

## On the Interaction of an Isolated State with the Known Infinite-dimensional Quantum System\*

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RECEIVED APRIL 16, 2003; ACCEPTED SEPTEMBER 12, 2003

The interaction of an isolated state  $|\Theta\rangle$  with a known infinite-dimensional quantum system  $S_\infty^b$  containing multiple eigenvalue bands is considered. An example is the interaction of an isolated molecular state with the electromagnetic field. This problem is the main subject of spectroscopy. Another example is the interaction of an isolated molecular state of a molecule situated on the surface of a solid with this solid. This is the subject of the surface state physics. Such problems are usually treated within the formalism of the perturbation expansion. Recently a new mathematical method for the treatment of such problems was suggested. This method produces correct solution of the combined system, however strong the interaction between the state  $|\Theta\rangle$  and the system  $S_\infty^b$ . Key quantities in this method are characteristic functions  $f_v(\varepsilon)$  and functions  $\omega_v(\varepsilon)$ . Functions  $f_v(\varepsilon)$  are constructed from the quantities describing unperturbed system  $S_\infty^b$  and from the known interaction of this system with the state  $|\Theta\rangle$ . Functions  $\omega_v(\varepsilon)$  are then expressed in terms of the characteristic functions  $f_v(\varepsilon)$ . An important mathematical problem is the calculation of the functions  $\omega_v(\varepsilon)$ , once functions  $f_v(\varepsilon)$  are known. A general mathematical solution to this problem is obtained for the case when characteristic functions  $f_v(\varepsilon)$  are polynomials. Since each function which is continuous in a finite interval can be approximated (to any desired degree of accuracy) with some polynomial, this solution presents an important mathematical tool for the practical application of the suggested method. Obtained results are illustrated with few model examples of the interaction of an isolated state with an infinite quantum system.

### Key words

interaction of quantum systems  
perturbation  
eigenvalues  
eigenstates

## INTRODUCTION

The aim of this paper is to provide and verify a solution to a particular mathematical problem that arises in a novel approach for the treatment of an important class of quantum systems. We will formulate this problem and give its solution in the third section of this paper. But first we present a short description of quantum systems to be considered and of this new method for the treatment of those systems.

Consider the interaction of an isolated state  $|\Theta\rangle$  that has the eigenvalue  $E$  with an infinite quantum system  $S_\infty^b$ . This system may contain one or several eigenvalue bands in the intervals  $I_\nu = [a_\nu, b_\nu]$  ( $\nu = 1, \dots, \kappa$ ). Union  $D = \bigcup_\nu I_\nu$  of those intervals defines range of the continuous eigenvalues of  $S_\infty^b$ . In addition to those eigenvalue bands, system  $S_\infty^b$  may contain some isolated eigenvalues and eigenstates. The solution to the unperturbed system  $S_\infty^b$  is assumed to be known, and one is interested in the

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\* Dedicated to Professor Nenad Trinajstić on the occasion of his 65<sup>th</sup> birthday.

properties of a state  $|\Theta\rangle$  subject to the interaction with this system. Mathematically, this problem requires the solution of the combined system  $S_\infty = S_1^a \oplus S_\infty^b$ , where  $S_1^a$  represents one-dimensional system containing a single state  $|\Theta\rangle$  with the eigenvalue  $E$ . This combined system can be described by the eigenvalue equation

$$\mathbf{H}|\Psi\rangle = \varepsilon|\Psi\rangle, \quad (1a)$$

where  $\mathbf{H}$  is a hermitian operator

$$\mathbf{H} = E|\Theta\rangle\langle\Theta| + \mathbf{B} + \beta \mathbf{V}. \quad (1b)$$

In this expression  $\mathbf{B}$  is a hermitian operator which describes unperturbed system  $S_\infty^b$ ,  $\mathbf{V}$  is hermitian operator which describes the interaction between the state  $|\Theta\rangle$  and this system (normalized in an appropriate way), while  $\beta$  is a parameter that measures interaction strength or coupling between the state  $|\Theta\rangle$  and the system  $S_\infty^b$ .

There are numerous problems in physics and chemistry of this type. An example is the interaction of an atom or a molecule with the electromagnetic field. This atom or a molecule can be approximated with a finite number of discrete eigenvalues  $E_\nu$  and corresponding eigenstates  $|\Theta_\nu\rangle$ . Those eigenstates interact with one-photon states  $|\Theta_\nu, \mathbf{k}\varpi\rangle$ , where  $|\mathbf{k}\varpi\rangle$  represents a state containing one photon with momentum  $\mathbf{k}$  and polarization  $\varpi$ . States  $|\Theta_\nu, \mathbf{k}\varpi\rangle$  interact with two-photon states  $|\Theta_\nu, \mathbf{k}\varpi, \mathbf{k}'\varpi'\rangle$ , which in turn interact with three-photon states, *etc.*<sup>1</sup> Consider properties of the particular molecular state  $|\Theta_\mu\rangle \equiv |\Theta\rangle$  subject to the interaction with all such single- and multi-photon states. To a very good approximation, one can neglect all states containing more than one photon, and one can associate system  $S_\infty^b$  with the set of all one-photon states  $|\Theta_\nu, \mathbf{k}\varpi\rangle$ . The solution to this system is known, since the states  $|\mathbf{k}\varpi\rangle$  are essentially plane waves, while  $|\Theta_\nu\rangle$  are eigenstates of the isolated molecule, which are assumed to be known. Each molecular state  $|\Theta_\nu\rangle$  generates an eigenvalue band containing all one-photon states  $|\Theta_\nu, \mathbf{k}\varpi\rangle$  with all possible values of the photon momentum  $\mathbf{k}$  and polarization  $\varpi$ . Eigenvalues of this eigenvalue band are confined to the interval  $I_\nu = [E_\nu, \infty)$ . Concerning the state  $|\Theta_\mu\rangle \equiv |\Theta\rangle$ , it interacts with other molecular states  $|\Theta_\eta\rangle$  only indirectly, through the intermediate interaction with the one-photon states  $|\Theta_\nu, \mathbf{k}\varpi\rangle$ . If the eigenvalue  $E$  of the state  $|\Theta\rangle$  is relatively isolated from other eigenvalues of this molecule, one can to a very good approximation neglect other molecular states. Hence, one has formally the problem of the interaction of a single state  $|\Theta\rangle$  with a known infinite system  $S_\infty^b$ . In this example, the system  $S_\infty^b$  contains only eigenvalue bands and no isolated states.

Another example is the interaction of an atom or a molecule situated on a surface of a solid with this solid. The solid represents system  $S_\infty^b$  and one is interested in the properties of an isolated atomic or molecular state

$|\Theta\rangle$  subject to the interaction with this solid. Usually the system  $S_\infty^b$  contains a number of eigenvalue bands  $I_\nu$  and in addition, it may contain some isolated eigenvalues.<sup>2,3</sup> Those isolated eigenvalues represent possible surface states. In principle, the solution to the solid alone can be obtained by numerous other methods.<sup>2</sup> Hence, one has again the problem of the interaction of a single state  $|\Theta\rangle$  with a known infinite system  $S_\infty^b$ . This time however the system  $S_\infty^b$  besides eigenvalue bands may also contain some isolated states.

In this and similar situations one has a general problem of the interaction of an isolated state with a known infinite system containing eigenvalue bands. There are important characteristic properties of such an interaction. In general, if an isolated state  $|\Theta\rangle$  interacts with an eigenvalue band, this interaction shifts eigenvalue  $E$  of this state to a new position  $\varepsilon_0$ . In the perturbation approach this level shift is a second order effect.<sup>1,4</sup> In addition, if the unperturbed eigenvalue  $E$  is embedded in some eigenvalue band of the system  $S_\infty^b$ , shifted eigenvalue  $\varepsilon_0$  is not sharp and it has an uncertainty  $\Delta\varepsilon_0$ . If the interaction between the state  $|\Theta\rangle$  and this system is relatively weak, the shape of this shifted eigenvalue is that of the universal resonance curve.<sup>1,4,5</sup> Further, if the combined system is initially prepared in the state  $|\Theta\rangle$ , due to the interaction with the system  $S_\infty^b$  there is an exponential decay of this state.<sup>1,4</sup> There are also well-defined probabilities for the transition of this state into various states of the system  $S_\infty^b$ . For example, if the state  $|\Theta\rangle$  is an excited molecular state, it has well-defined probability for the transition into each particular eigenvalue band  $\nu$  that contains all one-photon states  $|\Theta_\nu, \mathbf{k}\varpi\rangle$ . Transition to this eigenvalue band represents transition of the molecular state  $|\Theta\rangle$  into molecular state  $|\Theta_\nu\rangle$  with simultaneous emission of one photon.<sup>1</sup> Probability of this transition is an important experimental quantity and it determines the intensity of the corresponding spectral line.

All above properties are usually obtained in the first or second order of the perturbation expansion approach.<sup>1,4</sup> Though this approach is very powerful and very general, in the case of strong coupling it suffers from a serious drawback of slow convergence. If the coupling is sufficiently strong, perturbation series may diverge and the entire method fails. Even if the coupling is not strong, one may be interested in the fine details of the interaction. In some cases, those fine details can not be obtained with only few leading terms of the perturbation expansion. Therefore, some other approach for the treatment of such systems is required.

## THE METHOD

Recently a new method for the treatment of such systems was suggested.<sup>6</sup> This method provides an exact solution to the interaction of an isolated state  $|\Theta\rangle$  with a

known infinite system  $S_\infty^b$ . There is no power series expansion, and the derived relations are valid, however strong the interaction between the state  $|\Theta\rangle$  and this system.<sup>6</sup>

One finds that the combined system  $S_\infty$  may contain two kinds of the eigenvalues and eigenstates. Each  $\varepsilon \in D$ , which is an eigenvalue of the unperturbed system  $S_\infty^b$ , is also an eigenvalue of the combined system. We call such eigenvalues and the corresponding eigenstates *embedded* eigenvalues and eigenstates. Those eigenstates depend on the continuous parameter  $\varepsilon \in D$  and they are normalized to a delta-function. In addition to the embedded eigenvalues, combined system may contain few eigenvalues  $\varepsilon_1 \in \bar{D}$ , where  $\bar{D}$  is a complement of  $D$ . Those eigenvalues and the corresponding eigenstates are isolated, and they are normalized to a unity.<sup>6</sup> Isolated eigenstates of the combined system may exist even in the case when the unperturbed system  $S_\infty^b$  contains no isolated states.

For the sake of simplicity, consider the case when the system  $S_\infty^b$  contains no isolated states. In this case, system  $S_\infty^b$  can be described by the eigenvalue equation

$$\mathbf{B}|\Phi_\nu(k,l)\rangle = \lambda_\nu(k) |\Phi_\nu(k,l)\rangle, \quad \nu = 1, \dots, \kappa. \quad (2a)$$

where  $\mathbf{B}$  is a hermitian operator, index  $\nu$  labels various eigenvalue bands, and each  $\lambda_\nu(k)$  is a nondecreasing function of a parameter  $k$  confined to the interval  $I_\nu = [a_\nu, b_\nu]$ , i.e.  $\lambda_\nu(k) \in I_\nu$ . Parameter  $l$  labels possible degeneracies inside eigenvalue band  $\nu$ . This parameter may be continuous and/or discrete. If it is continuous, eigenstates  $|\Phi_\nu(k,l)\rangle$  are orthonormalized according to

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

and similarly for the case when this parameter is discrete.

Generalization to the case when the system  $S_\infty^b$  in addition to the eigenvalue bands contains also isolated states is straightforward.<sup>7</sup> This generalization provides no new features regarding the subject of this paper.

