Journal of Mathematical Chemistry, Vol. 39, No. 1, January 2006 (© 2005)
DOI: 10.1007/s10910-005-9010-8

Interaction of an isolated state with an infinite quantum system containing several one-parameter eigenvalue bands: II. time-dependent case

Tomislav P. Živković

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

Received 24 September 2004; revised 4 October 2004

Time-dependent properties of a state $|\Theta\rangle$ that interacts with an infinite dimensional quantum system $\boldsymbol{S}_{\infty}^{b}$ containing several one-parameter eigenvalue bands $\lambda_{\nu}(k) \in I_{\nu} \equiv [a_{\nu}, b_{\nu}]$ are considered. This is done by a new mathematical method that 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 one obtains standard results that are usually obtained within the formalism of the perturbation expansion method. In particular, if the eigenvalue E of the state $|\Theta\rangle$ is embedded inside the range $D = \bigcup_{\nu} I_{\nu}$ of the unperturbed eigenvalues, time evolution of the state $|\Theta(t)\rangle$ that is initially prepared in the state $|\Theta(0)\rangle \equiv |\Theta\rangle$ has typical exponential decay behavior. One also reproduces standard results concerning probabilities of the transition of the state $|\Theta(t)\rangle$ at infinite time ($t = \infty$) into various eigenvalue bands. However, if the interaction is strong, one finds much more complex and much more complicated behavior.

KEY WORDS: Interaction of quantum systems, time dependent perturbation, transition probabilities

1. Introduction

Consider the interaction of a state $|\Theta\rangle$ with an infinite quantum system $\boldsymbol{S}_{\infty}^{b}$ that contains a finite number of one-parameter eigenvalue bands. The solution to the unperturbed system $\boldsymbol{S}_{\infty}^{b}$ is assumed to be known, and one is interested in the properties of the state $|\Theta\rangle$ subject to the interaction with this system. Mathematically, this problem requires the solution of the combined system $\boldsymbol{S}_{\infty} = \boldsymbol{S}_{1}^{a} \oplus \boldsymbol{S}_{\infty}^{b}$, where $\boldsymbol{S}_{1}^{a}$ represents one-dimensional system containing a single state $|\Theta\rangle$ with the eigenvalue E. In the previous paper time-independent properties of the combined system $\boldsymbol{S}_{\infty}$ were considered [1]. The solution to this system was obtained by a new mathematical method that provides exact expressions for the eigenvalues and eigenstates of $\boldsymbol{S}_{\infty}$[1,2]. Unlike standard perturbation expansion approach, this method involves no power series expansion, and the results

obtained are valid, however strong the interaction between the systems $\boldsymbol{S}_1^a$ and $\boldsymbol{S}_\infty^b$.

We will generalize the original approach to the time-dependent case. Of particular interest is the time development of the state $|\Theta(t)\rangle$ that is at time $t = 0$ prepared in the state $|\Theta(0)\rangle \equiv |\Theta\rangle$. Important quantities to calculate are the decay of a state $|\Theta(t)\rangle$ and probabilities for the transition of this state at time t into various eigenvalue bands. Exact expressions for all those quantities will be derived.

The method described in this and in a previous paper [1] is still restricted, since the infinite system $\boldsymbol{S}_\infty^b$ is required to contain only a finite number of one-parameter eigenvalue bands. However, this restriction is not so serious. Those eigenvalue 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 this and in the previous paper can be generalized in a rather straightforward way to the case when the system $\boldsymbol{S}_\infty^b$ contains any number of arbitrary eigenvalue bands [3]. If the system $\boldsymbol{S}_\infty^b$ 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 $\boldsymbol{S}_\infty^b$ can be described [3].

Numerous problems in physics and chemistry can be analyzed in terms of the interaction of a single state with an infinite quantum system [1–7]. In particular, one can in this way analyze the interaction of an isolated molecular state $|\Theta\rangle$ (system $\boldsymbol{S}_1^a$) with the electromagnetic field (system $\boldsymbol{S}_\infty^b$). This problem is a main subject of spectroscopy [4,5]. In a similar way one can analyze the interaction of an isolated molecular state $|\Theta\rangle$ (system $\boldsymbol{S}_1^a$) of a molecule situated on the surface of some solid with this solid (system $\boldsymbol{S}_\infty^b$) [6]. This problem is one of the main subjects of the surface state physics [6,7]. In general, the suggested method can be applied to each case where an isolated state interacts with an infinite quantum system.

2. Mathematical formulation of a problem

Let us formulate in more mathematical terms the problem to be treated in a present paper. Consider first the time-independent case [1]:

System $\boldsymbol{S}_1^a$ is one-dimensional and it is described by the eigenvalue equation

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

where $\mathbf{A} = E|\Theta\rangle\langle\Theta|$ is a Hermitian operator. We refer to the state $|\Theta\rangle$ as a local state. With this system is associated one-dimensional space X_1^a spanned by $|\Theta\rangle$.

System $\boldsymbol{S}_{\infty}^{b}$ is infinite-dimensional and it is described by the eigenvalue equation

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

where $\mathbf{B}$ is a Hermitian operator. Formally, system $\boldsymbol{S}_{\infty}^{b}$ consists of κ subsystems $\boldsymbol{S}_{\infty}^{b\nu}$, i.e. $\boldsymbol{S}_{\infty}^{b} = \cup_{\nu}\boldsymbol{S}_{\infty}^{b\nu}$. Each subsystem $\boldsymbol{S}_{\infty}^{b\nu}$ is characterized by a single one-parameter eigenvalue band represented by the eigenvalue function $\lambda_{\nu}(k)$. This function is continuous and monotonic in the interval $[k_{a\nu}, k_{b\nu}]$. All eigenvalues of $\boldsymbol{S}_{\infty}^{b\nu}$ are hence confined to the eigenvalue interval $I_{\nu} = [a_{\nu}, b_{\nu}]$. If $\lambda_{\nu}(k)$ is monotonic increasing one has $a_{\nu} = \lambda_{\nu}(k_{a\nu})$ and $b_{\nu} = \lambda_{\nu}(k_{b\nu})$, while if it is monotonic decreasing one has $a_{\nu} = \lambda_{\nu}(k_{b\nu})$ and $b_{\nu} = \lambda_{\nu}(k_{a\nu})$. Union $D = \cup_{\nu} I_{\nu}$ of all intervals I_{ν} defines range of continuous eigenvalues of $\boldsymbol{S}_{\infty}^{b}$. We also consider point-set $\bar{D}$ which is defined as a complement of D. With the system $\boldsymbol{S}_{\infty}^{b}$ is associated an infinite-dimensional space X_{∞}^{b}, while with each subsystem $\boldsymbol{S}_{\infty}^{b\nu}$ is associated an infinite-dimensional space $X_{\infty}^{b\nu}$, subspace of X_{∞}^{b}.

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

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

We formally consider $\boldsymbol{S}_{\infty}^{b}$ as the unperturbed system. An arbitrary interaction between $\boldsymbol{S}_{1}^{a}$ and $\boldsymbol{S}_{\infty}^{b}$ 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 $\mathbf{V}$ has nonvanishing matrix elements between the state $|\Theta\rangle \in X_{1}^{a}$ and the states $|\Phi_{\nu}(k)\rangle \in X_{\infty}^{b}$. Eigenvalue equation describing combined system $\boldsymbol{S}_{\infty} = \boldsymbol{S}_{1}^{a} \oplus \boldsymbol{S}_{\infty}^{b}$ subject to this interaction is

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

where

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

In the time-dependent case instead of the eigenvalue equation (3a) one has time-dependent eigenvalue equation

$$i\hbar\frac{\partial}{\partial t}|\Psi(t)\rangle = \mathrm{H}|\Psi(t)\rangle. \tag{4}$$

3. The method

In a previous paper [1] a new method for the solution of the eigenvalue equation (3) was suggested. This method provides an exact solution to this equation. There is no power series expansion, and the derived relations are valid, however strong the interaction between the state $|\Theta\rangle$ and the system $\boldsymbol{S}_{\infty}$.

One finds that the combined system $\boldsymbol{S}_\infty$ may contain two qualitatively different types of solutions [1]. Each $\varepsilon \in D$ contained in the range D of the unperturbed eigenvalues is also an eigenvalue of the perturbed eigenvalue equation (3a). Eigenvalues $\varepsilon \in D$ and corresponding eigenstates $|\Psi_\nu(\varepsilon)\rangle$ are *embedded* eigenvalues and eigenstates. Eigenvalue equation (3a) may also have some discrete eigenvalues $\varepsilon_I \in \bar{D}$ with the corresponding eigenstates $|\Psi_I\rangle$. Those are *isolated* eigenvalues and eigenstates.

Properties of the combined system $\boldsymbol{S}_\infty$ can be expressed in terms of characteristic functions $f_\nu(\varepsilon)$ and in terms of derived functions $\omega_\nu(\varepsilon)$ [1]. With each eigenvalue band ν is associated *characteristic* function $f_\nu(\varepsilon)$:

$$f_\nu(\varepsilon) = \left.\frac{\langle\Theta|\mathbf{V}|\Phi_\nu(k)\rangle\langle\Phi_\nu(k)|\mathbf{V}|\Theta\rangle}{|\mathrm{d}\lambda_\nu(k)/\mathrm{d}k|}\right|_{\varepsilon=\lambda_\nu(k)} \cdot \begin{cases} 1 & \text{if } \varepsilon \in I_\nu \\ 0 & \text{if } \varepsilon \notin I_\nu \end{cases}. \tag{5a}$$

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

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

where P denotes principal Cauchy integral value [8]. In particular, if $f_\nu(\varepsilon)$ is polynomial inside the interval I_ν, one can obtain function $\omega_\nu(\varepsilon)$ in a closed analytic form [9].

Functions $f_\nu(\varepsilon)$ and $\omega_\nu(\varepsilon)$ combine into global functions $f(\varepsilon)$ and $\omega(\varepsilon)$, respectively [1]

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

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

$$h(\varepsilon) \equiv \beta^2\omega(\varepsilon) + E - \varepsilon. \tag{6}$$

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

3.1. Time-independent case

In order to solve time-dependent eigenvalue equation (4), one has first to consider the time-independent eigenvalue equation (3a). Each isolated eigenvalue $\varepsilon_I \in \overline{D}$ of this equation is a root of the auxiliary function $h(\varepsilon)$ [1]

$$\beta^2\omega(\varepsilon_I) + E - \varepsilon_I = 0, \quad \varepsilon_I \in \overline{D}. \tag{7}$$

Once eigenvalue ε_I is known, one can easily obtain the corresponding isolated eigenstate $|\Psi_I\rangle$ in a closed form [1]. In particular, probability $w_I^a = |\langle\Theta|\Psi_I\rangle|^2$ to find the state $|\Theta\rangle$ in the isolated eigenstate $|\Psi_I\rangle$, i.e. probability for the state $|\Theta\rangle$ to have eigenvalue ε_I equals

$$w_I^a = \frac{1}{1-\beta^2\omega'(\varepsilon_I)}, \tag{8}$$

where $\omega'(\varepsilon_I) = \mathrm{d}\omega(\varepsilon_I)/\mathrm{d}\varepsilon_I$ is derivative of a global function $\omega(\varepsilon)$ in a point $\varepsilon = \varepsilon_I$.

