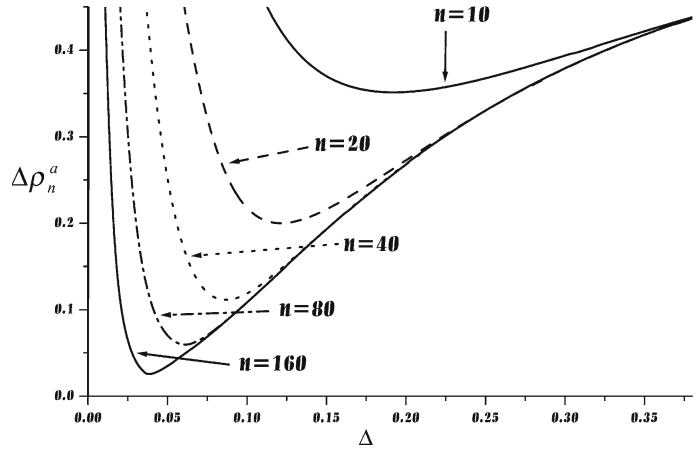

Figure 10. The method of the moving Gaussian window. Standard deviations $\Delta\rho_n^a(\Delta)$ are plotted as functions of the resolution Δ for the system considered in figure 9. This is done for five selected finite systems $\boldsymbol{S}_{n+1}$. Cases $n=10$, $n=20$, $n=40$, $n=80$ and $n=160$ are considered.

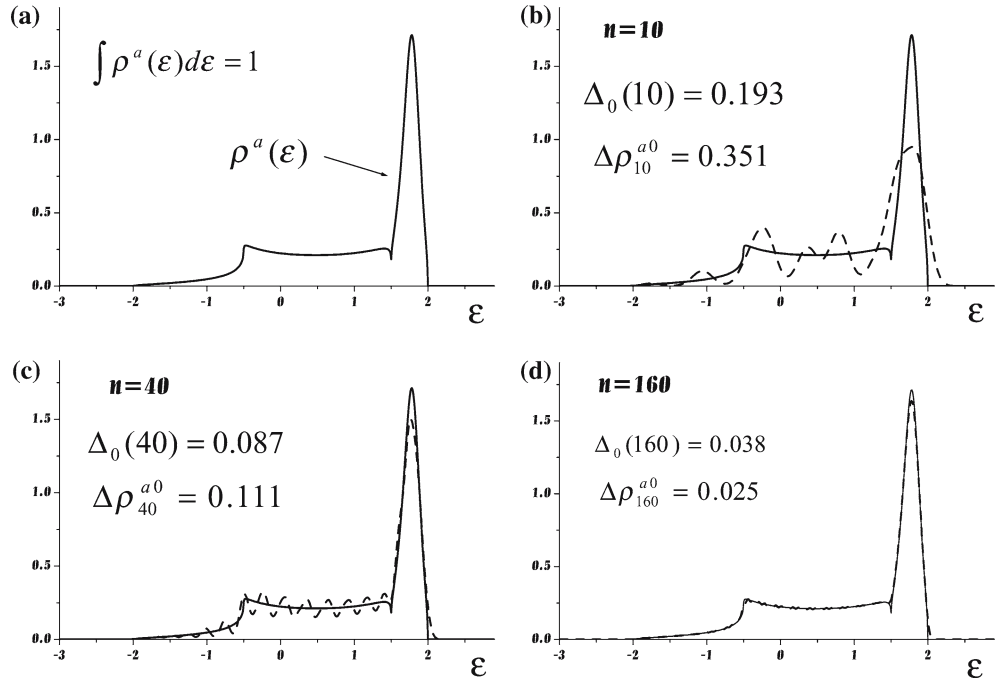

Figure 11. System analyzed in figure 9 by the method of normalized probabilities reconsidered by the method of the moving Gaussian window. Density distribution $\rho^a(\varepsilon)$ (solid lines) is compared with optimum finite system density distributions $\rho_n^{a0}(\varepsilon)$ (dashed lines). (a) Density distribution $\rho^a(\varepsilon)$, (b) comparison for $n=10$, (c) comparison for $n=40$, (d) comparison for $n=160$.

contains right isolated eigenvalue ε_R with the probability w_R^a in addition to the density $\rho^a(\varepsilon)$. One finds $\varepsilon_R = 2.3189$, $w_R^a = 0.5024$ and $w_D^a = 0.4976$. In accord with the completeness requirement one has $w_R^a + w_D^a = 1$. In figures 12(b–d) this eigenvalue distribution is compared with results obtained from selected finite systems in a standard way. In particular, density $\rho^a(\varepsilon)$ is compared with optimum densities $\rho_n^{a0}(\varepsilon)$, while isolated eigenvalue ε_R and the corresponding probability w_R^a are compared with related values $\varepsilon_{n+1}(n)$ and $w_{n+1}^a(n)$, respectively. If n is as low as $n = 10$, optimum width $\Delta_0(10) = 0.447$ of the Gaussian window is relatively large and one has $\Delta\rho_{10}^{a0} = 0.062$. In this case one finds $\varepsilon_{11}(10) = 2.3180$ and $w_{11}^a(10) = 0.5055$. This is in relatively good agreement with exact values $\varepsilon_R = 2.3189$ and $w_R^a = 0.5024$. However, finite chain density $\rho_{10}^{a0}(\varepsilon)$ is not such a good approximation of the exact density $\rho^a(\varepsilon)$ (see figure 12(b)). If n increases to $n = 40$, optimum width of the Gaussian window decreases to $\Delta_0(40) = 0.149$, while standard deviation decreases to $\Delta\rho_{40}^{a0} = 0.021$. The agreement between $\rho_{40}^{ao}(\varepsilon)$

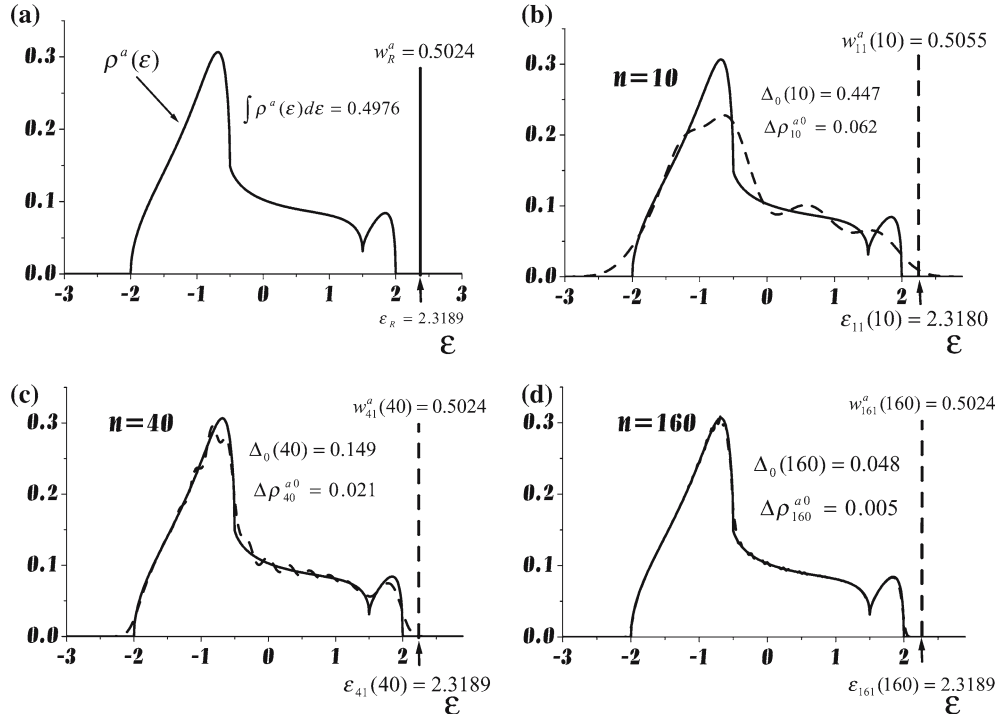

Figure 12. Gaussian window method applied to the system containing an isolated eigenstate. Density distribution $\rho^a(\varepsilon)$ (solid lines) is compared with optimum finite system density distributions $\rho_n^{a0}(\varepsilon)$ (dashed lines). In addition, isolated eigenvalue ε_R and the corresponding probability w_R^a are compared with related finite system quantities $\varepsilon_k(n)$ and $w_k^a(n)$ (vertical columns). (a) Eigenvalue distribution $\rho(\varepsilon)$ for the parameter choice **B** and for the values $E = 1$ and $\beta = 1.5$. This distribution corresponds to the point (•) in figure 7(a). (b) comparison for $n = 10$, (c) comparison for $n = 40$, (d) comparison for $n = 160$.

and $\rho^a(\varepsilon)$ substantially improves. One also finds $\varepsilon_{41}(40) = 2.3189$ and $w^a_{41}(40) = 0.5024$ which agrees up to all four significant figures with theoretical values for ε_R and w^a_R (figure 12(c)). Finally, if n increases to $n = 160$, optimum width of the Gaussian window decreases to $\Delta_0(160) = 0.048$ and one finds $\Delta\rho^{a0}_{160} = 0.005$. Finite chain density $\rho^{a0}_{160}(\varepsilon)$ is in an excellent agreement with the density $\rho^a(\varepsilon)$ (figure 12(d)).