If the unperturbed system contains no isolated states, properties of the combined system  $S_\infty$  are expressed in terms of the functions  $f_\nu(\varepsilon)$  and  $\omega_\nu(\varepsilon)$ .<sup>6,7</sup> With each eigenvalue band  $\nu$  is associated *characteristic* function  $f_\nu(\varepsilon)$ , and this function in turn determines corresponding function  $\omega_\nu(\varepsilon)$ . Function  $f_\nu(\varepsilon)$  is defined according to<sup>6,7</sup>

$$f_\nu(\varepsilon) = \frac{\int \left| \langle \Theta | \mathbf{V} | \Phi_\nu(k,l) \rangle \right|^2 dl}{d\lambda_\nu(k) / dk} \Bigg|_{\varepsilon=\lambda_\nu(k)} \cdot \begin{cases} 1 & \text{if } \varepsilon \in I_\nu \\ 0 & \text{if } \varepsilon \notin I_\nu \end{cases}, \quad \nu = 1, \dots, \kappa. \quad (3)$$

This expression applies to the case when  $l$  is a continuous degeneracy index. Integration over  $l$  should be replaced with an appropriate summation if  $l$  is discrete.

Function  $f_\nu(\varepsilon)$  ( $\nu = 1, \dots, \kappa$ ) incorporates essential features of the interaction of the state  $|\Theta\rangle$  with the eigenvalue band  $\nu$  of the system  $S_\infty^b$ . If the solution to this system is known (eigenstates  $|\Phi_\nu(k,l)\rangle$  and the corresponding eigenvalue functions  $\lambda_\nu(k)$ ), one can easily obtain derivatives  $d\lambda_\nu(k)/dk$  and matrix elements  $\langle \Theta | \mathbf{V} | \Phi_\nu(k,l) \rangle$ . It is a matter of a simple integration and/or summation to obtain each function  $f_\nu(\varepsilon)$  from those quantities. However, for our present discussion it is not important how those functions are constructed. All we need are some general properties of those functions. According to (3), each characteristic function  $f_\nu(\varepsilon)$  ( $\nu = 1, \dots, \kappa$ ) is positive almost everywhere in the interval  $I_\nu$  and it vanishes outside this interval. One also finds that  $f_\nu(\varepsilon)$  is integrable<sup>6,7</sup>

$$f_\nu(\varepsilon) \geq 0, \quad \varepsilon \notin I_\nu \Rightarrow f_\nu(\varepsilon) = 0, \quad \int f_\nu(\varepsilon) d\varepsilon < \infty. \quad (4a)$$

Once characteristic functions  $f_\nu(\varepsilon)$  are known, functions  $\omega_\nu(\varepsilon)$  are expressed in terms of those functions according to<sup>6,7</sup>

$$\omega_\nu(\varepsilon) = P \int \frac{f_\nu(\lambda)}{\varepsilon - \lambda} d\lambda, \quad \nu = 1, \dots, \kappa. \quad (5a)$$

where  $P$  denotes principal Cauchy integral value.<sup>8</sup>

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

$$f(\varepsilon) = \sum_\nu f_\nu(\varepsilon), \quad \omega(\varepsilon) = \sum_\nu \omega_\nu(\varepsilon) \quad (6)$$

Function  $f(\varepsilon)$  is nonzero almost everywhere in the range  $D$  and it vanishes outside this range. In analogy to (4a) one finds

$$f(\varepsilon) \geq 0, \quad \varepsilon \notin D \Rightarrow f(\varepsilon) = 0, \quad \int f(\varepsilon) d\varepsilon < \infty. \quad (4b)$$

while (5a) and (6) imply

$$\omega(\varepsilon) = P \int \frac{f(\lambda)}{\varepsilon - \lambda} d\lambda \quad (5b)$$

Since  $f(\varepsilon) \geq 0$ , first derivative  $\omega^{(1)}(\varepsilon)$  of  $\omega(\varepsilon)$  is negative for each  $\varepsilon \notin D$

$$\omega^{(1)}(\varepsilon) = - \int \frac{f(\lambda)}{(\varepsilon - \lambda)^2} d\lambda < 0, \quad \varepsilon \in \bar{D} \quad (7)$$

This is an important property of the function  $\omega(\varepsilon)$ . This property does not apply to the case  $\varepsilon \in D$ . Namely, if  $\varepsilon \in D$ , one has to integrate (5b) over the point  $\lambda = \varepsilon$  where subintegral function usually diverges. Hence one has to take principal Cauchy integral value, and derivative of  $\omega(\varepsilon)$  is not expressed in the simple form (7). In general, inside the range  $D$  derivative of  $\omega(\varepsilon)$  can assume any positive and negative value.

In addition to the above functions, we also define auxiliary function  $h(\varepsilon)$

$$h(\varepsilon) \equiv \beta^2 \omega(\varepsilon) + E - \varepsilon \quad (8)$$

Due to (7), this function is monotonically decreasing in each interval  $I \subseteq \bar{D}$ .

### Time Independent Properties of the Combined System

In the time-independent case combined system  $S_\infty$  is described by the eigenvalue Eq. (1) where  $|\Psi\rangle$  may be an embedded as well as an isolated eigenstate of this system. Concerning isolated eigenvalues and eigenstates, one finds that each isolated eigenvalue  $\varepsilon_1 \in \bar{D}$  is the root of the function  $h(\varepsilon)$ , i.e. it satisfies<sup>6</sup>

$$\beta^2 \omega(\varepsilon_1) + E - \varepsilon_1 = 0, \quad \varepsilon_1 \in \bar{D}. \quad (9a)$$

Since  $h(\varepsilon)$  is monotonically decreasing in  $\bar{D}$ , in each open interval  $(b_v, a_\mu) \subseteq \bar{D}$  can exist at most one isolated eigenvalue  $\varepsilon_1$ . This eigenvalue exists if and only if

$$h(b_v + 0) > 0 \text{ and } h(a_\mu - 0) < 0, \quad (b_v, a_\mu) \subseteq \bar{D}. \quad (9b)$$

In above expressions we use shorthand notation

$$y(x_0 + 0) \equiv \lim_{x \rightarrow x_0 + 0} y(x), \quad y(x_0 - 0) \equiv \lim_{x \rightarrow x_0 - 0} y(x).$$

in order to denote right and left limits of the function  $y(x)$  in a point  $x = x_0$ .

Note that if  $b_v = -\infty$  first condition in (9b) is automatically satisfied, while if  $a_\mu = \infty$  second condition in (9b) is automatically satisfied. This follows from  $\omega(\pm\infty) = 0$ . Further, if the boundary point  $b_v$  or  $a_\mu$  is finite and if the function  $\omega(\varepsilon)$  diverges in this point, corresponding condition in (9b) is satisfied for each  $\beta \neq 0$  and for each  $E$ . In particular, if both boundary points are finite and if  $\omega(\varepsilon)$  diverges in those points, eigenvalue  $\varepsilon_1 \in (b_v, a_\mu)$  exists for each  $\beta \neq 0$  and for each  $E$ . Thus in some cases relations (9b) present no restriction on the existence of the isolated eigenvalue  $\varepsilon_1 \in (b_v, a_\mu)$ , while in some other cases those relations provide nontrivial conditions for the existence of this eigenvalue.

Once eigenvalue  $\varepsilon_1$  is known, one can easily obtain the corresponding isolated eigenstate  $|\Psi_1\rangle$  in a closed form.<sup>6,7</sup> Of a special interest is the probability  $w_1^a = |\langle \Theta | \Psi_1 \rangle|^2$  to find the state  $|\Theta\rangle$  in this eigenstate. This probability equals<sup>6</sup>

$$w_1^a = \frac{1}{1 - \beta^2 \omega^{(1)}(\varepsilon_1)} \quad (10)$$

where  $\omega^{(1)}(\varepsilon_1)$  is a first derivative of  $\omega(\varepsilon)$  in a point  $\varepsilon = \varepsilon_1$ .

Relation (9a) implicitly defines each isolated eigenvalue  $\varepsilon_1$  as a function of parameters  $E$  and  $\beta$ , i.e.  $\varepsilon_1 \equiv$

$\varepsilon_1(E, \beta)$ . Using this relation and expression (10), one finds<sup>6</sup>

$$\frac{\partial \varepsilon_1}{\partial E} = w_1^a(\varepsilon_1) > 0, \quad \frac{\partial \varepsilon_1}{\partial \beta} = 2\beta \omega(\varepsilon_1) w_1^a(\varepsilon_1), \quad \varepsilon_1 \in \bar{D}. \quad (11a)$$

Those relations determine the rate of change of the isolated eigenvalue  $\varepsilon_1$  as one changes eigenvalue  $E$  and/or coupling parameter  $\beta$ . It is interesting to note that the derivative of  $\varepsilon_1$  with respect to the eigenvalue  $E$  equals probability  $w_1^a$ .

Using (10) and (11a) one also finds derivatives of the probability  $w_1^a \equiv w_1^a(E, \beta)$  with respect to  $E$  and  $\beta$ :

$$\frac{\partial w_1^a}{\partial E} = \beta^2 \omega^{(2)}(\varepsilon_1) w_1^a(\varepsilon_1)^3, \quad (11b)$$

$$\frac{\partial w_1^a}{\partial \beta} = 2\beta w_1^a(\varepsilon_1)^2 [\omega^{(1)}(\varepsilon_1) + \beta^2 \omega(\varepsilon_1) \omega^{(2)}(\varepsilon_1) w_1^a(\varepsilon_1)] \quad (11c)$$

In the above expressions  $\omega^{(2)}(\varepsilon_1)$  is a second derivative of a function  $\omega(\varepsilon)$  in a point  $\varepsilon = \varepsilon_1$ .

Concerning embedded eigenstates, one can show that probability density  $\rho^a(\varepsilon)$  to find the state  $|\Theta\rangle$  with the eigenvalue  $\varepsilon \in D$  equals<sup>6,7</sup>

$$\rho^a(\varepsilon) = \frac{\beta^2 f(\varepsilon)}{\pi^2 \beta^4 f(\varepsilon)^2 + (\beta^2 \omega(\varepsilon) + E - \varepsilon)^2}, \quad \varepsilon \in D. \quad (12)$$

Relations (10) and (12) define eigenvalue distribution of the state  $|\Theta\rangle$ . If one performs the measurement of the eigenvalue on this state, one should obtain the eigenvalue  $\varepsilon_1 \notin D$  with the probability  $w_1^a$  and the eigenvalue  $\varepsilon \in D$  with the probability density  $\rho^a(\varepsilon)$ . Those quantities satisfy completeness relation<sup>6,7</sup>

$$\sum_I w_1^a + \int \rho^a(\varepsilon) d\varepsilon = 1 \quad (13)$$

Properties (11) and above completeness relation imply the corresponding dependence of the density  $w_1^a = \int \rho^a(\varepsilon) d\varepsilon$  on the parameters  $E$  and  $\beta$ . Thus one finds

$$\frac{\partial}{\partial E} \int \rho^a(\varepsilon) d\varepsilon = -\beta^2 \sum_I \omega^{(2)}(\varepsilon_1) w_1^a(\varepsilon_1)^3 \quad (11d)$$

and similarly for the derivative with respect to the coupling parameter  $\beta$ .

