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Exact analytical solution of the N-level Landau–Zener-type bow-tie model

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Abstract. The non-stationary Schrödinger equation in a finite basis of states is considered for the Hamiltonian matrix linearly depending on time. Exact analytical solutions of asymptotic transition probabilities are obtained for a bow-tie model, in which an arbitrary number of linear time-dependent diabatic potential curves cross at one point and only a particular horizontal curve has interactions with the others. Based on the contour integral method used, some mathematical aspects such as a possible generalization of the Whittaker functions are also briefly discussed.

1. Introduction

Exactly solvable model problems which describe interactions among several closely coupled states (channels) are of interest for many branches of physics. They could be subdivided into non-stationary and stationary models stemming respectively from the time-dependent and time-independent Schrödinger equations. Another subdivision is the one- into two-state and multistate models.

The difficulties in obtaining exact solutions increase from non-stationary to stationary and from two-state to multistate models. Historically the first and most famous model is due to the independent papers by Landau (1932) and Zener (1932). Since in the same year Majorana (1932) also suggested and solved such a model, probably the more justifiable name would be the Landau–Zener–Majorana model, but we use the traditional terminology below‡. This was the non-stationary two-state model. Since that time a number of *non-stationary two-state models* were suggested (Nikitin and Umanskii 1984, Demkov and Ostrovsky 1988). Some *stationary two-state models* were also solved exactly (Osherov and Voronin 1994, Osherov and Nakamura 1996), among which the recent achievement in the case of the stationary Landau–Zener–Stueckelberg problem by Zhu and Nakamura should be noted (Nakamura and Zhu 1996, Nakamura 1996, Zhu and Nakamura 1994, 1995).

As for the *multistate models*, the number of exact solutions remains quite limited even in the non-stationary formulation§. The solutions of some (resonance) three-state models are generated by the solutions of two-state models (see Hioe 1984 and references therein).

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‡ As a curiosity we refer also to the paper by Wannier (1965) who 33 years later considered the same model apparently unaware of the other publications on the subject.

§ It seems that the only exactly solvable *stationary multistate model* known nowadays is the quantum version of the Demkov–Osherov model (1967).

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The class of N-state models for an arbitrary number N originates from the problem of a particle with the spin $j = \frac{1}{2}(N-1)$ in a time-dependent magnetic field. According to the idea put forward by Majorana (1932) and developed further by a number of authors (Hight *et al* 1977, Sanctuary 1979, Hioe 1987, Kazansky and Ostrovsky 1996), in this case the problem is *exactly reducible to the two-state model* (for arbitrary-field time-dependence of the field) and all varieties of exact solutions available for the latter can be applied. The other multistate model (with an infinite number of states) reducible to a two-state model was put forward recently by Demkov and Ostrovsky (1995) and developed further by Demkov *et al* (1995).

Among the specific time-dependencies the most natural one seems to be a generalization of the simplest Landau–Zener case. It presumes a time-dependent Hamiltonian of the form $H(t) = Bt + A$, where A and B are time-independent Hermitian $N \times N$ matrices which generally do not commute. We choose the basis of states in which the matrix $\mathbf{B}$ is diagonal: $\mathbf{B}_{jk} = \beta_j \delta_{jk}$. The diagonal elements of the Hamiltonian matrix $H_{jj} = \beta_j t + \varepsilon_j$ ($\varepsilon_j \equiv A_{jj}$) are named *diabatic potential curves*. They are linear in the Landau–Zener model with the slopes β_j. The non-diagonal elements $H_{jk} = A_{jk} \equiv V_{jk}$ describe the *coupling* between the diabatic basis states. These couplings are time-independent in the Landau–Zener model.

In general, the Laplace transformation is useful for solving the problems with linear time-dependence. This transformation plainly reduces the problem to the first-order differential equation in the case when only one coefficient β_j is non-zero. This corresponds to the Demkov–Osherov model† (Demkov and Osherov 1967 and references therein): one slanted diabatic potential curve crosses a parallel set of horizontal‡ curves.

The objective of the present paper is to explore a somewhat less evident, exactly solvable, case known as the *bow-tie model*. In this model all diagonal elements of the matrix $\mathbf{A}$ are assumed to be zero ($\varepsilon_j \equiv 0$). Hence all diabatic potential curves cross at the same moment which is chosen as zero on the time axis. The additional assumption§ which makes the model solvable refers to the couplings: all states are coupled only to one singled out (zeroth) state: $V_{jk} = 0$ if both k and j differ from zero. It is convenient to make the zeroth diabatic potential curve horizontal ($\beta_0 = 0$) by the appropriate phase transformation.