Above examples illustrate general behavior of the density $\rho^a(\varepsilon)$ and finite chain densities $\rho^{a0}_n(\varepsilon)$. As n increases those finite chain densities converge to the infinite chain density $\rho^a(\varepsilon)$ and one has $\lim_{n\to\infty} \rho^{a0}_n(\varepsilon) = \rho^a(\varepsilon)$.

Above examples illustrate the suggested method in the case when the system $\mathcal{S}^b_\infty$ represents the set of $\kappa = 2$ infinite Hückel chains and when the local state $|\Theta\rangle$ interacts only with the first site of those chains. There is nothing special about this choice. The suggested method is rather general and it applies to an arbitrary system $\mathcal{S}^b_\infty$ that contains a finite number of one-parameter eigenvalue bands. The interaction between the local state $|\Theta\rangle$ and this system can be of any kind.

5. Conclusion

Exact treatment of the interaction of an isolated state $|\Theta\rangle$ with the known infinite dimensional quantum system $\mathcal{S}^b_\infty$ is generalized to the case when the system $\mathcal{S}^b_\infty$ contains a finite number of one-parameter eigenvalue bands. Formally, this requires the solution of the combined system $\mathcal{S}_\infty = \mathcal{S}^a_1 \oplus \mathcal{S}^b_\infty$ where $\mathcal{S}^a_1$ is one-dimensional system containing a single state $|\Theta\rangle$ with the eigenvalue E. In the original treatment of this problem, the system $\mathcal{S}^b_\infty$ was assumed to contain a single one-parameter eigenvalue band [1]. Each eigenstate $|\Phi(k)\rangle$ of such a system is nondegenerate. This assumption is rather restrictive and there are very few infinite quantum systems with such a property. In particular, electromagnetic field forms a degenerate eigenvalue band and the same applies to the eigenvalues and eigenstates of a three-dimensional solid. Since an arbitrary (multiparameter) eigenvalue band can be approximated to any desired degree of accuracy with a finite number of one-parameter eigenvalue bands, generalization presented in this paper is crucial in order to describe in a closed form interaction of a single state with an arbitrary infinite dimensional quantum system [7].

It is shown that combined system $\mathcal{S}_\infty$ contains embedded eigenstates $|\Psi_\nu(\varepsilon)\rangle$ with continuous eigenvalues $\varepsilon \in D$, where D is a range containing all eigenvalues of the unperturbed infinite system $\mathcal{S}^b_\infty$. This range may contain one or several nonoverlapping intervals. In addition to embedded eigenvalues and eigenstates, combined system may contain isolated eigenstates $|\Psi_I\rangle$ with discrete eigenvalues $\varepsilon_I \notin D$.

Closed expressions for the embedded and isolated solutions of the combined system are derived. Unlike standard perturbation expansion approach, those expressions involve no approximation, and they apply to each coupling of

the system S_1^a with the system S_∞^b, however strong. In particular, closed expressions for the spectral (eigenvalue) distribution of the state $|\Theta\rangle$ that interacts with the infinite quantum system S_∞^b are obtained.

The method is illustrated with a simple model describing the interaction of a single state $|\Theta\rangle$ (system S_1^a) with several infinite one-dimensional solids in the nearest-neighbor tight-binding approximation (system S_∞^b). This model is sufficiently complex in order to illustrate and verify all derived expressions. In particular, key completeness relation is verified. This relation is verified with several examples involving an extremely large interval of coupling constants. In addition, the interaction of the system S_1^a with finite one-dimensional solids that contains n atoms (system S_n^b) is considered. Since the corresponding combined system $S_{n+1} = S_1^a \oplus S_n^b$ is finite-dimensional, it can be solved by standard diagonalization methods. In this way one can compare all results that apply to an infinite system S_∞ (obtained using expressions derived in this paper) with corresponding results for finite system S_{n+1} (obtained independently in the standard way). As n increases, the results for the system S_{n+1} are shown to converge to the corresponding results for the system S_∞. This provides a direct verification of the suggested method. For the sake of simplicity, in the numerical examples only the case when the system S_n^b contains two infinite chains is considered. This does not present any restriction on the general validity of derived expressions.

Obtained results and their generalization [7,8] can be applied to all cases where one considers an isolated state $|\Theta\rangle$ in the interaction with an infinite quantum system S_∞^b. This includes, among others, a general problem of the interaction of an isolated molecular state with electromagnetic field. Investigation of such an interaction is a main problem of spectroscopy. Another example is the interaction of an isolated molecular state of a molecule situated on a surface of some solid with this solid. Investigation of such an interaction is a main problem of the surface state physics. In the present paper time-independent properties of the state $|\Theta\rangle$ that interacts with the infinite system S_∞^b are considered. Time-dependent properties are considered in the following paper [6].

From the mathematical and conceptual point of view, the main result of the present paper is the generalization of the notion of the fractional shift to the case when the system S_∞^b contains a finite number of one-parameter eigenvalue bands. This generalization is a precondition of the final generalization to arbitrary infinite dimensional systems S_∞^b [7]. In the suggested method fractional shift is a key quantity for the derivation of many properties of the combined system S_∞. It is therefore highly important that the notion of the fractional shift can be unambiguously defined for arbitrary quantum systems.

Appendix A

A.1. System $\mathcal{S}_\infty$ as the $n \to \infty$ limit of finite dimensional systems $\mathcal{S}_{n+1}$

In order to solve eigenvalue equation (3), we approximate infinite dimensional system $\mathcal{S}_\infty \equiv \mathcal{S}_1^a \oplus \mathcal{S}_\infty^b$ with a finite dimensional system $\mathcal{S}_{n+1} \equiv \mathcal{S}_1^a \oplus \mathcal{S}_n^b$ containing $n+1$ eigenvalues. This can be done by first replacing unperturbed infinite system $\mathcal{S}_\infty^b$ with n-dimensional system $\mathcal{S}_n^b$. Next one introduces the interaction between the systems $\mathcal{S}_1^a$ and $\mathcal{S}_n^b$. The solution to the finite dimensional combined system $\mathcal{S}_{n+1}$ can be obtained in the closed form [13]. One has to derive an appropriate $n \to \infty$ limit of this solution. Provided this limit is well defined, it represents the solution to the system $\mathcal{S}_\infty$.

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

$$\mathbf{B}\left|\Phi_{\nu,i}\right\rangle = \lambda_{\nu,i}\left|\Phi_{\nu,i}\right\rangle, \quad i = 1, \ldots, m_\nu, \quad \nu = 1, \ldots, \kappa, \tag{A.1a}$$

where

$$\sum_{\nu}^{\kappa} m_\nu = n. \tag{A.1b}$$

The eigenstates $\left|\Phi_{\nu,i}\right\rangle$ of this system can be orthonormalized according to

$$\left\langle \Phi_{\nu,i} \,\middle|\, \Phi_{\mu,j} \right\rangle = \delta_{ij}\delta_{\nu\mu}. \tag{A.1c}$$

System $\mathcal{S}_n^b$ thus defined is a union of κ subsystems $\mathcal{S}_{m_\nu}^{b\nu}$ $(\nu = 1, \ldots, \kappa)$.