If  $E \in D$  is an interior point of the range  $D$  and if the interaction parameter  $\beta$  is relatively small (the resonance approximation),<sup>6</sup> expression (12) reduces to<sup>6</sup>

$$\rho^a(\varepsilon) \approx \rho^{a0}(\varepsilon) = \frac{\beta^2 f(\varepsilon_0)}{\pi^2 \beta^4 f(\varepsilon_0)^2 + (\varepsilon - \varepsilon_0)^2} \quad (14a)$$

where  $\varepsilon_0$  is a solution of the relation

$$\beta^2 \omega(\varepsilon_0) + E - \varepsilon_0 = 0, \quad \varepsilon_0 \in D. \quad (14b)$$

Density  $\rho^{a0}(\varepsilon)$  describes a universal resonance curve.<sup>5</sup> This curve has maximum in the point  $\varepsilon = \varepsilon_0$  and it has the width  $\Delta\varepsilon_0$  (Ref. 6)

$$\Delta\varepsilon_0 = 2\pi\beta^2 f(\varepsilon_0) \quad (14c)$$

Neglecting terms of the order  $O(\beta^4)$  in the coupling parameter  $\beta$ , one can approximate  $\varepsilon_0$  as

$$\varepsilon_0 \approx E + \beta^2\omega(E) \quad (14b')$$

This reproduces well known result that in the case of the weak coupling eigenvalue  $E$  shifts to a new position  $\varepsilon_0$ . This shifted eigenvalue has a finite uncertainty  $\Delta\varepsilon_0$  in the shape of the universal resonance curve.<sup>1,4,5</sup>

#### Time Dependent Properties of the Combined System

In addition to the eigenvalue Eq. (1), one can consider time dependent equation

$$i\hbar \frac{\partial}{\partial t} |\Psi(t)\rangle = H |\Psi(t)\rangle \quad (15)$$

Each solution of this equation is a linear combination

$$|\Psi(t)\rangle = \sum_I c_I |\Psi_I\rangle \exp(-i\varepsilon_I t / \hbar) + \sum_{\mu} \int c_{\mu}(\varepsilon) |\Psi_{\mu}(\varepsilon)\rangle \exp(-i\varepsilon t / \hbar) d\varepsilon \quad (16)$$

where  $|\Psi_I\rangle$  and  $|\Psi_{\mu}(\varepsilon)\rangle$  are isolated and embedded eigenstates of the time-independent eigenvalue Eq. (1), while  $c_I$  and  $c_{\mu}(\varepsilon)$  are unknown coefficients and unknown functions to be determined from the initial conditions.

Usually the system  $S_{\infty}$  is at time  $t = 0$  prepared in the state  $|\Theta\rangle$  and one is interested in the time evolution  $|\Theta(t)\rangle$  of this state. The state  $|\Theta(t)\rangle$  is a solution of (15) and it satisfies initial condition  $|\Theta(0)\rangle = |\Theta\rangle$ . One finds<sup>6,7</sup>

$$|\Theta(t)\rangle = \sum_I \sqrt{w_I^a} |\Psi_I\rangle \exp(-i\varepsilon_I t / \hbar) + \sum_{\mu} \int \langle \Psi_{\mu}(\varepsilon) | \Theta \rangle |\Psi_{\mu}(\varepsilon)\rangle \exp(-i\varepsilon t / \hbar) d\varepsilon, \quad (17a)$$

where

$$\sum_{\mu} |\langle \Psi_{\mu}(\varepsilon) | \Theta \rangle|^2 = \rho^a(\varepsilon). \quad (17b)$$

The probability  $w^a(t)$  to find the state  $|\Theta(t)\rangle$  at time  $t$  in the initial state  $|\Theta\rangle$  is a square of the amplitude  $\langle \Theta | \Theta(t) \rangle$

$$w^a(t) = |\langle \Theta | \Theta(t) \rangle|^2 \quad (18a)$$

This probability describes time-decay of a state  $|\Theta(t)\rangle$ . One finds<sup>6,7</sup>

$$\langle \Theta | \Theta(t) \rangle = \int \rho^a(\varepsilon) \exp(-i\varepsilon t / \hbar) d\varepsilon + \sum_I w_I^a \exp(-i\varepsilon_I t / \hbar) \quad (18b)$$

Similarly, the probability to find the state  $|\Theta(t)\rangle$  at time  $t$  in any of the states  $|\Phi_{\nu}(k, l)\rangle$  with the eigenvalue  $\lambda = \lambda_{\nu}(k)$  and in the eigenvalue interval  $d\lambda$  equals  $\rho_{\nu}^b(\lambda, t) d\lambda$ , where the probability density  $\rho_{\nu}^b(\lambda, t)$  is a square of the amplitude  $u_{\nu}^b(\lambda, t)$

$$\rho_{\nu}^b(\lambda, t) = |u_{\nu}^b(\lambda, t)|^2, \quad \lambda \in I_{\nu}. \quad (19a)$$

This probability density describes transition of a state  $|\Theta(t)\rangle$  to various states  $|\Phi_{\nu}(k, l)\rangle$  of a system  $S_{\infty}^b$ . One finds<sup>6,7</sup>

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

Amplitudes  $u_{\nu}^b(\lambda, t)$  can be also expressed in terms of the amplitude  $\langle \Theta | \Theta(t) \rangle$ <sup>6,7,9</sup>

$$u_{\nu}^b(\lambda, t) = -i \frac{\beta}{\hbar} \sqrt{f_{\nu}(\lambda)} \int_0^t \langle \Theta | \Theta(t) \rangle e^{i\lambda t/\hbar} dt \quad (20)$$

Integral

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

over all probability densities  $\rho_{\nu}^b(\lambda, t)$  ( $\lambda \in I_{\nu}$ ) is the probability to find the state  $|\Theta(t)\rangle$  at time  $t$  in any of the unperturbed states  $|\Phi_{\nu}(k, l)\rangle$  contained in the eigenvalue band  $\nu$ . In other words, this is the probability for the transition at time  $t$  of the state  $|\Theta(t)\rangle$  into the eigenvalue band  $\nu$ . Since at each time the state  $|\Theta(t)\rangle$  must be found with a certainty either in the original state  $|\Theta\rangle$  or in some eigenvalue band  $\nu$ , probabilities  $w^a(t)$  and  $w_{\nu}^b(t)$  satisfy the completeness relation<sup>6,7</sup>

$$w^a(t) + \sum_{\nu} w_{\nu}^b(t) = 1 \quad (21b)$$

This expression can be used as an efficient test for the consistency and correctness of the suggested method.

Usually one prepares the system  $S_{\infty}$  at time  $t = 0$  in the state  $|\Theta\rangle$ , and one measures various transitions of this state at some very large time. This corresponds to the measurement of the probability  $w^a(\infty)$  and probability densities  $\rho_{\nu}^b(\lambda, \infty)$ . Due to the properties of a Fourier transform,<sup>1</sup> for large enough times integral on the right hand side of the relation (18b) becomes negligibly small. Hence for such times

$$\langle \Theta | \Theta(t) \rangle = \sum_I w_I^a \exp(-i\varepsilon_I t / \hbar) \quad (18b')$$

If the system  $S_{\infty}$  contains no isolated eigenstates, one has  $w_I^a = 0$  and hence  $w^a(\infty) = 0$ . Thus for a large enough time the state  $|\Theta(t)\rangle$  performs a complete decay into available eigenvalue bands. In this case, there is

also a well defined limit  $\lim_{t \rightarrow \infty} \rho_v^b(\lambda, t) = \rho_v^b(\lambda, \infty)$ . However, if the system  $S_\infty$  contains some isolated eigenstates, the situation is qualitatively different. In the case when the system  $S_\infty$  contains only one isolated eigenvalue  $\varepsilon_1$  one has

$$w^a(\infty) = (w_1^a)^2 > 0$$

Thus even at infinite time there is a finite probability  $w^a(\infty) > 0$  to find a state  $|\Theta(\infty)\rangle$  in the original state  $|\Theta(0)\rangle \equiv |\Theta\rangle$ . The decay of the state  $|\Theta(t)\rangle$  is hence never complete. If the system  $S_\infty$  contains several isolated eigenvalues, situation is more complex. In this case, probability  $w^a(t)$  has no limit  $\lim_{t \rightarrow \infty} w^a(t)$ . According to (18b'), for large enough times this probability displays an oscillatory behavior.<sup>6,7</sup> However, since in each interval  $(b_v, a_{\mu}) \subseteq \bar{D}$  can be at most one isolated eigenvalue  $\varepsilon_i$ , mutual separation of those eigenvalues is relatively large. Oscillations of the probability  $w^a(t)$  are hence extremely fast. Such oscillations are hard to detect experimentally. If the experimental set up is not sensitive enough to detect such fast oscillations, one should observe a time-average of those oscillations. This time-average equals

$$\overline{w^a(\infty)} = \sum_I (w_1^a)^2 > 0$$

Similar conclusions apply to the probability densities  $\rho_v^b(\lambda, t)$  and to the probabilities  $w_v^b(t)$ .

Though one is usually interested in the properties of the system  $S_\infty$  in a limit  $t \rightarrow \infty$ , relations (18)–(21) can be used to analyze and theoretically explain more subtle experiments that involve measurement of various transition probabilities at any finite time. In the resonance approximation those relations simplify. In particular, in this approximation relations (18) reduce to<sup>6</sup>

$$w^a(t) \approx w^{a0}(t) = e^{-2\pi\beta^2 f(\varepsilon_0)t/\hbar} \quad (22a)$$

where  $\varepsilon_0$  is a solution of (14b). Function  $w^{a0}(t)$  describes well-known exponential decay of the initial state  $|\Theta\rangle$ .

In the same approximation relations (19) reduce to<sup>6,7</sup>

$$\rho_v^b(\lambda, t) \approx \rho_v^{b0}(\lambda, t) = \frac{\beta^2 f_v(\varepsilon_0)}{\pi^2 \beta^4 f^2(\varepsilon_0) + (\varepsilon_0 - \lambda)^2} \times \left[ e^{-2\pi\beta^2 f(\varepsilon_0)t/\hbar} - 2e^{-\pi\beta^2 f(\varepsilon_0)t/\hbar} \cos\left(\frac{(\varepsilon_0 - \lambda)t}{\hbar}\right) + 1 \right] \quad (22b)$$

In particular, transition probability to the eigenvalue band  $v$  is

$$w_v^b(t) \approx w_v^{b0}(t) = \int \rho_v^{b0}(\lambda, t) d\lambda = \frac{f_v(\varepsilon_0)}{f(\varepsilon_0)} [1 - e^{-2\pi\beta^2 f(\varepsilon_0)t/\hbar}], \quad v = 1, \dots, \kappa. \quad (22c)$$

Probabilities  $w^{a0}(t)$  and  $w_v^{b0}(t)$  satisfy completeness requirement (21b).

## FUNCTIONS $\omega_v(\varepsilon)$ IN THE CASE OF THE POLYNOMIAL TYPE FUNCTIONS $f_v(\varepsilon)$

In the above method, one has first to construct functions  $f_v(\varepsilon)$ . Once those functions are known, one has to calculate functions  $\omega_v(\varepsilon)$  according to (5a). Various time-dependent as well as time-independent properties of the combined system are then expressed in terms of those functions. Construction of the functions  $f_v(\varepsilon)$  is rather straightforward according to the expression (3). This expression involves a simple integration and/or summation over the degeneracy index  $l$ . If the eigenstates associated with the eigenvalue band  $v$  are nondegenerate, even that much calculation is not needed. Moreover, functions  $f_v(\varepsilon)$  can be considered as primitive elements describing the unperturbed system  $S_\infty^b$  and the interaction of the state  $|\Theta\rangle$  with this system. From this point of view, there is no need to calculate those functions and instead one can model those functions in an appropriate way.<sup>7</sup> Next step, calculation of functions  $\omega_v(\varepsilon)$ , is more complex and it requires calculation of the integrals (5a). This calculation is complicated by the fact that in the case  $\varepsilon \in I_v$  subintegral function in (5a) diverges in the point  $\lambda = \varepsilon$ . This is not a simple integral and one has to take a principal Cauchy integral value. It is hence important to have an efficient way for the calculation of this integral. We will now consider a special but highly important case when this integral can be calculated exactly.

