Counterintuitive transitions in the multistate Landau–Zener problem with linear level crossings

2004 J. Phys. A: Math. Gen. 37 10691

(http://iopscience.iop.org/0305-4470/37/44/016)

INSTITUTE OF PHYSICS PUBLISHING JOURNAL OF PHYSICS A: MATHEMATICAL AND GENERAL

J. Phys. A: Math. Gen. **37** (2004) 10691–10697 PII: S0305-4470(04)77933-0

Counterintuitive transitions in the multistate Landau–Zener problem with linear level crossings

N A Sinitsyn

Department of Physics, Texas A&M University, College Station, TX 778434242, USA

Received 16 March 2004
Published 20 October 2004
Online at stacks.iop.org/JPhysA/37/10691
doi:10.1088/0305-4470/37/44/016

Abstract

We generalize the Brundobler–Elser hypothesis in the multistate Landau–Zener problem to the case when instead of a state with the highest slope of the diabatic energy level there is a band of states with an arbitrary number of parallel levels having the same slope. We argue that the probabilities of counterintuitive transitions among such states are exactly zero.

PACS numbers: 02.30.Hq, 02.30.Ik, 31.50.Gh

The multistate Landau–Zener problem has been an active field of research during the last decade with various applications in condensed matter and atomic physics. The two-state problem with linear time dependence of diagonal elements of the Hamiltonian was solved exactly by Landau and Zener [1, 2]. The simplest generalization of the two-state problem is the Schrödinger equation of the form

$$\mathrm{i}\dot{\psi}(t) = (A + Bt)\psi(t), \tag{1}$$

where A and B are Hermitian $N \times N$ matrices with constant elements. The Hamiltonian of the model is $H = A + Bt$. The matrix B can be always chosen diagonal. The goal of the theory is to find the transition probabilities, namely the squared elements of the scattering matrix $\lim_{t'\to+\infty,t\to-\infty}|S_{ij}(t',t)|^2$ where i and j enumerate eigenstates (the so-called diabatic states) of the matrix B with time-dependent diabatic energies $E_i(t) = B_{ii}t + A_{ii} \equiv \beta_i t + \alpha_i$. Nondiagonal elements of the matrix A that couple diabatic states with the same slopes β_i can always be made zero by a time-independent change of the basis. It is convenient to visualize the time dependence of diagonal elements of any such model in the time–energy diagram like the one in figure 1. When all crossing points are well separated, one can try to solve the problem naively by a successive application of the two-state Landau–Zener formula at every two-level intersection. Even in this approximation, the dependence of transition probabilities on parameters can be very complicated since amplitudes of different paths leading to the same final states can interfere. The task becomes even more complicated when more than two levels can be close to each other simultaneously. Then even approximate estimates become very sophisticated [3]. In spite of this complexity, there have been a number of remarkable efforts to solve the model (1) exactly, at least for some special choices of parameters. Generally,

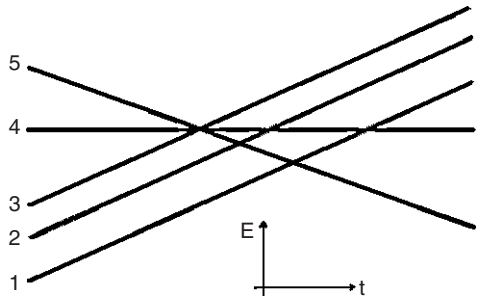

Figure 1. Diabatic energies of a five-state Landau–Zener model. The choice of parameters is as follows: $\beta_1 = \beta_2 = \beta_3 = 1$, $\beta_4 = 0$, $\beta_5 = -0.8$, $\alpha_1 = 0$, $\alpha_2 = 0.3$, $\alpha_3 = 0.5$, $\alpha_4 = 0$, $\alpha_5 = 0.4$.

this requires nontrivial approaches because to solve the nth-state model one must consider a nth-order differential equation with time-dependent coefficients.