Let the system $\mathcal{S}_n^b$ interact with the one-dimensional system $\mathcal{S}_1^a$ that contains a single eigenstate $|\Theta\rangle$ with the eigenvalue E. This system is described by the eigenvalue equation (1). An arbitrary interaction between $\mathcal{S}_1^a$ and $\mathcal{S}_n^b$ can be written in the form $\beta\mathbf{V}$ where $\mathbf{V}$ is a Hermitian operator fully described by matrix elements $\left\langle \Theta \middle| \mathbf{V} \middle| \Phi_{\nu,i} \right\rangle$ and where β is a coupling parameter. Combined system $\mathcal{S}_{n+1}$ may have cardinal eigenvalues $\varepsilon_k \notin \{\lambda_{\nu,i}\}$ as well as singular eigenvalues $\varepsilon_k \in \{\lambda_{\nu,i}\}$ [13]. One finds that $\varepsilon_k \notin \{\lambda_{\nu,i}\}$ is a (cardinal) eigenvalue of the combined system if and only if it is a root of the function $h_n(\varepsilon)$ [13]:

$$h_n(\varepsilon_k) \equiv \beta^2 \Omega(\varepsilon_k) + E - \varepsilon_k = 0, \tag{A.2a}$$

where

$$\Omega(\varepsilon) = \sum_{\nu}^{\kappa} \sum_{i}^{m_\nu} \frac{\left\langle \Theta \middle| \mathbf{V} \middle| \Phi_{\nu,i} \right\rangle \left\langle \Phi_{\nu,i} \middle| \mathbf{V} \middle| \Theta \right\rangle}{\varepsilon - \lambda_{\nu,i}}. \tag{A.2b}$$

We use index n in order to emphasize that function $h_n(\varepsilon)$ refers to a combined system $\mathcal{S}_{n+1}$ containing $n+1$ eigenvalues.

Each cardinal eigenvalue $\varepsilon_k \notin \{\lambda_{\nu,i}\}$ of $\mathcal{S}_{n+1}$ is nondegenerate and the corresponding normalized eigenstate is [13]

$$|\Psi_k\rangle = \frac{1}{\sqrt{Q_k}}\left[|\Theta\rangle + \beta\sum_{\nu=1}^{\kappa}\sum_{i=1}^{m_\nu}\frac{\langle\Phi_{\nu,i}\,|\,\mathbf{V}\,|\Theta\rangle}{\varepsilon_k-\lambda_{\nu,i}}\,|\Phi_{\nu,i}\rangle\right], \tag{A.3a}$$

where

$$Q_k = 1+\beta^2\sum_{\nu=1}^{\kappa}\sum_{i=1}^{m_\nu}\frac{\left|\langle\Phi_{\nu,i}\,|\,\mathbf{V}\,|\Theta\rangle\right|^2}{\left(\varepsilon_k-\lambda_{\nu,i}\right)^2}. \tag{A.3b}$$

Further, if $\lambda_j \equiv \lambda_{\nu,i}$ are unperturbed eigenvalues of $\mathcal{S}_n^b$ arranged in the nondecreasing order and if ε_k are perturbed eigenvalues (cardinal as well as singular) of $\mathcal{S}_{n+1}$ arranged in the nondecreasing order, those eigenvalues satisfy the interlacing rule [13]

$$\varepsilon_1 \leqslant \lambda_1 \leqslant \varepsilon_2 \leqslant \lambda_2 \leqslant \cdots \leqslant \lambda_n \leqslant \varepsilon_{n+1}. \tag{A.4a}$$

In addition, if all unperturbed eigenvalues λ_j are nondegenerate and if all matrix elements $\langle\Theta|\mathbf{V}|\Phi_{\nu,i}\rangle$ are nonzero, then the system $\mathcal{S}_{n+1}$ contains no singular solutions. In this case relations (A2)–(A3) produce all solutions of this system and interlacing rule (A4a) contains only strict inequalities

$$\varepsilon_1 < \lambda_1 < \varepsilon_2 < \lambda_2 < \cdots < \lambda_n < \varepsilon_{n+1}. \tag{A.4b}$$

One can form an infinite sequence of finite dimensional systems $\mathcal{S}_{n+1}$ in such a way that each system $\mathcal{S}_{n+1}$ contains only cardinal solutions and that in a limit $n\to\infty$ those systems converge to $\mathcal{S}_\infty$. The solution to $\mathcal{S}_\infty$ can be hence obtained as the $n\to\infty$ limit of the solutions to those intermediate systems. Since each $\mathcal{S}_{n+1}$ contains only cardinal solutions, relations (A2) and (A3) are sufficient to obtain all solutions to $\mathcal{S}_{n+1}$. However, though none of those intermediate systems contains a singular solution, $n\to\infty$ limit of those systems (system $\mathcal{S}_\infty$) may contain singular solutions [1]. Accordingly, with due caution one can in this way obtain all solutions of the combined system $\mathcal{S}_\infty$, cardinal as well as singular.

A.2. Eigenvalues and eigenstates of $\mathcal{S}_\infty$

In order for the system $\mathcal{S}_n^b$ to approximate infinite system $\mathcal{S}_\infty^b$, each subsystem $\mathcal{S}_{m_\nu}^{b\nu}$ of $\mathcal{S}_n^b$ should approximate corresponding subsystem $\mathcal{S}_\infty^{b\nu}$ of $\mathcal{S}_\infty^b$. In particular, for each ν in a limit $m_\nu\to\infty$ eigenvalues $\lambda_{\nu,i}$ $(i=1,\ldots,m_\nu)$ should be dense in the interval $I_\nu=[a_\nu,b_\nu]\subseteq D$. Hence in a limit $n\to\infty$ eigenvalues $\lambda_{\nu,i}$ of $\mathcal{S}_n^b$ are dense in the range D. In addition, since no eigenvalue of $\mathcal{S}_\infty^b$ is contained in the point set $\bar{D}$, no eigenvalue $\lambda_{\nu,i}$ of $\mathcal{S}_n^b$ can be contained in $\bar{D}$. Due to the interlacing rule, eigenvalues ε_k of the combined system $\mathcal{S}_{n+1}$ are also dense in

each interval I_ν. Hence, in a limit $n \to \infty$ each $\varepsilon \in D \equiv \cup I_\nu$ is a perturbed eigenvalue. By definition, this is an *embedded* eigenvalue of the combined system $\boldsymbol{S}_\infty$ [1]. This eigenvalue is part of a continuous band of eigenvalues, and the corresponding eigenstates can be written as $\left|\Psi_\mu(\varepsilon)\right\rangle$ where discrete index μ labels possible degeneracy of those eigenstates. Those eigenstates can be orthonormalized according to

$$\left\langle \Psi_\mu(\varepsilon) \,\middle|\, \Psi_{\mu'}(\varepsilon') \right\rangle = \delta_{\mu\mu'}\delta(\varepsilon - \varepsilon').$$

This is similar to the orthonormalization (2b) of the unperturbed eigenstates $|\Phi_\nu(k)\rangle$.

In addition to the embedded eigenvalues $\varepsilon \in D$, system $\boldsymbol{S}_\infty$ may contain some eigenvalues $\varepsilon_I \in \bar{D}$ outside the range D. Due to the interlacing rule (A.4), in each interval $I \subseteq \bar{D}$ one can have at most one eigenvalue $\varepsilon_I \in \bar{D}$. By definition, eigenvalue $\varepsilon_I \in \bar{D}$ and the corresponding eigenstate $|\Psi_I\rangle$ is an *isolated* eigenvalue and eigenstate, respectively. Since each ε_I is discrete, eigenstates $|\Psi_I\rangle$ can be normalized to unity. In this respect isolated eigenstates $|\Psi_I\rangle$ are similar to the local state $|\Theta\rangle \in X_1^a$ that is also normalized to unity.

A.3. Isolated eigenvalues and eigenstates

In the case of isolated eigenvalues ($\varepsilon_I \in \bar{D}$) it is relatively easy to obtain the $n \to \infty$ limit of relations (A.2) and (A.3). In particular, summation over i in (A.2b) is replaced with an integral, and one finds [1]

$$\Omega(\varepsilon) \to \omega(\varepsilon) = \sum_\nu \int_{k_{a\nu}}^{k_{b\nu}} \frac{\langle \Theta \,|\, \mathbf{V} \,|\, \Phi_\nu(k) \rangle \, \langle \Phi_\nu(k) \,|\, \mathbf{V} \,|\, \Theta \rangle}{\varepsilon - \lambda_\nu(k)} \mathrm{d}k, \quad \varepsilon \in \bar{D}.$$

Using expressions (4) this translates into relations (5). Hence and from (A2) one derives (8). In a similar way one derives all remaining relations concerning isolated eigenvalues and eigenstates. As implied by the interlacing rule, each isolated eigenstate is nondegenerate.

