

## Doubly periodical in time and energy exactly soluble system with two interacting systems of states

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**Abstract.** The time-dependent matrix Schrödinger equation  $\frac{1}{i\hbar} \frac{\partial \Psi}{\partial t} = \mathcal{H}(t)\Psi$  describing two bands of an infinite number of equidistant states with different energy spacings  $\omega_{\pm}$  in each band is studied. Both bands are linearly dependent on time  $t$ . The interaction  $v = (\sqrt{\omega_- \omega_+}/\pi) \tan \pi s$  between the bands is considered to be equal for any pair of states from each band. Using the Fourier series transformation the instant eigenvalues  $E(t, s)$  are calculated which reveal the double periodicity in the energy–time plane. The corresponding eigenvalue surface in the  $(E, t, s)$ -space, apart from the triple periodicity, shows quite unexpected symmetry properties relative to the exchange of  $t$  and  $s$ , and relative to some inversions in the  $(E, t)$  plane. The latter one leads to a new equivalence between weak and strong coupling, a new kind of pseudocrossing and a new concept of antiadiabatic states. The Fourier transformation reduces the problem to a  $2 \times 2$  first-order differential operator. The diagonalization of  $\mathcal{H}(t)$  for fixed  $t$  produces explicit expressions for the eigenvalues (adiabatic potential curves) and eigenstates (adiabatic basis). The time evolution operator is calculated both in the diabatic and adiabatic representations. The results are simplified for the special value of the interaction parameter.

### 1. Introduction

The time-dependent matrix Schrödinger equation is considered. Such operators are used, for instance, in atomic physics to describe molecule–molecule collisions. A broad class of quantum problems of practical importance can be described in terms of the transitions between two systems (bands) of parallel potential curves. The potential curves are understood here to be the eigenvalues of the Hamiltonian  $H(\lambda)$  which depends on some parameter  $\lambda$ .

In the static aspect of the problem the objects of interest are the peculiarities in  $\lambda$ -dependence of the potential curves and of the related eigenfunctions (adiabatic states). It is well known that, generally, the potential curves do not cross each other (Neumann–Wigner non-crossing rule, see e.g. Landau and Lifshitz [7]) provided that the related adiabatic state belongs to the same irreducible representation of the exact symmetry group of  $\mathcal{H}(\lambda)$ .

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However, so called avoided crossings (or pseudocrossings) can occur which often have a solid foundation in the physics of a specific system.

In the dynamic formulation,  $\lambda$  becomes a function of time  $t$  defined by the physical content of the problem. The object of interest is the matrix of the time propagator. In physical problems the adiabatic states vary rapidly with  $\lambda$  in some special regions of  $\lambda$  (near the avoided crossings of two or more potential curves). The alternative choice is the diabatic basis of states which represents a somewhat loosely defined notion. Generally it is chosen so that in the generating physical problem the basis functions vary smoothly with  $\lambda$ . The diabatic potential curves are defined as the diagonal elements of the Hamiltonian in the diabatic basis. These curves can cross each other at certain values of  $\lambda$  which indicates that, in the diabatic approximation, the physical system has higher symmetry than the exact Hamiltonian.

The simplest model of this type—the Landau–Zener model [6, 11]—describes the situation when the instantaneous Hamiltonian has only two energy levels. Pseudo-crossing of these levels is considered. The Demkov–Osherov model [2] describes the crossing of several parallel energy curves by one particular curve. Some generalizations of the Landau–Zener model were analysed recently by Brundobler and Elser [1]. An important problem is the intersection of the two families of potential curves. The complexity of the solution of this problem grows with the number of levels considered. The case of a large number of potential curves is interesting in some applications. For example, the interaction of two Rydberg series of energy levels can be approximated by two equidistant families of potential curves. This problem is considered in the present paper. It appears that it has a solution in terms of elementary functions for the limit when the number of curves in each band is infinite.

The important and unique property of the model considered here is its double periodicity in time and energy. Apparently this is the simplest non-trivial model of this kind and, therefore, it is worth full consideration. Hamiltonians that are periodic in time only have been considered by many authors and the concept of quasi-energy has been introduced in this respect. The quasi-energy  $\epsilon$  and the quasi-energetic states  $\Psi_\epsilon$  are defined by the condition  $\Psi_\epsilon(t + T_0) = \exp(i\epsilon T_0)\Psi_\epsilon(t)$ , where  $T_0$  is the period of the Hamiltonian  $\mathcal{H}(t)$  (see e.g. Manakov *et al* [8]). The energy shift periodicity has also been considered by some authors [10]. The general properties of systems that are periodic in time and energy can be understood using the investigating model.

Some examples of the physical realization of the band-crossing problem were discussed recently by Demkov and Ostrovsky [4]. The general properties of the potential curves were established and a special model with an infinite number of parallel and equidistant potential curves was formulated. A more detailed analysis of the latter model, in both its static and dynamic aspects, constitutes the main object of this paper. The model is generalized to the case when the curve spacing is different in each band. The dynamical properties of the model are investigated in this paper. A striking similarity between the time parameter  $t$ , interaction parameter  $s$  and energy parameter  $E$  has been discovered (see formulae (14) and (15)). The evolution operator is calculated.

It is convenient to formulate the model in the diabatic basis. Each band contains an infinite number of potential curves. The related diabatic states form the Hilbert space  $\ell_2$ .

Hence, the model Hamiltonian is defined in  $\ell_2 \oplus \ell_2$  space by the infinite matrix

$$\mathcal{H}(t) = \begin{pmatrix} \ddots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ \dots & \beta_+ t - \omega_+ & 0 & 0 & \dots & \dots & v & v & v & \dots \\ \dots & 0 & \beta_+ t & 0 & \dots & \dots & v & v & v & \dots \\ \dots & 0 & 0 & \beta_+ t + \omega_+ & \dots & \dots & v & v & v & \dots \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \ddots \\ \hline \ddots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ \dots & v & v & v & \dots & \dots & \beta_- t - \omega_- & 0 & 0 & \dots \\ \dots & v & v & v & \dots & \dots & 0 & \beta_- t & 0 & \dots \\ \dots & v & v & v & \dots & \dots & 0 & 0 & \beta_- t + \omega_- & \dots \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}. \quad (1)$$

The *adiabatic* potential curves are the diagonal matrix elements of  $\mathcal{H}$  in the chosen basis

$$E = D_{\pm, m} = \beta_{\pm} t + \omega_{\pm} m \quad m \in \mathbb{Z}.$$

They depend linearly on time  $t$  with the slopes  $\beta_{\pm}$ , with  $\omega_{\pm}$  the spacings between the potential curves in each band. The bands are labelled by the subscript  $\pm$ . The interaction is introduced only between the levels from the different bands. We assume that the interaction (or coupling) does not depend on the distance between the levels. So, in the  $v = 0$  limit the two infinite equidistant systems of parallel lines crossing each other form, in the  $(E, t)$ -plane, an infinite grid of parallelograms with an evident double periodicity.

We are going to study the related dynamical problem

$$\mathcal{H}(t)F(t) = \frac{1}{ic} \frac{\partial}{\partial t} F(t) \quad (2)$$

with the constant  $c$  introduced for convenience.

The common linear term can be removed from the diagonal of the matrix  $\mathcal{H}(t)$  with the help of the phase transformation

$$F(t) = e^{ic(\beta_+ + \beta_-)t^2/4} F_0(t).$$

The function  $F_0(t)$  satisfies the equation

$$\left( \mathcal{H}(t) - \frac{\beta_+ + \beta_-}{2} t \right) F_0(t) = \frac{1}{ci} \frac{\partial}{\partial t} F_0(t).$$

The matrix  $\mathcal{H}_0(t) = \mathcal{H}(t) - \frac{\beta_+ + \beta_-}{2} t$  is of the same form as (1) but with equal slopes for the adiabatic potential curves. Hence, it is sufficient to consider the operators  $\mathcal{H}(t)$  with  $\beta_+ = -\beta_- = \beta$  only. The same transformation can be used to obtain the equation with the following linear dependence of the Hamiltonian on time  $A + Bt$  with constant matrices  $A, B$ . This problem has been analysed recently by Brundobler and Elser [1].

We are going to use the symmetrical form of the Hamiltonian only. Dividing the operator  $\mathcal{H}$  by  $\beta$  one obtains the equation of the same form with  $\beta = 1$ , and new values of the parameters  $\omega_{\pm}$  and  $c$ . Hence, we can restrict our consideration, without losing generality,

to the operators  $\mathcal{H}(t)$  with unit slopes for the diabatic potential curves:

$$\mathcal{H}(t) = \begin{pmatrix} \ddots & \vdots & \vdots & \vdots & & \ddots & \vdots & \vdots & \vdots & \\ \dots & t - \omega_+ & 0 & 0 & \dots & \dots & v & v & v & \dots \\ \dots & 0 & t & 0 & \dots & \dots & v & v & v & \dots \\ \dots & 0 & 0 & t + \omega_+ & \dots & \dots & v & v & v & \dots \\ & \vdots & \vdots & \vdots & \ddots & & \vdots & \vdots & \vdots & \ddots \\ \hline \ddots & \vdots & \vdots & \vdots & & \ddots & \vdots & \vdots & \vdots & \\ \dots & v & v & v & \dots & \dots & -t - \omega_- & 0 & 0 & \dots \\ \dots & v & v & v & \dots & \dots & 0 & -t & 0 & \dots \\ \dots & v & v & v & \dots & \dots & 0 & 0 & -t + \omega_- & \dots \\ & \vdots & \vdots & \vdots & \ddots & & \vdots & \vdots & \vdots & \ddots \end{pmatrix}. \quad (3)$$

This operator was first analysed [4, 9] in the original (diabatic) representation for equal spacings between the energy levels in both bands, i.e. for  $\omega_+ = \omega_-$  only. The energy levels for the perturbed problem were calculated, and the whole set of the potential curves was analysed. The system of potential curves is a periodic function in time for this model. The important features of the time evolution were characterized.