This model received some attention in the literature where the essential advancements were made. Carroll and Hioe (1985, 1986a, b) motivated its study by applications to quantum optics associated with an atom driven by lasers. They employed a certain version of Laplace transformation and obtained the solution for the three-state case ($N = 3$). Later Brundobler and Elser (1993) noted that the approach used by Carroll and Hioe could be generalized to write down the solutions in the form of the contour integrals in the complex plane for arbitrary N. However, the explicit expressions of the transition probabilities for arbitrary N could not be derived.

Below we present the complete solution for arbitrary N which in fact looks more transparent than the solution for the $N = 3$ case given by Carroll and Hioe (1985, 1986a, b). From the mathematical point of view the study could be cast into a special generalization of the Whittaker functions and an analysis of the Stokes phenomenon for the special system of

† The solution of the Demkov–Osherov model was rederived using an alternative method by Kayanuma and Fukuchi (1985), but only for the single probability that the system remains at the initially populated slanted diabatic state. Note that these authors incorrectly classified the *exact* solution provided by Demkov and Osherov (1967) as approximate.

‡ Of course, a trivial phase transformation makes the horizontal curves slanted also but with the equal slopes.

§ Harmin (1991) considered the more-general bow-tie model in connection with the problem of level mixing in an intrashell Rydberg manifold by a time-dependent electric field. However, this model does not allow any exact solution.

first-order differential equations, or equivalently for a single high-order differential equation.

This paper is organized as follows. In section 2 exact analytical solutions are expressed in terms of contour integrals. In section 3 from these contour integrals explicit asymptotes of the solutions are derived for $t \to -\infty$, and thus we can apply initial conditions to them. Transition probabilities are finally obtained in section 4 in compact forms. These results are analysed in section 5 in connection with the Demkov–Osherov model. The new mathematical aspects we have found are discussed in section 6. Concluding remarks are provided in section 7.

2. Solution in terms of contour integrals

The following labelling of the diabatic basis states $|\psi_j\rangle$ is convenient for the subsequent formulation. We ascribe the subscript 0 to the singled-out horizontal diabatic state which interacts with all the other states. The other states are labelled by the subscripts of positive and negative integers. The states with positive slope β_j are labelled by positive subscripts j in order of increasing β_j. The states with negative β_j are labelled by negative indices j, the larger $|j|$ corresponding to the larger $|\beta_j|$. Namely, we have

$$\ldots \beta_{-3} < \beta_{-2} < \beta_{-1} < \beta_0 < \beta_1 < \beta_2 < \ldots . \tag{1}$$

We avoid the cases of degeneracy of two or more diabatic potential curves. Indeed, the bases in the degerate subspace could always be chosen so that only one state interacts with the zeroth state, and all the other states are completely decoupled.

Finally, the Hamiltonian matrix which we deal with here is given by

$$\begin{aligned} &H_{00} = 0 \qquad H_{jj} = \beta_j t \qquad H_{j0} = H_{0j} \equiv V_j \qquad (j \neq 0) \\ &H_{jk} = 0 \qquad \text{if } k \neq 0 \text{ and } j \neq 0. \end{aligned} \tag{2}$$

We presume that the phases of the basis states are chosen so that all the couplings V_j are real. The general solution of the non-stationary Schrödinger equation is expanded over the diabatic basis,

$$|\Psi(t)\rangle = \sum_j c_j(t)|\psi_j\rangle \tag{3}$$

where the coefficients have to satisfy the following system of equations†:

$$\mathrm{i}\frac{\mathrm{d}c_0}{\mathrm{d}t} = \sum_n V_n c_n \qquad \mathrm{i}\frac{\mathrm{d}c_j}{\mathrm{d}t} = \beta t c_j + V_j c_0 \qquad (j \neq 0). \tag{4}$$

Introducing $c_0(t) = t\tilde{c}_0(t)$ and switching to the new 'time' variable $\tau = \frac{1}{2}t^2$, we obtain

$$\mathrm{i}2\tau\frac{\mathrm{d}\tilde{c}_0}{\mathrm{d}\tau} = -\mathrm{i}\tilde{c}_0 + \sum_n V_n c_n \qquad \mathrm{i}\frac{\mathrm{d}c_j}{\mathrm{d}\tau} = \beta c_j + V_j \tilde{c}_0 \qquad (j \neq 0). \tag{5}$$

The Laplace transformation reduces this system to a single first-order differential equation (as in the Demkov–Osherov model) which is easily solved. Returning to the original variable, we obtain the following contour-integral representations (Brundobler and Elser 1993):

$$c_0(t) = Qt \int_{\mathcal{A}} \frac{\mathrm{d}u}{\sqrt{-u}} \exp\left(-\frac{1}{2}\mathrm{i}ut^2\right) \prod_n \left(\frac{-u+\beta_n}{-u}\right)^{\mathrm{i}h_n} \tag{6}$$

$$c_j(t) = -QV_j \int_{\mathcal{A}} \frac{\mathrm{d}u}{\sqrt{-u}} \exp\left(-\frac{1}{2}\mathrm{i}ut^2\right) \frac{1}{-u+\beta_j} \prod_n \left(\frac{-u+\beta_n}{-u}\right)^{\mathrm{i}h_n} \qquad (j \neq 0) \tag{7}$$

† Unless indicated otherwise, the sums and products below run over all integer indices labelling the basis states *except zero*.