A.4. Embedded eigenvalues and eigenstates

In the case of the embedded eigenvalues $\varepsilon \in D$ of the combined system $\boldsymbol{S}_\infty$, transition to the limit $n \to \infty$ of the relations (A.2) and (A.3) is more complex. Derivation of the correct $n \to \infty$ limit is complicated by the fact that infinitesimally close to each embedded eigenvalue $\varepsilon \in D$ there is an infinite number of unperturbed eigenvalues $\lambda \in D$. This limit was originally derived for the case when the system $\boldsymbol{S}_\infty^b$ contains a single one-parameter eigenvalue band $\lambda(k)$ [1].

In this case each state $|\Phi(k)\rangle$ is a nondegenerate eigenstate of the unperturbed system $\mathcal{S}_\infty^b$. We will generalize this result to the case when $\mathcal{S}_\infty^b$ contains several one-parameter eigenvalue bands $\lambda_\nu(k)$ $(\nu = 1, \ldots, \kappa)$.

A.4.1. Fractional shift

Key quantity in the treatment of embedded eigenstates is fractional shift $x(\varepsilon)$ [1]. Let us first consider this quantity in the case when the system $\mathcal{S}_\infty^b$ contains a single one-parameter eigenvalue band [1].

(a) case $\kappa = 1$:

If $\kappa = 1$ eigenvalue equation (2a) reduces to [1]

$$\mathbf{B}\,|\Phi(k)\rangle = \lambda(k)\,|\Phi(k)\rangle\,, \quad k \in [k_a, k_b]\,. \tag{A.5}$$

Let $\lambda(k)$ be monotonic increasing function of k. In this case all eigenvalues of the unperturbed system $\mathcal{S}_\infty^b$ are contained in the interval $D = [a, b]$ where $a = \lambda(k_a)$ and $b = \lambda(k_b)$. Partition the interval $[k_a, k_b]$ into n subintervals of equal length $\Delta k = (k_b - k_a)/n$. Midpoints of those subintervals are $k_i = k_a + (i - 1/2)\,\Delta k$ $(i = 1, \ldots, n)$. Next replace continuous functions $\lambda(k)$ and $\langle\Theta\,|\,\mathbf{V}\,|\Phi(k)\rangle$ with n discrete values sampled at those midpoints. Function $\lambda(k)$ is replaced with n discrete values $\lambda_i \equiv \lambda(k_i)$ $(i = 1, \ldots, n)$, while function $\langle\Theta\,|\,\mathbf{V}\,|\Phi(k)\rangle$ is replaced with n discrete values $\langle\Theta\,|\,\mathbf{V}\,|\Phi_i\rangle$ according to [1]

$$\langle\Theta\,|\,\mathbf{V}\,|\Phi_i\rangle = \langle\Theta\,|\,\mathbf{V}\,|\Phi(k_i)\rangle\,\sqrt{\Delta k}, \quad i = 1, \ldots, n. \tag{A.6}$$

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

$$\int |\Phi(k)\rangle\,\langle\Phi(k)|\,\mathrm{d}k \Leftrightarrow \sum_i |\Phi_i\rangle\,\langle\Phi_i|.$$

The above procedure approximates infinite-dimensional system $\mathcal{S}_\infty = \mathcal{S}_1^a \oplus \mathcal{S}_\infty^b$ where $\mathcal{S}_\infty^b$ contains one-parameter eigenvalue band $\lambda(k)$ with $(n+1)$-dimensional system $\mathcal{S}_{n+1} \equiv \mathcal{S}_1^a \oplus \mathcal{S}_n^b$. As n increases, this approximation improves and in a limit $n \to \infty$ it is exact. Since $\lambda(k)$ is monotonic increasing function of k, eigenvalues $\lambda_i \equiv \lambda(k_i)$ are nondegenerate. In addition, without loss of generality one can assume $\langle\Theta\,|\,\mathbf{V}\,|\Phi_i\rangle \neq 0$ $(i = 1, \ldots, n)$ [1]. According to the interlacing rule this implies $\lambda_{k-1} < \varepsilon_k < \lambda_k$ and each perturbed eigenvalue ε_k of the combined system is cardinal. Relations (A.2) and (A.3) are hence sufficient to provide all solutions to the combined system $\mathcal{S}_{n+1}$.

Let $\varepsilon_k \in D$ be an interior point of a range D. Using (A2.b) and (A.6) and assuming $\kappa = 1$ one can express quantity $\Omega(\varepsilon_k)$ as a sum of two components [1]

$$\Omega(\varepsilon_k) = \Omega^{(0)}(\varepsilon_k) + \Omega^{(1)}(\varepsilon_k), \tag{A.7a}$$

where

$$\Omega^{(0)}(\varepsilon_k)=\sum_{j=-N(n)}^{N(n)}\frac{\langle\Theta\,|\,\mathbf{V}\,|\Phi(k_{k+j})\rangle\langle\Phi(k_{k+j})\,|\,\mathbf{V}\,|\Theta\rangle}{\varepsilon_k-\lambda(k_{k+j})}\Delta k, \tag{A.7b}$$

$$\Omega^{(1)}(\varepsilon_k)=\sum_{j<-N(n)}\frac{\langle\Theta\,|\,\mathbf{V}\,|\Phi(k_{k+j})\rangle\langle\Phi(k_{k+j})\,|\,\mathbf{V}\,|\Theta\rangle}{\varepsilon_k-\lambda(k_{k+j})}\Delta k + \sum_{j>N(n)}\frac{\langle\Theta\,|\,\mathbf{V}\,|\Phi(k_{k+j})\rangle\langle\Phi(k_{k+j})\,|\,\mathbf{V}\,|\Theta\rangle}{\varepsilon_k-\lambda(k_{k+j})}\Delta k, \tag{A.7c}$$

and where $N(n)=\lfloor n^{1/3}\rfloor$ is the largest integer smaller than $n^{1/3}$.

Since $\varepsilon_k\in(\lambda_{k-1},\lambda_k)$ component $\Omega^{(0)}(\varepsilon_k)$ contains contributions to $\Omega(\varepsilon_k)$ from approximately $2n^{1/3}$ eigenvalues $\lambda_i\equiv\lambda(k_i)$ that are close to ε_k, while component $\Omega^{(1)}(\varepsilon_k)$ contains all remaining contributions. In a limit $n\to\infty$ component $\Omega^{(1)}(\varepsilon_k)$ converges to [1]

$$\Omega^{(1)}(\varepsilon_k)\to\omega(\varepsilon)=P\int_{k_a}^{k_b}\frac{\langle\Theta\,|\,\mathbf{V}\,|\Phi(k)\rangle\,\langle\Phi(k)\,|\,\mathbf{V}\,|\Theta\rangle}{\varepsilon-\lambda(k)}\mathrm{d}k, \tag{A.8}$$

where P denotes principal Cauchy integral value. Using definition (4) this can be expressed as (5d).

Concerning component $\Omega^{(0)}(\varepsilon_k)$, one can expand functions $\lambda(k)$ and $\langle\Theta\,|\,\mathbf{V}\,|\Phi(k)\rangle$ in the point $k=k_k\in[k_a,k_b]$ to obtain [1]

$$\lambda_{k+j}=\lambda_k+(\mathrm{d}\lambda/\mathrm{d}k)_k\,(\Delta k)\,j+O(j^2/n^2), \tag{A.9a}$$

$$\langle\Theta\,|\,\mathbf{V}\,|\Phi(k_{k+j})\rangle=\langle\Theta\,|\,\mathbf{V}\,|\Phi(k_k)\rangle+O(j/n), \tag{A.9b}$$

where $(\mathrm{d}\lambda/\mathrm{d}k)_k$ is a derivative of a function $\lambda(k)$ taken in a point $k=k_k$ and where $O(x)$ is a small quantity of the order x. Since the summation in (A.7b) is confined to $|j|\leqslant N(n)\approx n^{1/3}$ and since Δk is of the order $O(n^{-1})$, in a limit $n\to\infty$ small quantities $O(x)$ in (A.9) can be neglected [1]. In particular, in this limit eigenvalues λ_{k+j} are equidistant with the interval

$$\begin{aligned}\Delta\lambda_{k+j}&=\lambda_{k+j}-\lambda_{k+j-1}=(\mathrm{d}\lambda/\mathrm{d}k)_k\,\Delta k+O(j^2/n^2)\\&\approx\left(\mathrm{d}\lambda\big/\mathrm{d}k\right)_k\Delta k,\quad j\in\left[-n^{1/3},n^{1/3}\right],\end{aligned} \tag{A.9c}$$

while matrix elements $\langle\Theta\,|\,\mathbf{V}\,|\Phi(k_{k+j})\rangle\approx\langle\Theta\,|\,\mathbf{V}\,|\Phi(k_k)\rangle$ are constant.