We continue this investigation, concentrating our attention on the problem with different level spacings in the bands. Using a Fourier transformation, the matrix operator (1) is transformed to a  $2 \times 2$  first-order matrix differential operator over the interval. The differential form of the operator is independent of the interaction parameter  $v$ . The interaction is introduced by  $v$ -dependent boundary conditions at the end points of the interval. We show that the operator is self-adjoint. Normalized diabatic and adiabatic eigenfunctions are obtained (section 2).

The evolution operator, corresponding to the dynamical equation (2), is calculated for all values of the parameters using the modulated translational invariant form for the solution of the differential equation. Simplified formulae are derived for the case of equal spacings in the bands. This common value of the spacing can be assumed to equal unity because the scaling transformation  $t \rightarrow t/\omega$  transforms the problem with equal spacing  $\omega$  to the problem with unit spacing. Evolution in this case is investigated in detail. The evolution operator for the half period is of particular interest. Simplified formulae are presented for the case when the frequency of the transitions between the levels coincides with the two inverse periods of the Hamiltonian (section 3).

If the interaction parameter  $v$  is equal to  $\omega/\pi$ , then the system of the adiabatic curves is independent of the time. It is shown that the evolution operator on the period is also independent of the initial time and equals the diabatic evolution operator. The evolution operator over half a period is antidiagonal: the initial data with support on one of the family of energy levels are transformed during the half-period to certain initial data with support on the other family. During the second-half of the period the data are transformed back to the first family of energy levels. The shift occurs on one level only. The adiabatic evolution operator is calculated (section 4).

We do not need to separately consider the cases of  $\omega_+ \neq \omega_-$  and  $\beta_+ \neq \beta_-$ , when investigating the static eigenvalue problem for a given  $v, t$ . If the system of energy curves is not symmetric, then certain linear transformations of the  $(E, t)$ -plane can be performed and the parallelograms can be transformed into squares. Then the problem is reduced to  $\omega_+ = \omega_- = 1$ ,  $\beta_+ = \beta_- = 1$ . The values of  $\omega_+, \omega_-$  are important for the dynamical problem only.

## 2. Stationary problem

Consider the matrix operator  $\mathcal{H}(t)$  in  $\ell_2 \oplus \ell_2$ . The representation given by the matrix  $\mathcal{H}(t)$  (3) will be referred to as the *adiabatic* representation. The domain of the operator coincides with the set of all elements  $\Psi$  from  $\ell_2 \oplus \ell_2$ , which are solutions of the equation  $\mathcal{H}(t)\Psi = F$  for certain  $F \in \ell_2 \oplus \ell_2$ . More precisely, the element  $\Psi = (\psi_+, \psi_-) \in \ell_2 \oplus \ell_2$  belongs to the domain of  $\mathcal{H}(t)$  if and only if the following conditions are satisfied.

(i) The sums  $\text{vp} \sum_n \psi_{\pm,n}$  converge in the principal value sense:  $\text{vp} \sum_n \psi_{\pm,n} = \lim_{N \rightarrow \infty} \sum_{n=-N}^N \psi_{\pm,n}$ ;

(ii)  $\{(\pm t + m\omega_{\pm})\psi_{\pm,m} + v(\text{vp} \sum_n \psi_{\mp,n})\}_m \in \ell_2$ .

We define the action of the operator  $\mathcal{H}(t)$  as

$$\left( \mathcal{H}(t) \begin{pmatrix} \psi_+ \\ \psi_- \end{pmatrix} \right)_m = \begin{pmatrix} (t + m\omega_+)\psi_{+,m} + v(\text{vp} \sum_n \psi_{-,n}) \\ (-t + m\omega_-)\psi_{-,m} + v(\text{vp} \sum_n \psi_{+,n}) \end{pmatrix}.$$

We are going to use the Fourier transformation

$$\tilde{f}(\varphi) = \frac{1}{\sqrt{2\pi}} \sum_n e^{-in\varphi} f_n \quad f_n = \frac{1}{\sqrt{2\pi}} \int_0^{2\pi} e^{in\varphi} \tilde{f}(\varphi) d\varphi.$$

The Fourier transformation of the operator  $\mathcal{H}(t)$  will be denoted by  $\tilde{\mathcal{H}}(t)$ . This operator is defined on the two-component functions  $\tilde{\Psi} = (\tilde{\psi}_+, \tilde{\psi}_-) \in L_2(0, 2\pi) \oplus L_2(0, 2\pi)$ . The domain of the operator  $\tilde{\mathcal{H}}(t)$  consists of functions  $\tilde{\Psi}$  which are Fourier transformations of the elements from  $\ell_2 \oplus \ell_2$  satisfying conditions (i) and (ii). The second condition is satisfied only if  $\tilde{\psi}_{\pm} \in W_2^1(0, 2\pi)$ . It follows that the boundary values  $\tilde{\psi}_{\pm}(0), \tilde{\psi}_{\pm}(2\pi)$  exist and are finite and the first condition is fulfilled. For the functions  $\tilde{\psi}_{\pm}(\varphi)$  the second condition is equivalent to the conditions

$$\left( \pm t + i\omega_{\pm} \frac{d}{d\varphi} \right) \tilde{\psi}_{\pm} + 2\pi v \delta(\varphi) \frac{\tilde{\psi}_{\mp}(0) + \tilde{\psi}_{\mp}(2\pi)}{2} \in L_2(0, 2\pi).$$

These conditions are satisfied if and only if

$$\tilde{\psi}_{\pm} \in W_2^1(0, 2\pi)$$

and

$$i\omega_{\pm} (\tilde{\psi}_{\pm}(0) - \tilde{\psi}_{\pm}(2\pi)) + \pi v (\tilde{\psi}_{\mp}(0) + \tilde{\psi}_{\mp}(2\pi)) = 0.$$

The last conditions can be written in the form

$$\begin{pmatrix} \tilde{\psi}_+(0) \\ \tilde{\psi}_-(0) \end{pmatrix} = \Gamma \begin{pmatrix} \tilde{\psi}_+(2\pi) \\ \tilde{\psi}_-(2\pi) \end{pmatrix} \quad (4)$$

$$\Gamma = \begin{pmatrix} \frac{\omega_+\omega_- - (\pi v)^2}{\omega_+\omega_- + (\pi v)^2} & \frac{2i\omega_- \pi v}{\omega_+\omega_- + (\pi v)^2} \\ \frac{2i\omega_+ \pi v}{\omega_+\omega_- + (\pi v)^2} & \frac{\omega_+\omega_- - (\pi v)^2}{\omega_+\omega_- + (\pi v)^2} \end{pmatrix}. \quad (5)$$

We have proven that the operator  $\tilde{\mathcal{H}}(t)$  is the matrix differential operator

$$\tilde{\mathcal{H}}(t) = \begin{pmatrix} t + i\omega_+ \frac{\partial}{\partial \varphi} & 0 \\ 0 & -t + i\omega_- \frac{\partial}{\partial \varphi} \end{pmatrix} \quad (6)$$

with the domain of all functions from  $W_2^1(0, 2\pi) \oplus W_2^1(0, 2\pi)$  satisfying the boundary conditions (4).

We are going to show that the operator  $\tilde{H}(t)$  is equal to a matrix operator with the singular interaction at the origin:

$$\tilde{H}(t) = \begin{pmatrix} t + i\omega_+ \frac{\partial}{\partial \varphi} & 2\pi v \delta(\varphi) \\ 2\pi v \delta(\varphi) & -t + i\omega_- \frac{\partial}{\partial \varphi} \end{pmatrix}. \quad (7)$$

The correct mathematical definition of operator (7) can be given in the framework of the distribution theory for discontinuous test functions (see [5] for details). Operator  $\tilde{H}(t)$  is a matrix first-order differential operator of the form

$$\tilde{H}(t) = i\Omega \frac{\partial}{\partial \varphi} + V\delta(\varphi) + T$$

with the constant matrices

$$\Omega = \begin{pmatrix} \omega_+ & 0 \\ 0 & \omega_- \end{pmatrix} \quad T = \begin{pmatrix} t & 0 \\ 0 & -t \end{pmatrix} = t\sigma_3 \quad V = \begin{pmatrix} 0 & 2\pi v \\ 2\pi v & 0 \end{pmatrix} = 2\pi v\sigma_1$$

where

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

are the Pauli matrices. The domain of the operator  $\tilde{H}(t)$  consists of all vector valued two-component functions  $\tilde{\Psi}(\varphi) = (\tilde{\psi}_+(\varphi), \tilde{\psi}_-(\varphi))$ , which are solutions of the equation  $\tilde{H}(t)\tilde{\Psi} = \tilde{F}$  for certain functions  $\tilde{F} \in L_2(0, 2\pi) \oplus L_2(0, 2\pi)$ . Function  $\tilde{\psi}_\pm$  is a solution of the first-order diagonal matrix differential equations with constant coefficients at every point  $\varphi \neq 0, 2\pi$ :

$$i\Omega \frac{\partial}{\partial \varphi} \tilde{\Psi} + T\tilde{\Psi} = \tilde{F}. \quad (8)$$