Concerning embedded eigenstates of (3a), one finds that there exists an ortnonormalized set $\{|\Psi_\nu(\varepsilon)\rangle\}$ of those eigenstates that satisfies

$$\langle\Theta|\ \Psi_\nu(\varepsilon)\rangle = \sqrt{\rho_\nu^a(\varepsilon)}, \tag{9a}$$

where [1]

$$\rho_\nu^a(\varepsilon) = \frac{\beta^2 f_\nu(\varepsilon)}{\pi^2\beta^4 f^2(\varepsilon) + \left(\beta^2\omega(\varepsilon) + E - \varepsilon\right)^2}. \tag{9b}$$

Each $|\Psi_\nu(\varepsilon)\rangle$ is an eigenstate of the combined system with the eigenvalue $\varepsilon \in D$. Probability density $\rho^a(\varepsilon)$ to find the state $|\Theta\rangle$ with the eigenvalue $\varepsilon \in D$ is hence a sum $\sum_\nu |\langle\Theta|\Psi_\nu(\varepsilon)\rangle|^2$:

$$\rho^a(\varepsilon) \equiv \sum \rho_\nu^a(\varepsilon) = \frac{\beta^2 f(\varepsilon)}{\pi^2\beta^4 f^2(\varepsilon) + \left(\beta^2\omega(\varepsilon) + E - \varepsilon\right)^2}. \tag{10}$$

Expressions (9) and (10) are valid for each $\varepsilon \in D$, except for the anomal points $\varepsilon_a \in D$ that satisfy $f(\varepsilon_a) = 0$ and $h(\varepsilon_a) = 0$ [1]. Since each anomal point has to satisfy simultaneously two conditions, such points are rather rare. Unless otherwise specified, we will assume that the combined system $\mathbf{S}_\infty$ contains no anomal points.

If the interaction of the local state $|\Theta\rangle$ with the system $\boldsymbol{S}_\infty^b$ is weak (small β) and if $E \in D$ (resonance approximation [1]) one has

$$\rho^a(\varepsilon) \approx \rho^{a0}(\varepsilon) = \frac{\beta^2 f(\varepsilon_r)}{\pi^2\beta^4 f^2(\varepsilon_r) + (\varepsilon - \varepsilon_r)^2} \cdot \begin{cases} 1 & \text{if } \varepsilon \in D \\ 0 & \text{if } \varepsilon \notin D \end{cases}, \tag{11a}$$

where *resonant point* $\varepsilon_r \approx E + \beta^2\omega(E)$ is a root of the auxiliary function $h(\varepsilon)$ [1]

$$h(\varepsilon_r) \equiv \beta^2\omega(\varepsilon_r) + E - \varepsilon_r = 0, \quad \varepsilon_r \in D. \tag{11b}$$

Density $\rho^{a0}(\varepsilon)$ has the shape of the universal resonance curve [10] truncated at the boundaries of the range D. Universal resonance curve is usually obtained within the standard perturbation expansion approach that assumes weak interaction between the state $|\Theta\rangle$ and the system $\boldsymbol{S}_\infty^b$ [4,5,10].

Relations (7), (8) and (10) determine eigenvalue distribution of the local state $|\Theta\rangle$ subject to the interaction with the infinite system $\boldsymbol{S}_\infty^b$. If one performs the measurement of the eigenvalue on this state, one obtains result $\varepsilon_I \notin D$ with the probability w_I^a and the result $\varepsilon \in D$ with the probability density $\rho^a(\varepsilon)$. This eigenvalue distribution can be written in a compact form

$$\rho(\varepsilon) \equiv \rho^a(\varepsilon) + \sum_I w_I^a \delta(\varepsilon - \varepsilon_I). \tag{12}$$

The state $|\Theta\rangle$ must be found with certainty either with some eigenvalue $\varepsilon_I \notin D$ or with some eigenvalue $\varepsilon \in D$. Hence completeness relation [1]

$$\int \rho(\varepsilon)\mathrm{d}\varepsilon \equiv \int \rho^a(\varepsilon)\mathrm{d}\varepsilon + \sum_I w_I^a = 1. \tag{13}$$

Since the eigenstates $|\Psi_I\rangle$ and $|\Psi_\nu(\varepsilon)\rangle$ form a complete set in a space corresponding to the combined system $\boldsymbol{S}_\infty$, each state can be expressed in terms of those eigenstates. In particular, local state $|\Theta\rangle$ can be expressed in this way. One finds [1]

$$|\Theta\rangle = \sum_I \sqrt{w_I^a}|\Psi_I\rangle + \sum_\nu \int \sqrt{\rho_\nu^a(\varepsilon)}|\Psi_\nu(\varepsilon)\rangle \mathrm{d}\varepsilon. \tag{14}$$

Expressions (12)–(14) apply to the case when the system S_∞ contains no anomal points. Otherwise those expressions should be corrected with some additional terms [1–3]. More details concerning the solution of the time-independent eigenvalue equation (3a) can be found elsewhere [1].

3.2. *Time-dependent case*

Consider now time-dependent eigenvalue equation (4). Each solution of this equation can be expressed as a linear combination

$$|\Psi(t)\rangle = \sum_I c_I |\Psi_I\rangle \exp(-\mathrm{i}\varepsilon_I t/\hbar) + \sum_\nu \int c_\nu(\varepsilon)|\Psi_\nu(\varepsilon)\rangle \exp\left(-\mathrm{i}\varepsilon t/\hbar\right) \mathrm{d}\varepsilon, \tag{15}$$

where $|\Psi_I\rangle$ and $|\Psi_\nu(\varepsilon)\rangle$ are eigenstates of the time-independent eigenvalue equation (3a), while c_I and $c_\nu(\varepsilon)$ are unknown coefficients and unknown functions to be determined from the initial conditions. In general, one has $c_I = \langle\Psi_I|\Psi(0)\rangle$ and $c_\nu(\varepsilon) = \langle\Psi_\nu(\varepsilon)|\Psi(0)\rangle$. Of particular interest is the state $|\Theta(t)\rangle$ that is at time $t = 0$ prepared in the local state $|\Theta\rangle \in X_1^a$, that is $|\Theta(0)\rangle = |\Theta\rangle$. Using (14) and (15) one finds

$$|\Theta(t)\rangle = \sum_I \sqrt{w_I^a}|\Psi_I\rangle \exp(-\mathrm{i}\varepsilon_I t/\hbar) + \sum_\nu \int \sqrt{\rho_\nu^a(\varepsilon)}|\Psi_\nu(\varepsilon)\rangle \exp\left(-\mathrm{i}\varepsilon t/\hbar\right) \mathrm{d}\varepsilon. \tag{16}$$

Important quantities are the probability $w^a(t)$ to find the state $|\Theta(t)\rangle$ at time t in the initial state $|\Theta(0)\rangle = |\Theta\rangle$ and transition probabilities for the transition of a state $|\Theta(t)\rangle$ at time t into various eigenvalue bands. Concerning probability $w^a(t)$, this probability is a square of the amplitude $\langle\Theta|\Theta(t)\rangle$

$$w^a(t) = |\langle\Theta|\Theta(t)\rangle|^2 . \tag{17a}$$

Above expressions imply

$$\begin{aligned}\langle\Theta|\Theta(t)\rangle &= \int \rho(\varepsilon) \exp\left(-\mathrm{i}\varepsilon t/\hbar\right) \mathrm{d}\varepsilon \\ &\equiv \int \rho^a(\varepsilon) \exp\left(-\mathrm{i}\varepsilon t/\hbar\right) \mathrm{d}\varepsilon + \sum_I w_I^a \exp\left(-\mathrm{i}\varepsilon_I t/\hbar\right),\end{aligned} \tag{17b}$$

where density $\rho^a(\varepsilon)$ is given by (10), eigenstates ε_I are roots of (7), while probabilities w_I^a are given by (8). Expression (17b) is formally identical to the expression obtained previously [2] for the case when the system S_∞^b contains a single one-parameter eigenvalue band. According to this expression, probability amplitude $\langle\Theta|\Theta(t)\rangle$ to find the state $|\Theta(t)\rangle$ at time t in the initial state $|\Theta\rangle$ is a Fourier transform of the eigenvalue distribution $\rho(\varepsilon)$. Of particular interest is the $t \to \infty$ limit of this amplitude. For sufficiently big times the first term on the right hand side of (17b) becomes negligibly small. Hence

$$\lim_{t\to\infty} \langle\Theta|\Theta(t)\rangle = \sum_I w_I^a \exp\left(-\mathrm{i}\varepsilon_I t/\hbar\right). \tag{18a}$$

If the combined system contains no isolated eigenstates, after long enough time there is a complete decay of a state $|\Theta\rangle$ and hence $w^a(\infty) = 0$. This is a usual case that can be also obtained within the formalism of the perturbation expanse approach [4,5]. However, if the combined system contains one isolated eigenstate $|\Psi_I\rangle$ with a nonvanishing probability $w_I^a \neq 0$, one has $\lim_{t\to\infty} \langle\Theta|\Theta(t)\rangle = w_I^a \exp\left(-\mathrm{i}\varepsilon_I t/\hbar\right)$ and hence $w^a(\infty) = \left(w_I^a\right)^2 \neq 0$. Therefore, at infinite time the state $|\Theta(\infty)\rangle$ will be found with a finite probability $\left(w_I^a\right)^2$ in the initial state $|\Theta\rangle$. The situation is more complex if the combined system contains several isolated eigenstates. In this case one has

$$\lim_{t\to\infty} w^a(t) = \sum_I \left(w_I^a\right)^2 + 2\sum_{I<J} w_I^a w_J^a \cos\left(\frac{(\varepsilon_I - \varepsilon_J)t}{\hbar}\right). \tag{18b}$$

Accordingly, after long enough time the state $|\Theta\rangle$ will only partially decay, and in a limit $t \to \infty$ there will be an oscillatory probability to find the state $|\Theta(t)\rangle$ in the local state $|\Theta\rangle$. However, since in each interval $(a, b) \subseteq \overline{D}$ there can be at most one isolated eigenstate [1], all quantities $(\varepsilon_I - \varepsilon_J)$ $(\varepsilon_I \neq \varepsilon_J)$ are relatively large. Those oscillations are hence extremely fast. It is usually quite difficult to detect such fast oscillations experimentally. Instead one should detect a

time-average $\overline{w}^a(\infty)$ of those oscillations. Time average of a second term in (18b) equals zero, and hence

$$\overline{w}^a(\infty) = \sum_I \left(w_I^a\right)^2. \tag{18c}$$

This last case with fast oscillations of the probability $w^a(t)$ requires existence of at least two isolated eigenstates ε_I with significant probabilities w_I^a. Hence it can happen only in extreme conditions. If the coupling β is relatively small and if $E \in D$, combined system contains no isolated eigenstates [1]. This system may contain several isolated eigenstates $|\Psi_I\rangle$ with significant probabilities w_I^a only if this coupling is quite large. Those are conditions where standard perturbation expansion approach fails [1].