Hence and from the identity [14]

$$\frac{1}{x}+\sum_{j=1}^{\infty}\left(\frac{1}{x-j}+\frac{1}{x+j}\right)=\pi\cot(\pi x). \tag{A.10}$$

one finds [1]

$$\Omega^{(0)}(\varepsilon_k) \approx \pi \frac{\langle \Theta | \mathbf{V} | \Phi(k_k) \rangle \langle \Phi(k_k) | \mathbf{V} | \Theta \rangle}{(\mathrm{d}\lambda/\mathrm{d}k)_k} \cot(\pi x(\varepsilon_k)), \tag{A.11a}$$

where

$$x(\varepsilon_k) = \frac{\varepsilon_k - \lambda_{k-1}}{\lambda_k - \lambda_{k-1}}, \quad k = 2, \ldots, n. \tag{A.11b}$$

Quantity $x(\varepsilon_k)$ is a fractional shift of the perturbed eigenvalue $\varepsilon_k \in (\lambda_{k-1}, \lambda_k)$ relative to the unperturbed eigenvalue λ_{k-1}. Due to the interlacing rule and since the system $\mathcal{S}_{n+1}$ contains no singular eigenvalues, this quantity satisfies

$$0 < x(\varepsilon_k) < 1. \tag{A.11c}$$

In a limit $n \to \infty$ arguments ε_k of $x(\varepsilon_k)$ become dense in the interval $[a, b]$ and according to (A.11c) fractional shift $x(\varepsilon)$ may have any value in the interval $[0, 1]$. Also in this limit one has

$$\frac{\langle \Theta | \mathbf{V} | \Phi(k_k) \rangle \langle \Phi(k_k) | \mathbf{V} | \Theta \rangle}{(\mathrm{d}\lambda/\mathrm{d}k)_k} \to \left. \frac{\langle \Theta | \mathbf{V} | \Phi(k) \rangle \langle \Phi(k) | \mathbf{V} | \Theta \rangle}{\mathrm{d}\lambda / \mathrm{d}k} \right|_{\varepsilon = \lambda(k)} \equiv f(\varepsilon). \tag{A.12}$$

Combining above expressions one finds that in the case $\varepsilon = \varepsilon_k \in D$ relation (A.2a) can be approximated as $h_n(\varepsilon_k) \approx \beta^2 [\omega(\varepsilon_k) + \pi f(\varepsilon_k) \cot(\pi x(\varepsilon_k))] + E - \varepsilon_k = 0$. As n increases this approximation improves and in a limit $n \to \infty$ it is exact. This shows that in this limit fractional shifts $x(\varepsilon_k)$ $(k = 2, \ldots, n)$ converge to a function $x(\varepsilon)$ given by the relation (17a).

In the above derivation of the fractional shift correct treatment of the component $\Omega^{(0)}(\varepsilon_k)$ is essential. Crucial point in the evaluation of this component is the transition from the expression (A.7b) to the expression (A.11a). This transition is possible due to the properties (A.9) of discrete eigenvalues λ_i and discrete matrix elements $\langle \Theta | \mathbf{V} | \Phi(k_i) \rangle$. Neglecting terms of the order $O(j/n)$, matrix elements $\langle \Theta | \mathbf{V} | \Phi(k_{k+j}) \rangle$ are constant over the interval $j \in [-n^{1/3}, n^{1/3}]$. Hence one can factor out constant term $|\langle \Theta | \mathbf{V} | \Phi(k_{k+j}) \rangle|^2 \Delta k \approx |\langle \Theta | \mathbf{V} | \Phi(k_k) \rangle|^2 \Delta k = |\langle \Theta | \mathbf{V} | \Phi_k \rangle|^2$ under the summation sign in (A.7b). Next and according to (A.9c), neglecting terms of the order $O(j^2/n^2)$, unperturbed eigenvalues λ_{k+j} are equidistant over this interval. Using (A.10) one can sum remaining terms in (A.7b). One thus obtains expression (A.11a) for the quantity $\Omega^{(0)}(\varepsilon_k)$. In a limit $n \to \infty$ this expression is exact.

In order to generalize the notion of fractional shift to the case of multiple eigenvalue bands, the above two properties of discrete eigenvalues λ_i and discrete matrix elements $\langle \Theta | \mathbf{V} | \Phi_i \rangle$ should be retained. Hence finite systems $\mathcal{S}_{n+1}$ that approximate the system $\mathcal{S}_\infty$ should satisfy following two properties:

(i) Let $I_n = [a_n, b_n] \subset D$ be an interval containing $O(n^{1/3})$ unperturbed eigenvalues λ_i. Interval I_n depends on n, and as n increases dimension $d_n = b_n - a_n$ of this interval decreases. Neglecting higher order terms, eigenvalues λ_i contained in this interval should be equidistant.

(ii) Under the same conditions, matrix elements $\langle \Theta \,|\, \mathbf{V} \,|\, \Phi_i \rangle$ should be constant over this interval.

A more detailed analysis shows that it is not necessary for each interval $I_n \subset D$ containing $O(n^{1/3})$ unperturbed eigenvalues to satisfy above two conditions. Range D may contain some isolated points $\varepsilon_0 \in D$ such that if $\varepsilon_0 \in I$, this interval does not satisfy above conditions. This is acceptable, as long as there is a finite number of such points. Points that can violate properties (i) and (ii) are usually end points a_ν and b_ν of intervals I_ν.

Let us now generalize fractional shift to the next more complicated case:
(b) case $\lambda_1(k) = \lambda_2(k) = \cdots = \lambda_\kappa(k)$:

In this case system $\mathbf{S}_\infty^b$ contains κ one-parameter eigenvalue bands with the same eigenvalue function $\lambda(k) \equiv \lambda_\nu(k)$ $(\nu = 1, \ldots, \kappa)$. This can be considered as a single κ-degenerate eigenvalue band. Formally, this is a two-parameter eigenvalue band containing a continuous parameter k and a discrete parameter ν. In this case eigenvalue equation (2a) reduces to

$$\mathrm{B}\,|\Phi_\nu(k)\rangle = \lambda(k)\,|\Phi_\nu(k)\rangle\,, \quad k \in [k_a, k_b]\,, \quad \nu = 1, \ldots, \kappa. \tag{A.13}$$

Eigenvalues of the unperturbed system are again contained in the single interval $D = [a, b]$ where $a = \lambda(k_a)$ and $b = \lambda(k_b)$. However, this time each $\lambda(k) \in D$ is κ-degenerate.

Let n be a multiple of κ, i.e. let $n = m\kappa$ where m is an integer. In analogy to the case $\kappa = 1$, partition the interval $[k_a, k_b]$ into $m = n/\kappa$ subintervals of equal length $\Delta k = (k_b - k_a)/m$. In addition, partition each of those subintervals into κ smaller subintervals of length $\Delta = (k_b - k_a)/n = \Delta k/\kappa$. One thus obtains n subintervals of equal length Δ. Midpoints of those subintervals are $k_{\nu,i} = k_a + [(i-1)\kappa + (\nu - 1/2)]\,\Delta$ $(i = 1, \ldots, m;\ \nu = 1, \ldots, \kappa)$. Double indices (ν, i) can be replaced with a single index $l = (i-1)\kappa + \nu$ $(l = 1, \ldots, n)$. With this indexing convention one has $k_{\nu,i} \equiv k_l = k_a + (l - 1/2)\,\Delta$ $(l = 1, \ldots, n)$. Next approximate function $\lambda(k)$ with n values $\lambda_l \equiv \lambda(k_l)$ sampled at those n points. Since $\lambda(k)$ is monotonic increasing function of k, unperturbed eigenvalues λ_l are nondegenerate. In addition, those eigenvalues satisfy relations (A.9) In particular one has

$$\Delta\lambda_{k+l} = (\mathrm{d}\lambda/\mathrm{d}k)_k\,\Delta + O(l^2 n^{-2}) \approx \left(\mathrm{d}\lambda\big/\mathrm{d}k\right)_k \Delta, \quad l \in \lfloor -n^{1/3}, n^{1/3} \rfloor,$$

where $k \equiv (\mu, i)$ and $l = (\nu, j)$ are subject to the above indexing convention with an appropriate summation $(k+l)$. In a limit $n \to \infty$ unperturbed eigenvalues λ_{k+l} are equidistant in accord with the requirement (i).