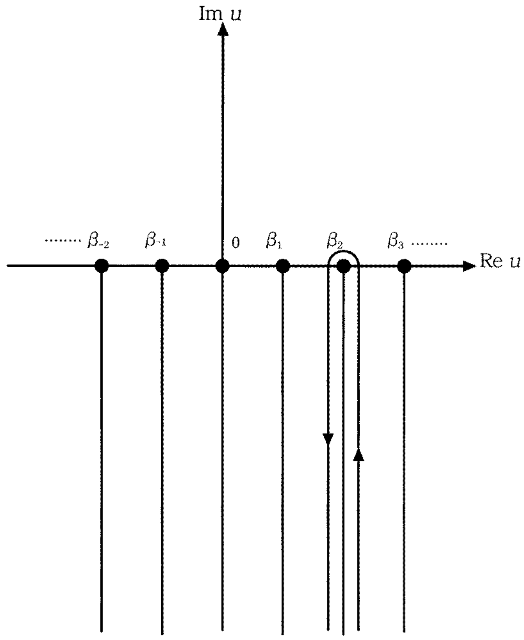

Figure 1. Branch points, cuts and integration contour at $t = -\infty$. This is the case for $k = 2$.

with $h_j = V_j^2/(2\beta_j)$. Note that the normalization factor Q and the integration contour $\mathcal{A}$ in the plane of the complex-valued variable u are to be the same in all integrals (6), (7). The complete set of linear independent solutions for the system (4) is obtained by different choices of $\mathcal{A}$ as discussed in the next section.

3. Linear independent solutions and initial conditions

The integrands in (6) and (7) have N branch points: β_k and 0. In the complex-u plane we draw the cuts from each of them downwards to $-\mathrm{i}\infty$. For each cut we introduce the corresponding integration contour $\mathcal{A}_k$ which starts from $-\mathrm{i}\infty$, encircles the branch point β_k counterclockwise and goes again to $-\mathrm{i}\infty$ (see figure 1). The solution (6), (7) with the integration over the contour $\mathcal{A}_k$ is denoted as $c_j^{(k)}(t)$.

Below we demonstrate that this solution corresponds to the initial population of the kth diabatic state. In order to do this we calculate $t \to -\infty$ asymptotes of the integrals in (6) and (7). The principal contribution to the asymptote comes from the vicinity of the branch point β_k, where only the exponential function and the factor $(u - \beta_k)^{\mathrm{i}h_k}$ are to be retained in the integrand; all other factors are replaced by their values at the point $u = \beta_k$. After that we come to the standard integral representation for the gamma-function (Gradshteyn and Ryzhik 1980),

$$\Gamma(z) = -\frac{1}{2\mathrm{i}\sin\pi z}\int_{\mathcal{C}} (-t)^{z-1}\mathrm{e}^{-t}\,\mathrm{d}t \tag{8}$$

where the integration contour $\mathcal{C}$ in the complex t plane starts from $+\infty$, encircles the point $t = 0$ counterclockwise and returns to $+\infty$. Finally, the $t \to -\infty$ asymptotes are obtained for $k = 0$ as

$$
\begin{aligned}
c_0^{(0)}(t) &= 2Q^{(0)}\left(\prod_{j<0} \mathrm{e}^{\pi h_j}\right)\sqrt{\pi\left[1+\exp\left(-2\pi\sum_j h_j\right)\right]} \\
&\quad\times\left(\prod_j |\beta_j|^{\mathrm{i}h_j}\right)\exp\left(-\mathrm{i}\arg\Gamma\left(\mathrm{i}\sum_j h_j+\frac{1}{2}\right)\right)D_0(t) \\
c_j^{(0)}(t) &= c_0^{(0)}(t)\mathrm{O}(t^{-1})
\end{aligned}
\qquad (9)
$$

and for $k \neq 0$

$$
\begin{aligned}
c_k^{(k)}(t) &= 2Q^{(k)}\mathrm{e}^{-\mathrm{i}\pi/2}\left(\prod_{j>k} \mathrm{e}^{-\pi h_j}\right)\sqrt{\pi[1-\exp(-2\pi h_k)]} \\
&\quad\times\left(\prod_j \beta_k^{-\mathrm{i}h_j}\right)\left(\prod_{j\neq k}|\beta_k-\beta_j|^{\mathrm{i}h_j}\right)\exp(\mathrm{i}\arg\Gamma(\mathrm{i}h_k))D_k(t) \\
c_j^{(k)}(t) &= c_k^{(k)}(t)\mathrm{O}(t^{-2}) \qquad (j\neq k) \\
c_0^{(0)}(t) &= c_k^{(k)}(t)\mathrm{O}(t^{-1}).
\end{aligned}
\qquad (10)
$$