Consider now probability to find the state $|\Theta(t)\rangle$ at time t in the state $|\Phi_\nu(k)\rangle$ with the eigenvalue $\lambda = \lambda_\nu(k)$ and in the eigenvalue interval $\mathrm{d}\lambda$. This probability can be written as $\rho_\nu^b(\lambda, t)\mathrm{d}\lambda$ where the probability density $\rho_\nu^b(\lambda, t)$ is a square of the corresponding amplitude $u_\nu^b(\lambda, t)$:

$$\rho_\nu^b(\lambda, t) = \left|u_\nu^b(\lambda, t)\right|^2. \tag{19a}$$

If the system $\boldsymbol{S}_\infty^b$ contains several eigenvalue bands, the state $|\Theta(t)\rangle$ may decay via different channels $|\Theta(t)\rangle \to |\Phi_\nu(k)\rangle$ $(\nu = 1, \ldots, \kappa)$. For example, one can consider the decay of some molecular state $|\Theta(t)\rangle$. In principle, this state may decay to each molecular state $|\Theta_f\rangle$ that has energy E_f lower than the energy E of the original state $|\Theta\rangle \equiv |\Theta(0)\rangle$. This decay is accompanied by the emission of a photon in the state $|\mathbf{k}\varpi\rangle$ where $\mathbf{k}$ denotes wavevector, while ϖ denotes photon polarization [11]. Accordingly, one has the transition $|\Theta(t)\rangle \to |\Theta_f \mathbf{k}\varpi\rangle$. In the above notation $|\Phi_\nu(k)\rangle \equiv |\Theta_f \mathbf{k}\varpi\rangle$ is the unperturbed state contained in the system $\boldsymbol{S}_\infty^b$ [12]. Transitions to various finale states $|\Theta_f\rangle$ are physically very different, they are usually well separated, and it is quite important to know relative probabilities of those transitions.

In reference [2] the system $\boldsymbol{S}_\infty^b$ containing a single one-parameter eigenvalue band was considered. In this case there is only one probability amplitude $u^b(\lambda, t)$ for the transition of the state $|\Theta(t)\rangle$ into various eigenstates $|\Phi(k)\rangle$ of $\boldsymbol{S}_\infty^b$. Following the same approach as in this reference, one finds in a more general case considered here

$$u_\nu^b(\lambda, t) = \beta\sqrt{f_\nu(\lambda)}\left[\int \frac{\rho^a(\varepsilon)\left[\mathrm{e}^{-\mathrm{i}(\varepsilon-\lambda)t/\hbar} - 1\right]}{\varepsilon - \lambda}\mathrm{d}\varepsilon + \sum_I w_I^a \frac{\left[\mathrm{e}^{-\mathrm{i}(\varepsilon_I-\lambda)t/\hbar} - 1\right]}{\varepsilon_I - \lambda}\right]. \tag{19b}$$

Using (17b) above amplitudes can be expressed in terms of the amplitude $\langle\Theta|\Theta(t)\rangle$ [13]

$$u_\nu^b(\lambda,t) = -\mathrm{i}\frac{\beta}{\hbar}\sqrt{f_\nu(\lambda)}\int_0^t \langle\Theta|\Theta(t)\rangle\, \mathrm{e}^{\mathrm{i}\lambda t/\hbar}\mathrm{d}t, \quad \nu = 1,\ldots,\kappa. \tag{19c}$$

This expression provides a direct connection between the amplitude $\langle\Theta\,|\Theta(t)\rangle$ that determines probability $w^a(t)$ with the amplitudes $u_\nu^b(\lambda,t)$ that determine probability densities $\rho_\nu^b(\lambda,t)$. In the case $\kappa = 1$ above expressions reduce to the expressions derived previously [2,13].

Expressions (19) determine transition probabilities for the transition of the state $|\Theta(t)\rangle$ at time t in the states $|\Phi_\nu(k)\rangle$. For $t = 0$ one finds $u_\nu^b(\lambda,0) = 0$ and hence $\rho_\nu^b(\lambda,0) = 0$. As t increases, one obtains nonvanishing probability densities $\rho_\nu^b(\lambda,t)$ to find the state $|\Theta(t)\rangle$ in the state $|\Phi_\nu(k)\rangle$ that has eigenvalue $\lambda = \lambda_\nu(k)$. Above expressions imply

$$\frac{\rho_\nu^b(\lambda,t)}{\rho_\mu^b(\lambda,t)} = \frac{f_\nu(\lambda)}{f_\mu(\lambda)}. \tag{20}$$

This shows that for each unperturbed eigenvalue λ the ratio of the probability densities to decay to different subsystems $\boldsymbol{S}_\infty^{b\nu}$ is independent on time.

If the combined system contains no isolated eigenstates, there is a well-defined limit $\rho_\nu^b(\lambda,\infty) = \lim_{t\to\infty}\rho_\nu^b(\lambda,t)$ to find local state $|\Theta\rangle$ after long enough time in the state $|\Phi_\nu(k)\rangle$. Otherwise for large times probability densities $\rho_\nu^b(\lambda,t)$ exhibit fast oscillations. Time scale of those oscillations is dictated by the quantities $(\lambda - \varepsilon_I)$. Since $\lambda \in D$ while $\varepsilon_I \in \overline{D}$, those quantities are usually large. Hence under normal conditions those oscillations are to fast to be detected experimentally. Instead one can detect only well defined limit $\bar{\rho}_\nu^b(\lambda,\infty)$ which is the average over those fast oscillations. This is similar to the analogous behavior of the probability $w^a(t)$ discussed above.

Probability to find the state $|\Theta(t)\rangle$ at time t in the subsystem $\boldsymbol{S}_\infty^{b\nu}$, i.e. to find it in any of the states $|\Phi_\nu(k)\rangle \in X_\infty^{b\nu}$ equals

$$w_\nu^b(t) = \int \rho_\nu^b(\lambda,t)\mathrm{d}\lambda. \tag{21a}$$

This expression can be evaluated either using relation (19b) or using relation (19c) that involves amplitude $\langle\Theta\,|\,\Theta(t)\rangle$. Rearranging integrations one finds equivalent expression

$$w_\nu^b(t) = \frac{\beta^2}{\hbar^2}\int_0^t \mathrm{d}t\int_0^t \mathrm{d}t'\langle\Theta(t')\,|\,\Theta\rangle\langle\Theta\,|\,\Theta(t)\rangle\tilde{f}_\nu(t-t'), \tag{21b}$$

where

$$\tilde{f}_\nu(t) = \int f_\nu(\lambda)\mathrm{e}^{\mathrm{i}\lambda t/\hbar}\,\mathrm{d}\lambda. \tag{21c}$$

Up to the normalization constant, function $\tilde{f}_\nu$ is inverse Fourier transform [4] of the characteristic function f_ν.

At each time t the state $|\Theta(t)\rangle$ must be found with a certainty either in the original state $|\Theta\rangle \in X_1^a$ or in some state $|\Phi_\nu(k)\rangle \in X_\infty^{b\nu}$ of any of κ subsystems $\boldsymbol{S}_\infty^{b\nu}$. Hence completeness relation

$$w^a(t) + \sum_\nu^\kappa w_\nu^b(t) = 1. \tag{22}$$

One can also consider $w^b(t) = \sum_\nu^\kappa w_\nu^b(t)$ which is a total probability to find the state $|\Theta(t)\rangle$ at time t in any of the subsystems $\boldsymbol{S}_\infty^{b\nu}$, i.e. to find it in a system $\boldsymbol{S}_\infty^b$.

Relation (22) is a key completeness relation that can be used as an efficient test for the validity of the suggested method in the time-dependent case.

Note that unlike the ratio (20) that involves probability densities and that does not depend on time, the ratio $w_\mu^b(t)/w_\nu^b(t)$ of total probabilities to decay via channels μ and ν usually depends on time.

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

In the case of the weak coupling there are two qualitatively different cases, the case $E \in \overline{D}$ and the case $E \in D$. There are also small intermediate regions close to the boundaries between D and $\bar{D}$.

If $E \in \overline{D}$ is an interior point in $\overline{D}$ and if β is sufficiently small, one has an isolated eigenvalue ε_I close to E that satisfies $w_I^a \approx 1$ [1]. Hence $\rho(\varepsilon) \approx \delta(\varepsilon - \varepsilon_I)$ and relation (17b) implies $w^a(t) \approx 1$. In conclusion, If $E \in \overline{D}$ is an interior point in $\overline{D}$ and if β is sufficiently small, the state $|\Theta\rangle$ is only slightly effected by the interaction with the system $\boldsymbol{S}_\infty^b$ and essentially it does not change with time.

Another possibility is $E \in D$ where E is an interior point in D. If the coupling β is sufficiently small, one has a resonance approximation [1]. In this case density $\rho^a(\varepsilon)$ is well approximated by the truncated universal resonance curve $\rho^{a0}(\varepsilon)$ and in addition $w_I^a \approx 0$ [1]. Hence and from (17b) amplitude $\langle\Theta \mid \Theta(t)\rangle$ reduces to

$$\langle\Theta \mid \Theta(t)\rangle \approx \mathrm{e}^{-\mathrm{i}\varepsilon_r t/\hbar}\mathrm{e}^{-\pi\beta^2 f(\varepsilon_r)t/\hbar}, \tag{23a}$$

where $\varepsilon_r \in D$ is a root of (11b). Probability $w^a(t)$ to find the state $|\Theta(t)\rangle$ at time t in the initial state $|\Theta\rangle$ is hence

$$w^a(t) \approx w^{a0}(t) = \mathrm{e}^{-2\pi\beta^2 f(\varepsilon_r)t/\hbar}. \tag{23b}$$

This expression describes well-known exponential decay of the state $|\Theta\rangle$.

Concerning probability densities $\rho_\nu^b(\lambda, t)$, one finds in a resonance approximation

$$\rho_\nu^b(\lambda, t) \approx \rho_\nu^{b0}(\lambda, t) = \frac{f_\nu(\varepsilon_r)}{f(\varepsilon_r)} \rho^{a0}(\lambda) \left[\mathrm{e}^{-2\pi\beta^2 f(\varepsilon_r)t/\hbar} - 2\mathrm{e}^{-\pi\beta^2 f(\varepsilon_r)t/\hbar} \cos\left((\varepsilon_r - \lambda)t/\hbar\right) + 1 \right]. \tag{24}$$

This expression is a product of three terms. First term is a ratio $f_\nu(\varepsilon_r)/f(\varepsilon_r)$ that determines relative probabilities of a transition via different channels (ν). In particular, if $\varepsilon_r \notin I_\nu$ one has $f_\nu(\varepsilon_r) = 0$ and there is no transition to the channel ν. Second term is density $\rho^{a0}(\lambda)$ that has a sharp peak in the resonant point $\lambda = \varepsilon_r$ and that satisfies $\int \rho^{a0}(\lambda)\mathrm{d}\lambda \approx 1$. Last term describes an exponential approach to the $t = \infty$ limit modified in an oscillatory way by the cos() function. This oscillatory modification is absent in the resonant point $\lambda = \varepsilon_r$ where $\rho^{a0}(\lambda)$ has a maximum. As one departs from this point, frequency of those oscillations increases, while probability $\rho_\nu^{b0}(\lambda, t)$ sharply decreases.