It follows that both components of the solution are continuous functions inside the interval; moreover,  $\tilde{\Psi} \in W_2^1(0, 2\pi) \oplus W_2^1(0, 2\pi)$ . Every function from the domain of this operator is a solution of the equation

$$i\Omega \frac{\partial}{\partial \varphi} \tilde{\Psi}(\varphi) + V\delta(\varphi)\tilde{\Psi}(\varphi) + T\tilde{\Psi}(\varphi) = \tilde{F}(\varphi). \quad (9)$$

This equation does not have any solution in the class of continuous functions  $\tilde{\Psi}$ . The natural assumption that the  $\delta$ -function is an even function can be used. This assumption leads to a formula for the delta function, defined on the discontinuous test functions [5]:

$$\delta[\psi] = \frac{\psi(+0) + \psi(2\pi)}{2}. \quad (10)$$

We then obtain boundary conditions for the function  $\tilde{\Psi}$  at the point  $\varphi = 0, 2\pi$  by integrating equation (9) from  $2\pi - \epsilon$  to  $+\epsilon$  with respect to the variable  $\varphi$  and considering the limit  $\epsilon \rightarrow 0$ :

$$i\Omega (\tilde{\Psi}(0) - \tilde{\Psi}(2\pi)) + V \frac{\tilde{\Psi}(0) + \tilde{\Psi}(2\pi)}{2} = 0.$$

These conditions can be written in the form

$$\tilde{\Psi}(0) = (\Omega - iV/2)^{-1}(\Omega + iV/2)\tilde{\Psi}(2\pi)$$

and coincide with the boundary conditions defined by the matrix  $\Gamma$  (5).

We note that the differential form of the operator is independent of the interaction parameter  $v$ . Only the boundary conditions contain this dependence. The matrix  $\Gamma$  has a simpler form if the following notations are used:

$$\frac{\pi v}{\sqrt{\omega_- \omega_+}} = \tan \pi s \rightarrow$$

$$\rightarrow \Gamma = \begin{pmatrix} \cos 2\pi s & i\sqrt{\frac{\omega_-}{\omega_+}} \sin 2\pi s \\ i\sqrt{\frac{\omega_+}{\omega_-}} \sin 2\pi s & \cos 2\pi s \end{pmatrix}.$$

If the spacings between the levels in the bands are equal i.e.  $\omega_+ = \omega_-$ , then the matrix  $\Gamma$  is unitary and can be written as an exponential:  $\Gamma = e^{2\pi i s \sigma_1}$ , where  $\sigma_1$  is the Pauli matrix.

The operator  $\tilde{\mathcal{H}}(t)$  is self-adjoint for all values of  $\omega_-$ ,  $\omega_+$ . Indeed, the boundary form of the operator is

$$\begin{aligned} \langle \langle \tilde{\mathcal{H}}(t) \tilde{\Psi}, \tilde{\Phi} \rangle \rangle - \langle \langle \tilde{\Psi}, \tilde{\mathcal{H}}(t) \tilde{\Phi} \rangle \rangle \\ = i \left[ \omega_+ \left\{ \tilde{\psi}_+(2\pi) \overline{\tilde{\phi}_+(2\pi)} - \tilde{\psi}_+(0) \overline{\tilde{\phi}_+(0)} \right\} \right. \\ \left. + \omega_- \left\{ \tilde{\psi}_-(2\pi) \overline{\tilde{\phi}_-(2\pi)} - \tilde{\psi}_-(0) \overline{\tilde{\phi}_-(0)} \right\} \right] = 0. \end{aligned}$$

Here  $\langle \langle *, * \rangle \rangle$  denotes the standard scalar product in  $L_2(0, 2\pi) \oplus L_2(0, 2\pi)$ . The adjoint operator  $\tilde{\mathcal{H}}^*(t)$  is defined by the same differential expression on a subset of functions from  $W_2^1(0, 2\pi) \oplus W_2^1(0, 2\pi)$ . Any element  $G$  from this domain defines a continuous form on the domain of the operator  $\tilde{\mathcal{H}}(t)$  by the formula  $\langle \langle \tilde{\mathcal{H}}F, G \rangle \rangle$  only if this element satisfies the same boundary conditions (4). Thus, the operator  $\tilde{\mathcal{H}}(t)$  is self-adjoint.

The operator  $\tilde{\mathcal{H}}(t)$  has a purely discrete spectrum (the adiabatic potential curves), which depends on the parameter  $t$ . The related eigenfunctions satisfy the equations

$$\begin{cases} t\tilde{\psi}_+ + i\omega_+ \frac{\partial}{\partial \varphi} \tilde{\psi}_+ = E\tilde{\psi}_+ \\ -t\tilde{\psi}_- + i\omega_- \frac{\partial}{\partial \varphi} \tilde{\psi}_- = E\tilde{\psi}_- \end{cases} \quad (11)$$

with the boundary conditions (4). The general solution of system (11) is

$$\begin{cases} \tilde{\psi}_+ = c_+ e^{i\pi(t-E)\varphi/\omega_+} \\ \tilde{\psi}_- = c_- e^{-i\pi(t+E)\varphi/\omega_-} \end{cases} \quad (12)$$

where the constants  $c_{\pm}$  can be calculated by substituting ansatz (12) into the boundary conditions (4):

$$\begin{pmatrix} \sqrt{\frac{\omega_+}{\omega_-}} e^{i\pi(t-E)/\omega_+} \cos \pi s \sin \frac{\pi(t-E)}{\omega_+} & e^{-i\pi(t+E)/\omega_-} \sin \pi s \cos \frac{\pi(t+E)}{\omega_-} \\ e^{i\pi(t-E)/\omega_+} \sin \pi s \cos \frac{\pi(t-E)}{\omega_+} & -\sqrt{\frac{\omega_-}{\omega_+}} e^{-i\pi(t+E)/\omega_-} \cos \pi s \sin \frac{\pi(t+E)}{\omega_-} \end{pmatrix} \begin{pmatrix} c_+ \\ c_- \end{pmatrix} = 0. \quad (13)$$

This linear system has solutions if and only if the determinant of the matrix is equal to zero. This condition defines the adiabatic spectrum of the problem:

$$\tan \frac{\pi(t-E)}{\omega_+} \tan \frac{\pi(t+E)}{\omega_-} + (\tan \pi s)^2 = 0. \quad (14)$$

We first discuss the system of potential curves for the case  $\omega_- = \omega_+ = 1$ . This will be referred to as the *symmetric* case. The dispersion (eigenvalue) equation for this case was first derived using the diabatic representation by Demkov and Ostrovsky [4]. Another form

of the dispersion equation, in this case, shows the striking similarity between the parameters  $t$  and  $s$ :

$$(\tan \pi E)^2 = \frac{(\tan \pi s)^2 + (\tan \pi t)^2}{1 + (\tan \pi s)^2 (\tan \pi t)^2}. \quad (15)$$

This formula defines a surface in the  $(E, s, t)$ -space which is triple periodic along all three axes with all three periods equal to one. The general shape of this surface is presented in figure 1. The equi-energy curves are shown by figure 2.

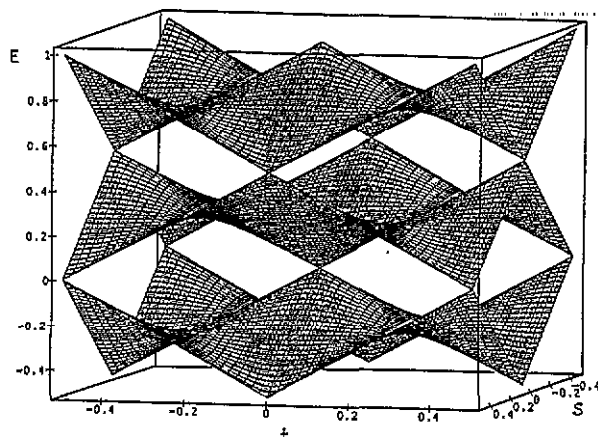


Figure 1. The system of potential surfaces for the symmetric case  $\omega_- = \omega_+ = 1$ . All properties considered in cases (1)–(9) can be seen.

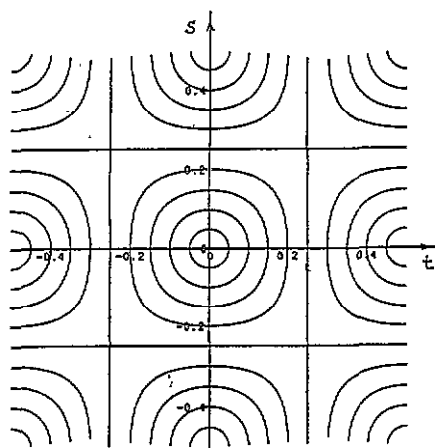


Figure 2. Equi-energy curves  $E = 0.5, 0.15, 0.20, 0.25, 0.30, 0.35, 0.40, 0.45$  for  $\omega_+ = \omega_- = 1$ . Transitions from the ellipse in the vicinity of the degenerate points to the rectangles in the iso-energetic region can be easily seen.

Let us consider the intersections of this surface with the planes defined by the equations



$\tan \pi s$ ,  $\tan \pi t$  and  $\tan \pi E$  equal to 0, 1 or infinity.