Here $D_j(t)$ are the standard asymptotic solutions given by

$$
D_j(t) = \left(\frac{2}{t^2}\right)^{\mathrm{i}h_j}\exp\left(-\frac{1}{2}\mathrm{i}\beta_j t^2\right) \qquad \text{and} \qquad D_0(t) = \left(\frac{2}{t^2}\right)^{-\mathrm{i}\sum_j h_j}. \qquad (11)
$$

With the proper choice of the normalization factors $Q^{(k)}$ we obtain (only the principal terms in the asymptotes are retained)

$$
c_j^{(k)}(t\to-\infty) = \delta_{jk}D_j(t) \qquad (12)
$$

which means that the choice of the integration contour $\mathcal{A}_k$ leads to the solution which physically corresponds to the initial population of kth state. These solutions form the *complete set*. The formulae for the normalization factors are

$$
\begin{aligned}
Q^{(0)} &= \tfrac{1}{2}\pi^{-1/2}\left(\prod_{j<0}\mathrm{e}^{-\pi h_j}\right)\left[1+\exp\left(-2\pi\sum_j h_j\right)\right]^{-1/2} \\
&\quad\times\left(\prod_j|\beta_j|^{-\mathrm{i}h_j}\right)\exp\left(\mathrm{i}\arg\Gamma\left(\mathrm{i}\sum_j h_j+\tfrac{1}{2}\right)\right) \\
Q^{(k)} &= \tfrac{1}{2}\pi^{-1/2}\left(\prod_{j>k}\mathrm{e}^{\pi h_j}\right)[1-\exp(-2\pi h_k)]^{-1/2}\left(\prod_j\beta_k^{\mathrm{i}h_j}\right) \\
&\quad\times\left(\prod_{j\neq k}|\beta_k-\beta_j|^{-\mathrm{i}h_j}\right)\exp(\mathrm{i}\arg\Gamma(\mathrm{i}h_k)+\tfrac{1}{2}\mathrm{i}\pi).
\end{aligned}
\qquad (13)
$$

It is important to note that the factors of the form $\beta_j^{\mathrm{i}h_k}$ contribute to the moduli when $j < 0$ (i.e. $\beta_j < 0$). Note also that the parameters h_j are positive for $j > 0$ and negative for $j < 0$ and that $\prod_{j<0}\mathrm{e}^{\pi h_j} = 1$ when there is no $\beta_j < 0$.

4. Transition probabilities: asymptotic solutions at $t \to \infty$

In order to obtain the transition probabilities we have to find the asymptotes of the solutions $c_j^{(k)}(t)$ for $t \to +\infty$. However, here we encounter a problem. For real t the contour integrals (6), (7) have different limits as $t \to 0^-$ and $t \to 0^+$. For the three-state case Carroll and Hioe (1985, 1986a, b) were able to calculate these limits explicitly and then to continue the general solution (presented as a linear combination of the basis solutions) through the point $t = 0$ by matching. This became possible because for $t \to \pm 0$ the right-hand sides in equations (7) for the three-state problem are expressible in terms of hypergeometric functions using known integrals of the form (Gradshteyn and Ryzhik 1980)

$$\int_0^\infty x^{\nu-1}(\beta + x)^{-\mu}(x+\gamma)^{-\rho}\,\mathrm{d}x = \beta^{-\mu}\gamma^{\nu-\rho}B(\nu, \mu - \nu + \rho)\,{}_2F_1\left(\mu, \nu; \mu + \rho; 1 - \frac{\gamma}{\beta}\right). \tag{14}$$

This manipulation is quite tedious, but can be done for the three-state problem. A difficulty in our context is that this treatment cannot be applied to the general multistate problem ($N > 3$).

Here we employ a different approach treating t as a complex variable. This allows us to circumvent the singular point $t = 0$ and also to develop a general outlook at the mathematical aspects of the problem.

We present complex-valued t and the integration variable u as $t = |t|\mathrm{e}^{\mathrm{i}\tilde{\tau}}$ and $u = |u|\mathrm{e}^{\mathrm{i}\varphi}$ respectively. The steepest descent direction $\varphi = \varphi_{st}$ for the integrals (6), (7) is governed by the following relation: $\varphi_{st} = \frac{3}{2}\pi - 2\tilde{\tau}$, which for $\tilde{\tau} = \pi$ gives $\varphi_{st} = -\frac{1}{2}\pi$ as discussed above.