According to (24) total probability $w_\nu^b(t)$ for the decay via channel ν equals

$$w_\nu^b(t) \approx w_\nu^{b0}(t) = \int \rho_\nu^{b0}(\lambda, t)\mathrm{d}\lambda = \frac{f_\nu(\varepsilon_r)}{f(\varepsilon_r)} \left[1 - \mathrm{e}^{-2\pi\beta^2 f(\varepsilon_r)t/\hbar} \right]. \tag{25}$$

Relations (23b) and (25) satisfy $w^{a0}(t) + \sum_\nu w_\nu^{b0}(t) = 1$ in accord with the completeness requirement (22). In addition one has

$$\frac{w_\nu^{b0}(t)}{w_\mu^{b0}(t)} = \frac{f_\nu(\varepsilon_r)}{f_\mu(\varepsilon_r)}, \tag{26}$$

which is similar to (20). Thus in the resonance approximation ratios of the probabilities to decay via different channels are independent of time. Unlike exact expression (20) this result is only approximate, and it depends on the validity of the resonance approximation. One has also

$$w^{b0}(t) \equiv \sum_\nu w_\nu^{b0}(t) = 1 - \mathrm{e}^{-2\pi\beta^2 f(\varepsilon_r)t/\hbar}. \tag{27}$$

In a resonance approximation after long enough time the state $|\Theta\rangle$ has completely decayed in the system $\boldsymbol{S}_\infty^b$, and one has $w^{b0}(\infty) = 1$.

Above results are in accord with the well-known results obtained in a standard way within the formalism of the perturbation expansion approach [4].

There is finally a third possibility when the local eigenvalue E is either a boundary point of the range D or very close to some boundary point of this range. In this case and if the coupling β is sufficiently small, the result is intermediate between the two cases considered above.

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

As an illustration of the method described above, consider a simple model described in reference [1]. In this model system $\boldsymbol{S}_\infty^b$ is the set of κ one-dimensional solids (subsystems $\boldsymbol{S}_\infty^{b\nu}$) in the nearest-neighbor tight-binding approximation [5,6]. With each site of the subsystem $\boldsymbol{S}_\infty^{b\nu}$ is associated a single state $|\nu, j\rangle$ ($j = 1, 2, \dots$). 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 [5]. Each subsystem $\boldsymbol{S}_\infty^{b\nu}$ represents an infinite Hückel chain. Eigenvalues $\lambda_\nu(k)$ and eigenstates $|\Phi_\nu(k)\rangle$ of such a chain are [1]

$$\lambda_\nu(k) = \alpha_\nu + 2\gamma_\nu \cos(k), \quad |\Phi_\nu(k)\rangle = \sqrt{\frac{2}{\pi}} \sum_{j=1}^{\infty} \sin(kj)\, |\nu, j\rangle, \quad 0 < k < \pi. \tag{28a}$$

According to (28a), each subsystem $\boldsymbol{S}_\infty^{b\nu}$ contains a single one-parameter eigenvalue band with the eigenvalue function $\lambda_\nu(k)$ in the interval I_ν

$$I_\nu = [a_\nu, b_\nu] \equiv [\alpha_\nu - 2\gamma_\nu, \lambda_\nu + 2\gamma_\nu], \qquad \nu = 1, \dots, \kappa. \tag{28b}$$

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

For the sake of simplicity assume that local state $|\Theta\rangle$ interacts only with first state $|\nu, 1\rangle$ of each Hückel chain. This interaction is completely determined by κ matrix elements $\beta_\nu = \langle\Theta|\mathbf{V}|\nu, 1\rangle$ where $\mathbf{V}$ is a hermitian operator that defines interaction between the state $|\Theta\rangle$ and a system $\boldsymbol{S}_\infty^b$. Without loss of generality one can impose the condition

$$\sum_{\nu}^{\kappa} \beta_\nu^2 = 1, \tag{29a}$$

This condition normalizes $\mathbf{V}$ according to $\langle\Theta|\,\mathrm{V}^2|\Theta\rangle = 1$ [1]. Using (28a) one finds

$$\langle\Theta|\,\mathrm{V}|\Phi_\nu(k)\rangle = \beta_\nu \sqrt{\frac{2}{\pi}} \sin(k). \tag{29b}$$

One can now solve combined system $\boldsymbol{S}_\infty$ with the method described in previous sections. First step in this method is the construction of characteristic and

derived functions of the system $\boldsymbol{S}_\infty$. One finds [1]

$$f_\nu(\varepsilon) = \frac{\beta_\nu^2}{2\pi\gamma_\nu}\sqrt{4 - g_\nu(\varepsilon)^2}\begin{cases} 1 & \text{if } \varepsilon \in I_\nu \\ 0 & \text{if } \varepsilon \notin I_\nu \end{cases}, \tag{30a}$$

$$\omega_\nu(\varepsilon) = \frac{\beta_\nu^2}{2\gamma_\nu}\begin{cases} \left(g_\nu(\varepsilon) + \sqrt{g_\nu(\varepsilon)^2 - 4}\right) & \text{if} \quad \varepsilon < a_\nu \\ g_\nu(\varepsilon) \quad \text{if} \quad \varepsilon \in I_\nu = [a_\nu, b_\nu] \\ \left(g_\nu(\varepsilon) - \sqrt{g_\nu(\varepsilon)^2 - 4}\right) & \text{if} \quad \varepsilon > b_\nu \end{cases}, \tag{30b}$$

where

$$g_\nu(\varepsilon) = \frac{\varepsilon - \alpha_\nu}{\gamma_\nu}. \tag{30c}$$

Expressions (30) provide all necessary information for the derivation of time-independent [1] as well as time-dependent properties of the combined system. We will now consider time-dependent case.

4.1. Numerical 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, 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 a single one-parameter eigenvalue band.

As a particular example, let the unperturbed system $\boldsymbol{S}_\infty^b$ be characterized by the parameters $\alpha_1 = 0, \alpha_2 = 0.5, \gamma_1 = 1$ and $\gamma_2 = 0.5$. Assume also that relative couplings of subsystems $\boldsymbol{S}_\infty^{b1}$ and $\boldsymbol{S}_\infty^{b2}$ with the local state $|\Theta\rangle$ are $\beta_1 = 0.7$ and $\beta_2 = \sqrt{1 - \beta_1^2} = 0.71414$, respectively. This last expression follows from the requirement (29a). In [1] above parameter choice is defined as parameter choice **B.** According to (28b), this parameter choice implies $I_1 = [-2,2]$ and $I_2 = [-0.5,1.5]$. Since $I_2 \subset I_1$ the range D coincides with the interval I_1. Point set $\bar{D}$ is hence a union of two intervals, left interval $\bar{I}_L = (-\infty, -2)$ and right interval $\bar{I}_R = (2, \infty)$. In addition, in the interval I_2 unperturbed eigenvalues λ as well as perturbed eigenvalues ε are degenerate. All other eigenvalues $\lambda \in D$ and $\varepsilon \in D$ are nondegenerate. It is crucial to demonstrate correct behavior of the suggested method in the case of degenerate eigenvalue bands, since this is the most important new feature not considered in the original approach involving a single one-parameter eigenvalue band [2]. Accordingly, let $E = 1$ which is an interior point of the interval $I_2 = [-0.5,1.5]$.

Consider time-evolution of a state $|\Theta(t)\rangle$ that is at time $t = 0$ prepared in a local state $|\Theta(0)\rangle \equiv |\Theta\rangle$. This state is given by relation (16) where probabilities

w_I^a and probability densities $\rho_\nu^a(\varepsilon)$ are given by expressions (8) and (9b), respectively. Of particular interest is the probability $w^a(t)$ to find the state $|\Theta(t)\rangle$ at time t in the initial state $|\Theta\rangle$ and probabilities $w_\nu^b(t)$ for the transition of this state at time t in the eigenvalue band ν. Probability $w^a(t)$ is given by expression (17), while probabilities $w_\nu^b(t)$ are integrals (21a) of probability densities $\rho_\nu^b(\lambda, t) = \left|u_\nu^b(\lambda, t)\right|^2$ where probability amplitudes $u_\nu^b(\lambda, t)$ are obtained either by equation (19b) or by equation (19c). Alternatively, one can use expression (21b).

4.1.1. Probability $w^a(t)$and transition probabilities $w_\nu^b(t)$

As a first example in figure 1 parameter choice **B** with local eigenvalue $E = 1$ and with coupling $\beta = 0.2$ is considered. This case corresponds to the point $(*)$ in figure 7(a) of reference [1]. Coupling $\beta = 0.2$ is relatively weak and those are conditions of a resonance approximation. Hence system $\boldsymbol{S}_\infty$ contains no isolated eigenstate and probability density $\rho^a(\varepsilon)$ has approximately the shape of the truncated universal resonance curve $\rho^{a0}(\varepsilon)$. This is shown in figure 1(a). In figure 1(b) are shown probabilities $w^a(t)$ and $w_\nu^b(t)$ (solid lines) as well as approximate probabilities $w^{a0}(t)$ and $w_\nu^{b0}(t)$ given by relations (23b) and (25), respectively (doted lines). The sum $w^a(t) + w_1^b(t) + w_2^b(t)$ is also shown (dashed line). All those quantities are shown as functions of time t. In a resonance approximation exact probabilities $w^a(t)$ and $w_\nu^b(t)$ are relatively well approximated with expressions for $w^{a0}(t)$ and $w_\nu^{b0}(t)$, respectively. In particular, $w^a(t)$ has the shape of the exponential decay $w^{a0}(t)$. As required by the completeness relation (22), for each time t the sum $w^a(t) + w_1^b(t) + w_2^b(t)$ equals unity.

In figure 2 parameter choice **B** with eigenvalue $E = 1$ is reconsidered, but this time coupling β is much stronger. In figure 2(a) one has $\beta = 0.9$ while in figure 2(b) one has $\beta = 1.5$. Those cases correspond, respectively, to the points $(\circ)$ and $(\bullet)$ in figure 7(a) of reference [1]. Eigenvalue distributions for those cases are shown in figures 11 and 12 of this reference, respectively. In both cases probabilities $w^a(t)$ and $w_\nu^b(t)$ (solid lines) as well as their sum $w^a(t)+w_1^b(t)+w_2^b(t)$ (dashed lines) are shown as functions of time t. In figure 2(a) (case $\beta = 0.9$) system $\boldsymbol{S}_\infty$ contains no isolated eigenstate and after long enough time there is a complete decay of the initial state $|\Theta\rangle$ into the system $\boldsymbol{S}_\infty^b$. Hence $\lim_{t\to\infty} w^a(t) = 0$. However, since the coupling is relatively strong, decay curve $w^a(t)$ differs substantially from the approximate exponential decay $w^{a0}(t)$ (doted line). This applies also to the transition probabilities $w_\nu^b(t)$, which differ significantly from approximate transition probabilities $w_\nu^{b0}(t)$.

In figure 2(b) coupling is as strong as $\beta = 1.5$. In this case system $\boldsymbol{S}_\infty$ contains a single isolated eigenstate $|\Psi_R\rangle$. One finds $\varepsilon_R = 2.3186$ and $w_R^a = 0.5024$. There is hence never complete decay of the initial state $|\Theta\rangle$ and one has $\lim_{t\to\infty} w^a(t) = \left(w_R^a\right)^2 = 0.2523 \neq 0$. In this case approximations $w^{a0}(t)$ and $w_\nu^{b0}(t)$ completely fail.