Each integral (5a) is of a type

$$K(\varepsilon) = P \int_a^b \frac{y(\lambda)}{\varepsilon - \lambda} d\lambda \quad (23)$$

Let the function  $y(\lambda)$  be a polynomial inside the interval  $I = [a, b]$ :

$$y(\lambda) = \begin{cases} F(\lambda) & \text{if } \lambda \in [a, b] \\ 0 & \text{if } \lambda \notin [a, b] \end{cases} \quad (24a)$$

where  $F(\lambda)$  is a polynomial

$$F(\lambda) = \sum_{i=0}^n c_i \lambda^i \quad (24b)$$

In this case integral (23) has an exact solution (see appendix):

$$K(\varepsilon) = F(\varepsilon) \ln \left| \frac{\varepsilon - a}{\varepsilon - b} \right| - G(\varepsilon), \quad (25a)$$

where

$$G(\varepsilon) = \sum_{k=1}^n c_k g_k(\varepsilon), \quad (25b)$$

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

$$g_k(\varepsilon) = \sum_{i=0}^{k-1} \frac{\varepsilon^i}{k-i} [b^{k-i} - a^{k-i}], \quad k = 1, 2, \dots \quad (25c)$$

Those polynomials satisfy recursive relation

$$g_1(\varepsilon) = b - a,$$

$$g_k(\varepsilon) = \varepsilon g_{k-1}(\varepsilon) + \frac{b^k - a^k}{k}, \quad k = 2, 3, 4, \dots \quad (26a)$$

First few polynomials  $g_k(\varepsilon)$  are

$$g_1(\varepsilon) = b - a, \quad g_2(\varepsilon) = (b - a)\varepsilon + \frac{1}{2}(b^2 - a^2),$$

$$g_3(\varepsilon) = (b - a)\varepsilon^2 + \frac{1}{2}(b^2 - a^2)\varepsilon + \frac{1}{3}(b^3 - a^3),$$

$$g_4(\varepsilon) = (b - a)\varepsilon^3 + \frac{1}{2}(b^2 - a^2)\varepsilon^2 + \frac{1}{3}(b^3 - a^3)\varepsilon + \frac{1}{4}(b^4 - a^4) \quad (26b)$$

Note that each function  $y(\varepsilon)$  which is continuous in a finite interval  $I = [a, b]$  can be approximated to any desired degree of accuracy with some polynomial in this interval. The assumption (24) is hence not a serious restriction to the possible application of the above expressions.

Besides function  $K(\varepsilon)$  we need also a derivative  $K^{(1)}(\varepsilon)$  of this function. One finds

$$K^{(1)}(\varepsilon) = F^{(1)}(\varepsilon) \ln \left| \frac{\varepsilon - a}{\varepsilon - b} \right| - F(\varepsilon) \frac{b - a}{(\varepsilon - b)(\varepsilon - a)} - G^{(1)}(\varepsilon), \quad (27)$$

where  $F^{(1)}(\varepsilon)$  and  $G^{(1)}(\varepsilon)$  are derivatives of polynomials  $F(\varepsilon)$  and  $G(\varepsilon)$ , respectively.

#### Analytical Properties of the Function $K(\varepsilon)$ and Consequences

Function  $K(\varepsilon)$  and its derivatives are continuous and derivable everywhere, except possibly in the boundary points  $a$  and  $b$  of the interval  $I = [a, b]$ . Qualitative behavior of those functions in the neighborhood of the boundary points is analyzed in the appendix. This behavior depends on the properties of the polynomial  $F(\varepsilon)$  in those points. In each boundary point polynomial  $F(\varepsilon)$  can differ from zero, or it can have zero of some integer order in this point.<sup>10</sup> For the sake of simplicity, if in a point  $\varepsilon = \varepsilon_0$  polynomial  $F(\varepsilon)$  is nonzero ( $F(\varepsilon_0) \neq 0$ ), we shall write  $y(\varepsilon_0) \neq 0$  and say that function  $y(\varepsilon)$  is nonzero in this point. Similarly, if  $F(\varepsilon)$  has in a point  $\varepsilon_0$  zero of the order  $s$ , we shall write  $y^{(s)}(\varepsilon_0) \neq 0$  and say that the function  $y(\varepsilon)$  has zero of the order  $s$  in this point (see appendix).

In the appendix we show that if  $y(b) \neq 0$  function  $K(\varepsilon)$  diverges logarithmically in the boundary point  $\varepsilon = b$ , first derivative  $K^{(1)}(\varepsilon)$  diverges as  $O(\xi^{-1})$  (where  $\xi = \varepsilon - b$ ) in this point, second derivative  $K^{(2)}(\varepsilon)$  diverges as  $O(\xi^{-2})$ , etc. However, if the function  $y(\varepsilon)$  has zero of the first order in the boundary point  $b$  ( $y(b) = 0$  and  $y^{(1)}(b) \neq 0$ ), function  $K(\varepsilon)$  is finite and continuous in this point, first derivative  $K^{(1)}(\varepsilon)$  diverges logarithmically in this point, second derivative  $K^{(2)}(\varepsilon)$  diverges as  $O(\xi^{-1})$ , etc.

Those results follow regular pattern. In particular, if the function  $y(\varepsilon)$  has zero of the order  $s > 1$  in the point  $\varepsilon = b$ ,  $K(\varepsilon)$  and  $K^{(1)}(\varepsilon)$  are both finite and continuous in this point. Analogous results apply to the left boundary point  $a$  of the interval  $I = [a, b]$ .

If the characteristic functions  $f_\nu(\varepsilon)$  are polynomials inside the corresponding intervals  $I_\nu$ , above properties have nontrivial consequences for the global function  $\omega(\varepsilon)$ , its derivatives, and for the probabilities  $w_1^a$  and  $w_c^a = \int \rho^a(\varepsilon) d\varepsilon$ .

Consider the interval  $(b_\nu, a_\mu) \subseteq \bar{D}$ . In this interval, isolated eigenvalue  $\varepsilon_1 \in (b_\nu, a_\mu)$  may exist. Conditions for the existence of this eigenvalue are given by relations (9b). In general, this eigenvalue is a function of parameters  $E$  and  $\beta$ , i.e.  $\varepsilon_1 \equiv \varepsilon_1(E, \beta)$ . According to (10), probability  $w_1^a$  is also a function of those parameters, i.e.  $w_1^a \equiv w_1^a(E, \beta)$ . If those parameters continuously change, eigenvalue  $\varepsilon_1$  may converge either to the boundary point  $b_\nu$  or to the boundary point  $a_\mu$  of the interval  $(b_\nu, a_\mu)$ . Consider convergence of this eigenvalue to the point  $\varepsilon = b_\nu$ . This is a right boundary point of the range  $D$ , and for sufficiently small  $\xi > 0$  one has  $b_\nu - \xi \in D$  and  $b_\nu + \xi \in \bar{D}$ . If in some interval on the left side of this point characteristic function  $f(\varepsilon)$  is a polynomial, properties of the function  $K(\varepsilon)$  and its derivatives apply to the function  $\omega(\varepsilon)$  and its derivatives in the neighborhood of the point  $\varepsilon = b_\nu$ . There are various possibilities.

If the function  $f(\varepsilon)$  is nonzero in the boundary point  $\varepsilon = b_\nu$ , function  $\omega(\varepsilon)$  diverges logarithmically in this point. First condition in (9b) is hence satisfied for each  $\beta \neq 0$  and for each  $E$ . If the second condition in (9b) is also satisfied, isolated eigenvalue  $\varepsilon_1 \in (b_\nu, a_\mu)$  exists. According to the relations (10) and (11), if  $\varepsilon_1$  converges to  $\varepsilon = b_\nu + 0$ , probability  $w_1^a$  converges to zero and derivatives  $\partial w_1^a / \partial E$  and  $\partial w_1^a / \partial \beta$  converge to zero. More precisely one finds

$$f(b_\nu) \neq 0 \Rightarrow$$

$$\omega(b_\nu + \xi) = O(\ln |\xi|) \rightarrow \infty, \quad \omega^{(1)}(b_\nu + \xi) = O(\xi^{-1}) \rightarrow \infty$$

$$w_1^a(b_\nu + \xi) = O(\xi) \rightarrow 0, \quad \frac{\partial w_1^a(b_\nu + \xi)}{\partial E} = O(\xi) \rightarrow 0,$$

$$\frac{\partial w_1^a(b_\nu + \xi)}{\partial \beta} = O(\xi \ln |\xi|) \rightarrow 0 \quad (28a)$$

where  $O(x)$  denotes a quantity of the order  $x$  and where symbols  $\rightarrow 0$  and  $\rightarrow \infty$  indicate the value of the corresponding expression in the limit  $\xi \rightarrow 0$ .

According to (28a), probability  $w_1^a \equiv w_1^a(E, \beta)$  is a continuous function of the eigenvalue  $E$ . As this eigenvalue decreases, probability  $w_1^a$  as well as derivative  $\partial w_1^a / \partial E$  also decreases. Similar conclusion applies to the probability  $w_1^a$  considered as a function of a parameter  $\beta$ .

One has qualitatively different situation if  $f(\varepsilon)$  has zero of the first order in the boundary point  $b = b_v$ . In this case one finds

$$f^{(1)}(b_v) \neq 0 \Rightarrow$$

$$\omega(b_v) = O(1), \quad \omega^{(1)}(b_v + \xi) = O(\ln|\xi|) \rightarrow \infty,$$

$$w_1^a(b_v + \xi) = O((\ln|\xi|)^{-1}) \rightarrow 0,$$

$$\frac{\partial w_1^a(b_v + \xi)}{\partial E} = O(\xi^{-1}(\ln|\xi|)^{-3}) \rightarrow \infty,$$

$$\frac{\partial w_1^a(b_v + \xi)}{\partial \beta} = O(\xi^{-1}(\ln|\xi|)^{-3}) \rightarrow \infty \quad \text{if } \beta > 0. \quad (28b)$$

Assume again that the second condition in (9b) is satisfied. Since the function  $\omega(\varepsilon)$  is now finite and continuous in the boundary point  $\varepsilon = b_v$ , first condition in the relation (9b) is nontrivial. There is a critical value  $E_b = b_v - \beta^2\omega(b_v)$  such that if  $E \leq E_b$  isolated eigenvalue  $\varepsilon_I$  does not exist. Hence  $w_1^a(E_b - 0) = 0$ . Since  $w_1^a \rightarrow 0$  if  $\xi \rightarrow 0$ , probability  $w_1^a \equiv w_1^a(E, \beta)$  is a continuous function of  $E$  in the point  $E = E_b$ . However, in this point derivative of  $w_1^a(E, \beta)$  with respect to  $E$  diverges as  $O(\xi^{-1}(\ln|\xi|)^{-3})$ .

Consider now probability  $w_1^a \equiv w_1^a(E, \beta)$  as a function of a coupling parameter  $\beta$ . First condition in (9b) implies existence of a critical point  $\beta_b = \sqrt{(b_v - E)/\omega(b_v)}$  if and only if  $(b_v - E)/\omega(b_v) > 0$ . There are two possibilities, either  $\omega(b_v) > 0$  and  $E < b_v$  (this is usually the case) or  $\omega(b_v) < 0$  and  $E > b_v$ . In the former case ( $\omega(b_v) > 0$ ) isolated eigenvalue  $\varepsilon_I$  does not exist for each  $\beta \leq \beta_b$ , while in a latter case ( $\omega(b_v) < 0$ ) this eigenvalue does not exist for each  $\beta \geq \beta_b$ . In both cases one finds that the probability  $w_1^a \equiv w_1^a(E, \beta)$  is a continuous function of  $\beta$  in the point  $\beta = \beta_b$ , while derivative of  $w_1^a(E, \beta)$  with respect to  $\beta$  diverges as  $O(\xi^{-1}(\ln|\xi|)^{-3})$  in this point. Another possibility is  $(b_v - E)/\omega(b_v) < 0$ . In this case, there is no critical point and probability  $w_1^a(E, \beta)$  as well as derivative of this probability with respect to  $\beta$  are continuous functions of  $\beta$  for each  $\beta > 0$ . In addition, in a limit  $\beta \rightarrow 0$  one has  $w_1^a \rightarrow 1$ .