	0	1	$\infty$
$\tan \pi s$	1	2	3
$\tan \pi t$	4	5	6
$\tan \pi E$	7	8	9

(1) Purely diabatic case  $E = \pm t + n$ . Rectangular grid of two mutually crossing infinite equidistant parallel straight lines in the  $(E, t)$ -plane.

(2)  $E = n \pm \frac{1}{4}$ , iso-energetic case, all lines are  $t$  independent parallel with the distance  $1/2$ .

(3) Antidiabatic case  $E = n + \frac{1}{2} \pm \frac{1}{4}$ . The rectangular grid with the crossing points in the centres of the diabatic grid (case (1)).

(4)  $E = \pm s + n$ . The energy curves form a rectangular grid in the  $(E, s)$  plane. If  $s$  is small, then this formula indicates the pseudocrossing splitting  $\Delta E = 2s$ .

(5)  $\tan \pi E = \pm 1$ . The energy  $E = n \pm \frac{1}{4}$  is independent of  $s$ . These lines correspond to the stationary points in the  $(E, t)$  plane. All  $E(s, t)$  cross at these points.

(6)  $\tan \pi E = \pm \cot \pi s \Rightarrow E = \pm s + n + \frac{1}{2}$ . Rectangular grid in the  $(E, s)$  plane between the grid in case (4).

(7) (a)  $\tan \pi s = 0$  and  $\tan \pi t = 0$ . The diabatic degeneration points. In the vicinity of these points the surface is close to a circular cone, which is the demonstration of the Neumann-Wigner theorem; (b)  $\cot \pi s = 0, \cot \pi t = 0 \rightarrow s = n + \frac{1}{2}, t = m + \frac{1}{2}$ . These points form a square-centred grid in each plane  $E = n$ .

(8) Either  $s = n \pm \frac{1}{4}$  or  $t = m \pm \frac{1}{4}$ . The rectangular grid in the  $(s, t)$  plane with the  $(\frac{1}{2}, \frac{1}{2})$ -size squares.

(9) Either  $\tan \pi s = 0 (s = n)$  and  $\cot \pi t = 0 (t = m + \frac{1}{2})$ , or  $\tan \pi t = 0 (t = n)$  and  $\cot \pi s = 0 (s = m + \frac{1}{2})$ . These are the adiabatic crossing points or the antidiabatic conic intersections in the  $(E, t, s)$ -space. The points form a square centred grid shifted by  $\frac{1}{2}$  in the  $t$  or  $s$  direction relative to case (7).

In the symmetric case the Hamiltonian is periodic with period one. More precisely, Hamiltonians corresponding to different  $t$  and  $t'$ ,  $t - t' = m \in \mathbb{Z}$  are unitary equivalent. The unitary transformation connecting these operators is the translation of the  $+$  and  $-$  components on the  $m$  units in the opposite directions. Note that in the diabatic basis this periodicity is hidden, but in the adiabatic representation it appears explicitly.

The system of the energy curves is invariant with respect to the shift of the parameters  $(s, t) \rightarrow (s \pm 1/2, t \pm 1/2)$ :

$$E(s \pm 1/2, t \pm 1/2) = E(s, t).$$

Note that a shift of the parameter  $s$  on  $1/2$ :  $s \rightarrow s + 1/2$  corresponds to the transformation of the parameter  $v$ :  $v \rightarrow \pi^2/v$ . The system of the energy levels is doubly periodic in the  $(t, E)$ -plane with the invariant translation vectors  $(\frac{1}{2}, \pm \frac{1}{2})$ :

$$(t, E) \rightarrow (t + \frac{1}{2}, E + \frac{1}{2})$$

$$(t, E) \rightarrow (t + \frac{1}{2}, E - \frac{1}{2}).$$

The structure of the potential curves in the non-symmetric case  $\omega_+ \neq \omega_-$  is similar (see figure 3). It is invariant under the translations by the vectors  $(\omega_-/2, \omega_-/2)$ ,  $(\omega_+/2, -\omega_+/2)$ :

$$(t, E) \rightarrow (t + \omega_-/2, E + \omega_-/2)$$

$$(t, E) \rightarrow (t + \omega_+/2, E - \omega_+/2).$$

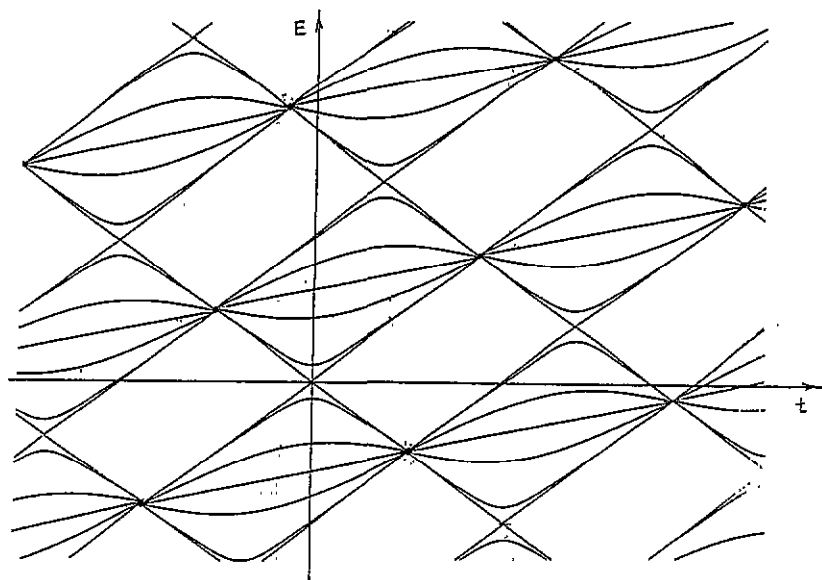


Figure 3. The system of potential curves for  $\omega_+ = 1, \omega_- = 1.7$ .

The system of energy levels for all values of the interaction parameter  $v$  (or  $s$ ) contains the points  $(t, E)$  of both of the types

$$(t, E) = \left(\frac{\omega_-}{4}, \frac{\omega_-}{4}\right) + l \left(\frac{\omega_-}{2}, \frac{\omega_-}{2}\right) + m \left(\frac{\omega_+}{2}, -\frac{\omega_+}{2}\right) \quad l, m \in \mathbb{Z}$$

$$(t, E) = \left(\frac{\omega_+}{4}, -\frac{\omega_+}{4}\right) + l \left(\frac{\omega_-}{2}, \frac{\omega_-}{2}\right) + m \left(\frac{\omega_+}{2}, -\frac{\omega_+}{2}\right) \quad l, m \in \mathbb{Z}.$$

We show that the dispersion (eigenvalue) equation is satisfied at the point  $(\omega_-/4, \omega_-/4)$  for all values of the interaction parameter  $v(s)$ :

$$\sin \frac{\pi(t-E)}{\omega_+} \sin \frac{\pi(t+E)}{\omega_-} (\cos \pi s)^2 + (\sin \pi s)^2 \cos \frac{\pi(t-E)}{\omega_+} \cos \frac{\pi(t+E)}{\omega_-}$$

$$= \sin 0 \sin \frac{\pi}{2} (\cos \pi s)^2 + (\sin \pi s)^2 \cos 0 \cos \frac{\pi}{2} = 0.$$

The other points from this lattice can be considered in the same way. These will be referred to as *stationary points*. They are important for further considerations of the dynamical problem.

The system of energy levels is symmetric with respect to the stationary points. Consider, for example, point  $(\omega_-/4, \omega_-/4)$ . Let  $(t, E)$  be a solution of the dispersion equation (14). Then, the symmetric point  $(t', E') = (-t + \omega_-/2, -E + \omega_-/2)$  is also a solution of the dispersion equation:

$$\tan \frac{\pi(t'-E')}{\omega_+} \tan \frac{\pi(t'+E')}{\omega_-} + (\tan \pi s)^2$$

$$= \tan \frac{\pi(-t+E)}{\omega_+} \tan \frac{\pi(-t'-E'+\omega_-)}{\omega_-} + (\tan \pi s)^2$$

$$= \tan \frac{\pi(t-E)}{\omega_+} \tan \frac{\pi(t+E)}{\omega_-} + (\tan \pi s)^2 = 0.$$

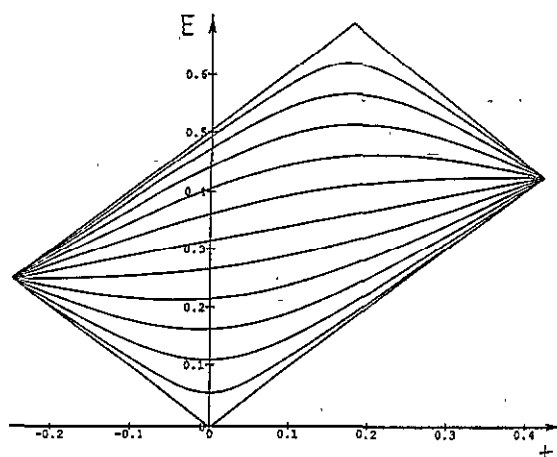


Figure 4. The potential curves in the main parallelogram for  $\omega_+ = 1$ ,  $\omega_- = 1.7$ ,  $s = n/24$ ,  $n = 1, 2, \dots, 11$ . Transition from the diabatic case ( $s = 0$ ) through the iso-energetic (linear) ( $s = \frac{1}{4}$ ) case to the antidiabatic case ( $s = \frac{1}{2}$ ) can be seen.