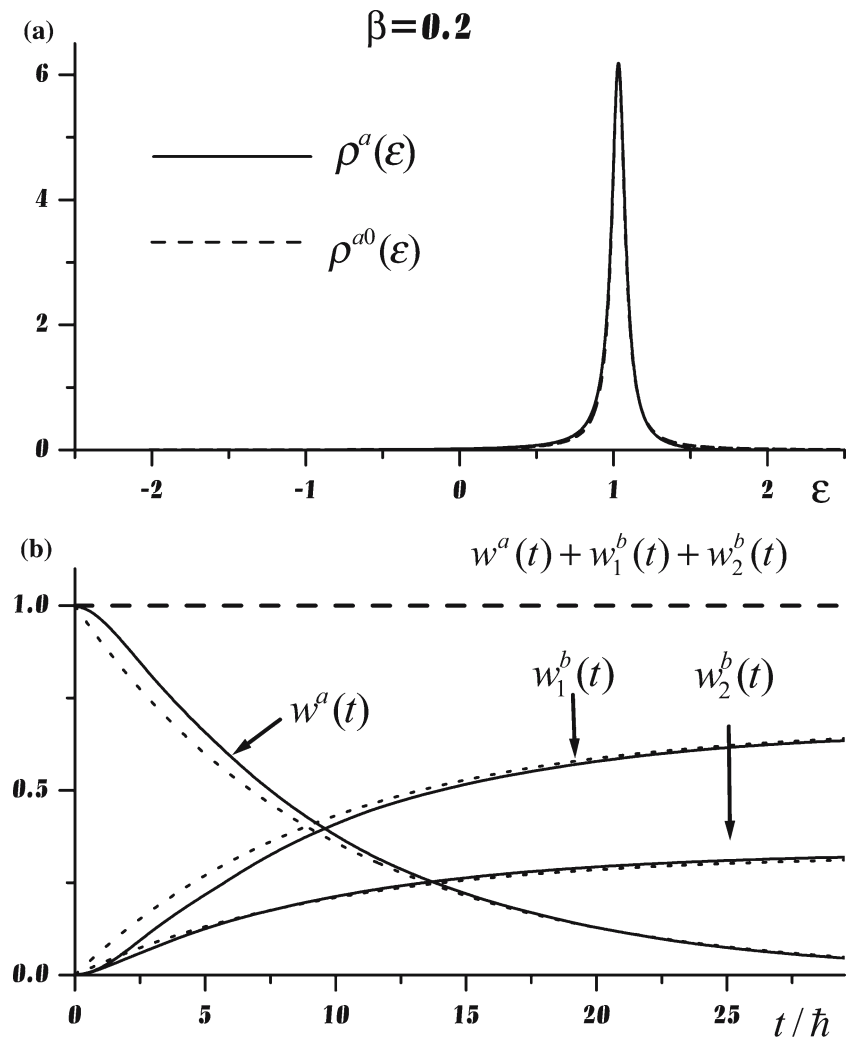

Figure 1. Time evolution of the state $|\Theta(t)\rangle$ for the parameter choice **B** with $E = 1$ and $\beta = 0.2$. Since $E \in D$ and since coupling β is relatively small, those are conditions of the resonance approximation. (a) Probability density $\rho^a(\varepsilon)$ (solid line) is very well approximated with the truncated universal resonance curve $\rho^{a0}(\varepsilon)$ (dashed line). (b) Probabilities $w^a(t)$ and $w_\nu^b(t)$ (solid lines) are very well approximated with probabilities $w^{a0}(t)$ and $w_\nu^{b0}(t)$ (doted lines).

In both cases shown in figure 2 for all times considered total probability $w^a(t)+\sum_\nu w_\nu^b(t)$ equals unity. This confirms completeness relation (22). One also finds that for large times probabilities $w^a(t)$ and $w_\nu^b(t)$ asymptotically converge to their respective limit values. For example, if $\beta = 0.9$ one finds $w^a(15\hbar) = 0.0152$, $w^a(20\hbar) = 0.0020$ and $w^a(25\hbar) = 0.0002$. Those values converge to zero and already for $t/\hbar = 15$ the decay of the state $|\Theta(t)\rangle$ is mainly completed.

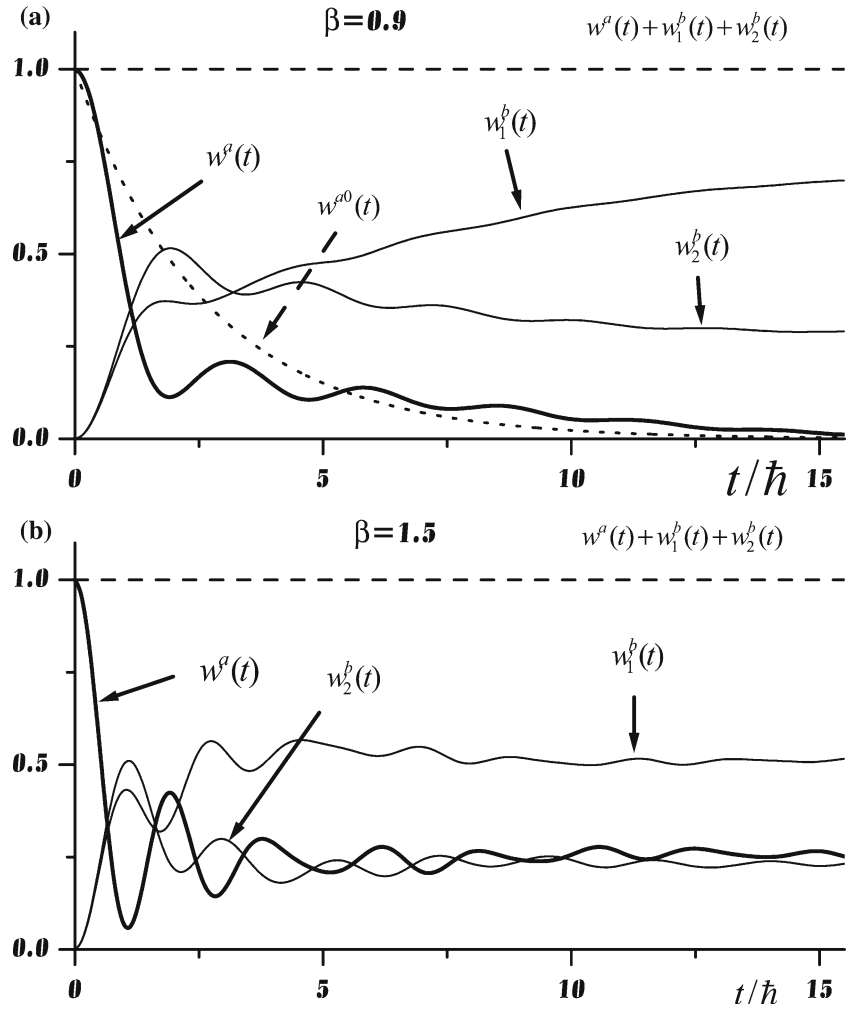

Figure 2. Time evolution of the state $|\Theta(t)\rangle$ for the parameter choice **B** with $E = 1$ and with two different values of the coupling β. Probabilities $w^a(t)$ and $w_\nu^b(t)$ (solid lines) as well as the sum $w^a(t) + \sum_\nu w_\nu^b(t)$ (dashed lines) are shown. (a) $\beta = 0.9$. The system contains no isolated eigenstate and hence $\lim_{t\to\infty} w^a(t) = 0$. The curve $w^a(t)$ differs significantly from the approximate exponential decay curve $w^{a0}(t)$ (doted line). (b) $\beta = 1.5$. The system contains an isolated eigenstate and hence $\lim_{t\to\infty} w^a(t) \neq 0$.

Accordingly, for $t/\hbar = 15$ probabilities $w_\nu^b(t)$ are also close to their limit values (see figure 2(a)). If however $\beta = 1.5$ one finds $w^a(15\hbar) = 0.2660$, $w^a(20\hbar) = 0.2482$ and $w^a(25\hbar) = 0.2473$. Due to the presence of the isolated eigenstate, those values converge to their limit value $w^a(\infty) = 0.2523$ much slower. One has to go as far as $t/\hbar = 100$ to obtain $w^a(t) = 0.2519$. Nevertheless, already for $t/\hbar = 15$ probabilities $w^a(t)$ and $w_\nu^b(t)$ are relatively close to their respective limit values (see figure 2(b)).

4.1.2. Comparison with finite combined systems $\boldsymbol{S}_{n+1}$

In figures 3 and 4 probabilities $w^a(t)$ and $w^b_\nu(t)$ from figure 2 are analyzed in more details. Combined system $\boldsymbol{S}_\infty$ containing two infinite chains can be approximated with a finite combined system $\boldsymbol{S}_{n+1}$ containing two finite chains of equal length $n/2$. Those finite systems can be solved by standard diagonalization methods. One thus finds n orthonormalized eigenstates $|\Phi_{\nu,i}\rangle \in X^{b\nu}_{n/2}$ and n corresponding eigenvalues $\lambda_{\nu,i}(n)$ of the associated unperturbed subsystems $\boldsymbol{S}^{b\nu}_{n/2}$ ($\nu = 1, 2$; $i = 1, \ldots, n/2$). In a time-dependent case one also finds eigenstate $|\Theta_n(t)\rangle$ of a finite system $\boldsymbol{S}_{n+1}$ that is at time $t = 0$ prepared in the local state $|\Theta\rangle$, $|\Theta_n(0)\rangle = |\Theta\rangle$. Hence probability $w^a_n(t) = |\langle\Theta \mid \Theta_n(t)\rangle|^2$ for a transition of a state $|\Theta_n(t)\rangle$ at time t into the initial state $|\Theta\rangle$, as well as discrete probabilities $w^{b\nu}_i(t) = \left|\langle\Phi_{\nu,i} \mid \Theta_n(t)\rangle\right|^2$ for the transition of the state $|\Theta_n(t)\rangle$ at time t into the states $|\Phi_{\nu,i}\rangle \in X^b_n$ of the system $\boldsymbol{S}^b_n$. Those discrete probabilities imply probabilities $w^b_{\nu,n}(t) = \sum_i w^{b\nu}_i(t)$ for the transition of a state $|\Theta_n(t)\rangle$ at time t into the subsystem $\boldsymbol{S}^{b\nu}_{n/2}$ ($\nu = 1, 2$). As n increases results obtained in a standard way using finite combined systems $\boldsymbol{S}_{n+1}$ should converge to the corresponding results for the infinite combined system $\boldsymbol{S}_\infty$.

In figure 3 probabilities $w^a(t)$ and $w^b_\nu(t)$ from figure 2(a) are compared in this way with finite-chain probabilities $w^a_n(t)$ and $w^b_{\nu,n}(t)$, respectively. This is done for three finite combined systems $\boldsymbol{S}_{n+1}$. As emphasized above, it is assumed that both chains of a finite system $\boldsymbol{S}_{n+1}$ contain the same number of sites. For example, in the case $n = 6$ each chain contains three sites. Cases $n = 6, 12$ and 24 are considered.