If  $f(\varepsilon)$  has zero of the second order in the boundary point  $b = b_v$ , then

$$f^{(2)}(b_v) \neq 0 \Rightarrow$$

$$\omega(b_v) = O(1), \quad \omega^{(1)}(b_v) = O(1), \quad w_1^a(b_v + 0) > 0,$$

$$\frac{\partial w_1^a(b_v + \xi)}{\partial E} = O(\ln|\xi|) \rightarrow \infty,$$

$$\frac{\partial w_1^a(b_v + \xi)}{\partial \beta} = O(\ln|\xi|) \rightarrow \infty \quad \text{if } \beta > 0. \quad (28c)$$

Since  $\omega(\varepsilon)$  is finite and continuous in the boundary point  $b = b_v$ , there is again a critical value  $E_b = b_v - \beta^2\omega(b_v)$  such that if  $E \leq E_b$  isolated eigenvalue  $\varepsilon_I$  does not exist. This time however derivative  $\omega^{(1)}(\varepsilon)$  is also finite and continuous in this point. According to (10) one has

$$w_1^a(b_v + 0) = \frac{1}{1 - \beta^2\omega^{(1)}(b_v)} > 0. \quad (29)$$

Probability  $w_1^a$  considered as a function of the eigenvalue  $E$  is hence discontinuous in a point  $E = E_b$ . In this point, probability  $w_1^a$  has a finite jump from  $w_1^a(E_b - 0) = 0$  to  $w_1^a(E_b + 0) = w_1^a(b_v + 0) > 0$ . This jump is given by relation (29).

Concerning the dependence of the probability  $w_1^a$  on the coupling parameter  $\beta$ , one has again two possibilities, either  $(b_v - E)/\omega(b_v) > 0$  or  $(b_v - E)/\omega(b_v) < 0$ . In the former case critical point  $\beta_b = \sqrt{(b_v - E)/\omega(b_v)}$  exists, while in the later case it does not exist. If a critical point  $\beta = \beta_b$  exists, probability  $w_1^a$  considered as a function of the coupling  $\beta$  is discontinuous in this point and it has a finite jump  $w_1^a(b_v + 0) > 0$  in this point. If the critical point does not exist, probability  $w_1^a$  considered as a function of  $\beta$  is continuous for each  $\beta$  and it has no jump.

If in the boundary point  $\varepsilon = b_v$  the function  $f(\varepsilon)$  has zero of some higher order, qualitative behavior of the probability  $w_1^a$  is similar to the behavior of this probability considered in a previous case.

Above we have analyzed properties of the probability  $w_1^a = w_1^a(E, \beta)$  in the case when, due to the continuous change of parameters  $E$  and  $\beta$ , eigenvalue  $\varepsilon_I \equiv \varepsilon_I(E, \beta)$  converges to the boundary point  $b_v$  of the interval  $(b_v, a_\mu) \subseteq \bar{D}$ . Similar results are obtained in the case when this eigenvalue converges to the boundary point  $a_\mu$  of this interval.

Note finally that due to the completeness requirement (13), those results imply corresponding behavior of the probability  $w_C^a = \int \rho^a(\varepsilon) d\varepsilon$  considered as a function of parameters  $E$  and  $\beta$ .

## EXAMPLE

In order to illustrate relations (25) for the calculation of the functions  $\omega_v(\varepsilon)$  and in order to verify above suggested method, consider a following simple example. Let the system  $S_\infty^b$  contain three eigenvalue bands in the intervals  $I_1 = [-1, 1]$ ,  $I_2 = [0, 1]$  and  $I_3 = [2, 3]$ . Intervals  $I_1$  and  $I_2$  partially overlap, while interval  $I_3$  is separated from those intervals. This example is general enough to illustrate various properties of the combined system. In particular, this combined system may contain three isolated eigenvalues, left isolated eigenvalue  $\varepsilon_L \in (-\infty, -1)$ , right isolated eigenvalue  $\varepsilon_R \in (3, \infty)$  and intermediate isolated eigenvalue  $\varepsilon_I \in (1, 2)$ .

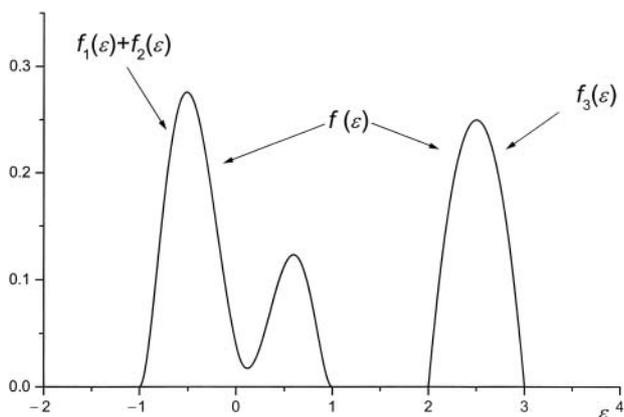


Figure 1. Characteristic function  $f(\varepsilon) = f_1(\varepsilon) + f_2(\varepsilon) + f_3(\varepsilon)$ . This function describes the interaction of the state  $|\Theta\rangle$  with three eigenvalue bands in the intervals  $I_1 = [-1, 1]$ ,  $I_2 = [0, 1]$  and  $I_3 = [2, 3]$ , respectively.

Since  $S_\infty^b$  contains three eigenvalue bands,  $f(\varepsilon)$  is a sum

$$f(\varepsilon) = f_1(\varepsilon) + f_2(\varepsilon) + f_3(\varepsilon) \quad (30a)$$

Let

$$f_v(\varepsilon) = \begin{cases} F_v(\varepsilon), & \varepsilon \in I_v \equiv [a, b], \\ 0 & \varepsilon \notin I_v. \end{cases} \quad (30b)$$

where functions  $F_v(\varepsilon)$  are polynomials. As a particular example consider following polynomials

$$\begin{aligned} F_1(\varepsilon) &= (\varepsilon^2 - 1)^2 (\varepsilon - 0.2)^2, & F_2(\varepsilon) &= \varepsilon^2 (\varepsilon - 1)^2, \\ F_3(\varepsilon) &= (\varepsilon - 2) (3 - \varepsilon). \end{aligned} \quad (30c)$$

Characteristic function  $f(\varepsilon)$  is shown in Figure 1. This function is positive almost everywhere in the range  $D = I_1 \cup I_2 \cup I_3$ , and it vanishes outside this range. Boundary points of this range are  $a_1 = -1$ ,  $b_1 = b_2 = 1$ ,  $a_3 = 2$  and  $b_3 = 3$ . Boundary point  $a_2 = 0$  of the interval  $I_2$  is not a boundary point of the range  $D$ , since this point is contained inside the interval  $I_1 = [-1, 1]$ . In the boundary points  $a_1$  and  $b_1$  function  $f(\varepsilon)$  has zero of the second order, while in a boundary points  $a_3$  and  $b_3$  it has zero of the first order.

Corresponding function  $\omega(\varepsilon)$  is a sum

$$\omega(\varepsilon) = \omega_1(\varepsilon) + \omega_2(\varepsilon) + \omega_3(\varepsilon) \quad (31a)$$

According to (25), individual functions  $\omega_v(\varepsilon)$  are

$$\omega_v(\varepsilon) = F_v(\varepsilon) \ln \left| \frac{\varepsilon - a_v}{\varepsilon - b_v} \right| - G_v(\varepsilon) \quad (31b)$$

Using (25) and (30c) one finds

$$G_1(\varepsilon) = 2\varepsilon^5 - 0.8\varepsilon^4 - \frac{9.76}{3}\varepsilon^3 + \frac{4}{3}\varepsilon^2 + \frac{2.8}{3}\varepsilon - \frac{6.4}{15},$$

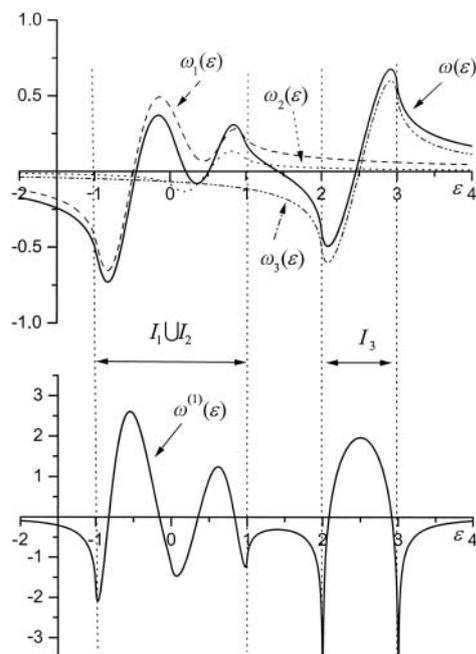


Figure 2. (a) Global function  $\omega(\varepsilon) = \omega_1(\varepsilon) + \omega_2(\varepsilon) + \omega_3(\varepsilon)$  (solid line) and individual functions  $\omega_v(\varepsilon)$  (other lines). (b) Derivative  $\omega^{(1)}(\varepsilon)$  of a global function  $\omega(\varepsilon)$ .

$$G_2(\varepsilon) = \varepsilon^3 - \frac{3}{2}\varepsilon^2 + \frac{1}{3}\varepsilon - \frac{1}{12}, \quad G_3(\varepsilon) = -\varepsilon + \frac{5}{2}. \quad (31c)$$

Global function  $\omega(\varepsilon)$  and individual functions  $\omega_v(\varepsilon)$  are shown in the upper part of the Figure 2. In the lower part of this figure is shown derivative  $\omega^{(1)}(\varepsilon)$  of the global function  $\omega(\varepsilon)$ . In accord with the relation (7), function  $\omega(\varepsilon)$  is monotonically decreasing in the intervals  $(-\infty, -1)$ ,  $(1, 2)$  and  $(3, \infty)$  outside the range  $D$ . However, inside this range derivative of  $\omega(\varepsilon)$  assumes positive as well as negative values. Each function  $f_v(\varepsilon)$  vanishes in the boundary points of the corresponding interval  $I_v$ . All three functions  $\omega_v(\varepsilon)$  are hence continuous on the entire real axis. Accordingly, global function  $\omega(\varepsilon)$  is also continuous for each real  $\varepsilon$ . However, this is not the case with derivative  $\omega^{(1)}(\varepsilon)$  of this function. Function  $f_3(\varepsilon)$  has zero of the first order in the boundary points of the interval  $I_3 = [2, 3]$ , and therefore derivative  $\omega_3^{(1)}(\varepsilon)$  of  $\omega_3(\varepsilon)$  diverges logarithmically in those points. As a consequence derivative  $\omega^{(1)}(\varepsilon)$  of a global function  $\omega(\varepsilon)$  also diverges in those points (see Eq. (28b)). This is clearly visible in the lower part of the Figure 2 where derivative  $\omega^{(1)}(\varepsilon)$  is shown.