Let us denote the solution of equation (14) inside the parallelogram with the vertices  $\{(0, 0), (\omega_-/4, \omega_-/4), (-\omega_+/4, \omega_+/4), ((\omega_- - \omega_+)/4, (\omega_- + \omega_+)/4)\}$  by  $E_{+,0}(t)$ . Let the potential curve be known in this cell for a fixed value of the interaction  $v$  (see figure 4). Then, the potential curves in the whole  $(t, E)$  plane can be restored using the invariance transformations described above. Firstly, we can continue this potential curve symmetrically with respect to the point  $(\omega_-/4, \omega_-/4)$  and it can then be continued using translations by the vectors  $n((\omega_- + \omega_+)/2, (\omega_- - \omega_+)/2)$ ,  $n \in \mathbb{Z}$ . Another curve is symmetric with respect to the point  $((\omega_- + \omega_+)/4, (\omega_- - \omega_+)/4)$ :

$$E_{-,0}(t) = -E_{+,0}\left(-t + \frac{\omega_- + \omega_+}{2}\right) + \frac{\omega_- - \omega_+}{2}.$$

Two series of solutions of the dispersion equation can be introduced:

$$E_{\pm,n}(t) = E_{\pm,0}\left(t - n\frac{\omega_- - \omega_+}{2}\right) + n\frac{\omega_- + \omega_+}{2} \quad n \in \mathbb{Z}.$$

In the case of the weak interaction  $v \rightarrow 0$ , the solutions  $E_{\pm,n}$  approach the diabatic curves

$$D_{\pm,m}(t) = \pm t + m\omega_{\pm} \quad m \in \mathbb{Z}.$$

For  $v = 0$  (no interaction occurs) we obtain the standard diabatic levels  $E = D_{\pm,m}$  with the crossing points

$$\left\{n\left(\frac{\omega_-}{2}, \frac{\omega_-}{2}\right) + m\left(\frac{\omega_+}{2}, -\frac{\omega_+}{2}\right); n, m \in \mathbb{Z}\right\}.$$

The infinite interaction ( $v = \infty$ ) defines the potential curves

$$E = \pm t + (m + \frac{1}{2})\omega_{\pm} \quad m \in \mathbb{Z},$$

with the crossings at the points

$$\left\{\left(\frac{\omega_+ + \omega_-}{4}, \frac{\omega_- - \omega_+}{4}\right) + n\left(\frac{\omega_-}{2}, \frac{\omega_-}{2}\right) + m\left(\frac{\omega_+}{2}, -\frac{\omega_+}{2}\right); n, m \in \mathbb{Z}\right\}.$$

The curves (actually the straight lines) obtained in the limit of superstrong interaction were named *antidiabatic* by Demkov and Ostrovsky ([4]). For the small interaction  $v \rightarrow 0$ , one

observes avoided crossings of the adiabatic curves in the neighbourhood of the crossings of the diabatic curves. For the large interaction  $v \rightarrow \infty$ , a similar picture can be observed close to the crossings of the antidiabatic curves. These antidiabatic avoided crossings were also obtained for the finite number of states within both bands (see [4]).

The linear dependence of the adiabatic curves on the parameter  $t$  occurs in the case  $v\pi/\sqrt{\omega_+\omega_-} = 1$ , ( $s = 1/4$ ). Solutions of the dispersion equation form the straight lines passing through the stationary points:

$$E_{\pm,n} = \frac{\omega_- - \omega_+}{\omega_- + \omega_+}t + (2n \pm \frac{1}{2})\frac{\omega_- \omega_+}{2(\omega_- + \omega_+)}.$$

We have, in this case,

$$\tan \pi \frac{t-E}{\omega_+} \tan \pi \frac{t+E}{\omega_-} = \tan \left( \frac{\pi}{2} + \frac{2t - \omega_-/2}{\omega_- + \omega_+} \right) \tan \left( \frac{2t - \omega_-/2}{\omega_- + \omega_+} \right) = -1$$

and the dispersion equation is satisfied. The potential lines are horizontal in the symmetric case  $\omega_- = \omega_+ = \omega$  and the spectrum of the Hamiltonian does not depend on  $t$ . This is referred to as the *isospectral* case:

$$E_{\pm,n}(t) = \omega(\pm \frac{1}{4} + n) \quad n \in \mathbb{Z}.$$

Another set of lines passing through the stationary points

$$\tilde{E}_{\pm,n}(t) = \frac{\omega_- + \omega_+}{\omega_- - \omega_+}t + (2n \pm \frac{1}{2})\frac{\omega_- \omega_+}{2(\omega_- - \omega_+)}$$

corresponds to the complex values of the interaction parameter  $\tan \pi s = i$ . These lines become vertical in the limit of equal spacing  $\omega_- = \omega_+$ .

As in the original Landau-Zener model, if the interaction is not equal to zero or infinity, i.e.  $s \neq 0, 1/2$ , then the energy curves intersect at the complex values of the time parameter  $t$ . These branching points of the  $E$  function in the complex  $t$ -plane play an important role in the calculations of the non-diabatical transitions when the factor in front of the time derivative tends to zero.

Consider the symmetric case for simplicity i.e.  $\omega_+ = \omega_- = 1$ . The intersection occurs at the points with the same values of the energy parameter  $E$ , as the intersection of the diabatic and antidiabatic curves, i.e. at the points with  $E_1 = 0, \pm 1, \pm 2, \dots$  or  $E_2 = \pm 1/2, \pm 3/2, \pm 5/2, \dots$ . Let  $|s| \ll 1$ , then the first set of the energy values corresponds to the time parameter with real part  $\text{Re } t = n, n \in \mathbb{Z}$ . The imaginary part of  $t$  is defined by the equation

$$(\tan \pi s)^2 + (\tan \pi t)^2 = 0.$$

The solution is given by

$$t = \pm i \frac{\tanh^{-1}(\tan \pi s)}{\pi} + n \quad n \in \mathbb{Z}.$$

A numerical solution for this equation is presented in figure 5. Solutions from the second set are defined by the values of  $t$  with real part  $\text{Re } t = 1/2 + n, n \in \mathbb{Z}$ . The corresponding equation

$$(\cot \pi t)^2 + (\tan \pi s)^2 = 0$$

defines the solution

$$t = \pm i \frac{\tanh^{-1}(\tan \pi s)}{\pi} + 1/2 + n \quad n \in \mathbb{Z}.$$

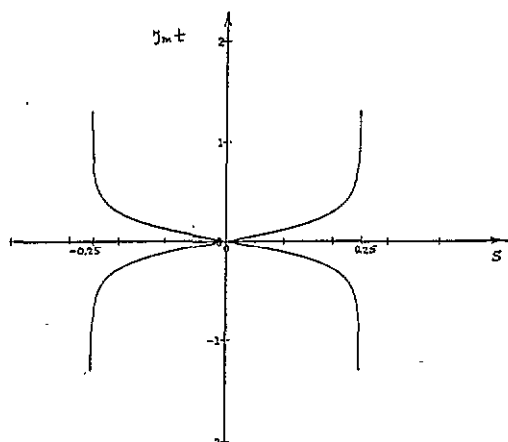


Figure 5. Complex intersection of the energy surfaces for the symmetric case  $\omega_+ = \omega_- = 1$ . These intersections tend to infinity, approaching the iso-energetic case.

The same phenomenon is observed close to the intersection of the antidiabatic curves. Suppose that the interaction is strong, i.e.  $|s - 1/2| \ll 1$ . The energy curves intersect at the same values of the energy parameter. The corresponding equations for the parameter  $t$  are

$$(\cot \pi s)^2 + (\tan \pi t)^2 = 0$$

and

$$(\cot \pi s)^2 + (\cot \pi t)^2 = 0.$$

The solutions are equal to

$$t = \pm i \frac{\tanh^{-1} \cot \pi s}{\pi} + 1/2 + n$$

and

$$t = \pm i \frac{\tanh^{-1}(\cot \pi s)}{\pi} + n.$$

All the branching points tend to infinity in the isospectral case when all eigenenergies are independent of time.

The time-dependent adiabatic basis  $\{\tilde{\Psi}^{\pm, n}\}$ , which diagonalizes the operator  $\tilde{\mathcal{H}}(t)$ , can be calculated using the solutions of equation (13). The formulae are presented below for the symmetric case  $\omega_- = \omega_+ = 1$  only, to avoid complicated expressions. The structure of the formulae corresponding to the general case is essentially the same, although no periodicity with respect to the time variable occurs in the general case. The upper index  $(\pm, n)$  corresponds to the energy level  $E_{\pm, n}$ , but the lower index denotes the first and the second components of the vector valued function. The matrix  $\mathcal{H}(t)$  is real in the diabatic representation. Hence, the basis can also be chosen real in the diabatic representation. We shall use this property to fix the phase of the eigenfunctions. Such a normalized adiabatic basis is

$$\tilde{\Psi}_{\pm}^{\pm, n}(\varphi) = \frac{\text{sign}(\sin \pi(t \pm 1/4)) \sin \pi(t \pm E_{+,0}(t)) \cos \pi s e^{-i\pi(t \mp E_{+,0}(t))}}{\sqrt{2\pi} \sqrt{(\cos \pi s)^2 (\sin \pi(t \pm E_{+,0}(t)))^2 + (\sin \pi s)^2 (\cos \pi(t \mp E_{+,0}(t)))^2}} \times e^{i(t \mp E_{+,0}(t) - n)\varphi}$$

$$\tilde{\psi}_{\pm}^{\pm,n}(\varphi) = \frac{\text{sign}(\sin \pi(t \pm 1/4)) \cos \pi(t \mp E_{+,0}(t)) \sin \pi s e^{i\pi(t \pm E_{+,0}(t))}}{\sqrt{2\pi} \sqrt{(\cos \pi s)^2 (\sin \pi(t \pm E_{+,0}(t)))^2 + (\sin \pi s)^2 (\cos \pi(t \mp E_{+,0}(t)))^2}} \times e^{-i(t \pm E_{+,0}(t) + n)\varphi}. \quad (16)$$

The adiabatic basis is periodic with period two, but the period of the Hamiltonian is equal to one in the symmetric case under consideration. This means that Berry's phase in this case is equal to  $\pi$ . Note that the coefficients in front of the exponentials are independent of the index  $n$ .