In figure 3(a) probability $w^a(t)$ (solid line) is compared with finite-chain probabilities $w^a_6(t)$, $w^a_{12}(t)$ and $w^a_{24}(t)$ (other lines). This figure illustrates convergence of finite-chain probabilities $w^a_n(t)$ to the theoretical infinite-chain probability $w^a(t)$ with the increase of n. For small times t probabilities $w^a_n(t)$ follow theoretical curve $w^a(t)$. However, each curve $w^a_n(t)$ at some large enough time t' separates from $w^a(t)$. As n increases this separation point also increases. One has approximately $t'/\hbar \approx 2$ if $n = 6$, $t'/\hbar \approx 5$ if $n = 12$ and $t'/\hbar \approx 10$ if $n = 24$. In addition, one finds that with the increase of n the agreement between $w^a_n(t)$ and $w^a(t)$ improves for each $t < t'$. Accordingly, probabilities $w^a_n(t)$ converge to the probability $w^a(t)$ for an infinite system $\boldsymbol{S}_\infty$, i.e., for each t one has $\lim_{n\to\infty} w^a_n(t) = w^a(t)$.

In figure 3(b) analogous comparison is done for the transition probability $w^b_1(t)$ (solid line) and the corresponding finite-chain probabilities $w^b_{1,6}(t)$, $w^b_{1,12}(t)$ and $w^b_{1,24}(t)$ (other lines). In figure 3(c) the same is done for the transition probability $w^b_2(t)$. In both cases one has similar behavior as in the case of the probability $w^a(t)$. Each finite chain probability $w^b_{\nu,n}(t)$ reproduces the corresponding infinite-chain probability $w^b_\nu(t)$ up to some point $t = t'$. If $t < t'$ probability $w^b_{\nu,n}(t)$ is virtually identical to the theoretical limit probability $w^b_\nu(t)$. However, if $t > t'$ probability $w^b_{\nu,n}(t)$ deviates significantly from $w^b_\nu(t)$. As n

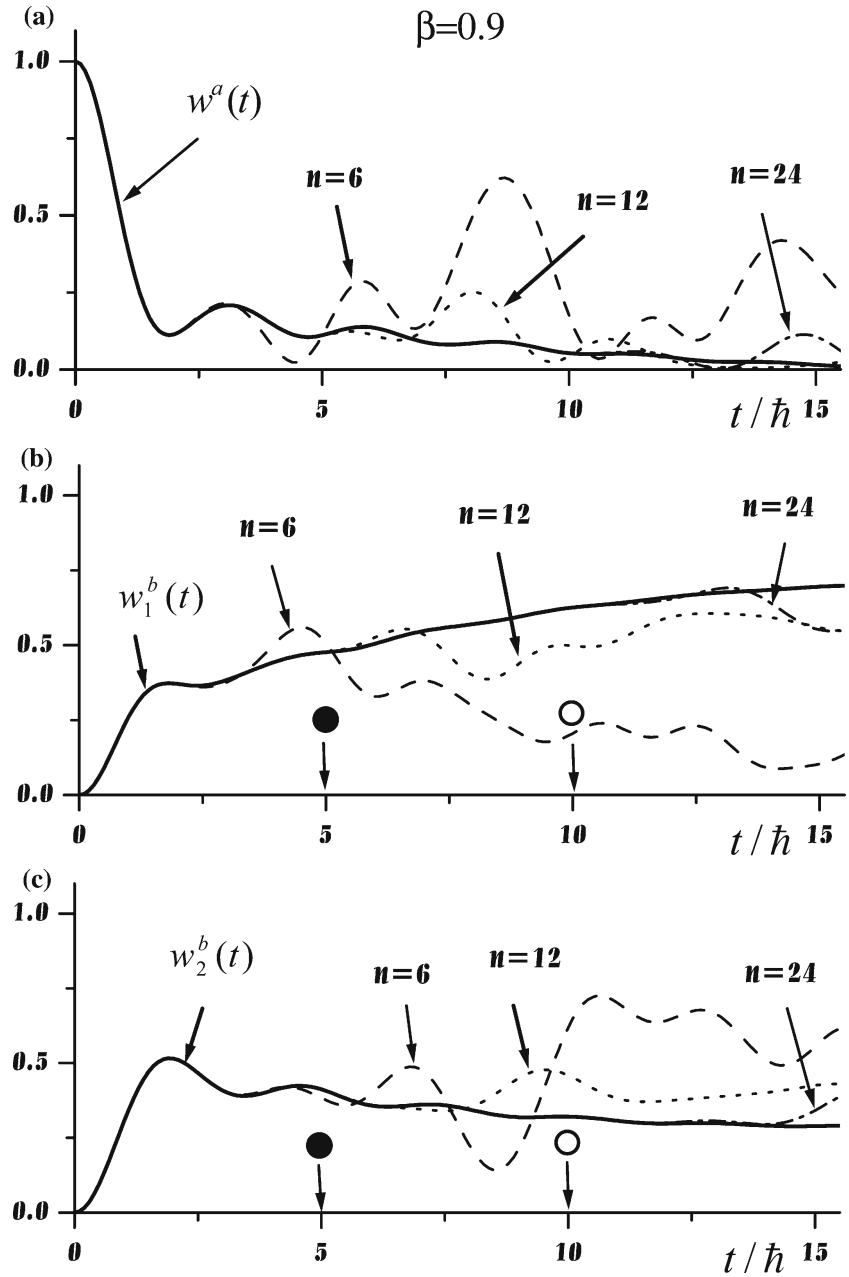

Figure 3. Comparison of probabilities $w^a(t)$ and $w_\nu^b(t)$ from figure 2(a) (solid lines) with corresponding probabilities $w_n^a(t)$ and $w_{\nu,n}^b(t)$ for selected finite combined systems $\boldsymbol{S}_{n+1}$ (other lines). Cases $n = 6, 12$ and 24 are considered. (a) Comparison of the probability $w^a(t)$ with finite-chain probabilities $w_n^a(t)$. (b) Comparison of the probability $w_1^b(t)$ with finite-chain probabilities $w_{1,n}^b(t)$. (c) Comparison of the probability $w_2^b(t)$ with finite chain probabilities $w_{2,n}^b(t)$.

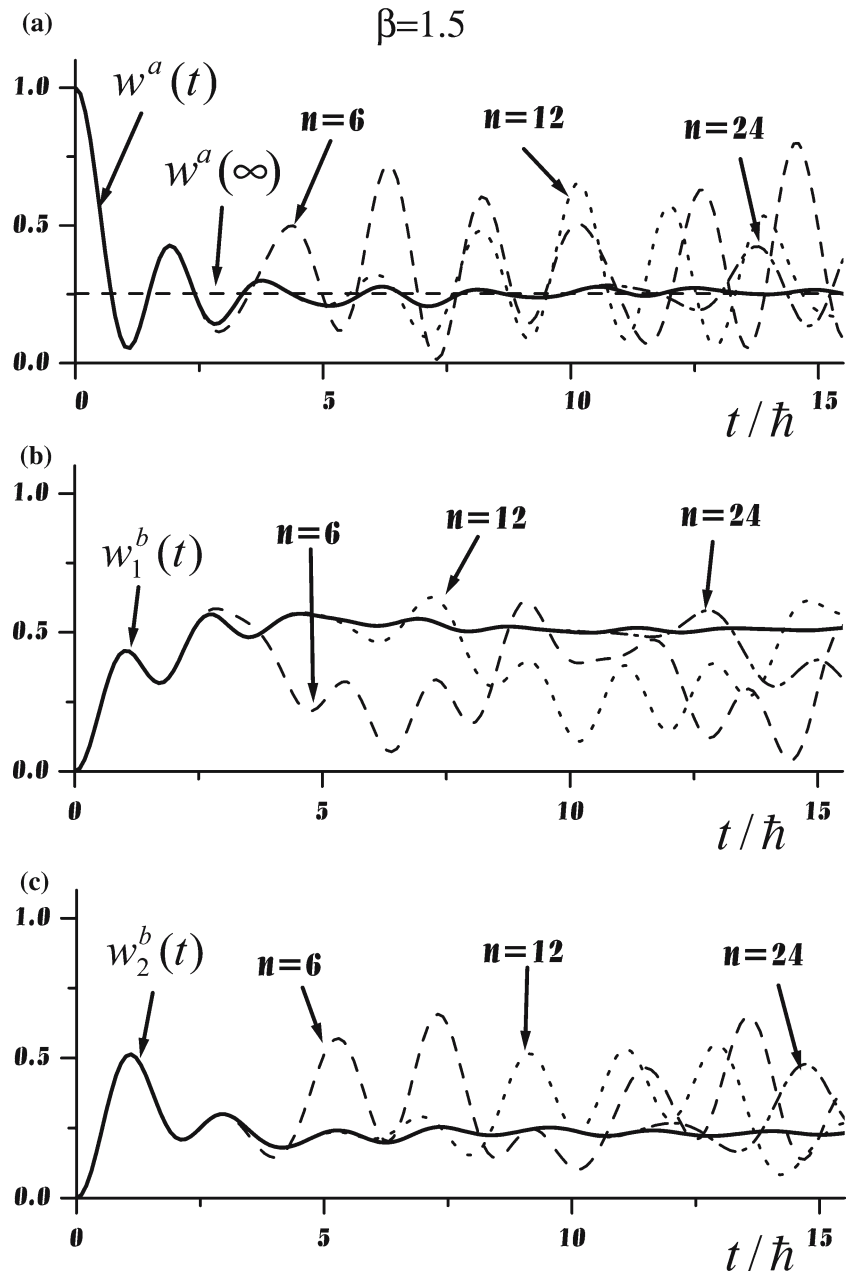

Figure 4. Comparison of probabilities $w^a(t)$ and $w_v^b(t)$ from figure 2(b) (solid lines) with corresponding probabilities $w_n^a(t)$ and $w_{v,n}^b(t)$ for selected finite combined systems $\boldsymbol{S}_{n+1}$ (other lines). Cases $n = 6$, 12 and 24 are considered. (a) Comparison of the probability $w^a(t)$ with finite-chain probabilities $w_n^a(t)$. Horizontal line denotes asymptotic limit value $w^a(\infty) = \lim_{t\to\infty} w^a(t) = (w_R^a)^2$. (b) Comparison of the probability $w_1^b(t)$ with finite-chain probabilities $w_{1,n}^b(t)$. (c) Comparison of the probability $w_2^b(t)$ with finite-chain probabilities $w_{2,n}^b(t)$.

increases the point $t = t'$ also increases. One again finds that probabilities $w^b_{\nu,n}(t)$ converge to the probability $w^b_\nu(t)$ for an infinite system $\boldsymbol{S}_\infty$, i.e., for each t one has $\lim_{n\to\infty} w^b_{\nu,n}(t) = w^b_\nu(t)$.

Figure 4 is identical to the figure 3, except that in figure 4 probabilities $w^a(t)$ and $w^b_\nu(t)$ from figure 2(b) are reconsidered. Those probabilities are compared with corresponding finite-chain probabilities $w^a_n(t)$ and $w^b_{\nu,n}(t)$. This time coupling is as strong as $\beta = 1.5$ and the combined system $\boldsymbol{S}_\infty$ contains an isolated eigenstate. One again finds convergence of a finite-chain probabilities $w^a_n(t)$ to the theoretical infinite-chain probability $w^a(t)$, as well as convergence of finite-chain transition probabilities $w^b_{\nu,n}(t)$ to the corresponding infinite-chain transition probabilities $w^b_\nu(t)$. In addition, in figure 4(a) is shown a theoretical limit $w^a(\infty) = \left(w^a_R\right)^2 = 0.2523$ (horizontal dashed line). This limit is asymptotic value of the curve $w^a(t)$.