As t moves along the semicircular path in the upper half-plane of complex t, $\tilde{\tau}$ decreases from π to 0 and consequently φ_{st} increases from $-\frac{1}{2}\pi$ to $\frac{3}{2}\pi$. This means that the steepest descent direction (and hence the ends of the integration contours in (6), (7)) is rotated counterclockwise over 2π. In the course of this rotation the integration contour

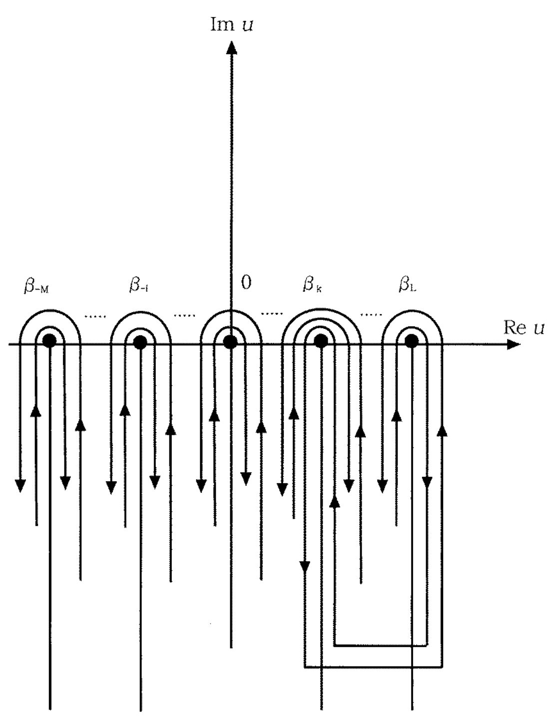

Figure 2. Deformation of the integration contour at $t = +\infty$ for the kth initial state.

'hooks' on all the branch points of the integrand. Deforming the contour we can present the final integration path for $t \to +\infty$ as a sum of the integrals over the contours $\mathcal{A}_k$ (figure 2). Asymptotic calculations for each contour proceed as above (section 3). The correct evaluation of the integral in the vicinity of each branch point implies identification of the related sheet of the Riemann surface. This is straightforwardly achieved by tracing the deformations of the contour. This is the key feature of the calculations here which does not pose essential difficulties. Of course, the asymptotes of the solutions $c_j^{(k)}(t)$ at $t \to +\infty$ are presented as (only principal terms in the asymptotes are retained)

$$c_j^{(k)}(t \to +\infty) = S_{jk} D_j(t) \tag{15}$$

and the probability of the transition from the diabatic state k to the diabatic state j is defined as $P_{k\to j} = |S_{jk}|^2$. The final results are listed below:

$$P_{0\to 0} = \left[1 - \prod_{n>0} p_n - \prod_{n<0} p_n\right]^2 \tag{16}$$

$$P_{0\to j} = P_{j\to 0} = \left(\prod_{n>j} p_n\right)(1-p_j)\left(\prod_{n>0} p_n + \prod_{n<0} p_n\right) \qquad (j > 0) \tag{17}$$

$$P_{0\to j} = P_{j\to 0} = \left(\prod_{n<j} p_n\right)(1-p_j)\left(\prod_{n>0} p_n + \prod_{n<0} p_n\right) \qquad (j < 0) \tag{18}$$

$$P_{j\to j} = \left[1 + \left(\prod_{n>j} p_n\right)p_j - \prod_{n>j} p_n\right]^2 \qquad (j > 0) \tag{19}$$

$$P_{j\to k} = \left(\prod_{n>j} p_n\right)\left(\prod_{n>k} p_n\right)(1-p_j)(1-p_k) \qquad (j > 0, k > 0) \tag{20}$$

$$P_{j\to k} = \left(\prod_{n>j} p_n\right)\left(\prod_{n<k} p_n\right)(1-p_j)(1-p_k) \qquad (j > 0, k < 0) \tag{21}$$

$$P_{j\to j} = \left[1 + \left(\prod_{n<j} p_n\right)p_j - \prod_{n<j} p_n\right]^2 \qquad (j < 0) \tag{22}$$

$$P_{j\to k} = \left(\prod_{n<j} p_n\right)\left(\prod_{n>k} p_n\right)(1-p_j)(1-p_k) \qquad (j < 0, k > 0) \tag{23}$$

$$P_{j\to k} = \left(\prod_{n<j} p_j\right)\left(\prod_{n<k} p_k\right)(1-p_j)(1-p_k) \qquad (j < 0, k < 0) \tag{24}$$

where

$$p_j = \exp(-2\pi|h_j|) = \exp\left(-\frac{\pi V_j^2}{|\beta_j|}\right). \tag{25}$$

The unitarity of the transition matrix implies that

$$\sum_{k>0} P_{j\to k} + \sum_{k<0} P_{j\to k} + P_{j\to 0} + P_{j\to j} = 1 \tag{26}$$

$$\sum_{j>0} P_{0\to j} + \sum_{j<0} P_{0\to j} + P_{0\to 0} = 1. \tag{27}$$

These relations are easily checked by employing the useful formulae below

$$\sum_{j>0}\left[\left(\prod_{n>j} \mathrm{e}^{-2\pi h_n}\right)(1 - \mathrm{e}^{-2\pi h_j})\right] = 1 - \prod_{n>0} \mathrm{e}^{-2\pi h_n} \tag{28}$$

$$\sum_{j<0}\left[\left(\prod_{n<j}\mathrm{e}^{2\pi h_n}\right)(1-\mathrm{e}^{2\pi h_j})\right]=1-\prod_{n<0}\mathrm{e}^{2\pi h_n}. \tag{29}$$

5. Analysis of the results

Equations (16)–(24) give the complete solution of the problem for an arbitrary number of states. For the three-state case the results obtained by Carroll and Hioe (1986b) are reproduced.