Although a few important classes of exactly solvable models of the type (1) have been known for a long time [4, 5], the interest towards exact results in the multistate Landau–Zener problem has grown up after the work of Brundobler and Elser [6], who noticed that for any model of the form (1) there are elements of the transition probability matrix that can be found by a simple application of the two-state Landau–Zener formula at every intersection of diabatic energies. Particularly, they presented an empirical formula for the diagonal element of the scattering matrix for the state whose diabatic energy level has the highest slope, i.e. if k is the index of the state with $\beta_k = \max(\beta_1 \dots \beta_N)$ or $\beta_k = \min(\beta_1 \dots \beta_N)$ then

$$|S_{kk}(+\infty, -\infty)| = \exp\left(-\pi \sum_{i\ (i\neq k)} \frac{|A_{ki}|^2}{|\beta_k - \beta_i|}\right). \tag{2}$$

Formula (2) is confirmed by all known exactly solvable models with finite number of states [4, 5, 7–10] and by multiple numerical checks. Brundobler and Elser [6] speculated that this finding probably indicates that the whole problem (1) can be solved exactly or at least can be understood in terms of the two-level crossings. Various exact solutions and approximations seem to support this idea [10, 11]. Recent work [12] demonstrated that (2) follows from a simple analytical continuation of the asymptotic solution into the complex time, although such a procedure fails to predict correctly other elements of the scattering matrix. The goal of the present work is to demonstrate that the Brundobler–Elser hypothesis can be generalized to some nondiagonal elements of the scattering matrix and to explain why analytical continuation of amplitudes into the complex times provides correct predictions for some elements of the scattering matrix.

Assume that instead of one state with the highest slope of diabatic energy level there is a band of an arbitrary number of states having the same highest slope so that diabatic energies in this band are different only by constant parameters α_m. If we assume a 'semiclassical' approximation where a transition between any two states happen only at the corresponding crossing point of their diabatic energies then there are elements of the transition probability matrix that would be zero in this approximation. Such transitions, if they happen, are called counterintuitive transitions [13]. Thus, in the model shown in figure 1, transitions from the state 1 to states 2 and 3 and from the state 2 to the state 3 are counterintuitive.

Generally, for the model (1), if $\beta_m = \beta_n = \max(\beta_1 \dots \beta_N)$ then the transition from the state m to the state of the same band n would be counterintuitive if $\alpha_m < \alpha_n$. Correspondingly, if $\beta_m = \beta_n = \min(\beta_1 \dots \beta_N)$ then the transition is counterintuitive if $\alpha_m > \alpha_n$. We argue

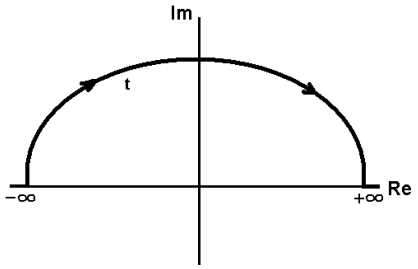

Figure 2. The deformed time contour for the evolution from large negative to large positive times with $t = R\exp(\mathrm{i}\phi)$, $R \to \infty$, $0 \leqslant \phi \leqslant \pi$.

that in the multistate Landau–Zener model with linear time dependence of diabatic energies such counterintuitive transitions have exactly zero probability, i.e. without assuming any semiclassical approximation for any model of type (1), if the transition from the state m to the state n is counterintuitive, then

$$|S_{nm}(+\infty, -\infty)| = 0. \tag{3}$$

The 'no-go' equation (3) and the Brundobler–Elser conjecture (2) can be understood by the approach similar to the one used by Landau in the two-state calculations [1]. Since we are interested in the asymptotic magnitude of the amplitudes we can analytically extend the evolution (1) to imaginary time and choose the evolution path so that always $|t| \to \infty$. The distances between instantaneous eigenenergies $\epsilon_i(t)$ of the Hamiltonian remain always large in this case, namely of the order of $|(\beta_i - \beta_j)t| \gg |A_{ij}|$ for the states $i \neq j$ and hence we can use the adiabatic approximation

$$\psi_i(t) = \mathrm{e}^{-\mathrm{i}\int_{t_0}^{t} \epsilon_i(t)\,\mathrm{d}t}\psi_i(t_0), \tag{4}$$

where the state ψ_i has the leading asymptotic $\psi_i \sim \exp(-\mathrm{i}\beta_i t^2/2)$ at $t \to -\infty$.