4.1.3. Probability densities $\rho^b_\nu(\lambda, t)$

In figures 3 and 4 expressions (17) for the probability $w^a(t)$ as well as corresponding expressions for the transition probabilities $w^b_\nu(t)$ are verified. Each transition probability $w^b_\nu(t)$ is a global probability for the transition of the state $|\Theta(t)\rangle$ at time t into the eigenvalue band ν. This global probability is integral (21a) of the probability density $\rho^b_\nu(\lambda, t)$. In order to verify fine details of the transition to the eigenvalue band ν, one has to verify probability density $\rho^b_\nu(\lambda, t)$ alone. This can be done by comparing probability density $\rho^b_\nu(\lambda, t)$ with corresponding finite-chain probability densities using the method of the moving Gaussian window [1].

In the case of a finite system S_{n+1} containing two chains of equal length $n/2$ one can consider probability densities $\rho^b_{\nu,n}(\lambda, \Delta, t)$ defined as

$$\rho^b_{\nu,n}(\lambda, \Delta, t) = \sum_i w^{b\nu}_i(t)\, g\left(\lambda - \lambda_{\nu,i}(n), \Delta\right), \quad \nu = 1, 2, \tag{31a}$$

where $g(\varepsilon, \Delta)$ is a normalized Gaussian centered at $\varepsilon = 0$ and with the width Δ [1]

$$g(\varepsilon, \Delta) = \frac{1}{\Delta\sqrt{\pi}} \mathrm{e}^{-\left(\frac{\varepsilon}{\Delta}\right)^2}, \quad \int g(\varepsilon, \Delta)\mathrm{d}\varepsilon = 1. \tag{31b}$$

Relations (31) describe the moving Gaussian window method [1] applied to the time-dependent case. Probability density $\rho^b_{\nu,n}(\lambda, \Delta, t)$ represents measurement performed with the resolution Δ at time t on a finite system $\boldsymbol{S}_{n+1}$. This is a smeared up measurement of the probabilities $w^{b\nu}_i(t)$ for the transition of the state $|\Theta_n(t)\rangle$ at time t in the states $|\Phi_{\nu,i}\rangle \in X^{b\nu}_{n/2}$ of the subsystem $\boldsymbol{S}^{b\nu}_{n/2}$. This probability density should be compared with probability density $\rho^b_\nu(\lambda, t)$ for an infinite system $\boldsymbol{S}_\infty$. The agreement between $\rho^b_{\nu,n}(\lambda, \Delta, t)$ and $\rho^b_\nu(\lambda, t)$ can be

estimated with a standard deviation

$$\Delta\rho^{b}_{\nu,n}(\Delta,t)=\sqrt{\int\left(\rho^{b}_{\nu,n}(\lambda,\Delta,t)-\rho^{b}_{\nu}(\lambda,t)\right)^{2}\,\mathrm{d}\lambda}. \tag{32}$$

Density $\rho^{b}_{\nu,n}(\lambda,\Delta,t)$ depends on the resolution Δ, and there is an optimum resolution $\Delta\equiv\Delta^{\nu}_{0}(n,t)$ such that the above standard deviation assumes a minimum value. This minimum value equals $\Delta\rho^{b0}_{\nu,n}(t)\equiv\Delta\rho^{b}_{\nu,n}(\Delta^{\nu}_{0}(n,t),t)$. We also denote the corresponding probability density as $\rho^{b0}_{\nu,n}(\lambda,t)\equiv\rho^{b}_{\nu,n}(\lambda,\Delta^{\nu}_{0}(n,t),t)$. As n increases, $\Delta^{\nu}_{0}(n,t)$ should converge to zero, densities $\rho^{b0}_{\nu,n}(\lambda,t)$ should converge to $\rho^{b}_{\nu}(\lambda,t)$ and standard deviations $\Delta\rho^{b0}_{\nu,n}(t)$ should converge to zero. For details and the rational behind the moving Gaussian window method see reference [1].

In figures 5 and 6 probability densities $\rho^{b}_{\nu}(\lambda,t)$ for the system $\boldsymbol{S}_{\infty}$ defined with the parameter choice **B** and with local eigenvalue $E=1$ and coupling $\beta=0.9$ are analyzed with the above moving Gaussian window method. This is the same system that is considered in figure 3.

In figure 5 probability density $\rho^{b}_{1}(\lambda,t)$ for the transition of the state $|\Theta(t)\rangle$ into the eigenvalue band $\nu=1$ is considered. This density is compared with the corresponding finite chain densities $\rho^{b0}_{1,n}(\lambda,t)$ for three selected times t ($t/\hbar=5, t/\hbar=10$ and $t/\hbar=40$). First two values correspond to the points (•) and (○) in figure 3(b). Third value ($t/\hbar=40$) corresponds to relatively large time when the density $\rho^{b}_{1}(\lambda,t)$ is quite close to its limit value $\rho^{b}_{1}(\lambda,\infty)$ (figure 5(e,f)). The comparison of the density $\rho^{b}_{1}(\lambda,t)$ and finite chain densities $\rho^{b0}_{1,n}(\lambda,t)$ is done for two values of $n, n=24$ (figure 5(a,c,e)) and $n=240$ (figure 5(b,d,f)). In order to simplify notation, in the following expressions for the resolutions $\Delta^{\nu}_{0}(n,t)$ and for standard deviations $\Delta\rho^{b0}_{\nu,n}(t)$ reduced Planck constant associated with the parameter t is omitted.

Consider first the case $n=24$. In this case optimum Gaussian window is relatively large and one finds $\Delta^{1}_{0}(n,5)=0.23$, $\Delta^{1}_{0}(n,10)=0.17$ and $\Delta^{1}_{0}(n,40)=0.39$. The resolution is not very good and the agreement between finite chain densities $\rho^{b0}_{1,24}(\lambda,t)$ and densities $\rho^{b}_{1}(\lambda,t)$ is only qualitative. In particular, finite chain density $\rho^{b0}_{1,24}(\lambda,40)$ differs significantly from the theoretical infinite chain density $\rho^{b}_{1}(\lambda,40)$. Standard deviations $\Delta\rho^{b0}_{1,24}(t)$ are hence also relatively large, and one finds $\Delta\rho^{b0}_{1,24}(5)=0.054$, $\Delta\rho^{b0}_{1,24}(10)=0.151$ and $\Delta\rho^{b0}_{1,24}(40)=0.631$ (see figures 5(a,c,e)). If one increases n 10-fold optimum resolution substantially improves and one finds $\Delta^{1}_{0}(n,5)=0.04$, $\Delta^{1}_{0}(n,10)=0.03$ and $\Delta^{1}_{0}(n,40)=0.03$. Accordingly, the agreement between $\rho^{b}_{1}(\lambda,t)$ and $\rho^{b0}_{1,240}(\lambda,t)$ also improves and standard deviations $\Delta\rho^{b0}_{1,240}(t)$ significantly decrease. One finds $\Delta\rho^{b0}_{1,240}(5)=0.003$, $\Delta\rho^{b0}_{1,240}(10)=0.007$ and $\Delta\rho^{b0}_{1,240}(40)=0.013$. As shown in figure 5(b,d,f)), there is almost no noticeable difference between theoretical densities $\rho^{b}_{1}(\lambda,t)$ and finite chain densities $\rho^{b0}_{1,240}(\lambda,t)$.

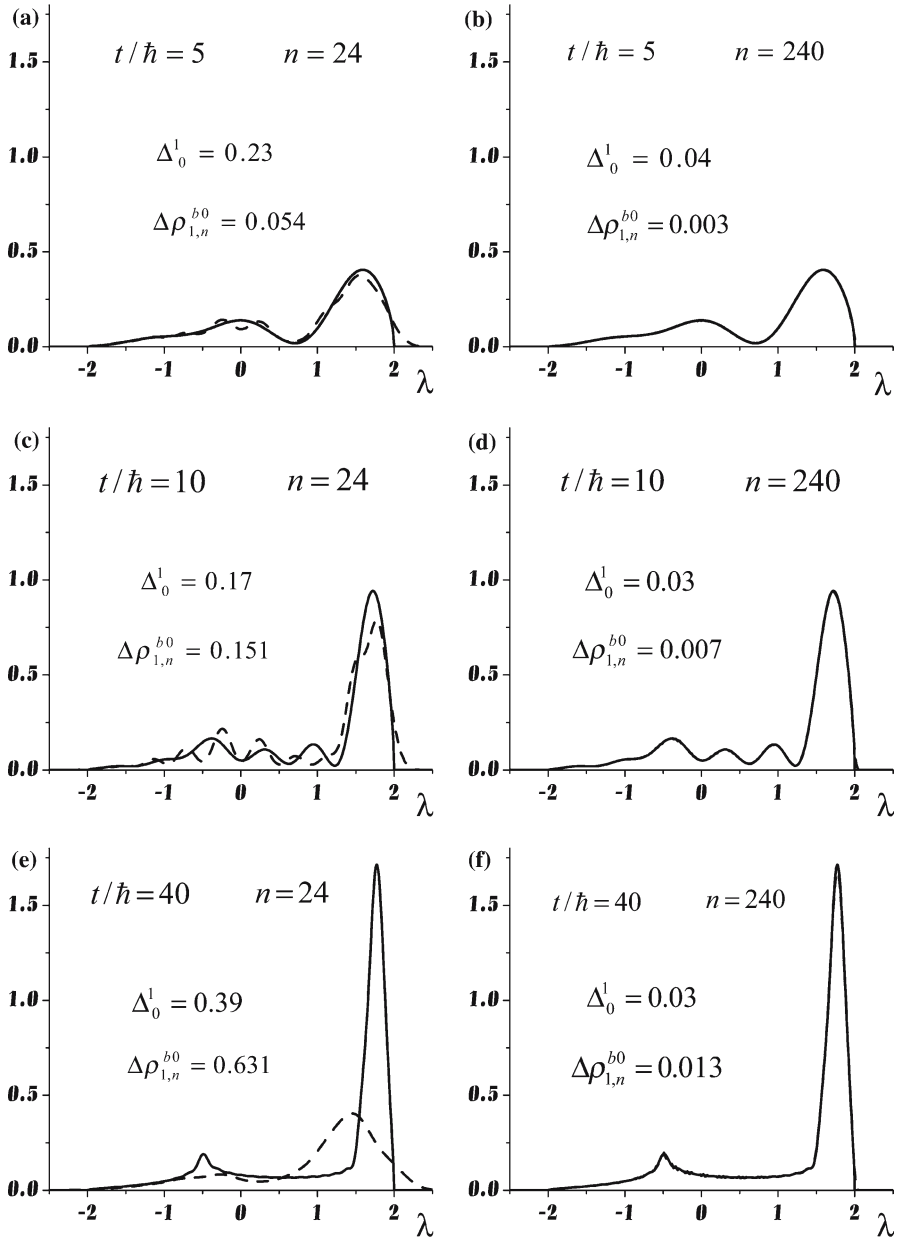

Figure 5. Probability densities $\rho_1^b(\lambda, t)$ for the transition into the band $\nu = 1$ (solid lines) and corresponding finite chain densities $\rho_{1,n}^{b0}(\lambda, t)$ (dashed lines) for the system defined with parameter choice **B** and with local eigenvalue $E = 1$ and coupling $\beta = 0.9$. Those quantities are shown as functions of the unperturbed eigenvalue λ for three selected values of time t: $t/\hbar = 5, t/\hbar = 10$ and $t/\hbar = 40$. In (a), (c) and (e) finite system $\boldsymbol{S}_{24+1}$ is considered, while in (b), (d) and (f) finite system $\boldsymbol{S}_{240+1}$ is considered.