The characteristic feature of the present model is that all the transition probabilities are expressed via products of the factors p_j and $1-p_j$. Note that $\mathcal{P}_j \equiv p_j^2$ is the probability that the system remains at the initially populated diabatic potential curve in the plain Landau–Zener model when only two states interact (in our case the interacting states would be zeroth and jth). The similar situation appears in the Demkov–Osherov (1967) model. In the latter the structure of the transition probability formulae is particularly simple since they are factorized into products of the probabilities for transition ($\mathcal{P}_j$) and non-transition $(1-\mathcal{P}_j)$. This allowed Demkov and Osherov (1967) to transparently interpret the general formulae in terms of the pair-wise interactions and transitions. The possibility of this simple interpretation in the Demkov–Osherov model stems from the fact that the crossings between the pairs of states are separated at least in the weak-coupling limit. On the contrary, within the present model such an interpretation is difficult because for all values of the model parameters the interaction region corresponds to the vicinity of $t=0$ where *all N states cross simultaneously* and it is not possible to present the time-propagation as the sequence of pair-wise transitions.

However, just the 'concentrated' character of the interaction allows us to think that the interference effects are not operative in the present model†. This tentatively explains why the expressions (16)–(24) are still relatively simple, whereas in the more general situation (in the presence of interference effects) the overall probability would take a complicated function of the system parameters (couplings and slopes) (Nakamura 1987, Zhu and Nakamura 1996a, b).

As is easily seen from equations (16)–(24), in the diabatic limit ($p_j \to 1$) the system remains with unit probability in the initially populated diabatic state. The adiabatic case deserves more detailed discussion.

At first we consider the *adiabatic potential curves* $E_{\mathrm{ad}}(t)$, which are defined as the eigenvalues of the Hamiltonian matrix $H(t)$ at fixed time t. The function $E_{\mathrm{ad}}(t)$ is given implicitly by equation

$$\left(\prod_j(\beta_j t-E_{\mathrm{ad}})\right)\left[E_{\mathrm{ad}}+\sum_j\frac{V_j^2}{\beta_j t-E_{\mathrm{ad}}}\right]=0 \tag{30}$$

(note that this is a reparametrization of equation (11) in the paper by Demkov and Osherov (1967), since the Hamiltonians in both models have a similar structure but different time-dependence). Considering the point $t=0$ we see that it has $(N-2)$ solutions $E_{\mathrm{ad}}=0$ and a pair of solutions given by

$$E_{\mathrm{ad}}=\pm\sqrt{\sum_j V_j^2}. \tag{31}$$

† The absence of the interference effects is characteristic also to the Demkov–Osherov model and for some other as yet unsolved model which embraces the latter and the bow-tie model, see the discussion by Brundobler and Elser (1993).

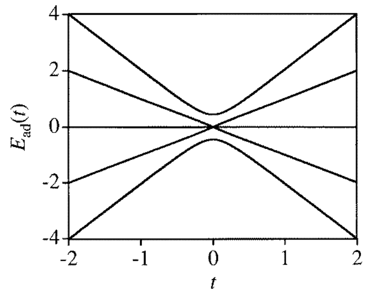

Figure 3. Adiabatic potential curves in the case of $N = 5$ with $V_1 = V_{-1} = 0.1$, $V_2 = V_{-2} = 0.3$, $\beta_1 = -\beta_{-1} = 1.0$, and $\beta_2 = -\beta_{-2} = 2.0$.

This implies that $(N - 2)$ *adiabatic* potential curves cross at $t = 0$ with the value $E = 0$. Only two 'outer' (i.e. uppermost and lowermost) adiabatic potential curves exhibit the conventional avoided-crossing pattern. Thus the well known Neumann–Wigner non-crossing rule for adiabatic potential curves (Landau and Lifshitz 1977) does not hold here due to the specific structure of the Hamiltonian with sparse couplings†. As an illustration we consider the 'symmetric' case under the reflection with respect to $E = 0$ for $N = 5$ ($V_1 = V_{-1}$, $V_2 = V_{-2}$, $\beta_1 = -\beta_{-1}$, $\beta_2 = -\beta_{-2}$), which is reduced to a biquadratic equation with the solutions‡

$$E_{ad}(t) = \pm\left[\frac{1}{2}\left(\beta_1^2 t^2 + \beta_2^2 t^2 + 2V_1^2 + 2V_2^2 \pm\sqrt{(\beta_1^2 t^2 - \beta_2^2 t^2 + 2V_1^2 - 2V_2^2)^2 + 16V_1^2 V_2^2}\right)\right]^{1/2} \qquad E_{ad}(t) \equiv 0. \tag{32}$$

