Exact transition probabilities in a 6-state Landau-Zener system with path interference

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We identify a nontrivial multistate Landau-Zener model for which transition probabilities between any pair of diabatic states can be determined analytically and exactly. In the semiclassical picture, this model features the possibility of interference of different trajectories that connect the same initial and final states. Hence, transition probabilities are generally not described by the incoherent successive application of the Landau-Zener formula. We discuss reasons for integrability of this system and provide numerical tests of the suggested expression for the transition probability matrix.
The multistate version of the two-state Landau-Zener model is one of the most fundamental systems in nonstationary quantum mechanics, which finds numerous applications in atomic and condensed matter physics. It considers the evolution of \( N \) states described by the Schrödinger equation with parameters that change linearly with time:

\[
i\frac{d\psi}{dt} = \left( \hat{A} + \hat{B}t \right) \psi. \tag{1}\]

Here, \( \psi \) is the state vector in a space of \( N \) states; \( \hat{A} \) and \( \hat{B} \) are constant Hermitian \( N \times N \) matrices. One can always choose the, so-called, diabatic basis in which the matrix \( \hat{B} \) is diagonal, and if any pair of its elements are degenerate then the corresponding off-diagonal element of the matrix \( \hat{A} \) can be set to zero, that is

\[
B_{ij} = \delta_{ij} \beta_i, \quad A_{nm} = 0 \text{ if } \beta_n = \beta_m, \quad n \neq m \in (1, \ldots, N). \tag{2}\]

Constant parameters \( \beta_i \) are called the slopes of diabatic levels; nonzero off-diagonal elements of the matrix \( \hat{A} \) in the diabatic basis are called the coupling constants, and the diagonal elements of the Hamiltonian, \( H_{ii} = \beta_i t + \epsilon_i \), where \( \epsilon_i \equiv A_{ii} \), are called the diabatic energies.

The goal of the multistate Landau-Zener theory is to find the scattering \( N \times N \) matrix \( \hat{S} \), whose element \( S_{nm} \) is the amplitude of the diabatic state \( n \) at \( t \to +\infty \), given that at \( t \to -\infty \) the system was in the \( n'-\)th diabatic state. In most cases, only the related matrix \( \hat{P} \), \( P_{n'\to n} = |S_{nm}|^2 \), called the matrix of transition probabilities, is of interest. Generally, for \( N > 2 \), the analytical solution of the model is unknown. Nevertheless, a number of exactly solvable cases with specific forms of matrices \( \hat{A} \) and \( \hat{B} \) have been derived.

Several influential results in the multistate Landau-Zener theory have been originally proposed as conjectures based on intuition and numerical calculations. This includes the solution of the generalized bow-tie model, Brundobler-Elser formula, and the no-go rule. The subsequent search for the proofs not only confirmed these conjectures but also advanced our understanding of solvable systems in nonstationary quantum mechanics beyond the multistate Landau-Zener model.

In this article, we introduce one more system of the type, which matrix of transition probabilities can be written explicitly. This model describes the system of \( N = 6 \) interacting states with the Hamiltonian

\[
\hat{H} = \begin{pmatrix}
\beta t + \epsilon_1 & 0 & 0 & -g_1 & -g_2 \\
0 & \beta t & 0 & g_1 & 0 & -g_3 \\
0 & 0 & \beta t - \epsilon_2 & g_2 & g_3 & 0 \\
0 & g_1 & g_2 & \epsilon_1 & 0 & 0 \\
-g_1 & 0 & g_3 & 0 & 0 & 0 \\
-g_2 & -g_3 & 0 & 0 & -\epsilon_2 & 0
\end{pmatrix}, \tag{3}
\]

where parameters \( \epsilon_1, \epsilon_2, g_1, g_2, g_3, \beta \) are arbitrary constants and \( t \) is time.

It is convenient to illustrate parameters of this model on a diagram that plots diabatic energies as functions of time and marks the pairwise intersections of diabatic levels by corresponding coupling constants, as shown in Fig. 1. For the Hamiltonian, this diagram shows that the model describes two crossing bands of energy levels, with three levels in each band.