Approximation (4) becomes exact in the limit $t \to \infty$ but it is valid generally only if there are no other solutions that become exponentially large in comparison with the state ψ_i to which it is applied. Suppose that the state ψ_0 has the largest slope of the diabatic energy β_0 at $t \to -\infty$ and is initially occupied. In this case, it is convenient to choose the time path as shown in figure 2 with $t = R\exp(\mathrm{i}\phi)$ where $R \to \infty$ and ϕ decreases from π to zero.One can always change variables so that $\beta_0 = 0$ and $\beta_i < 0$ for states with slopes $\beta_i \neq \beta_0$ [6]. When ϕ changes in the interval from $3\pi/4$ to $\pi/4$, the amplitudes of states with slopes $\beta_i < 0$ are decreasing exponentially and become suppressed by the factor $\exp(C(\phi)\beta_i|t|^2/2)$ where $\beta_i < 0$ and $C(\phi)$ is a positive coefficient that depends only on the angle. We choose the asymptotics so that at the angle $\phi = 3\pi/4$ the state ψ_0 is dominating over all others, i.e. is exponentially large in comparison to them. Then, the states with $\beta_i < 0$ should not affect the adiabatic approximation in the interval $3\pi/4 > \phi > \pi/4$ since they can only decrease there. One can see that the condition that at $\phi = 3\pi/4$ the state ψ_0 is dominating also leads to the vanishing of the amplitudes of other states with $\beta_i < 0$ in the interval $\pi < \phi < 3\pi/4$ so that it is not forbidden to choose $|\psi_0(-\infty)| = 1$ and $|\psi_i(-\infty)| \to 0$ $(i \neq 0)$.

At the last part of the contour $\pi/4 > \phi > 0$ amplitudes of states with $\beta_i < 0$ grow from almost zero value when the angle ϕ decreases to zero, but at $\phi = 0$ time becomes real and, hence, amplitudes cannot be larger than unity. So in this part of the contour such amplitudes

have not enough time to become exponentially large. It means that they still remain small or comparable with ψ_0 at this interval and formula (4) should be valid for the state ψ_0 during the whole evolution. Substituting the energy up to the first-order correction in $1/|t|$

$$\epsilon_0(t) \sim \alpha_0 + \sum_i \frac{|A_{i0}|^2}{(\beta_0 - \beta_i)t} \tag{5}$$

into the formula for the transition probability

$$|S_{00}|^2 = \frac{|\psi_0(+\infty)|^2}{|\psi_0(-\infty)|^2} = \exp\left(-2\,\mathrm{Im}\left(\int_C \epsilon_0(t)\,\mathrm{d}t\right)\right) \tag{6}$$

we find the Brundobler–Elser result (2). It is clear from this analysis why formula (2) is generally not valid for other diagonal elements of the scattering matrix. If an initially filled state does not have the highest slope of the energy level there are states with higher slopes whose amplitudes grow exponentially and become large in the interval $3\pi/4 > \phi > \pi/4$ of the contour so that the adiabatic approximation becomes invalid in application to ψ_0. To treat this case properly, one should investigate the Stokes phenomenon near all crossing points of diabatic energies [11].

This analysis becomes more complicated if there is more than one state having the same largest energy slope β_0. If such states have also larger constant part of the diabatic energy $\alpha_m > \alpha_0$ they can grow in the first half of the contour as $\exp(C'(\phi)\alpha_m|t|)$, i.e. faster than the initially filled state ψ_0, but being initially vanishing, amplitudes of such states can grow only due to transitions from the other states. They are coupled directly only to states that are suppressed by much stronger exponents $\exp(C(\phi)\beta_i|t|^2/2)$ ($\beta_i < 0$) at first half of the time contour; therefore we do not expect that they become large in comparison with ψ_0 up to $\phi = \pi/2$. In the second part of the path, $\pi/2 < \phi < 0$ states with such an asymptotic $\exp(-\mathrm{i}\alpha t)$ already decrease exponentially and become suppressed in comparison with ψ_0; therefore we can expect that they do not break the approximation (4) for the state ψ_0 and have vanishing amplitudes at the end of the evolution. This is exactly in agreement with (3).