Figure 3 shows the adiabatic potential curves for some values of the parameters. Three curves cross at the point $t = 0$, while two 'outer' curves exhibit a pseudocrossing pattern in agreement with our general conclusion. Interestingly, two slanted 'inner' adiabatic curves are very close to their rectilinear diabatic counterparts, although some difference exists.

The *dynamics* in the adiabatic limit $p_j \to 0$ is in correspondence with the potential curve behaviour. Namely, if the initially populated state corresponds to the minimum (maximum) slope β_j, then the population is transferred to the diabatic state with maximum (minimum) value of β_j with unit probability. For all other ('inner') curves the formulae (16)–(24) give unit probability for $j \Rightarrow j$ transition *in the diabatic basis*.

Brundobler and Elser (1993) had put forward (on a semi-empirical basis) the hypothesis that for the most general structure of the matrix $\mathbf{A}$ (see the introduction) the probability that the system remains in the initially populated diabatic jth state is given by a simple formula§

$$P_{j\to j} = \prod_k \exp\left(-\frac{2\pi|V_{jk}|^2}{|\beta_j - \beta_k|}\right) \tag{33}$$

provided that this state corresponds to the extremum (maximum or minimum) slope β_j. This hypothesis is confirmed within the present model. Indeed, if the (horizontal) 0-state

† Since this feature is present only for $N > 3$, it was not manifested in the three-state case considered by Carroll and Hioe (1985, 1986a, b).

‡ Note that the solution $E(t) \equiv 0$ appears for any number of states in the symmetric case.

§ The product in (29) runs over all values of the index *including zero*; the notations from the introduction are used.

corresponds to the maximum (minimum) slope (i.e. if all $\beta_j < 0$ or all $\beta_j > 0$), then the non-transition probability is

$$P_{0\to 0} = \prod_n \mathrm{e}^{-4\pi|h_n|}. \tag{34}$$

If some slanted (jth) state corresponds to the maximum (minimum) slope, then

$$P_{j\to j} = \mathrm{e}^{-4\pi|h_j|} \tag{35}$$

which also agrees with (33).

There are evident common features between the Demkov–Osherov and the present bow-tie models. First, the structure of the Hamiltonian matrices is similar: in both cases the non-zero matrix elements are on diagonal, one column and one row. This feature was used in the derivation of equation (30). The second point is that both problems are solved by the same general framework of the Laplace method and complex contour integration. However, in the Demkov–Osherov model the integrand contains time-dependence via the factor $\exp(-\mathrm{i}ut)$, which obviously makes the complex-valued integration variable u similar to the energy. Respectively, the branch points correspond to the energy values specific for the model, namely to the horizontal diabatic potential curves (see the introduction). In the bow-tie solution, on the other hand, the factor $\exp(-\frac{1}{2}\mathrm{i}ut^2)$ emerges in the integrand, and u could be interpreted as a variable representing a *slope* of the linear diabatic potential curve. The branch points correspond to the slopes of the actual model diabatic potential curves. The latter situation seems quite unusual, being specific to the bow-tie model.

6. Mathematical aspects

The standard two-state Landau–Zener model is described by a system of two first-order differential equations which is equivalent to one second-order differential equation. Zener (1932) solved the latter in terms of the parabolic cylinder functions. Here, as an illustration, we write down the expression for the function $c_0^{(0)}(t)$ in terms of the Whittaker function† for the case when the slanted potential curve has negative slope β:

$$c_0^{(0)}(t) = 2^{\frac{1}{4}} t^{-\frac{1}{2}} |\beta|^{-\mathrm{i}h-\frac{1}{4}} \mathrm{e}^{\frac{1}{2}\pi h} \exp(-\tfrac{1}{4}\mathrm{i}\beta t^2) W_{\mathrm{i}h+\frac{1}{4}\,\frac{1}{4}}(-\tfrac{1}{2}\mathrm{i}\beta t^2) \tag{36}$$

which is straightforwardly obtainable from the formulae (6) and (13) using the well known integral representation (Gradshteyn and Ryzhik 1980)

$$W_{\lambda\mu}(\xi) = \frac{\xi^{\mu+\frac{1}{2}} \mathrm{e}^{-\frac{1}{2}\xi}}{\Gamma(\mu-\lambda-\frac{1}{2})} \int_0^\infty \mathrm{e}^{-\xi\tau} \tau^{\mu-\lambda-\frac{1}{2}} (1+\tau)^{\mu+\lambda-\frac{1}{2}}\, \mathrm{d}\tau. \tag{37}$$

Note that our derivation for the multistate case has the two-state analogue in the treatment by Majorana (1932) who did not resort to the special functions but operated with the contour integrals.