Consider now matrix elements $\langle\Theta|\mathbf{V}|\Phi_\nu(k)\rangle$. In analogy to (A.6) one may try to replace functions $\langle\Theta|\mathbf{V}|\Phi_\nu(k)\rangle$ with n discrete values $\langle\Theta|\mathbf{V}|\Phi_{\nu,i}\rangle$ according to

$$\langle\Theta|\mathbf{V}|\Phi_{\nu,i}\rangle=\langle\Theta|\mathbf{V}|\Phi_\nu(k_{\nu,i})\rangle\sqrt{\Delta k},\quad i=1,\ldots,m_\nu,\quad \nu=1,\ldots,\kappa, \tag{A.6'}$$

where proportionality constant ($\sqrt{\Delta k}$) is due to the requirement

$$\int|\Phi_\nu(k)\rangle\langle\Phi_\nu(k)|\,dk\Leftrightarrow\sum_i|\Phi_{\nu,i}\rangle\langle\Phi_{\nu,i}|,\quad \nu=1,\ldots,\kappa.$$

If $\mu\neq\nu$ one usually has $\langle\Theta|\mathbf{V}|\Phi_\nu(k)\rangle\neq\langle\Theta|\mathbf{V}|\Phi_\mu(k)\rangle$. Hence matrix element $\langle\Theta|\mathbf{V}|\Phi_l\rangle\equiv\langle\Theta|\mathbf{V}|\Phi_{\nu,i}\rangle$ may be quite different from adjacent matrix elements $\langle\Theta|\mathbf{V}|\Phi_{l\pm1}\rangle$ and straightforward sampling of those matrix elements in the points $k=k_l$ violates condition (ii). However, for each $k\in[k_a,k_b]$ unperturbed eigenstates $|\Phi_\nu(k)\rangle$ ($\nu=1,\ldots,\kappa$) are κ-degenerate, and one can use any set of κ orthonormalized eigenstates $|\Phi'_\nu(k)\rangle$ that are linear combinations of initial unperturbed eigenstates $|\Phi_\nu(k)\rangle$, instead of those initial eigenstates. One can exploit this flexibility in order to satisfy condition (ii).

Without loss of generality one can assume that matrix elements $a_\nu\equiv\langle\Theta|\mathbf{V}|\Phi_\nu(k)\rangle$ ($\nu=1,\ldots,\kappa$) are real and nonnegative. If this is not the case, it can be accomplished by simple adjustment of the phases of eigenstates $|\Phi_\nu(k)\rangle$.

Consider transformed eigenstates

$$|\Phi'_\nu(k)\rangle=\sum_\mu^\kappa O_{\nu\mu}(k)\,|\Phi_\mu(k)\rangle,\quad \nu=1,\ldots,\kappa, \tag{A.14}$$

where $\mathbf{O}$ is an orthogonal matrix with matrix elements $O_{\mu\nu}$. Since $\mathbf{O}$ is orthogonal and since initial eigenstates $|\Phi_\nu(k)\rangle$ are orthonormalized, transformed eigenstates $|\Phi'_\nu(k)\rangle$ are also orthonormalized. Choose matrix $\mathbf{O}$ in such a way that those eigenstates satisfy

$$\langle\Theta|\mathbf{V}|\Phi'_\nu(k)\rangle=g(k),\quad \nu=1,\ldots,\kappa, \tag{A.15}$$

where $g(k)$ is a real continuous function of k that does not depend on ν. In section (d) we will show that such a choice is always possible. Let $X(k)$ be κ-dimensional space corresponding to the eigenvalue $\lambda(k)$. This space is spanned by original eigenstates $|\Phi_\nu(k)\rangle$ as well as by transformed eigenstates $|\Phi'_\nu(k)\rangle$. Projection operator $\mathbf{P}(k)$ on this space can be expressed in terms of the eigenstates $|\Phi_\nu(k)\rangle$ as well as in terms of the eigenstates $|\Phi'_\nu(k)\rangle$:

$$\mathbf{P}(k)=\sum_\nu^\kappa|\Phi_\nu(k)\rangle\langle\Phi_\nu(k)|=\sum_\nu^\kappa|\Phi'_\nu(k)\rangle\langle\Phi'_\nu(k)|. \tag{A.16}$$

Hence and from (A.15)

$$g(k)=\left[\frac{1}{\kappa}\sum_{\nu}^{\kappa}\langle\Theta\,|\,\mathbf{V}\,|\Phi_\nu(k)\rangle\,\langle\Phi_\nu(k)\,|\,\mathbf{V}\,|\Theta\rangle\right]^{1/2}, \tag{A.17a}$$

One can write this expression in a compact form

$$g(k)=\left[\frac{1}{\kappa}\,\langle\Theta\,|\,\mathbf{V}\mathbf{P}(k)\mathbf{V}\,|\Theta\rangle\right]^{1/2}. \tag{A.17b}$$

Since matrix elements $\langle\Theta\,|\,\mathbf{V}\,|\Phi_\nu(k)\rangle$ are by assumption continuous in the interval $[k_a, k_b]$, relation (A.17a) implies that function $g(k)$ is also continuous in this interval. Hence, one can sample matrix elements $\langle\Theta\,|\,\mathbf{V}\,|\Phi'_\nu(k)\rangle$ in the points k_l in such a way that the condition (ii) is satisfied. In particular, one can replace functions $\langle\Theta\,|\,\mathbf{V}\,|\Phi'_\nu(k)\rangle$ with n discrete values sampled at n points k_l according to

$$\langle\Theta\,|\,\mathbf{V}\,|\Phi'_{\nu,i}\rangle=\langle\Theta\,|\,\mathbf{V}\,|\Phi'_\nu(k_{\nu,i})\rangle\sqrt{\Delta k}=g(k_{\nu,i})\sqrt{\Delta k},\quad (\nu,i)\equiv l=1,\ldots,n. \tag{A.6''}$$

Since $g(k)$ is continuous, one finds in analogy to (A.9b)

$$\langle\Theta\,|\,\mathbf{V}\,|\Phi'_{k+l}\rangle\approx\langle\Theta\,|\,\mathbf{V}\,|\Phi'_k\rangle,\quad l\in\lfloor-n^{1/3},n^{1/3}\rfloor.$$

Requirement (ii) is now satisfied. One can again express $\Omega(\varepsilon_k)\equiv\Omega(\varepsilon_{\mu,j})$ as a sum of components $\Omega^{(0)}(\varepsilon_k)$ and $\Omega^{(1)}(\varepsilon_k)$. In analogy to (A.8) and (A.11) one finds

$$\Omega^{(1)}(\varepsilon_k)\to\omega(\varepsilon)=\kappa P\int\frac{\langle\Theta\,|\,\mathbf{V}\,|\Phi'_\mu(k)\rangle\langle\Phi'_\mu(k)\,|\,\mathbf{V}\,|\Theta\rangle}{\varepsilon-\lambda(k)}\mathrm{d}k,$$

$$\Omega^{(0)}(\varepsilon_k)\approx\kappa\pi\frac{\langle\Theta\,|\,\mathbf{V}\,|\Phi'_\mu(k_k)\rangle\langle\Phi'_\mu(k_k)\,|\,\mathbf{V}\,|\Theta\rangle}{(\mathrm{d}\lambda/\mathrm{d}k)_k}\cot(\pi x(\varepsilon_k)).$$

Using identity (A.16) one can express those quantities in terms of the original unperturbed eigenstates $|\Phi_\nu(k)\rangle$. Hence

$$\Omega^{(1)}(\varepsilon)\to\omega(\varepsilon)=P\sum_{\nu}\int\frac{\langle\Theta\,|\,\mathbf{V}\,|\Phi_\nu(k)\rangle\,\langle\Phi_\nu(k)\,|\,\mathbf{V}\,|\Theta\rangle}{\varepsilon-\lambda(k)}\mathrm{d}k,\quad \varepsilon\in D, \tag{A.18a}$$

$$\Omega^{(0)}(\varepsilon)\to\pi\sum_{\nu}\frac{\langle\Theta\,|\,\mathbf{V}\,|\Phi_\nu(k)\rangle\,\langle\Phi_\nu(k)\,|\,\mathbf{V}\,|\Theta\rangle}{\mathrm{d}\lambda/\mathrm{d}k}\Bigg|_{\varepsilon=\lambda(k)}\cot(\pi x(\varepsilon))=\pi f(\varepsilon)\cot(\pi x(\varepsilon)), \tag{A.18b}$$

where $f(\varepsilon)=\sum_\nu f_\nu(\varepsilon)$ and where

$$f_\nu(\varepsilon)=\left.\frac{\langle\Theta\,|\,\mathbf{V}\,|\,\Phi_\nu(k)\,\rangle\,\langle\,\Phi_\nu(k)\,|\,\mathbf{V}\,|\,\Theta\rangle}{\mathrm{d}\lambda(k)/\mathrm{d}k}\right|_{\varepsilon=\lambda(k)}\cdot\begin{cases}1 & \text{if}\quad \varepsilon\in[a,b],\\ 0 & \text{if}\quad \varepsilon\notin[a,b].\end{cases}\tag{A.18c}$$

Combining above results one derives expression (17a) for the fractional shift $x(\varepsilon)$. This generalizes this expression to the case when the system $\boldsymbol{S}^b_\infty$ contains several one-parameter eigenvalue bands which all have the same eigenvalue function $\lambda(k)$.