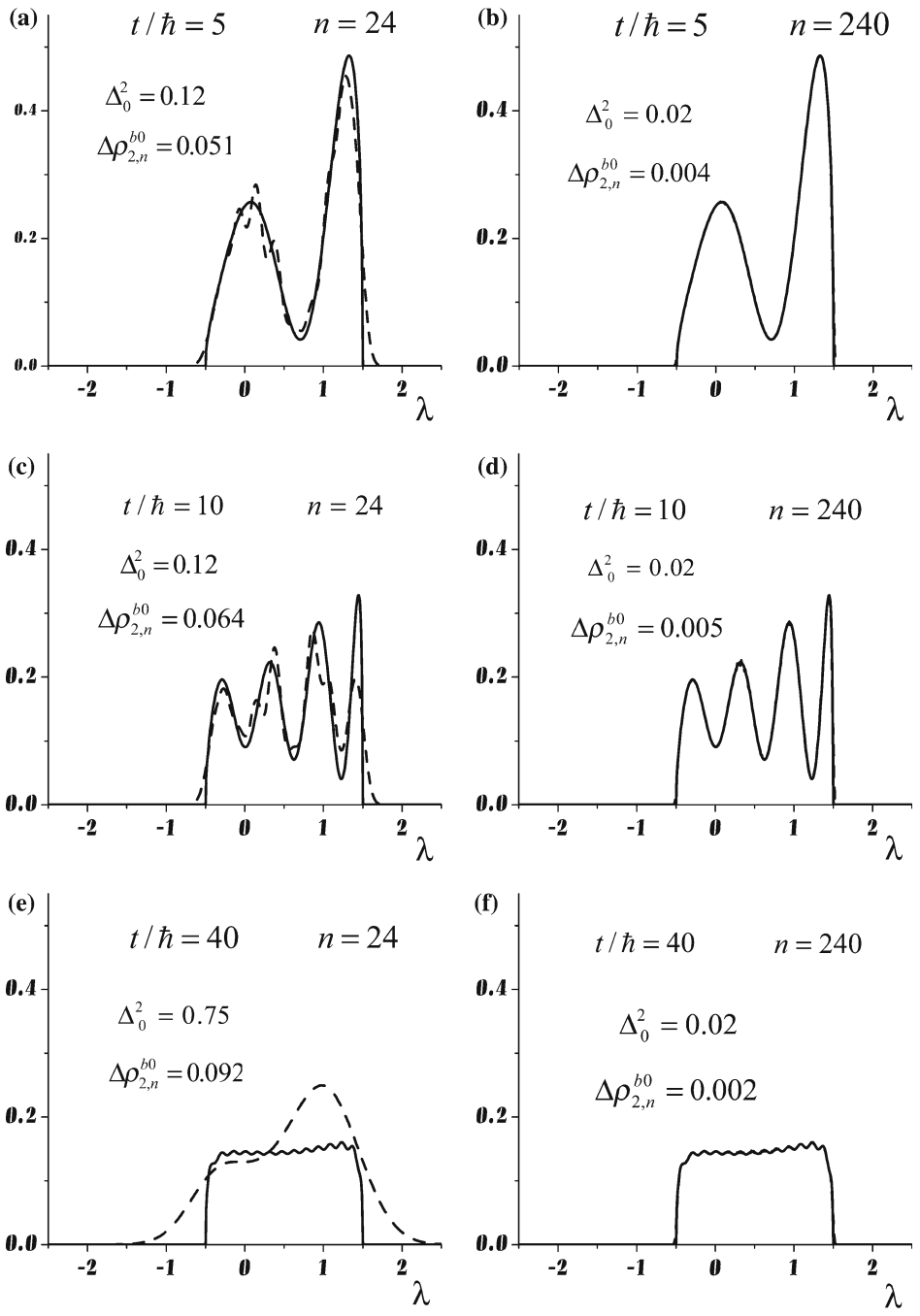

Figure 6. The same as figure 5, but this time probability densities for the transition into the band $\nu = 2$ are considered.

In figure 6 are compared in the same way theoretical densities $\rho_2^b(\lambda, t)$ for the transition of the state $|\Theta(t)\rangle$ into the eigenvalue band $\nu = 2$ with the corresponding finite chain densities $\rho_{2,n}^{b0}(\lambda, t)$. The values $t/\hbar = 5$ and $t/\hbar = 10$ correspond to the points (•) and (○) in figure 3(c). The value $t/\hbar = 40$ again corresponds to relatively large time when the density $\rho_2^b(\lambda, 40)$ is quite close to its limit value $\rho_2^b(\lambda, \infty)$ (figure 6(e,f)).

If n is as small as $n = 24$ optimum width of the Gaussian window is relatively large and one finds $\Delta_0^2(n, 5) = 0.12$, $\Delta_0^2(n, 10) = 0.12$ and $\Delta_0^2(n, 40) = 0.75$. Corresponding standard deviations are $\Delta\rho_{2,24}^{b0}(5) = 0.051$, $\Delta\rho_{2,24}^{b0}(10) = 0.064$ and $\Delta\rho_{2,24}^{b0}(40) = 0.092$. The agreement between $\rho_2^b(\lambda, t)$ and $\rho_{2,24}^{b0}(\lambda, t)$ is only qualitative. Especially bad is this agreement in the case $t/\hbar = 40$ when the width of the optimum Gaussian window is very large. However, if n increases 10-fold, optimum resolution as well as the agreement between densities $\rho_2^b(\lambda, t)$ and $\rho_{2,n}^{b0}(\lambda, t)$ substantially improves. Thus one finds $\Delta\rho_{2,240}^{b0}(5) = 0.004$, $\Delta\rho_{2,240}^{b0}(10) = 0.005$ and $\Delta\rho_{2,240}^{b0}(40) = 0.002$. As shown in figure 6(b,d,f), there is no noticeable difference between densities $\rho_2^b(\lambda, t)$ and finite chain densities $\rho_{2,240}^{b0}(\lambda, t)$.

The above example illustrates general property of densities $\rho_\nu^b(\lambda, t)$ and corresponding finite chain densities $\rho_{\nu,n}^{b0}(\lambda, t)$. For each time t the agreement between finite chain densities $\rho_{\nu,n}^{b0}(\lambda, t)$ and theoretical infinite chain densities $\rho_\nu^b(\lambda, t)$ improves with the increase of n and in a limit $n \to \infty$ it is exact. In other words, for each time t one has $\lim_{n\to\infty} \rho_{\nu,n}^{b0}(\lambda, t) = \rho_\nu^b(\lambda, t)$. This verifies in a most direct way expressions (19) for probability densities $\rho_\nu^b(\lambda, t)$.

5. Conclusion

Exact treatment of the interaction of an isolated state $|\Theta\rangle$ with the known infinite dimensional quantum system $\boldsymbol{S}_\infty^b$ is generalized to the case when the system $\boldsymbol{S}_\infty^b$ contains a finite number of one-parameter eigenvalue bands. Time-dependent properties of the combined system $\boldsymbol{S}_\infty = \boldsymbol{S}_1^a \oplus \boldsymbol{S}_\infty^b$ where $\boldsymbol{S}_1^a$ is one-dimensional system containing a single state $|\Theta\rangle$ with the eigenvalue E are considered. Since an arbitrary (multiparameter) eigenvalue band can be approximated to any desired degree of accuracy with a finite number of one-parameter eigenvalue bands, results obtained in this paper are crucial in order to describe in a closed form interaction of a single state with an arbitrary infinite dimensional quantum system [3].

Closed expressions for the time evolution of the state $|\Theta(t)\rangle$ that is at time $t = 0$ prepared in the state $|\Theta(0)\rangle \equiv |\Theta\rangle$ are derived. In particular, exact expression for the amplitude $\langle\Theta \mid \Theta(t)\rangle$ and hence for the probability $\rho^a(t) = |\langle\Theta \mid \Theta(t)\rangle|^2$ to find the state $|\Theta(t)\rangle$ at time t in the initial state $|\Theta(0)\rangle \equiv |\Theta\rangle$ is obtained. In the limit of weak coupling, probability $\rho^a(t)$ reduces to the well-known exponential decay of the state $|\Theta(t)\rangle$. However, if the coupling is not small, a more complex decay pattern is obtained. In addition, exact expressions

for the amplitudes $\langle \Phi_\nu(k)|\ \Theta(t)\rangle$ that determine probability of a transition of the state $|\Theta(t)\rangle$ at time t in a state $|\Phi_\nu(k)\rangle \in X_\infty^{b\nu}$ are also obtained. In conclusion, the suggested method provides exact and closed expressions for the solution of the combined system $\boldsymbol{S}_\infty$ in the time-dependent version. There is no power series expansion, no convergence problem, and this method applies to an arbitrary strong interaction between $\boldsymbol{S}_1^a$ and $\boldsymbol{S}_\infty^b$.

The method is illustrated with a simple model describing the interaction of a single state $|\Theta\rangle$ (system $\boldsymbol{S}_1^a$) with several infinite one-dimensional solids in the nearest-neighbor tight-binding approximation (system $\boldsymbol{S}_\infty^b$). This model is sufficiently complex in order to illustrate and verify all derived expressions. In particular, completeness relation (22) is verified. This relation is verified with several examples involving an extremely large interval of coupling constants. In addition, the interaction of the system $\boldsymbol{S}_1^a$ with finite one-dimensional solids that contain n sites (system $\boldsymbol{S}_n^b$) is considered. Since the corresponding combined system $\boldsymbol{S}_{n+1} = \boldsymbol{S}_1^a \oplus \boldsymbol{S}_n^b$ 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 $\boldsymbol{S}_\infty$ (obtained using expressions derived in this paper) with corresponding results for finite system $\boldsymbol{S}_{n+1}$ (obtained independently in the standard way). As n increases, the results for the system $\boldsymbol{S}_{n+1}$ are shown to converge to the corresponding results for the system $\boldsymbol{S}_\infty$. This provides a direct verification of the suggested method. For the sake of simplicity, in the numerical examples only the case when the system $\boldsymbol{S}_n^b$ contains two infinite chains is considered. However, this does not present any restriction on the general validity of derived results.

Obtained results and their generalization [3] can be applied to all cases where one considers an isolated state $|\Theta\rangle$ in the interaction with an infinite quantum system $\boldsymbol{S}_\infty^b$. This includes, among others, a general problem of the interaction of an isolated molecular state with the electromagnetic field as well as the interaction of an isolated molecular state of a molecule situated on a surface of some solid with this solid.

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[11] Neglecting the possibility of the simultaneous emission of two or more photons. If the decay is spontaneous, the probability of such multiphoton emissions is usually negligible.

[12] Due to the degeneracy of the one-photon states $|\mathbf{k}\varpi\rangle$, the set of all states $|\Theta_f \mathbf{k}\varpi\rangle$ with all possible photon states $|\mathbf{k}\varpi\rangle$ defines a multi-parameter eigenvalue band and not a one-parameter eigenvalue band as considered here. However, generalization to multi-parameter eigenvalue bands is straightforward.

[13] In the expression in [2] that corresponds to the present expression (19c) one reduced Planck constant $\hbar$ is missing.