Our arguments in support of (2) and (3) are certainly very intuitive and every step in the mathematically rigorous proof requires more detailed justification. However, we note that (3) is also confirmed by all known exactly solvable classes featuring the possibility of counterintuitive transitions, namely by the Demkov–Osherov model [4], the generalized bow-tie model [8] and the model of two crossing bands of parallel levels [9]. Besides, we performed a number of numerical simulations with arbitrary choices of parameters. As we found, all of them support our hypothesis (3). For example, in figure 3, we show the time dependence of the probabilities to find the system at states 2 and 3 in the model demonstrated schematically in figure 1 if initially only the state 1 is occupied. One can deduce that generally during the evolution these probabilities can be rather high (>0.1) and show oscillating behaviour, but asymptotically at $t \to +\infty$ they vanish. Numerically we can simulate the evolution only in the finite time interval. This corresponds to the error in calculation of the transition amplitude of the order of $\sim 1/T$, where T is the time of the evolution. We kept other calculational errors not larger than that value. For the evolution from $t = -500$ to 500 and the same parameters as in figure 1 we find $|S_{21}|^2 = 5.18 \times 10^{-7}$ and $|S_{31}|^2 = 3.11 \times 10^{-7}$. In comparison $|S_{11}|^2 = 0.234$, $|S_{41}|^2 = 0.295$ and $|S_{51}|^2 = 0.472$. We also note that although counterintuitive transitions have vanishing probabilities, the presence of the states 2 and 3 does affect other elements of the scattering matrix. Thus if we set all couplings of states 2 and 3 with all other states to zero, then numerically calculated nondiagonal transition probabilities are $|S_{41}|^2 = 0.672$ and $|S_{51}|^2 = 0.094$, which is different from our previous numerical result.

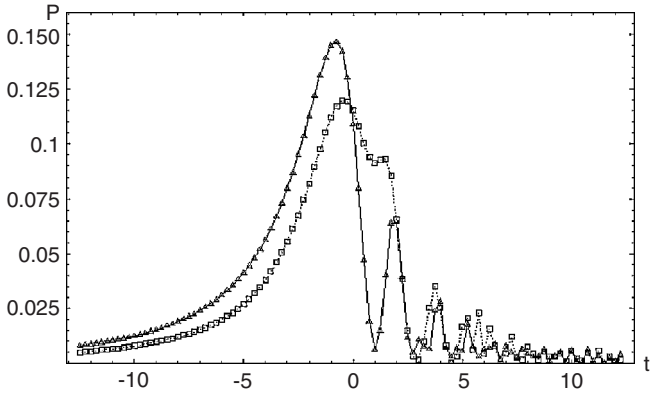

Figure 3. Time dependence of the counterintuitive transition probabilities for the model in figure 1. Triangles correspond to $P(t) = |S_{21}(t, -\infty)|^2$ and boxes show $P(t) = |S_{31}(t, -\infty)|^2$. The choice of nondiagonal elements of the Hamilton operator is $H_{12} = H_{13} = H_{23} = 0$, $H_{34} = 0.8$, $H_{35} = 0.3 + 0.24\mathrm{i}$, $H_{24} = 0.1 + 0.7\mathrm{i}$, $H_{25} = 0.5 + 0.1\mathrm{i}$, $H_{14} = 0.4 + 0.12\mathrm{i}$, $H_{15} = 0.25 + 0.2\mathrm{i}$, $H_{45} = 0.6 + 0.9\mathrm{i}$. The other elements are obtained by employing Hermitian properties of the matrix H.

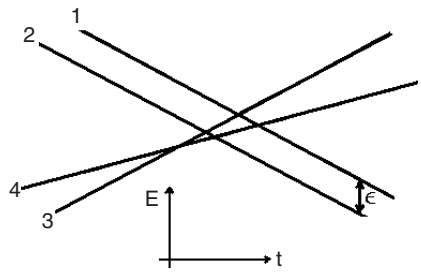

Figure 4. Diabatic levels of a four-state model. The matrix elements of the Hamilton operator are chosen as follows: $H_{11} = -t$, $H_{22} = -t - \epsilon$, $H_{33} = t$, $H_{44} = 0.5t - 0.5$, $H_{12} = 0$, $H_{13} = 0.4 - 0.1\mathrm{i}$, $H_{14} = 0.6$, $H_{23} = 0.4 + 0.5\mathrm{i}$, $H_{24} = 0.2 + 0.3\mathrm{i}$. The other elements are obtained by employing Hermitian properties of the matrix H.

As another example, consider a four-state model shown in figure 4. Obviously, for $\epsilon > 0$ the transition from state 1 to state 2 is counterintuitive but for $\epsilon < 0$ it is not. Figure 5 shows numerically calculated final probabilities to find the system in all four states for the evolution from $t = -600$ to 600 when initially only state 1 is populated.