#### Time Independent Properties of the Combined System

Expressions (30)–(31) provide all necessary information for the description of the combined system. In particular, in the boundary points of the range  $D$  one has

$$\begin{aligned} \omega(a_1) &= -0.49707, & \omega(b_1) &= 0.18296, \\ \omega(a_3) &= -0.38854, & \omega(b_3) &= 0.57361. \end{aligned}$$

According to (9b) left isolated eigenvalue  $\varepsilon_L \in (-\infty, -1)$  exists if and only if

$$E < a_1 - \beta^2 \omega(a_1) \equiv -1 + 0.49707 \beta^2 \quad (32a)$$

right isolate eigenvalue  $\varepsilon_R \in (3, \infty)$  exists if and only if

$$E > b_3 - \beta^2 \omega(b_3) \equiv 3 - 0.57361 \beta^2 \quad (32b)$$

while intermediate isolated eigenvalue  $\varepsilon_1 \in (1, 2)$  exists if and only if

$$b_1 - \beta^2 \omega(b_1) \equiv 1 - 0.18296 \beta^2 < E < a_3 - \beta^2 \omega(a_3) \equiv 2 + 0.38854 \beta^2 \quad (32c)$$

If the coupling  $\beta$  is small and if the unperturbed eigenvalue  $E$  is an interior point of the range  $D$ , this eigenvalue shifts to a new position  $\varepsilon_0$  with resulting eigenvalue uncertainty. In addition, in this case density  $\rho^a(\varepsilon)$  has a shape of the universal resonance curve. Those results are usually obtained within the standard perturbation expansion approach.<sup>1,4</sup> We reproduce those results using exact expression (12) for this density. An example is shown in Figure 3. In Figure 3(a) combined system with  $E = 0.7$  and  $\beta = 0.1$  is considered. This is relatively weak coupling. As a result of the interaction with the system  $S_\infty^b$ , eigenvalue  $E = 0.7$  of the state  $|\Theta\rangle$  is slightly shifted with additional uncertainty  $\Delta\varepsilon$ . This effect is clearly visible in Figure 3(b). This figure shows the same density  $\rho^a(\varepsilon)$  as in Figure 3(a), but amplified approximately 100-fold in the horizontal direction and decreased approximately 10-fold in the vertical direction. As required, density  $\rho^a(\varepsilon)$  has the shape of the uni-

versal resonance curve. According to (14b), this curve has a maximum at the position  $\varepsilon_0 = 0.70209$ . Expression (14b') produces the value  $\varepsilon_0 \approx 0.70223$ , which is an excellent approximation to the true value. In Figure 3(c) is given another example with  $E = 2.1$  and  $\beta = 0.1$ . The shape of the curve  $\rho^a(\varepsilon) \approx \rho^{a0}(\varepsilon)$  is emphasized in Figure 3(d). Density  $\rho^{a0}(\varepsilon)$  has maximum in the point  $\varepsilon_0 = 2.09507$ , while approximate expression (14b') produces the value  $\varepsilon_0 \approx 2.09509$ . As implied by conditions (32), in those two examples there are no isolated eigenstates. Hence, one finds  $\int \rho^a(\varepsilon) d\varepsilon = 1$  in accord with (13).

Example with relatively strong coupling is shown in Figure 4. In this figure, the case  $E = 0.7$  as in Figure 3 is considered. However, this time coupling is as strong as  $\beta = 1.5$ . The shape of the density  $\rho^a(\varepsilon)$  is now substantially different from the universal resonance curve. In addition, one finds  $\int \rho^a(\varepsilon) d\varepsilon = 0.6018 < 1$ . Moreover, condition (32c) is satisfied and hence relation (9a) has a solution  $\varepsilon_1 \in (1, 2)$ . Using the function  $\omega(\varepsilon)$  as given by (31), one finds  $\varepsilon_1 = 1.0396$ . Inserting this value into (10) where  $\omega^{(1)}(\varepsilon)$  is calculated according to (27), one obtains  $w_1^a = 0.3982$ . Hence  $w_1^a + \int \rho^a(\varepsilon) d\varepsilon = 1$  in accord with the completeness relation (13).

Completeness relation is verified in more details in Figure 5. In Figure 5(a) the case  $E = 0.7$  is considered and probabilities  $w_c^a = \int \rho^a(\varepsilon) d\varepsilon$ ,  $w_L^a$ ,  $w_R^a$  and  $w_1^a$  are plotted as functions of the coupling parameter  $\beta$ . In addition, total probability  $\sum_1 w_1^a + \int \rho^a(\varepsilon) d\varepsilon$  (which according to (13) should equal unity) is also plotted. According to conditions (32), in the case  $E = 0.7$  intermediate isolated eigenvalue  $\varepsilon_1$  exists if and only if  $\beta > \beta_1 = 1.2805$ , left isolated eigenvalue  $\varepsilon_L$  exists if and only if  $\beta > \beta_L = 1.8493$ , while right isolated eigenvalue  $\varepsilon_R$  exists if and

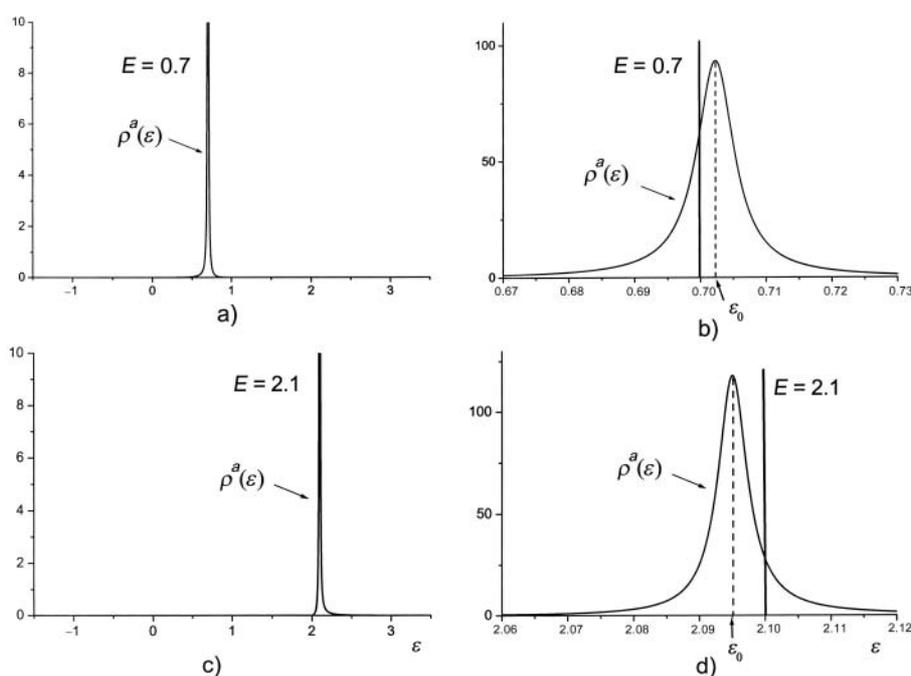


Figure 3. Probability density  $\rho^a(\varepsilon) = \sum_\nu |\langle \Theta | \psi_\nu(\varepsilon) \rangle|^2$  to find the state  $|\Theta\rangle$  with the eigenvalue  $\varepsilon$  in the case  $\beta = 0.1$  and for two different values of the eigenvalue  $E$ . This coupling is relatively weak and density  $\rho^a(\varepsilon)$  has the shape of the universal resonance curve. In (a) and (b) the case  $E = 0.7$  is considered, while in (c) and (d) the case  $E = 2.1$  is considered. In both cases one has  $w_c^a = \int \rho^a(\varepsilon) d\varepsilon = 1$ .

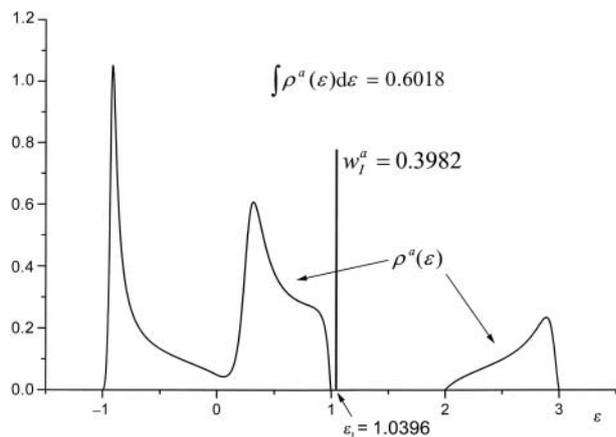


Figure 4. Probability density  $\rho^a(\varepsilon)$  to find the state  $|\Theta\rangle$  with the eigenvalue  $\varepsilon$  in the case  $E = 0.7$  and  $\beta = 1.5$ . This is relatively strong coupling and density  $\rho^a(\varepsilon)$  has no resemblance to the universal resonance curve. One finds  $w_C^a = \int \rho^a(\varepsilon) d\varepsilon = 0.6018 < 1$  and combined system has local eigenstate  $|\Psi_I\rangle$  with the eigenvalue  $\varepsilon_I = 1.0396$ . Probability  $w_I^a = |\langle \Theta | \Psi_I \rangle|^2$  equals  $w_I^a = 0.3982$  and hence  $w_C^a + w_I^a = 1$  in accord with the completeness requirement.

only if  $\beta > \beta_R = 2.0024$ . For small enough  $\beta$  there is no isolated eigenstate, density  $\rho^a(\varepsilon)$  has the shape of the universal resonance curve and one has  $w_C^a = \int \rho^a(\varepsilon) d\varepsilon = 1$ . In particular, in a point  $\beta = 0.1$  one has situation shown in Figure 3(a) and 3(b). As  $\beta$  increases, in a point  $\beta = \beta_I$  the probability  $w_C^a$  sharply decreases and intermediate isolated eigenstate  $|\Psi_I\rangle$  with the eigenvalue  $\varepsilon_I = b_1 + 0$  and probability  $w_I^a \neq 0$  appears. Since the function  $f(\varepsilon)$  has zero of the second order in the point  $b_1 = 1$ , derivative  $\omega^{(1)}(\varepsilon)$  is finite and continuous in this point. Hence, probability  $w_I^a$  has a finite jump in this point. Using (29) one finds this jump to equal  $w_I^a(\beta_I + 0) = 0.3671$ . Probability  $w_C$  decreases for the same amount, and one finds  $w_C^a + w_I^a = 1$  in accord with (13). In the point  $\beta = 1.5$  one has situation shown in Figure 4 with probabilities  $w_C^a = \int \rho^a(\varepsilon) d\varepsilon = 0.6018$  and  $w_I^a = 0.3982$ . As  $\beta$  further increases, in the point  $\beta = \beta_L$  left isolated eigenstate  $|\Psi_L\rangle$  with the eigenvalue  $\varepsilon_L = a_1 - 0$  appears. Since the function  $f(\varepsilon)$  has in the point  $a_1 = -1$  zero of the second order, there is again finite jump of the probability  $w_L$  in this point. One finds  $w_L^a(\beta_L + 0) = 0.1446$ . Probability  $w_C^a = \int \rho^a(\varepsilon) d\varepsilon$  decreases for the same amount, and hence  $w_C^a + w_I^a + w_L^a = 1$ . Finally in a point  $\beta = \beta_R$  right isolated eigenstate  $|\Psi_R\rangle$  with the eigenvalue  $\varepsilon_R = b_3 + 0$  appears. However, in a point  $b_3 = 3$  function  $f(\varepsilon)$  has zero of the first order. Derivative  $\omega^{(1)}(\varepsilon)$  hence diverges as  $O(\ln|\varepsilon - b_3|)$  in this point. According to (28b), probability  $w_R^a$  is continuous in this point, but its derivative diverges. This behavior is visible in Figure 5(a). Unlike probabilities  $w_I^a$  and  $w_L^a$ , probability  $w_R^a$  has no jump in the point  $\beta = \beta_R$ , though its derivative diverges in this point.