In the adiabatic representation this basis has the form

$$\begin{aligned} \Psi^{\pm,n} &= \left( \{\psi_{+,j}^{\pm,n}\}_{j \in \mathbb{Z}}, \{\psi_{-,j}^{\pm,n}\}_{j \in \mathbb{Z}} \right) \\ \psi_{+,j}^{\pm,n} &= \frac{\text{sign}(\sin \pi(t \pm 1/4)) (-\cos 2\pi t + \cos 2\pi E_{+,0}(t))}{2\pi \sqrt{(\cos \pi s)^2 (\sin^2 \pi(t \pm E_{+,0}(t)))^2 + (\sin \pi s)^2 (\cos \pi(t \mp E_{+,0}(t)))^2}} \\ &\quad \times \frac{\cos \pi s}{t \mp E_{+,0}(t) - n + j} \\ \psi_{-,j}^{\pm,n} &= \frac{\text{sign}(\sin \pi(t \pm 1/4)) (\sin 2\pi t \pm \sin 2\pi E_{+,0}(t))}{2\pi \sqrt{(\cos \pi s)^2 (\sin \pi(t \pm E_{+,0}(t)))^2 + (\sin \pi s)^2 (\cos \pi(t \mp E_{+,0}(t)))^2}} \\ &\quad \times \frac{\sin \pi s}{t \pm E_{+,0}(t) + n - j}. \end{aligned} \quad (17)$$

This last formula is valid for all  $t$ , such that  $t \pm E_{\pm,0}(t) \notin \mathbb{Z}$ , and is equivalent to the equations (2.1)–(2.6) from the [4] up to the normalization factor, which was not considered there. We obtain this formula using the definition of the delta function (10). This shows again that the chosen definition of the delta function is natural. The existence of a *sign* factor makes the time periodicity of the  $\psi$ — equal to two instead of one.

The adiabatic basis has the simplest form at the stationary points  $t = 1/4 + n/2$ ,  $n \in \mathbb{Z}$ . The basis vectors have a Fourier representation in the form

$$\begin{aligned} \tilde{\Psi}^{+,n}(1/4, \varphi) &= \frac{1}{\sqrt{2\pi}} \begin{pmatrix} \cos \pi s \\ i \sin \pi s e^{-i\varphi/2} \end{pmatrix} e^{-in\varphi} \\ \tilde{\Psi}^{-,n}(1/4, \varphi) &= \frac{\text{sign}(\sin 2\pi s)}{\sqrt{2\pi}} \begin{pmatrix} -i \sin \pi s e^{+i\varphi/2} \\ -\cos \pi s \end{pmatrix} e^{-in\varphi} \\ \tilde{\Psi}^{+,n}(3/4, \varphi) &= \frac{\text{sign}(\sin 2\pi s)}{\sqrt{2\pi}} \begin{pmatrix} -i \sin \pi s e^{i\varphi/2} \\ -\cos \pi s e^{-i\varphi} \end{pmatrix} e^{-in\varphi} \\ \tilde{\Psi}^{-,n}(3/4, \varphi) &= \frac{1}{\sqrt{2\pi}} \begin{pmatrix} -\cos \pi s e^{i\varphi} \\ -i \sin \pi s e^{-i\varphi/2} \end{pmatrix} e^{-in\varphi}. \end{aligned} \quad (18)$$

Although the potential curves are  $s$ — independent at the stationary points, the adiabatic states explicitly depend on the interaction. They can be compared with the diabatic states, e.g. at the point  $t = 1/4$  we obtain

$$\tilde{\Psi}_d^{+,n}(1/4, \varphi) = \frac{1}{\sqrt{2\pi}} \begin{pmatrix} 1 \\ 0 \end{pmatrix} e^{-in\varphi}, \quad \tilde{\Psi}_d^{-,n}(1/4, \varphi) = \frac{1}{\sqrt{2\pi}} \begin{pmatrix} 0 \\ 1 \end{pmatrix} e^{-in\varphi}.$$

### 3. Time evolution

We now consider the time evolution governed by the operator  $\mathcal{H}(t)$ :

$$\mathcal{H}(t)F(t) = \frac{1}{ic} \frac{\partial}{\partial t} F(t). \quad (19)$$

This equation corresponds to the differential equation in the Fourier representation

$$\begin{cases} \left(t + \frac{i}{c} \frac{\partial}{\partial t}\right) \tilde{f}_+(t, \varphi) + i\omega_+ \frac{\partial}{\partial \varphi} \tilde{f}_+(t, \varphi) = 0 \\ \left(-t + \frac{i}{c} \frac{\partial}{\partial t}\right) \tilde{f}_-(t, \varphi) + i\omega_- \frac{\partial}{\partial \varphi} \tilde{f}_-(t, \varphi) = 0 \end{cases} \quad (20)$$

with the boundary conditions

$$\begin{pmatrix} \tilde{f}_+(t, 0) \\ \tilde{f}_-(t, 0) \end{pmatrix} = \Gamma \begin{pmatrix} \tilde{f}_+(t, 2\pi) \\ \tilde{f}_-(t, 2\pi) \end{pmatrix}. \quad (21)$$

Both equations are decoupled and do not depend on the interaction  $v$  (or  $s$ ) except for the boundary conditions at  $\varphi = 0, 2\pi$ . Therefore, the general solution of equation (20) has the modulated translational invariant form

$$\tilde{f}_{\pm}(t, \varphi) = g_{\pm} \left( t - \frac{\varphi}{c\omega_{\pm}} \right) e^{\pm i c t^2 / 2}. \quad (22)$$

Thus, the initially prepared, arbitrary wave packet  $g$  shifts as time increases in the positive direction along the  $\varphi$  axis. Note that the  $+$  and  $-$  components are moving with different speeds. The component shapes are not changed but additional phases are gained which differ for  $+$  and  $-$  components. At the boundaries the components are mixed by the discrete transformations. Substitution into the boundary conditions gives a functional equation on the functions  $g_{\pm}$ :

$$\begin{pmatrix} g_+(t) \\ g_-(t) \end{pmatrix} = \begin{pmatrix} e^{-i c t^2 / 2} & 0 \\ 0 & e^{i c t^2 / 2} \end{pmatrix} \Gamma \begin{pmatrix} e^{i c t^2 / 2} & 0 \\ 0 & e^{-i c t^2 / 2} \end{pmatrix} \begin{pmatrix} g_+(t - 2\pi / c\omega_+) \\ g_-(t - 2\pi / c\omega_-) \end{pmatrix}. \quad (23)$$

The time-dependent problem can be solved in the following way. From the initial data at time  $t$ , one can define functions  $g_{\pm}$  on the intervals  $(t - 2\pi / c\omega_+, t)$  and  $(t - 2\pi / c\omega_-, t)$ ; then using the functional equation (23) these functions can be calculated on the whole half-axis  $(t, \infty)$ . The functional equation connects the values of the  $+$  and  $-$  components of the function  $g$  at different points. The solution procedure can be simplified in the symmetric case when the functional equation is solvable by iterations. Let  $\omega_- = \omega_+ = \omega$ ,  $\tau = 2\pi / c\omega$ . Iterating equation (23) we obtain a formula which connects the values of the functions  $g_{\pm}(t)$  at points  $t + n\tau$  and  $t$ :

$$\begin{pmatrix} g_+(t + n\tau) \\ g_-(t + n\tau) \end{pmatrix} = W_n(t) \begin{pmatrix} g_+(t) \\ g_-(t) \end{pmatrix}$$

where

$$\begin{aligned} W_n(t) &= G(t + n\tau) G(t + (n-1)\tau) \cdots G(t + \tau) \\ G(t) &= \begin{pmatrix} e^{-i c t^2 / 2} & 0 \\ 0 & e^{i c t^2 / 2} \end{pmatrix} \Gamma \begin{pmatrix} e^{i c t^2 / 2} & 0 \\ 0 & e^{-i c t^2 / 2} \end{pmatrix}. \end{aligned} \quad (24)$$