When diabatic energy levels in each band are well separated from each other, i.e. \( \epsilon_1, \epsilon_2 \gg g_1, g_2, g_3 \), one can justify the semiclassical approach to estimate transition amplitudes. During time intervals for which all levels are well separated, diabatic states are almost eigenstates of the Hamiltonian. The adiabatic theorem predicts then that transitions between such states are
The intersection with the level-6 without changing the diabatic state, then it turns to the level-4 at the corresponding intersection at the level-4. Semiclassically, there is only a single trajectory that connects these states. It starts at the level-2, passes through 

\[ p_j = e^{-2\pi |g_j|^2}/\beta \]  

(4) 

the system will remain in the same diabatic state after the level crossing. Respectively, the probability to turn to another level is 

\[ q_j = 1 - p_j. \]  

By applying the LZ-formula to pairs of diabatic level crossings according to their appearance in a chronological order one can estimate the amplitude of a semiclassical trajectory. For example, consider the process in Fig. [1] that starts at the level-2 and ends at the level-4. Semiclassically, there is only a single trajectory that connects these states. It starts at the level-2, passes through the intersection with the level-6 without changing the diabatic state, then it turns to the level-4 at the corresponding intersection and then goes through the intersection with the level-3 without changing the level. The amplitude of such a process is given by 

\[ S_{42} = \sqrt{p_3(1 - p_1)p_2}e^{i\phi_d + \phi_{LZ}}. \]  

(5) 

where \( \phi_d \) is the dynamic phase of a trajectory: 

\[ \phi_d = \int (\beta_{k(t)} + \epsilon_{k(t)}) dt, \]  

(6) 

and \( \phi_{LZ} \) is the “LZ-phase” that the system accumulates after transitions through the crossing points. Time-dependence of indexes in \( \phi \) indicates that different parts of a trajectory generally correspond to system’s presence at levels with different values of the index \( k \) and consequently different values of parameters \( \beta_k \in (0, \beta) \) and \( \epsilon_k \in (-\epsilon_2, 0, \epsilon_1) \). Since there is only a single trajectory connecting levels 4 and 2, the phase factor does not influence the corresponding transition probability: 

\[ P_{2\rightarrow 4} = p_3(1 - p_1)p_2. \]  

(7) 

The situation becomes more complex when there are more than one trajectory connecting initial and final states. In our case, such trajectories start from either the level 1 or 6 and end at either the level 3 or 4. In an arbitrary nonintegrable model, relative dynamic phases of different trajectories change violently with changing parameters. However, the model with the Hamiltonian \( \{3\} \) is tuned so that different trajectories connecting the same initial and final states acquire the same dynamic phase. Consider, e.g. transitions from the level-1 to the level-4. One can find that the blue-color trajectory in Fig. [1] spends the same amount of time at the level-1 with the constant part of the diabatic energy equal to \( \epsilon_1 \) as the red trajectory spends at the level-4 with the same value of the constant part of the diabatic energy, etc. Another way to see that the dynamic phase is the same for both paths is to use the property that the dynamic phase difference between two trajectories is proportional to the area between them \( \{10\} \). In Fig. [1] the blue and the red trajectories enclose two plaquettes of equal size but different sign. Hence, despite the trajectory amplitude interference, the dynamic phase drops out of the final expression for the transition probabilities in the model \( \{3\} \).

The role of the LZ-phase in the independent crossing approximation was discussed by Demkov and Ostrovsky in \( \{10\} \). They showed that the effect of this phase can be trivially included by assuming that, at each pairwise crossing point, if a system remains at the initial diabatic level it does not gain an additional phase factor but, if it changes the diabatic state, the amplitude of the trajectory acquires an additional factor \( i \). We found that this rule is not sufficient for our case because it was derived for real positive coupling constants. In the model in Fig. [1] all coupling constants appear with opposite sings at different intersection points. To account for this case, consider a simple Landau-Zener system:

\[ i \frac{d}{dt}a = \beta_1 ta + \epsilon|a|b, \quad i \frac{d}{dt}b = \beta_2 tb + \epsilon|b|a, \]  

(8) 

where we explicitly separated the absolute value and the phase of the coupling constant. By a change of variables, \( b \rightarrow be^{-i\phi_y} \), the system \( \{8\} \) transforms into the one with a real positive coupling:

\[ i \frac{d}{dt}a = \beta_1 ta + |a|b, \quad i \frac{d}{dt}b = \beta_2 tb + |b|a. \]  