Another example is shown in Figure 5(b). In this figure, the case  $E = 1.5$  is considered. This eigenvalue is

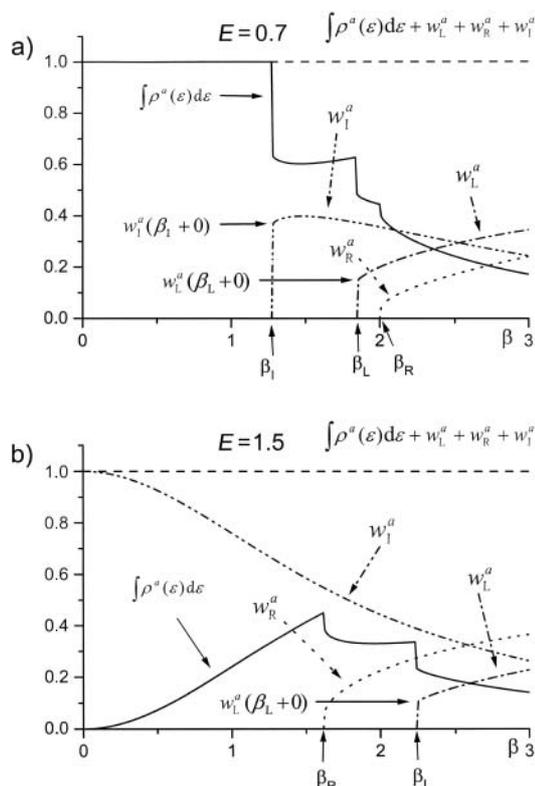


Figure 5. Illustration of the completeness requirement for the case  $E = 0.7$  (Figure 5(a)) and for the case  $E = 1.5$  (Figure 5(b)). Probabilities  $w_C^a = \int \rho^a(\varepsilon) d\varepsilon$ ,  $w_L^a$ ,  $w_R^a$  and  $w_I^a$  are plotted as functions of the interaction parameter  $\beta$ . Sum of those probabilities equals one, in accord with the completeness requirement.

inside the interval  $(1, 2) \in \bar{D}$ . According to the conditions (32), in the case  $E = 1.5$  left isolated eigenvalue  $\varepsilon_L$  exists if and only if  $\beta > \beta_L = 2.2426$ , right isolated eigenvalue  $\varepsilon_R$  exists if and only if  $\beta > \beta_R = 1.6171$ , while intermediate isolated eigenvalue  $\varepsilon_I$  exists for each value of  $\beta$ . This last result follows also from  $E \in (1, 2) \in \bar{D}$ . For small  $\beta$  isolated eigenstate  $|\Psi_I\rangle$  is essentially perturbed state  $|\Theta\rangle$  and hence  $w_I^a \approx 1$ . Also for small  $\beta$  the contribution  $w_C^a = \int \rho^a(\varepsilon) d\varepsilon$  is relatively small. As  $\beta$  increases, probability  $w_I^a$  decreases while probability  $w_C^a$  increases. In the point  $\beta = \beta_R$  right isolated eigenstate  $|\Psi_R\rangle$  appears, while in the point  $\beta = \beta_L$  left isolated eigenstate  $|\Psi_L\rangle$  appears. One again finds that in a point  $\beta_R$  probability  $w_R^a$  considered as a function of  $\beta$  is continuous, while its derivative diverges. However, probability  $w_L^a$  has a finite jump  $w_L^a(\beta_L + 0) = 0.1031$  in a point  $\beta_L$ .

In all cases considered in Figure 5, one has  $w_C^a + \sum_I w_I^a = 1$ , in accord with the completeness requirement. Verification of this requirement is a strong indication that the suggested method is correct. One can also verify this method in an explicit and more direct way.<sup>6,7</sup> The fact that the completeness relation is satisfied in the relatively large interval  $\beta \in [0, 3]$  shows that this method does not fail even in the case of extremely strong interactions.

Note finally that standard perturbation expansion method can not reproduce results shown in Figure 5. For example, consider the probability  $w_c^a(\beta) = \int \rho^a(\varepsilon) d\varepsilon$  in Figure 5(a). This probability is not an analytic function of  $\beta$  in the point  $\beta = \beta_1$ . Hence, no power series expansion of  $w_c^a(\beta)$  in a point  $\beta = 0$  can converge beyond this point. More formally, in the interval  $[0, \beta_1]$  probability  $w_c^a(\beta) = 1$  is constant, and analytic continuation of this function beyond this point is again  $w_c^a(\beta) = 1$ . This is obviously wrong, since one has  $w_c^a(\beta) < 1$  for each  $\beta > \beta_1$ .

### Time Dependent Properties of the Combined System

Time dependent properties of the combined system can be analyzed in a similar way. An example is shown in Figure 6 where we again assume  $E = 0.7$ . In this figure, probabilities  $w^a(t)$  to find the state  $|\Theta(t)\rangle$  at time  $t$  in the initial state  $|\Theta(0)\rangle \equiv |\Theta\rangle$  for two different values of the coupling  $\beta$  are considered. In Figure 6(a) coupling is relatively weak ( $\beta = 0.1$ ) and this probability has the shape of the well known exponential decay. In Figure 6(b) coupling is quite strong ( $\beta = 1.0$ ) and the decay of a state  $|\Theta\rangle$  deviates substantially from a standard exponential shape. Those two cases correspond to the points  $\beta = 0.1$  and  $\beta = 1.0$ , respectively, in Figure 5(a). In both cases no isolated eigenstate exists, and the probability  $w^a(t)$  is ob-

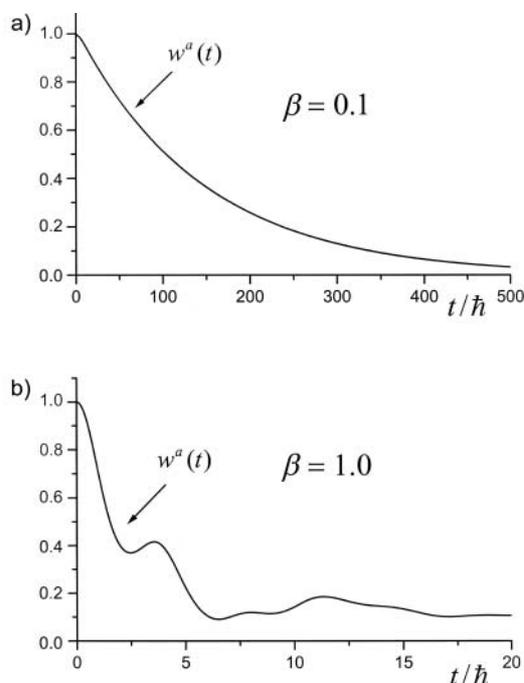


Figure 6. Probability  $w^a(t) = |\langle \Theta | \Theta(t) \rangle|^2$  to find the state  $|\Theta(t)\rangle$  at time  $t$  in the initial state  $|\Theta(0)\rangle \equiv |\Theta\rangle$  for the case  $E = 0.7$  and for two different values of the coupling  $\beta$ . (a) Coupling  $\beta = 0.1$  is relatively weak. Probability  $w^a(t)$  has a shape of the standard exponential decay. (b) Coupling  $\beta = 1$  is relatively strong. The shape of the probability  $w^a(t)$  deviates from that of the standard exponential decay.

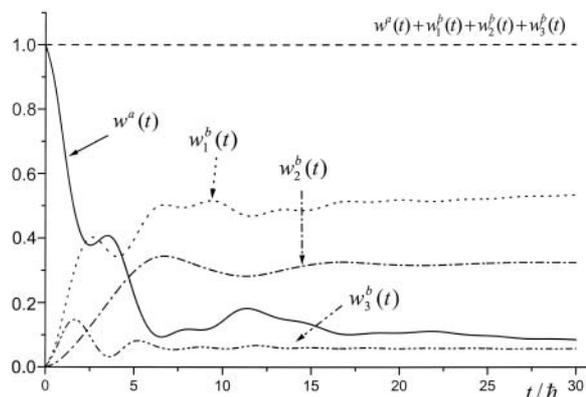


Figure 7. Probability  $w^a(t)$  and transition probabilities  $w_v^b(t)$  for the case  $E = 0.7$  and  $\beta = 1$ . Total probability  $w^a(t) + \sum_v w_v^b(t)$  is in accord with the completeness requirement (21b).

tained using relation (18) where  $w_1^a = 0$ . Note that in the case  $\beta = 1.0$  there is a temporary increase of the probability  $w^a(t)$  close to the point  $t/\hbar \approx 4$  and another temporary increase close to the point  $t/\hbar \approx 11$ . No classical decay mechanism can explain this behavior, and this is essentially a quantum effect.

In Figure 7 the case  $E = 0.7$  and  $\beta = 1.0$  from Figure 6(b) is considered in more details. In this figure in addition to the probability  $w^a(t)$  for the decay of the state  $|\Theta(t)\rangle$ , probabilities  $w_v^b(t)$  for the transition of this state into eigenvalue bands  $\nu$  ( $\nu = 1, 2, 3$ ) are also shown. Those probabilities are integrals (21a), where densities  $\rho_v^b(\lambda, t)$  are calculated using relations (19). Total probability  $w^a(t) + \sum_v w_v^b(t)$  is also given. As required by the completeness relation (21b), this total probability equals unity for all times considered. One also finds that for large times those probabilities asymptotically converge to their limit values. This follows from the fact that the combined system contains no isolated eigenstates. Thus if  $t/\hbar = 200$  one finds  $w^a(t) = 0.00255$ ,  $w_1^b(t) = 0.60232$ ,  $w_2^b(t) = 0.34410$  and  $w_3^b(t) = 0.05103$ . This is relatively large time and the decay of the state  $|\Theta(t)\rangle$  is almost completed ( $w^a(t)$  is quite small). Accordingly, probabilities  $w_v^b(t)$  are close to their asymptotic values. Those probabilities satisfy  $w^a(t) + \sum_v w_v^b(t) = 1$  in accord with completeness relation (21b).

## CONCLUSIONS

Recently a new approach for the treatment of the interaction of an isolated state  $|\Theta\rangle$  with a known infinite system  $S_\infty^b$  containing multiple eigenvalue bands was suggested.<sup>6</sup> Unlike the standard perturbation method, this approach involves no power series expansion, and it produces correct results, however strong the interaction between the state  $|\Theta\rangle$  and this infinite system. Key quantities in this new approach are functions  $f_\nu(\varepsilon)$  and  $\omega_\nu(\varepsilon)$ . Various properties of the combined system are expressed in terms of those functions. Characteristic functions

$f_v(\varepsilon)$  are fundamental, while each function  $\omega_v(\varepsilon)$  is expressed in terms of the corresponding function  $f_v(\varepsilon)$ . An important mathematical problem is the calculation of the functions  $\omega_v(\varepsilon)$ , once characteristic functions  $f_v(\varepsilon)$  are known. A general mathematical solution to this problem is obtained in the case when characteristic functions  $f_v(\varepsilon)$  are polynomials. Since each function which is continuous in some finite interval can be approximated (to any desired degree of accuracy) with some polynomial, this solution presents an important mathematical tool for the practical application of the suggested method. Obtained results are illustrated with few examples. Completeness relations in time-independent as well as in time-dependent case are verified. Verification of those relations provides rather strong support for the validity of the derived expressions and also for the validity of the suggested approach.

With the above mathematical method for the construction of the functions  $\omega_v(\varepsilon)$  once polynomial-like functions  $f_v(\varepsilon)$  are known, the entire approach reduces essentially to the initial construction of functions  $f_v(\varepsilon)$ . Those functions can be relatively easily constructed from the quantities describing unperturbed system  $S_\infty^b$  and the interaction of this system with the state  $|\Theta\rangle$ . There is however possibility of a different approach, especially in the case when the unperturbed system  $S_\infty^b$  is not exactly known. In this case, one can consider those functions as primitive elements and one can model those functions in an appropriate way. With such an approach, rather complex systems can be treated in some kind of a semiempirical method.