We shall calculate the evolution operator  $U(t, t+T)$  for the positive values of  $T > 0$ . The following notations will be used:  $T = m\tau + a$ ,  $m \in \mathbb{Z}$ ,  $0 \leq a < \tau$ . Firstly we shall define the values of the functions  $g_{\pm}(s)$  on the interval  $(t+T-\tau, t+T)$  from their values on the interval  $(t-\tau, t)$ :

$$\begin{aligned} \begin{pmatrix} g_+(t+T-b) \\ g_-(t+T-b) \end{pmatrix} &= \left\{ \chi_{b < a} W_{m+1}(t-b+a-\tau) \begin{pmatrix} g_+(t-b+a-\tau) \\ g_-(t-b+a-\tau) \end{pmatrix} \right. \\ &\quad \left. + \chi_{b > a} W_m(t-b+a) \begin{pmatrix} g_+(t-b+a) \\ g_-(t-b+a) \end{pmatrix} \right\}. \end{aligned} \quad (25)$$

Here  $\chi$  denotes the characteristic function

$$\chi_{b < a}(s) = \begin{cases} 1, & b < a \\ 0, & b > a \end{cases} \quad \chi_{b > a}(s) = \begin{cases} 0, & b < a \\ 1, & b > a \end{cases} \quad 0 \leq b < \tau.$$

Now the evolution operator acts in the Fourier representation:

$$\begin{aligned} \begin{pmatrix} \tilde{f}_+(t+T, \varphi) \\ \tilde{f}_-(t+T, \varphi) \end{pmatrix} &= \tilde{U}(t, t+T) \begin{pmatrix} \tilde{f}_+(t, \varphi) \\ \tilde{f}_-(t, \varphi) \end{pmatrix} \\ &= \begin{pmatrix} e^{2\pi i(t+T)^2} & 0 \\ 0 & e^{-2\pi i(t+T)^2} \end{pmatrix} \left\{ \chi_{\varphi/c\omega < a} W_{m+1} \left( t - \frac{\varphi}{c\omega} + a - \tau \right) \right. \\ &\quad \times \begin{pmatrix} e^{-2\pi i\tau^2} & 0 \\ 0 & e^{2\pi i\tau^2} \end{pmatrix} \begin{pmatrix} \tilde{f}_+(t, \varphi - c\omega(a - \tau)) \\ \tilde{f}_-(t, \varphi - c\omega(a - \tau)) \end{pmatrix} + \chi_{\varphi/c\omega > a} W_m \left( t - \frac{\varphi}{c\omega} + a \right) \\ &\quad \times \begin{pmatrix} e^{-2\pi i\tau^2} & 0 \\ 0 & e^{2\pi i\tau^2} \end{pmatrix} \begin{pmatrix} \tilde{f}_+(t, \varphi - c\omega\tau) \\ \tilde{f}_-(t, \varphi - c\omega\tau) \end{pmatrix} \left. \right\}. \end{aligned} \quad (26)$$

Using the shift operator  $T_\theta \tilde{f}(t, \varphi) = \tilde{f}(t, \varphi - \theta)$  the evolution operator can be written in the form

$$\begin{aligned} \tilde{U}(t, t+T) &= \begin{pmatrix} e^{2\pi i(t+T)^2} & 0 \\ 0 & e^{-2\pi i(t+T)^2} \end{pmatrix} \left\{ \chi_{\frac{\varphi}{c\omega} < a} W_{m+1} \left( t - \frac{\varphi}{c\omega} + a - \tau \right) \right. \\ &\quad \times \begin{pmatrix} e^{-2\pi i\tau^2} & 0 \\ 0 & e^{2\pi i\tau^2} \end{pmatrix} T_{c\omega(a-\tau)} + \chi_{\frac{\varphi}{c\omega} > a} W_m \left( t - \frac{\varphi}{c\omega} + a \right) \\ &\quad \times \begin{pmatrix} e^{-2\pi i\tau^2} & 0 \\ 0 & e^{2\pi i\tau^2} \end{pmatrix} T_{c\omega a} \left. \right\}. \end{aligned} \quad (27)$$

The form of the evolution operator for zero values of  $a$  is of particular interest. The expression for the evolution operator can be simplified in this case:

$$\tilde{U}(t, t+m\tau) = \begin{pmatrix} e^{2\pi i(t+m\tau)^2} & 0 \\ 0 & e^{-2\pi i(t+m\tau)^2} \end{pmatrix} W_m \left( t - \frac{\varphi}{c\omega} \right) \begin{pmatrix} e^{-2\pi i\tau^2} & 0 \\ 0 & e^{2\pi i\tau^2} \end{pmatrix}. \quad (28)$$

The spacing between the levels can be chosen to be equal to unity, i.e.  $\omega = 1$ . The parameter  $\tau = 2\pi/c\omega$  has a simple meaning: this is the period related to the level spacing  $\omega$  in the bands. The other period is also intrinsic for the system: the period of the Hamiltonian. As shown in section 2, this period is equal to one assuming that the time scaling is performed to fix  $\omega = 1$ . The presence of two periods makes the dynamics quite complicated as formula (27) shows. Even the propagator over an integer number of periods (28) is not expressed in simple terms.

Considerable simplification is achieved in the case when the periods differ by a rational factor. We choose  $c = 4\pi$ , then  $\tau = \frac{1}{2}$ . The evolution operator on the half period and on the period is equal, respectively, to

$$\tilde{U}(t, t+1/2) = \begin{pmatrix} ie^{2\pi i\tau} \cos 2\pi s & e^{-i\varphi^2/4\pi} e^{2i\varphi(t+1/2)} e^{-2\pi i\tau} \sin 2\pi s \\ -ie^{i\varphi^2/4\pi} e^{-2i\varphi(t+1/2)} e^{2\pi i\tau} \sin 2\pi s & -ie^{-2\pi i\tau} \cos 2\pi s \end{pmatrix} \quad (29)$$

$$\begin{aligned} \tilde{U}(t, t+1) &= \begin{pmatrix} e^{4\pi i\tau} (\cos 2\pi s)^2 + e^{i\varphi} (\sin 2\pi s)^2 & \\ -ie^{i\varphi^2/4\pi} e^{-2i\varphi(t+1/2)} (1 - e^{4\pi i\tau} e^{-i\varphi}) \sin 4\pi s/2 & \\ -ie^{-i\varphi^2/4\pi} e^{2i\varphi(t+1/2)} (1 - e^{-4\pi i\tau} e^{i\varphi}) \sin 4\pi s/2 & \\ e^{-4\pi i\tau} (\cos 2\pi s)^2 + e^{-i\varphi} (\sin 2\pi s)^2 & \end{pmatrix} \end{aligned} \quad (30)$$

The evolution operator between the stationary points is of particular interest:

$$\tilde{U}(1/4, 3/4) = \begin{pmatrix} P - \cos 2\pi s & -ie^{-i\varphi^2/4\pi} e^{3i\varphi/2} \sin 2\pi s \\ -ie^{i\varphi^2/4\pi} e^{-3i\varphi/2} \sin 2\pi s & -\cos 2\pi s \end{pmatrix} \quad (31)$$



$$\tilde{U}(1/4, 5/4) = \begin{pmatrix} -(\cos 2\pi s)^2 + e^{i\varphi}(\sin 2\pi s)^2 & -ie^{-i\varphi^2/4\pi} e^{2i\varphi} \cos \varphi/2 \sin 4\pi s \\ -ie^{i\varphi^2/4\pi} e^{-2i\varphi} \cos \varphi/2 \sin 4\pi s & -(\cos 2\pi s)^2 + e^{-i\varphi}(\sin 2\pi s)^2 \end{pmatrix}. \quad (32)$$

One can see that the evolution operator for the half-integer  $T$  with respect to the shift of variables  $s \rightarrow s + 1/2, t \rightarrow t + 1/2$  has the property

$$\tilde{U}_s(t + 1/2, t + 1/2 + T) = \begin{pmatrix} e^{i\varphi/2} & 0 \\ 0 & e^{-i\varphi/2} \end{pmatrix} \tilde{U}_{s+1/2}(t, t + T) \begin{pmatrix} e^{-i\varphi/2} & 0 \\ 0 & e^{i\varphi/2} \end{pmatrix}. \quad (33)$$

#### 4. Isospectral case

We now consider the special case when  $\pi v = 1, \omega = 1, c = 4\pi$ . The energy spectrum of the Hamiltonian  $\mathcal{H}(t)$  is independent of the parameter  $t$  in this case. The energy curves are horizontal and equidistant.

The evolution operator for  $T = 1$  (i.e. over the system period) is also independent of  $t$ :

$$\tilde{U}(t, t + 1) = \begin{pmatrix} e^{i\varphi} & 0 \\ 0 & e^{-i\varphi} \end{pmatrix}. \quad (34)$$

In the original diabatic representation this evolution operator has a very simple form:

$$U(t, t + 1) = \left( \begin{array}{cccc|cccc} \ddots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ \dots & 0 & 1 & 0 & \dots & \dots & 0 & 0 & 0 & \dots \\ \dots & 0 & 0 & 1 & \dots & \dots & 0 & 0 & 0 & \dots \\ \dots & 0 & 0 & 0 & \dots & \dots & 0 & 0 & 0 & \dots \\ & \vdots & \vdots & \vdots & \ddots & & \vdots & \vdots & \vdots & \ddots \\ \hline \ddots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ \dots & 0 & 0 & 0 & \dots & \dots & 0 & 0 & 0 & \dots \\ \dots & 0 & 0 & 0 & \dots & \dots & 1 & 0 & 0 & \dots \\ \dots & 0 & 0 & 0 & \dots & \dots & 0 & 1 & 0 & \dots \\ & \vdots & \vdots & \vdots & \ddots & & \vdots & \vdots & \vdots & \ddots \end{array} \right). \quad (35)$$

Only the subdiagonal and superdiagonal are not equal to zero. This form of the evolution operator defines shifts of the  $+$  and  $-$  components of the function in the negative and positive directions of the index  $n$  respectively. As a result, the system evolves along the adiabatic potential curves, i.e. along the horizontal straight lines.