(9) 

This means that the transition amplitude from the diabatic state described by the amplitude \( a \) into the other diabatic state is different in models \( \{8\} \) and \( \{9\} \) by a phase factor \( e^{-i\phi_y} \). In application to the multistate Landau-Zener models, this means that
FIG. 2. (Color online) (a-b) Typical dependence of adiabatic energies (eigenstates of the Hamiltonian matrix) on time $t$. The model in (a) corresponds to the Hamiltonian (1) and (b) corresponds to the Hamiltonian (13). The case (a) features three exact level crossings at $t = 0$ while these degeneracies are lifted in the case (b). (c-d) Transition probabilities from the level-1 as functions of the level separation for $\epsilon_1 = \epsilon$, $\epsilon_2 = 1.5\epsilon$, $g_1 = 0.25$, $g_2 = 0.3$, $g_3 = 0.35$, $\beta = 1$. The case (c) corresponds to the model (a) and (d) corresponds to the model (b). (e-f) Transition probabilities from the level-2 as functions of the level separation for $g_1 = g_2 = g_3 = 0.3$, $\epsilon_1 = \epsilon_2 = \epsilon$, $\beta = 1$. The case (e) corresponds to (a), and (f) corresponds to (b). All discrete points correspond to results of direct numerical simulations of the evolution from $t = -1000$ to $t = 1000$, and solid lines are theoretical predictions of Eq. (12). Details of the numerical algorithm are discussed in the supplementary material for Ref. [14].
each time a semiclassical trajectory switches between different diabatic levels, its amplitude acquires a phase factor $i e^{-i \phi_i}$, were $\phi_i$ is the phase of the coupling constant at a corresponding level intersection. Following this rule, we should assume for the model in Fig. 1 that whenever a trajectory changes levels, it acquires a phase factor $\pm i$ for, respectively, positive and negative values of the couplings at intersections.

Applying this rule to the transition from the level-1 to the level-4 we find two contributing amplitudes:

$$S_{41}^{\text{red}} = (-1)^2 2^{3/2} (1 - p_2)(1 - p_3)(1 - p_1) p_2, \quad S_{41}^{\text{blue}} = -i^{3/2} \sqrt{p_2(1 - p_1)(1 - p_3)(1 - p_2)}.$$  \hspace{1cm} (10)

The sum of those amplitudes is identically zero, i.e., trajectories interfere destructively so that the transition from the level-1 to the level-4 is forbidden: $P_{1 \rightarrow 4} = 0$. For the transition from the level-1 to the level-3 we find:

$$S_{31}^{\text{red}} = (-1)^2 2^{3/2} (1 - p_2)(1 - p_3)(1 - p_1) (1 - p_2), \quad S_{31}^{\text{blue}} = -i^{3/2} \sqrt{p_2(1 - p_1)(1 - p_3)p_2}.$$  \hspace{1cm} (11)

Amplitudes (11) interfere constructively, so that $P_{1 \rightarrow 3} = (1 - p_3)(1 - p_1)$. We are now in a position to summarize the prediction of the independent crossing approximation for the form of the transition probability matrix:

$$\hat{P} = \begin{pmatrix} p_2 p_1 & q_2 q_3 p_1 & q_1 q_3 & 0 & p_2 q_1 p_3 & q_2 p_3 & 0 \\ 0 & p_3 p_1 & p_3 q_1 q_2 & p_3 q_1 p_2 & 0 & q_3 \\ 0 & 0 & q_1 & q_1 p_2 & p_1 p_2 & 0 \\ q_1 & 0 & p_1 q_3 p_2 & p_1 q_3 q_2 & p_1 q_3 & 0 \\ q_2 p_1 & p_2 q_3 p_1 & 0 & q_1 q_3 & q_2 q_1 p_3 & p_2 p_3 \end{pmatrix}, \quad q_n \equiv 1 - p_n.$$ \hspace{1cm} (12)

So far, our derivation of the transition probability matrix was purely semiclassical. It is expected to be predictive only for sufficiently large values of parameters $\epsilon_1$ and $\epsilon_2$. In what follows, we are going to claim that for the model with the Hamiltonian (3) the matrix (12) is actually exact, i.e. it is valid for arbitrary values of all parameters.