One can see that the probability to remain in state 1 does not depend on ϵ, in agreement with the Brundobler–Elser conjecture. A small deviation from the Brundobler–Elser formula can be seen for two points with ϵ closest to zero. However, this should be explained due to the fact that $\epsilon = 0$ is the critical point and it takes much more time for probabilities to saturate in its vicinity, but in simulations the time interval had to be finite. At negative ϵ all other probabilities strongly depend on the distance between states 1 and 2. This can be explained partly even in the independent crossing approximation as due to the interference among different semiclassical paths leading to the same final state. However, for $\epsilon > 0$, the independent crossing approximation does not predict any dependence of probabilities on ϵ if initially only state 1 is populated. Nevertheless, one can deduce from figure 5 that in addition to state 1 only the transition probabilities to state 2 become flat and have indistinguishable from zero magnitudes in agreement with (3). Transition probabilities to states 3 and 4 strongly

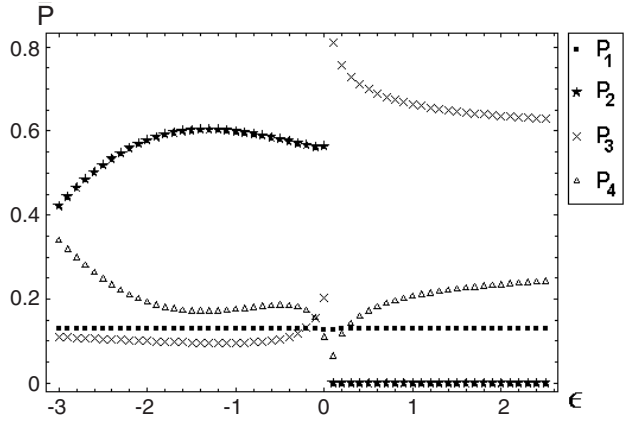

Figure 5. Transition probabilities to all states in the model in figure 4 as functions of the distance ϵ between levels 2 and 1. Long before level crossings the probability of state 1 is set to unity. The transition probabilities are represented by boxes, state 1; stars, state 2; crossed lines, state 3; triangles, state 4.

depend on ϵ there. This indicates that simulations were performed for the range of parameters where the independent crossing approximation fails unless its predictions become exact for some reason.

In conclusion, the generalization of the Brundobler–Elser hypothesis is proposed which states that counterintuitive transitions in the multistate Landau–Zener model with the linear time dependence of diabatic energies are asymptotically forbidden. It is confirmed by all numerical tests and by all known exact solutions. In addition, we demonstrated that this result can be explained by continuation of the time path into the complex plain, i.e. by the same approach as the one proposed by Landau to solve the two-state model. As in any known exact solution of the multistate Landau–Zener model, formula (3) coincides with predictions of the independent crossing approximation. This fact points to the common origin of all such exact results.

Acknowledgments

The author is grateful to V L Pokrovsky for useful discussions. This work was supported by NSF under the grant DMR0072115 and DMR 0103455 and by Telecommunication and Informatics Task Force at Texas A&M University.

References

[1] Landau L D 1932 *Physik Z. Sowjetunion* **2** 46
[2] Zener C 1932 *Proc. R. Soc.* A **137** 696
[3] Gefen Y and Thouless D J 1987 *Phys. Rev. Lett.* **59** 1752–5
Mullen K, BenJacob E, Gefen Y and Schuss Z 1989 *Phys. Rev. Lett.* **62** 2543–6
Lubin D, Gefen Y and Goldhirsch I 1990 *Phys. Rev.* B **41** 4441–55
[4] Demkov Yu N and Osherov V I 1967 *Zh. Exp. Teor. Fiz.* **53** 1589
Demkov Yu N and Osherov V I 1968 *Sov. Phys.–JETP* **26** 916 (Engl. Transl.)
[5] Carroll C E and Hioe F T 1986 *J. Phys. A: Math. Gen.* **19** 1151–61
[6] Brundobler S and Elser V 1993 *J. Phys. A: Math. Gen.* **26** 1211–27
[7] Ostrovsky V N and Nakamura H 1997 *J. Phys. A: Math. Gen.* **30** 6939–50

[8] Demkov Y N and Ostrovsky V N 2001 *J. Phys. B: At. Mol. Opt. Phys.* **34** 2419–35
[9] Usuki T 1997 *Phys. Rev.* B **56** 13360
[10] Sinitsyn N A 2002 *Phys. Rev.* B **66** 205303
[11] Aoki T, Kawai T and Takei Y 2002 *J. Phys. A: Math. Gen.* **35** 2401–30
[12] Shytov A V 2003 *Preprint* cond-mat/0312011
[13] Yurovsky V A, Ben-Reuven A, Julienne P S and Band Y B 1999 *J. Phys. B: At. Mol. Opt. Phys.* **32** 1845