Although the N-state problem is equivalent to an Nth order differential equation, it seems to be more convenient to cast the discussion to the system of N first-order differential equations. Comparing (36) and (6), (7) we can say that we have developed a generalization of the Whittaker functions for the high-order differential equation or the equivalent system of first-order equations. The generalized functions are defined in the complex-t plane. The integral representations (6), (7) of these generalized functions are convenient for the analysis of the asymptotic behaviour. The asymptotes of the linear independent solutions are expressed as linear combinations of the functions $D_j(t)$ (equation (11)). The coefficients in

† A solution in terms of the Whittaker functions was employed by Wannier (1965).

these linear combinations differ from sector to sector of the t-plane and vary discontinuously when the border between the two adjacent sectors is crossed. In this respect we recognize some sort of generalization of the Stokes phenomenon well known for the second-order differential equations. The derivation of the transition probabilities given above is equivalent to the determination of the Stokes constants.

It is easy to understand the positions of the aforementioned sectors and the method for detailed treatment of the Stokes phenomenon. Our analysis in section 4 in fact means that we have developed a procedure of analytical continuation of the solutions from the negative t semi-axis to the positive t semi-axis via the upper t half plane† We have shown that if the solution for $t < 0$ is given by the contour integral over the single contour $\mathcal{A}_k$, then for $t > 0$ *the same solution* is given by the integral over a certain complicated contour which can be represented as a succession of integrations over loops of the form $\mathcal{A}_k$ but lying on different sheets of the Riemann surface. This means that the integrals of the form (6), (7) with $\mathcal{A} \Rightarrow \mathcal{A}_k$ for $t > 0$ and for $t < 0$ represent in fact *different solutions* of the system (4). These integrals are generally discontinuous at the point $t = 0$. Note that Carroll and Hioe (1985, 1986a, b) incorrectly interpreted this situation as discontinuities in the *individual* basic solutions of the system (5).

Now consider the kth vector solution (i.e. set of the functions $c_j^{(k)}(t)$ for fixed k and all j) which are given by the integrals (6) and (7) with the integration contour $\mathcal{A}_k$. As $\tilde{\tau}$ decreases from π, the integration contour is rotated respectively (see section 4). For $\tilde{\tau} = \frac{3}{4}\pi$ it 'hooks' on the branch points β_n for $n > k$. This implies that the coefficients in the asymptotes change discontinuously at $\tilde{\tau} = \frac{3}{4}\pi$ which is the border of the sector discussed above. The next discontinuity appears for $\tilde{\tau} = \frac{1}{4}\pi$, where the branch points β_n for $n < k$ start to contribute to the asymptotic formulae. The more detailed study of asymptotes in the complex-t plane is possible along these lines, but it is beyond the scope of the present work.

7. Conclusion

The remarkable feature of the exact solution obtained in the present paper is that it contains an arbitrary (although finite) number of states N. The similar situation is met for the Demkov–Osherov model (and also for the spin-j model, see the introduction). In principle this feature allows us to make a transition to an infinite number of states ($N \to \infty$), namely to a continuous spectrum. This operation was carried out within the Demkov–Osherov model, where it implies a plain replacement of the dense band of states by a continuum. Formally, the similar transformation could be carried out also in our expressions (16)–(24). Consider, for instance, the survival probability $P_{0\to 0}$ (16). Its continuous analogue could be written as

$$P_{0\to 0} = \left[1 - \exp\left(-2\pi \int_{\beta_n > 0} h_n \, \mathrm{d}n \right) - \exp\left(-2\pi \int_{\beta_n < 0} |h_n| \, \mathrm{d}n \right) \right]^2. \tag{38}$$

If the states other than the zeroth are concerned, one has to consider the respective probability densities in the continuum. In any case, however, the physical interpretation of the continua in the bow-tie model is not clear, unfortunately.

For the conventional discrete state bow-tie model, the feasibility of physical application is supported by the most recent paper by Harshawardhan and Agarwal (1997) (published after submission of the present work). It is devoted to the analysis of population transfer in the three-level system placed in a frequency-modulated electromagnetic field. Some

† Analytical continuation via the lower t halfplane leads to the same results on the $t > 0$ semi-axis. This means that the solutions do not have branch points in the whole complex t plane.

attention is paid to the case of three-level crossing; note that the Hamiltonian structure exactly corresponds to the bow-tie model. It is also interesting that the specially constructed diabatization procedure for the potential curves in the three-body Coulomb problem produces some three-level crossings (Tolstikhin *et al* 1996; see figure 3).

The mathematical aspects such as the generalization of Whittaker functions touched upon in section 6 deserve further detailed analyses.

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