In order to understand what is special about the model (3), it is instructive to compare this model with a similar one that has the Hamiltonian

$$\hat{H}' = \begin{pmatrix} \beta t + \epsilon_1 & 0 & 0 & 0 & g_1 & g_2 \\ 0 & \beta t & 0 & g_1 & 0 & g_3 \\ 0 & 0 & \beta t - \epsilon_2 & g_2 & g_3 & 0 \\ 0 & g_1 & g_2 & \epsilon_1 & 0 & 0 \\ g_1 & 0 & g_3 & 0 & 0 & 0 \\ g_2 & g_3 & 0 & 0 & 0 & -\epsilon_2 \end{pmatrix},$$ \hspace{1cm} (13)

which is different from (3) only by removal of the minus signs in front of some coupling constants. Our discussion about interference and cancellation of the relative dynamic phase equally applies to the model (13). For example, transitions that correspond to a single allowed semiclassical path, such as from the level-2 to any other state, should have the same probabilities in both models. The only semiclassical difference is that now constructive and destructive interference correspond to different transitions.

Nevertheless, models (3) and (13) show very different behavior beyond the semiclassical limit. The crucial difference between them becomes apparent if we plot eigenstates of their Hamiltonians (adiabatic energies) as functions of the parameter $t$, as shown in Figs. 2(a,b). Figure 2(a) corresponds to the model (3). It demonstrates that at $t = 0$ the system experiences three pairs of adiabatic crossings of adiabatic energies. In contrast, Figure 2(b) shows that, in the model (13), those pairwise degeneracies are lifted. Returning to the diabatic basis, we find that the moment $t = 0$ also corresponds to the crossings between diabatic levels: 1 and 4, 2 and 5, 3 and 6. Such crossing levels are not coupled to each other directly, however, higher order processes can and do induce transitions between them. Nevertheless, the symmetry of the model (3) is sufficient to completely decouple those pairs of states at $t = 0$ but in the model (13) mini-gaps open up. Such mini-gaps are the signatures of the breakdown of the semiclassical approximation.

Let us compare now the transition probabilities in models (3) and (13) as functions of the level separation, as we illustrate in Figs. 2(c-f) for different initial conditions and different ratios of $\epsilon_1/\epsilon_2$. In the case of the model (3), numerically obtained transition probabilities are found to be independent of the values of the parameters $\epsilon_1$ and $\epsilon_2$, and they perfectly agree with the theoretical prediction (12). In contrast, in the model (13), transition probabilities generally depend on $\epsilon_1$, and $\epsilon_2$ nontrivially and saturate only in the limit $\epsilon_1, \epsilon_2 \gg g_1, g_2, g_3$, as it is expected from the semiclassical approximation.

Comparison of the models (3) and (13) does support the conjecture that the transition probability matrix (12) is the exact nonperturbative solution of the multistate Landau-Zener problem with the Hamiltonian (3). As an additional numerical proof, we provide Fig. 3 that compares the theoretical prediction (12) with numerical simulations of the model (3) with different choices of the coupling constants. All our numerical tests have shown perfect agreement with Eq. (12).

In conclusion, we identified and explored the Landau-Zener-like model of two crossing bands, for which we determined the matrix of transition probabilities. This model shows a relatively complex behavior due to the possibility of semiclassical path
interference leading to either constructive or destructive interference. Our numerical simulations confirm that the transition probability matrix, which we derived in a semiclassical framework, is exact i.e. it describes an arbitrary choice of the model parameters.

Our model was identified on the basis of its similarity with other known exactly solvable systems, such as the reducible 6-state model [8] and the generalized bow-tie model [10]. For such previously solved systems, the semiclassically derived and exact expressions for transition probabilities coincide. Two properties are also shared by our model with these systems: (i) the absence of the dynamic phase effect on transition probabilities in the semiclassical framework and (ii) the exact crossing of adiabatic energies at intersections of diabatic states without direct couplings. This finding suggests that our model and the previously solved systems [8, 10] are likely the instances of a more general class of solvable models that share the same properties. It should be interesting to identify new candidate systems of the type of Eq. (1) with properties (i-ii) and test them for integrability. Further progress in this direction will be also achieved by deriving a mathematically rigorous proof of Eq. (12).

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