We now consider the evolution in the adiabatic basis, associated with the matrix  $\mathcal{H}(t)$ , which in this case has the form

$$\tilde{\psi}_+^{\pm, n} = \frac{1}{2\sqrt{\pi}} e^{-i\pi(t \mp 1/4)} e^{i(t \mp \frac{1}{4})\varphi} e^{-in\varphi} \quad \tilde{\psi}_-^{\pm, n} = \frac{\pm 1}{2\sqrt{\pi}} e^{i\pi(t \pm 1/4)} e^{-i(t \pm \frac{1}{4})\varphi} e^{-in\varphi}. \quad (36)$$

We use the notation for the operator  $U(t, t + 1)$  in this basis given by

$$u_{n,m}^{\alpha,\beta}(t, t + 1) = \langle U(t, t + 1) \Psi^{\beta, m}(t), \Psi^{\alpha, n}(t + 1) \rangle$$

where  $\alpha, \beta$  denote  $+$  or  $-$ . This infinite matrix can be easily calculated using the Fourier representation for the functions  $\Psi^{\pm, n}$  and operator  $U(t, t + 1)$ :

$$\begin{pmatrix} u_{n,m}^{+,+}(t, t + 1) & u_{n,m}^{-,+}(t, t + 1) \\ u_{n,m}^{+,-}(t, t + 1) & u_{n,m}^{-,-}(t, t + 1) \end{pmatrix} = \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}.$$

Operator  $u$  does not depend on the parameter  $t$ .

Now we are going to calculate the evolution operator for the half-period  $U(t, t + 1/2)$  in the Fourier representation which depends on  $t$ :

$$\bar{U}(t, t + 1/2) = \begin{pmatrix} 0 & e^{-i(\varphi^2/4\pi) + 2i\varphi t + i\varphi - 2\pi i t} \\ -e^{i(\varphi^2/4\pi) - 2i\varphi t - i\varphi + 2\pi i t} & 0 \end{pmatrix}. \quad (37)$$

It can be written in the form

$$\begin{aligned} \bar{U}(t, t + 1/2) &= \begin{pmatrix} e^{-i\varphi^2/8\pi} & 0 \\ 0 & e^{i\varphi^2/8\pi} \end{pmatrix} \begin{pmatrix} 0 & e^{+2i\varphi t + i\varphi - 2\pi i t} \\ -e^{-2i\varphi t - i\varphi + 2\pi i t} & 0 \end{pmatrix} \begin{pmatrix} e^{i\varphi^2/8\pi} & 0 \\ 0 & e^{-i\varphi^2/8\pi} \end{pmatrix} \\ &= \begin{pmatrix} e^{-i\varphi^2/8\pi} & 0 \\ 0 & e^{i\varphi^2/8\pi} \end{pmatrix} \bar{Q}(t, t + 1/2) \begin{pmatrix} e^{i\varphi^2/8\pi} & 0 \\ 0 & e^{-i\varphi^2/8\pi} \end{pmatrix}. \end{aligned} \quad (38)$$

This form of the evolution operator shows that during half of the period the initial data which have a zero '+' component ( $f_{+,n}(0) = 0$ ) are transformed into the function with the zero '-' component ( $f_{-,n}(1/2) = 0$ ) and *vice versa*. If one starts from the localized initial data, for example  $f_{-,n}(0) = \delta(n)$ , then, after the half-period, it will be delocalized in the original diabatic representation

$$f_{+,m}(1/2) = \frac{1}{2\pi} \int_0^{2\pi} e^{-i(\varphi^2/4\pi) + 2i\varphi t + i\varphi - 2\pi i t} e^{-i(n-m)\varphi} d\varphi.$$

After the second half of the period the function will be localized and the '+' component will again be equal to zero.

We shall calculate the evolution operator in the adiabatic basis for  $t = 1/4$ . Corresponding bases are

$$\begin{cases} \tilde{\Psi}^{+,n}(1/4, \varphi) = \frac{1}{2\sqrt{\pi}} \begin{pmatrix} 1 \\ ie^{-i\varphi/2} \end{pmatrix} e^{-in\varphi} \\ \tilde{\Psi}^{-,n}(1/4, \varphi) = \frac{1}{2\sqrt{\pi}} \begin{pmatrix} -ie^{i\varphi/2} \\ -1 \end{pmatrix} e^{-in\varphi} \\ \tilde{\Psi}^{+,n}(3/4, \varphi) = \frac{1}{2\sqrt{\pi}} \begin{pmatrix} -ie^{i\varphi/2} \\ -e^{-i\varphi} \end{pmatrix} e^{-in\varphi} \\ \tilde{\Psi}^{-,n}(3/4, \varphi) = \frac{1}{2\sqrt{\pi}} \begin{pmatrix} -e^{i\varphi} \\ -ie^{-i\varphi/2} \end{pmatrix} e^{-in\varphi}. \end{cases} \quad (39)$$

We are now going to calculate the operator  $Q$  in the adiabatic bases. It is possible to consider a new Fourier transformation, associated with the adiabatic basis. A variable, conjugated to the index  $n$ , will be denoted by  $p$ , and the operator  $Q$  in this Fourier representation will be denoted by  $\tilde{q}$ . Operator  $\tilde{q}$  corresponding to the evolution between the stationary points is the operator of multiplication by the matrix

$$\tilde{q}(1/4, 3/4) = \tilde{q}(3/4, 5/4) = \begin{pmatrix} i \cos p/2 & -ie^{-ip/2} \sin p/2 \\ -ie^{ip/2} \sin p/2 & -i \cos p/2 \end{pmatrix}. \quad (40)$$

One can easily verify that

$$Q(3/4, 5/4)Q(1/4, 3/4) = U(1/4, 5/4)$$

due to the diagonal form of the evolution operator in the diabatic Fourier basis.

## 5. Conclusions

The presence of two periods is characteristic for the model under consideration. In the non-symmetric case, the periods are  $\tau_+ = 2\pi/c\omega_+$  and  $\tau_- = 2\pi/c\omega_-$ . The adiabatic potential curves and the Hamiltonian are not periodic in  $t$ .

In the symmetric case  $\omega_+ = \omega_-$  these periods coincide, but a new period appears, i.e. that of the adiabatic potential curves. Alternatively, it could be said that in the symmetric case the adiabatic potential curves are symmetric both in translations over time and energy. In the non-symmetric case the translational symmetry is somewhat more complicated: the elementary cell is a parallelogram on the  $(t, E)$ -plane.

In the dynamic problem the periods do not appear on the same footing, as is seen, for instance, from formula (20). The explicit expression for the evolution operator generally looks quite complicated and deserves further analysis. Physically, it could be expected that in the general double periodic case the time propagation does not follow a regular pattern.

The formulae are much more transparent when the periods are in a simple ratio. The evolution pattern is particularly lucid and regular in the isospectral case. The latter represents a regime with an interaction of intermediate strength. The more detailed analysis of the physically important adiabatic and antiadiabatic limits could be the object of further consideration.

It is rather interesting that the solution of the dynamic problem can be expressed through trigonometric functions only. For a two-state Landau-Zener case, which seems to be simpler, the propagator can be expressed only through the functions of a parabolic cylinder. Hence, the periodization of the model simplifies the problem considered to that which could be expected from other examples.

The model considered here presents a kind of quantization of  $(1+1)$  spacetime and allows 'continualization' when the periods of time and energy (which then plays the role of the space coordinate) tend to zero. If the coupling constant  $v$  is equal to zero, then we come to the wave equation case when propagation of the signal proceeds with constant velocities in both directions. The propagation becomes more complicated for the non-zero coupling. The unexpected feature is the  $s$ - $t$  symmetry and the antiadiabatic limit which returns us to the zero coupling case when the coupling tends to infinity. These additional symmetries need further investigation.

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## References

- [1] Brundobler S and Elser V 1993 *J. Phys. A: Math. Gen.* **26** 1211
- [2] Demkov Yu N and Osherov V I 1967 *Zh. Eksp. Teor. Fiz.* **53** 1589
- [3] Demkov Yu N and Ostrovsky V N 1988 *Zero-Range Potentials and their Applications in Atomic Physics* (New York: Plenum)
- [4] Demkov Yu N and Ostrovsky V N 1994 Crossings of two bands of potential curves *J. Phys. B: At. Mol. Phys.* submitted
- [5] Kurasov P and Boman J 1994 Distributions for the discontinuous test functions and differential operators with the generalized coefficients (in preparation)

- [6] Landau L 1932 *Phys. Z. Sowj.* 2 26
- [7] Landau L D and Lifshitz E M 1965 *Quantum Mechanics* (Oxford: Pergamon)
- [8] Manakov N L, Ovsiannikov V D and Rapoport L P 1986 *Phys. Rep.* 141 319
- [9] Ostrovsky V N 1973 Crossings of two systems of potential curves *Electronic and Atomic Collisions: Proc. VIII ICPEAC* (Beograd) Abstracts p 133
- [10] Presnyakov L P and Urnov A M 1970 *J. Phys. B: At. Mol. Phys.* 3 1267
- [11] Zener C 1932 *Proc. R. Soc. A* 137 696