(c) Fractional shift in the general case

Consider now a general case when the system $\boldsymbol{S}^b_\infty$ is described by the eigenvalue equation (2a) where eigenstates $|\Phi_\nu(k)\rangle$ are orthonormalized according to (2b). In this case range D contains a finite number of intervals such that in each of those intervals eigenvalues $\lambda_\nu(k)$ are exactly $\eta\leqslant\kappa$ degenerate. Quantity η depends on the interval and it can be as small as $\eta=1$ and as large as $\eta=\kappa$. With an appropriate change of variables, each such interval can be treated as a η-degenerate band considered in case (b) above. Accordingly, a general case can be piecewise reduced to the previous case. One thus finds that all relations derived above are still valid, provided expression (A.18c) is generalized to the expression (4a).

One final point. Above we have assumed that each $\lambda_\nu(k)$ is monotonic increasing function of k. In this case $\mathrm{d}\lambda_\nu/\mathrm{d}k\geqslant 0$ and hence $\mathrm{d}\lambda_\nu/\mathrm{d}k=\left|\mathrm{d}\lambda_\nu/\mathrm{d}k\right|$. If $\lambda_\nu(k)$ is monotonic decreasing function of k, one has $\mathrm{d}\lambda_\nu/\mathrm{d}k\leqslant 0$. With the substitution $k'=-k$ monotonic decreasing function $\lambda_\nu(k)$ is transformed into monotonic increasing finction which can be treated in the way described above. One thus finds that in both cases one should use absolute value $\left|\mathrm{d}\lambda_\nu/\mathrm{d}k\right|$ of the derivative $\mathrm{d}\lambda_\nu/\mathrm{d}k$. Hence definition (4a) which includes both possibilities.

(d) Construction of the eigenstates $\left|\Phi'_\kappa(k)\right\rangle$ that satisfy (A.15)

It remains to show that unperturbed system $\boldsymbol{S}^b_\infty$ contains a complete set of eigenstates $\left|\Phi'_\nu(k)\right\rangle$ that satisfy (A.15).

Consider eigenvalue equation (A.13). Adjust phases of eigenstates $|\Phi_\nu(k)\rangle$ in such a way that all matrix elements $a_\nu\equiv\langle\Theta\,|\,\mathbf{V}\,|\Phi_\nu(k)\,\rangle$ are real and nonnegative and arrange matrix elements a_ν in a nondecreasing order, $a_1\leqslant a_2\leqslant\cdots\leqslant a_\kappa$. Chose any $\nu\neq\kappa$ and replace eigenstates $|\Phi_\kappa(k)\rangle$ and $|\Phi_\nu(k)\rangle$ with eigenstates $\left|\Phi'_\kappa(k)\right\rangle$ and $\left|\Phi'_\nu(k)\right\rangle$ according to

$$\begin{aligned}\left|\Phi'_\kappa(k)\right\rangle&=|\Phi_\kappa(k)\rangle\cos\alpha+|\Phi_\nu(k)\rangle\sin\alpha,\\ \left|\Phi'_\nu(k)\right\rangle&=-|\Phi_\kappa(k)\rangle\sin\alpha+|\Phi_\nu(k)\rangle\cos\alpha.\end{aligned}\tag{A.19a}$$

This is an orthogonal transformation. Since original eigenstates $|\Phi_\kappa(k)\rangle$ and $|\Phi_\nu(k)\rangle$ are orthonormalized, transformed eigenstates $\left|\Phi'_\kappa(k)\right\rangle$ and $\left|\Phi'_\nu(k)\right\rangle$ are also orthonormalized. Corresponding matrix elements a_κ and a_ν transform

according to

$$a'_\kappa = a_\kappa \cos\alpha + a_\nu \sin\alpha, \quad a'_\nu = -a_\kappa \sin\alpha + a_\nu \cos\alpha. \tag{A.19b}$$

This transformation represents a rotation of a two-dimensional vector with the components a_κ and a_ν by the angle α. Hence $g'(k) = g(k)$, i.e. orthogonal transformation (A.19a) does not change the value of the quantity $g(k)$. Since $a_\kappa \geqslant g(k)$ there exist an angle α such that $a'_\kappa = g(k)$. This angle satisfies

$$\cos\alpha = \frac{g a_\kappa \pm a_\nu \sqrt{a_\kappa^2 + a_\nu^2 - g^2}}{a_\kappa^2 + a_\nu^2}. \tag{A.19c}$$

In conclusion, transformation (A.19a) where α satisfies (A.19c) transforms initial eigenstate $|\Phi_\kappa(k)\rangle$ into new eigenstate $\left|\Phi'_\kappa(k)\right\rangle$ in such a way that $a'_\kappa \equiv \left\langle\Theta\left|\mathbf{V}\right|\Phi'_\kappa(k)\right\rangle = g(k)$ and $g'(k) = g(k)$. This determines first eigenstate $\left|\Phi'_\kappa(k)\right\rangle$. One can apply the same procedure to the remaining $\kappa - 1$ eigenstates to obtain second transformed eigenstate $\left|\Phi'_{\kappa-1}(k)\right\rangle$. After repeating this procedure $\kappa - 1$ times, one constructs the set of κ eigenstates $\left|\Phi'_\mu(k)\right\rangle$ that satisfy (A.15). Since in each step one has an orthogonal transformation of a type (A.19a), transformed eigenstates $\left|\Phi'_\mu(k)\right\rangle$ are expressed in terms of the original eigenstates $|\Phi_\nu(k)\rangle$ according to (A.14) where $\mathbf{O}(k)$ is an orthogonal matrix.

Above construction proves that, if the matrix elements $\langle\Theta\,|\,\mathbf{V}\,|\Phi_\nu(k)\,\rangle$ are real and nonnegative (which can be assumed without loss of generality), there exists an orthogonal transformation $\mathbf{O}(k)$ of the original eigenstates $|\Phi_\nu(k)\rangle$ such that transformed eigenstates $\left|\Phi'_\nu(k)\right\rangle$ satisfy (A.15). Transformation $\mathbf{O}(k)$ with such property is not unique and there exists many orthonormalized sets $\left\{\left|\Phi'_\nu(k)\right\rangle\right\}$ that satisfy (A.15). However, what is important is the existence of at least one such set.

A.4.2. Calculation of the density $\rho^a(\varepsilon)$

Consider the case (b) from the previous section ($\lambda_1(k) = \lambda_2(k) = \cdots \lambda_\kappa(k)$) and let $\varepsilon_k \in D$ be an eigenvalue of the finite combined system $\boldsymbol{S}_{n+1}$. Using indexing convention $k \equiv (\mu, j)$ and $l \equiv (\nu, i)$ the corresponding normalized eigenstate $|\Psi_k\rangle \equiv \left|\Psi_{\mu,j}\right\rangle$ of this system can be written as

$$|\Psi_k\rangle = \frac{1}{\sqrt{Q_k}}\left[|\Theta\rangle + \beta \sum_l \frac{\left\langle\Phi'_l\,\middle|\,\mathbf{V}\,\middle|\Theta\right\rangle}{\varepsilon_k - \lambda_l}\left|\Phi'_l\right\rangle\right]. \tag{A.3a'}$$