## APPENDIX

### Calculation of the Function $\omega_v(\varepsilon)$ in the Case of the Polynomial-type Function $f_v(\varepsilon)$

Each function  $\omega_v(\varepsilon)$  is an integral of the type

$$K(\varepsilon) = P \int_a^b \frac{y(\lambda)}{\varepsilon - \lambda} \quad (\text{A1})$$

By definition<sup>8</sup>

$$P \int_a^b \frac{y(\lambda)}{\varepsilon - \lambda} = \lim_{h \rightarrow 0} \left[ \int_a^{\varepsilon-h} \frac{y(\lambda)}{\varepsilon - \lambda} d\lambda + \int_{\varepsilon+h}^b \frac{y(\lambda)}{\varepsilon - \lambda} d\lambda \right] \quad (\text{A2})$$

Let inside the interval  $I = [a, b]$  function  $y(\lambda)$  be a polynomial, *i.e.*

$$y(\lambda) = \begin{cases} F(\lambda) & \text{if } \lambda \in [a, b] \\ 0 & \text{if } \lambda \notin [a, b] \end{cases} \quad (\text{A3a})$$

where

$$F(\lambda) = \sum_{i=0}^n c_i \lambda^i. \quad (\text{A3b})$$

One has

$$P \int_a^b \frac{y(\lambda)}{\varepsilon - \lambda} d\lambda = F(\varepsilon) P \int_a^b \frac{d\lambda}{\varepsilon - \lambda} - P \int_a^b \frac{F(\varepsilon) - F(\lambda)}{\varepsilon - \lambda} d\lambda \quad (\text{A4})$$

Consider first integral on the right hand side of this expression. If  $\varepsilon \in [a, b]$  and if  $b - \varepsilon \geq \varepsilon - a$  one finds

$$\int_a^{\varepsilon-h} \frac{d\lambda}{\varepsilon - \lambda} + \int_{\varepsilon+h}^b \frac{d\lambda}{\varepsilon - \lambda} = \int_a^{2\varepsilon-b} \frac{d\lambda}{\varepsilon - \lambda} + \int_{2\varepsilon-b}^{\varepsilon-h} \frac{d\lambda}{\varepsilon - \lambda} + \int_{\varepsilon+h}^b \frac{d\lambda}{\varepsilon - \lambda} = \int_a^{2\varepsilon-b} \frac{d\lambda}{\varepsilon - \lambda} = \ln \frac{\varepsilon - a}{b - \varepsilon}$$

The same result is obtained if  $b - \varepsilon < \varepsilon - a$ . Hence

$$P \int_a^b \frac{d\lambda}{\varepsilon - \lambda} = \ln \frac{\varepsilon - a}{b - \varepsilon} \quad \varepsilon \in [a, b].$$

If however  $\varepsilon \notin [a, b]$  then

$$P \int_a^b \frac{d\lambda}{\varepsilon - \lambda} = \int_a^b \frac{d\lambda}{\varepsilon - \lambda} = \ln \frac{\varepsilon - a}{\varepsilon - b} \quad \varepsilon \notin [a, b].$$

Hence and from (A4)

$$K(\varepsilon) = F(\varepsilon) \ln \left| \frac{\varepsilon - a}{\varepsilon - b} \right| - \sum_{k=0}^n c_k g_k(\varepsilon), \quad (\text{A5a})$$

where

$$g_k(\varepsilon) = P \int_a^b \frac{\varepsilon^k - \lambda^k}{\varepsilon - \lambda} d\lambda. \quad (\text{A5b})$$

Using identity<sup>10</sup>

$$\varepsilon^k - \lambda^k = (\varepsilon - \lambda)(\varepsilon^{k-1} + \varepsilon^{k-2}\lambda + \varepsilon^{k-3}\lambda^2 + \dots + \varepsilon\lambda^{k-2} + \lambda^{k-1})$$

singularity  $\lambda = \varepsilon$  in (A5b) is removed and one finds

$$g_k(\varepsilon) = \int_a^b \frac{(\varepsilon - \lambda)}{\varepsilon - \lambda} \sum_{i=1}^k \varepsilon^{k-i} \lambda^{i-1} d\lambda = \sum_{i=1}^k \varepsilon^{k-i} \int_a^b \lambda^{i-1} d\lambda = \sum_{i=0}^{k-1} \frac{\varepsilon^i}{k-i} [b^{k-i} - a^{k-i}] \quad (\text{A5c})$$

This proves relation (25). Relations (26) and (27) are now trivial to derive.

### Properties of the Function $K(\varepsilon)$ in the Neighborhood of Boundary Points

Function  $K(\varepsilon)$  is continuous and derivable everywhere, except possibly in the boundary points  $a$  and  $b$  of the interval  $I = [a, b]$ . Qualitative behavior of this function in the neighborhood of those points depends on the properties of the polynomial  $F(\varepsilon)$  in those points. In general, polynomial  $F(\varepsilon)$  can differ from zero in a boundary point, or it can have a zero of some integer order in this point.

By definition, a function  $y(\varepsilon)$  has zero of the order  $s > 0$  in the point  $\varepsilon = \varepsilon_0$  if<sup>10</sup>

$$\lim_{\varepsilon \rightarrow \varepsilon_0} \left| \frac{y(\varepsilon)}{(\varepsilon - \varepsilon_0)^s} \right| = c > 0 \quad (\text{A6a})$$

In general,  $s$  can be any positive real number. However, in the case of polynomials it is a positive integer. Moreover, expression (A6a) implies that polynomial  $F(\varepsilon)$  has zero of the order  $s$  in the point  $\varepsilon = \varepsilon_0$  if and only if  $F(\varepsilon_0) = 0$  and if in addition

$$p < s \Rightarrow F^{(p)}(\varepsilon_0) = 0, \quad F^{(s)}(\varepsilon_0) \neq 0. \quad (\text{A6b})$$

In other words, polynomial  $F(\varepsilon)$ , as well as all derivatives of this polynomial that are lower than  $s$ , vanish in the point  $\varepsilon = \varepsilon_0$ .

Following results generalize in a natural way to rather arbitrary functions  $y(\varepsilon)$ , not just those that are identical to some polynomial in the interval  $I = [a, b]$ .<sup>7</sup> In order to formulate those results, we will use simplified notation and terminology. If the polynomial  $F(\varepsilon)$  is non-zero in a boundary point  $\varepsilon = b$ , we will write  $y(b) \neq 0$  and say that the function  $y(\varepsilon)$  is nonzero in this point. Strictly, this is not true, since if  $F(b) \neq 0$ , function  $y(\varepsilon)$  has two limits in this point, left limit  $y(b - 0) = F(b)$  and right limit  $y(b + 0) = 0$ . In a similar way, if the polynomial  $F(\varepsilon)$  has zero of the order  $s$  in the boundary point  $\varepsilon = b$ , we will write  $y^{(s)}(b) \neq 0$  and say that function  $y(\varepsilon)$  has zero of the order  $s$  in this point.

Consider now the case  $y(b) \neq 0$ . Since  $\lim_{\varepsilon \rightarrow 0} \varepsilon \ln(\varepsilon) = 0$  one finds

$$K(b + \xi) = O(\ln |\xi|), \quad K^{(1)}(b + \xi) = O(\xi^{-1}),$$

$$K^{(2)}(b + \xi) = O(\xi^{-2}). \quad (\text{A7a})$$

where  $\xi$  is a small quantity and where  $O(x)$  is a quantity of the order  $x$ . In other words, if the function  $y(\varepsilon)$  is non-zero in a boundary point  $b$  (or  $a$ ), the function  $K(\varepsilon)$  diverges logarithmically in this point, first derivative  $K^{(1)}(\varepsilon)$  of this function diverges as  $O(\xi^{-1})$  in this point, while second derivative  $K^{(2)}(\varepsilon)$  diverges as  $O(\xi^{-2})$  in this point.

If the function  $y(\varepsilon)$  has zero of the first order in the point  $\varepsilon = b$  ( $F(b) = 0$  and  $F^{(1)}(b) \neq 0$ ) one finds

$$K(b) = -G(b), \quad K^{(1)}(b + \xi) = O(\ln |\xi|),$$

$$K^{(2)}(b + \xi) = O(\xi^{-1}). \quad (\text{A7b})$$

In this case, function  $K(\varepsilon)$  is finite and continuous in the boundary point, first derivative  $K^{(1)}(\varepsilon)$  diverges logarithmically in this point, while second derivative diverges as  $O(\xi^{-1})$  in this point.

If the function  $y(\varepsilon)$  has zero of the second order in the point  $\varepsilon = b$  ( $F(b) = 0$ ,  $F^{(1)}(b) = 0$  and  $F^{(2)}(b) \neq 0$ ) then

$$K(b) = -G(b), \quad K^{(1)}(b) = -G^{(1)}(b),$$

$$K^{(2)}(b + \xi) = O(\ln |\xi|). \quad (\text{A7c})$$

In this case, function  $K(\varepsilon)$  as well as its first derivative  $K^{(1)}(\varepsilon)$  are finite and continuous in the boundary point, while second derivative diverges logarithmically in this point.

Finally, if the function  $y(\varepsilon)$  has zero of the order  $s > 2$  in the point  $\varepsilon = b$ , function  $K(\varepsilon)$  as well as its first and second derivatives is finite and continuous in this point.

*Acknowledgement.*— This work was supported in part by the Ministry of Science and Technology of the Republic of Croatia, Project No 0098043.

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## SAŽETAK

**O interakciji izoliranoga stanja s poznatim beskonačno-dimenzionalnim kvantnim sustavom****Tomislav P. Živković**

Razmatrana je interakcija izoliranoga stanja  $|\Theta\rangle$  s beskonačno-dimenzionalnim kvantnim sustavom  $S_\infty^b$  koji sadrži više vrpca vlastitih vrijednosti. Jedan je primjer interakcija izoliranoga stanja molekule s elektromagnetskim poljem. Taj je problem glavni predmet spektroskopije. Drugi je primjer interakcija izoliranoga stanja molekule koja se nalazi na površini čvrstog tijela s tim tijelom. To je predmet fizike površina. Takvi se problemi obično tretiraju formalizmom perturbacijskoga razvoja. Nedavno je predložena nova metoda za studiranje takvih problema. Ta metoda daje točna rješenja kombiniranoga sustava, koliko god bila jaka interakcija stanja  $|\Theta\rangle$  i sustava  $S_\infty^b$ . Ključne veličine u toj metodi su karakteristične funkcije  $f_\nu(\varepsilon)$  i funkcije  $\omega_\nu(\varepsilon)$ . Funkcije  $f_\nu(\varepsilon)$  konstruiraju se iz veličina koje opisuju neperturbirani sustav  $S_\infty^b$  i iz poznate interakcije toga sustava sa stanjem  $|\Theta\rangle$ . Funkcije  $\omega_\nu(\varepsilon)$  se tada izračunavaju iz karakterističnih funkcija  $f_\nu(\varepsilon)$ . Važan je matematički problem izračunavanje funkcija  $\omega_\nu(\varepsilon)$  iz poznatih funkcija  $f_\nu(\varepsilon)$ . Dobiveno je opće rješenje toga problema za slučaj kada su karakteristične funkcije  $f_\nu(\varepsilon)$  polinomi. Pošto se svaka funkcija koja je neprekidna u konačnome intervalu može aproksimirati (po volji točno) s nekim polinomom, to rješenje predstavlja važno matematičko sredstvo za praktičnu primjenu predložene metode. Dobiveni su rezultati ilustrirani s nekoliko primjera interakcije izoliranoga stanja s beskonačnim kvantnim sustavom.

$$f(\varepsilon) = \sum_{\nu} f_{\nu}(\varepsilon), \quad \omega(\varepsilon) = \sum_{\nu} \omega_{\nu}(\varepsilon), \quad \omega_{\nu}(\varepsilon) = P \int \frac{f_{\nu}(\lambda)}{\varepsilon - \lambda} d\lambda.$$

$$b^2 \omega(\varepsilon_1) + E - \varepsilon_1 = 0, \quad w_1^a = \frac{1}{1 - \beta^2 \omega^{(1)}(\varepsilon_1)}, \quad \varepsilon_1 \notin D.$$

$$r^a(\varepsilon) = \frac{\beta^2 f(\varepsilon)}{\pi^2 \beta^4 f(\varepsilon)^2 + (\beta^2 \omega(\varepsilon) + E - \varepsilon)^2}, \quad \varepsilon \in D.$$

$$\rho_{\nu}^b(l, t) = \sqrt{2} u_{\nu}^b(l, t) \sqrt{2}, \quad l \in I_{\nu}.$$

$$u_{\nu}^b(l, t) =$$

$$\left[ \int \frac{\rho^a(\varepsilon) [e^{-i(\varepsilon-\lambda)t/h} - 1]}{\varepsilon - \lambda} d\varepsilon + \sum_l w_l^a \frac{[e^{-i(\varepsilon_1-\lambda)t/h} - 1]}{\varepsilon_1 - \lambda} \right].$$