This can be expressed as a sum of three terms

$$|\Psi_k\rangle = \frac{1}{\sqrt{Q_k}}\left[|\Theta\rangle + \beta\left|\Psi_k^{(0)}\right\rangle + \beta\left|\Psi_k^{(1)}\right\rangle\right], \tag{A.20a}$$

where

$$\left|\Psi_k^{(0)}\right\rangle = \sum_{l=-M(n)}^{M(n)} \frac{\left\langle \Phi'_{k+l} \left| \mathbf{V} \right| \Theta \right\rangle}{\varepsilon_k - \lambda_{k+l}} \left|\Phi'_{k+l}\right\rangle, \tag{A.20b}$$

$$\left|\Psi_k^{(1)}\right\rangle = \sum_{l<-M(n)} \frac{\left\langle \Phi'_{k+l} \left| \mathbf{V} \right| \Theta \right\rangle}{\varepsilon_k - \lambda_{k+l}} \left|\Phi'_{k+l}\right\rangle + \sum_{l>M(n)} \frac{\left\langle \Phi'_{k+l} \left| \mathbf{V} \right| \Theta \right\rangle}{\varepsilon_k - \lambda_{k+l}} \left|\Phi'_{k+l}\right\rangle, \tag{A.20c}$$

and where

$$Q_k = 1 + \beta^2 \left\langle \Psi_k^{(0)} \middle| \Psi_k^{(0)} \right\rangle + \beta^2 \left\langle \Psi_k^{(1)} \middle| \Psi_k^{(1)} \right\rangle. \tag{A.20d}$$

Choose $M(n) = \lfloor n^{2/3} \rfloor$ to be the largest integer smaller than $n^{2/3}$. Function $\left|\Psi_k^{(0)}\right\rangle$ contains contributions to the perturbed eigenstate $|\Psi_k\rangle$ from $\approx 2n^{2/3}$ unperturbed states $\left|\Phi'_{k+l}\right\rangle \in X_n^b$ whose eigenvalues λ_{k+l} are close to ε_k, while function $\left|\Psi_k^{(1)}\right\rangle$ contains contributions from $\approx n$ remaining states $\left|\Phi'_{k+l}\right\rangle \in X_n^b$.

In order to calculate quantity Q_k that determines normalization of the eigenstate $|\Psi_k\rangle$ one has to evaluate scalar products

$$\left\langle \Psi_k^{(0)} \middle| \Psi_k^{(0)} \right\rangle = \sum_{l=-M(n)}^{M(n)} \frac{\left\langle \Theta \left| \mathbf{V} \right| \Phi'_{k+l} \right\rangle \left\langle \Phi'_{k+l} \left| \mathbf{V} \right| \Theta \right\rangle}{(\varepsilon_k - \lambda_{k+l})^2}, \tag{A.21a}$$

$$\left\langle \Psi_k^{(1)} \middle| \Psi_k^{(1)} \right\rangle = \sum_{l<-M(n)} \frac{\left\langle \Theta \left| \mathbf{V} \right| \Phi'_{k+l} \right\rangle \left\langle \Phi'_{k+l} \left| \mathbf{V} \right| \Theta \right\rangle}{(\varepsilon_k - \lambda_{k+l})^2} + \sum_{l>M(n)} \frac{\left\langle \Theta \left| \mathbf{V} \right| \Phi'_{k+l} \right\rangle \left\langle \Phi'_{k+l} \left| \mathbf{V} \right| \Theta \right\rangle}{(\varepsilon_k - \lambda_{k+l})^2}. \tag{A.21b}$$

All terms under summation sign in (A.21a) satisfy $|l| \leqslant n^{2/3}$. Hence and according to (A.15) matrix elements $\left\langle \Theta \left| \mathbf{V} \right| \Phi'_{k+l} \right\rangle \approx \left\langle \Theta \left| \mathbf{V} \right| \Phi'_k \right\rangle$ are constant. Further, (A.10) implies

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

Hence and from (A6″) one derives [1]

$$\left\langle \Psi_k^{(0)} \middle| \Psi_k^{(0)} \right\rangle \approx \frac{\kappa}{\Delta\lambda_k} \frac{\left\langle \Theta \left| \mathbf{V} \right| \Phi'_\mu(k_k) \right\rangle \left\langle \Phi'_\mu(k_k) \left| \mathbf{V} \right| \Theta \right\rangle}{\mathrm{d}\lambda/\mathrm{d}k_k} \frac{\pi^2}{\sin^2(\pi x(\varepsilon_k))}.$$

Intervals $\Delta\lambda_k$ scale as $O(n^{-1})$. Hence if $\left\langle \Theta \left| \mathbf{V} \right| \Phi'_\mu(k_k) \right\rangle \neq 0$ scalar product $\left\langle \Psi_k^{(0)} \middle| \Psi_k^{(0)} \right\rangle$ scales at least as $O(n)$. In a similar way one finds $\left\langle \Psi_k^{(1)} \middle| \Psi_k^{(1)} \right\rangle \leqslant$

$O(n^{2/3})$ [1]. In a limit $n \to \infty$ one can neglect $\left\langle \Psi_k^{(1)} \middle| \Psi_k^{(1)} \right\rangle$ relative to $\left\langle \Psi_k^{(0)} \middle| \Psi_k^{(0)} \right\rangle$. This implies $Q_k \approx \beta^2 \left\langle \Psi_k^{(0)} \middle| \Psi_k^{(0)} \right\rangle$. Further, according to (A.3a) probability $w_k^a = |\langle \Theta \,|\, \Psi_k \rangle|^2$ to find the state $|\Psi_k\rangle$ in a local state $|\Theta\rangle$ is $w_k^a = 1/Q_k$. Hence

$$w_k^a = \Delta\lambda_k \frac{(\mathrm{d}\lambda/\mathrm{d}k)_k}{\beta^2 \kappa \left\langle \Theta \middle| \mathbf{V} \middle| \Phi'_\mu(k_k) \right\rangle \left\langle \Phi'_\mu(k_k) \middle| \mathbf{V} \middle| \Theta \right\rangle} \frac{\sin^2(\pi x(\varepsilon_k))}{\pi^2}. \tag{A.22}$$

In a limit $n \to \infty$ one has $w_k^a \to \rho^a(\varepsilon) d\varepsilon$ where $\rho^a(\varepsilon) \equiv \sum_\mu \left| \left\langle \Theta \middle| \Psi_\mu(\varepsilon) \right\rangle \right|^2$. Also in this limit $\mathrm{d}\varepsilon = \mathrm{d}\lambda$ [1]. Hence and from (A.22) and (A.16) one derives expression (19). This proves this expression for the case when the system $\mathcal{S}_\infty^b$ is described by the eigenvalue equation (A.13).

This result can be generalized to an arbitrary case of multiple eigenvalue bands using the same approach described in the previous section concerning the derivation of the fractional shift $x(\varepsilon)$.

A.4.3. Degeneracy of the eigenstates $\Psi_\mu(\varepsilon)$

Relations (18) and (21.a) imply

$$\sum_\mu \rho_\mu^a(\varepsilon) = \sum_\mu \left| \left\langle \Theta \middle| \Psi_\mu(\varepsilon) \right\rangle \right|^2.$$

For each $\varepsilon \in D$ functions $\left|\Psi_\mu(\varepsilon)\right\rangle$ are defined up to the unitary transformation. Flexibility in the choice of the orthonormalized set $\left\{\left|\Psi_\mu(\varepsilon)\right\rangle\right\}$ suggests that it should be possible to choose this set in such a way as to satisfy $\langle \Theta \,|\, \Psi_\nu(\varepsilon) \rangle = \sqrt{\rho_\nu^a(\varepsilon)}$. By carefully analyzing relations (A.20b) and (A.20c) one finds that this is indeed the case.

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[10] Strictly $I_\nu = (a_\nu, b_\nu)$, since there are no eigenstates $|\Phi_\nu(0)\rangle$ and $|\Phi_\nu(\pi)\rangle$ corresponding to the values $k = 0$ and $k = \pi$, respectively. This slight imprecision has no serious consequences on the subsequent discussion.

[11] In reference [1], which treats special case $\kappa = 1$, there are few errors. Expression (58b) in this reference that involves derivative $\omega'(\varepsilon)$ (for the special case $\alpha_v \equiv \alpha = 0$ and $\gamma_v \equiv \gamma = 1$) and that corresponds to the present expression (36b) is in error for one minus sign. In addition, in figure 13 case $\beta = 0.9$ in this reference, one should replace $\varepsilon_R = 24804$ with $\varepsilon_R = 2.24804$.
[12] This convention differs slightly from the one applied in reference [1]. The difference is in a treatment of those eigenvalues $\varepsilon_k(n) \in D$ that are adjacent to some boundary points of D. However, there can be at most 2κ boundary points, and as n increases the contribution of those points decreases relative to the contribution of all other points. In a limit $n \to \infty$ those two conventions are identical.
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