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2006 J. Phys. A: Math. Gen. 39 14887

(http://iopscience.iop.org/0305-4470/39/48/004)

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

J. Phys. A: Math. Gen. **39** (2006) 14887–14893 doi:10.1088/0305-4470/39/48/004

Landau–Zener transition in photoassociation of cold atoms: strong interaction limit

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Received 4 August 2006, in final form 20 October 2006
Published 15 November 2006
Online at stacks.iop.org/JPhysA/39/14887

Abstract

The nonlinear Landau–Zener problem for two-mode photoassociation of cold atoms is studied. Based on an exact nonlinear Volterra integral equation for molecular state probability, a limit nonlinear first-order differential equation is applied to construct the first-order approximation to the solution of the problem at a strong coupling limit. An accurate approximate expression for the final transition probability to the molecular state is derived. The non-transition probability turns out to be inversely proportional to the Landau–Zener parameter in contrast to the linear two-state case when the dependence is exponential.

PACS numbers: 32.80.Bx, 34.50.Rk, 03.75.Nt

The system of nonlinear semiclassical equations describing the time evolution of atomic and molecular states in the process of molecule production in an atomic Bose–Einstein condensate [1] via one-colour Raman photoassociation [2] or by magnetic-field Feshbach resonance [3] in the rotating wave approximation reads [4, 5]

$$\mathrm{i}\frac{\mathrm{d}a_1}{\mathrm{d}t} = U(t)\,\mathrm{e}^{-\mathrm{i}\delta(t)}\bar{a}_1 a_2, \qquad \mathrm{i}\frac{\mathrm{d}a_2}{\mathrm{d}t} = \frac{U(t)}{2}\,\mathrm{e}^{\mathrm{i}\delta(t)} a_1 a_1, \tag{1}$$

where a_1 and a_2 are the atomic and molecular states' amplitudes, respectively, $\delta(t)$ is the detuning modulation function and $U(t)$ is the Rabi frequency of the field.

We have previously shown that, for models with constant field amplitude, $U = U_0 =$ const, this system at the initial condition $a_2(-\infty) = 0$ is equivalent to the following nonlinear Volterra integral equation for the molecular state probability $p = |a_2|^2$ [6]:

$$p(t) = \frac{U_0^2}{2}\int_{-\infty}^{t} K(t,x)(1 - 8p(x) + 12p^2(x))\,\mathrm{d}x, \tag{2}$$

where the *kernel* $K(t,x)$ is given by

$$K(t,x) = (C_\delta(t) - C_\delta(x))\cos(\delta(x)) + (S_\delta(t) - S_\delta(x)\sin(\delta(x)) \tag{3}$$

with the functions C_δ and S_δ defined as

$$C_\delta(t) = \int_{-\infty}^{t} \cos(\delta(x))\,\mathrm{d}x, \qquad S_\delta(t) = \int_{-\infty}^{t} \sin(\delta(x))\,\mathrm{d}x. \tag{4}$$

In the case of small U_0^2, this equation allows one to construct the solution of the problem in the form of uniformly convergent series using Picard's successive approximations [7]. The opposite limit of strong interaction, however, cannot be treated by the same approach. In our previous work [8], we studied this limit with the help of some limit nonlinear first-order equation. In the present paper, we will show that a more elaborate study of the strong interaction regime can be carried out on the basis of Volterra's (exact) integral equation (2). Below we present such a treatment which, notably, also justifies the application of the limit equation that we have used earlier. Though we here restrict ourselves to the consideration of the Landau–Zener model only, the presented approach is general and, slightly modified, can be applied in the case of other analogous level-crossing models.

In the Landau–Zener model, the field amplitude is constant and the frequency detuning linearly passes through zero: $U = U_0 = \text{const}$, $\delta_t = 2\delta_0 t$ [9]. Equation (2) can be rewritten in the following form of a Volterra integral equation of the second kind:

$$p(t) = \frac{\lambda}{4} f(t) - 4\lambda \int_{-\infty}^{t} K(t,x)\left(p(x) - \frac{3}{2}p^2(x)\right)\mathrm{d}x, \tag{5}$$

where $\lambda = U_0^2/\delta_0$ is the Landau–Zener parameter and the *forcing* function has the form

$$f(t) = \frac{\pi}{2\delta_0}\left\{\left[\frac{1}{2} + C\left(\sqrt{\frac{2\delta_0}{\pi}}t\right)\right]^2 + \left[\frac{1}{2} + S\left(\sqrt{\frac{2\delta_0}{\pi}}t\right)\right]^2\right\}, \tag{6}$$

where C and S are the Fresnel functions [10].

It is not difficult to see that, in the case of strong coupling when $\lambda \gg 1$, the forcing function $f(t)$ specified by formula (6) cannot serve as an acceptable initial approximation in practical calculations using Picard's successive approximations, since for the given case $p_0(+\infty) = \lambda f(+\infty)/4 = \lambda\pi/4 \gg 1$. For this reason, other approaches are to be searched for. Consider integral equation (2) transformed by substitution $p = p_0 + u$ with some function $p_0(t)$ which will be defined later. For the function $u(t)$ we have the following integral equation:

$$u(t) = f_0(t) - 4\lambda \int_{-\infty}^{t} K(t,x)\left[(1 - 3p_0(x))u(x) - \frac{3}{2}u^2(x)\right]\mathrm{d}x, \tag{7}$$

with the forcing function $f_0(t)$ defined as

$$f_0(t) = -p_0 + \frac{\lambda}{2}\int_{-\infty}^{t} K(t,x)\big(1 - 8p_0(x) + 12p_0^2(x)\big)\,\mathrm{d}x. \tag{8}$$

It is evident that the better the approximation $p_0(t)$ is the smaller the $f_0(t)$ will become (f_0 will be identically zero if p_0 is the exact solution of equation (2)). It can be easily checked that the function $f_0(t)$ obeys the following linear inhomogeneous differential equation:

$$f_0''' - \frac{f_0''}{t} + 4t^2 f_0' = -\left\{p_0''' - \frac{p_0''}{t} + 4[t^2 + \lambda(1 - 3p_0)]p_0' + \frac{\lambda}{2t}\big(1 - 8p_0 + 12p_0^2\big)\right\}. \tag{9}$$

Note that the homogeneous part of this equation does not depend on λ. Hence, in order to get a solution as small as possible, we demand the terms proportional to λ and the term $4t^2 p_0'$ that is not restricted in the infinite time interval to cancel the inhomogeneous part, which is enclosed in braces. For $p_0(t)$ this gives the *limit* nonlinear first-order equation used in [8]:

$$4[t^2 + \lambda(1 - 3p_0)]p_0' + \frac{\lambda}{2t}\big(1 - 8p_0 + 12p_0^2\big) = 0. \tag{10}$$

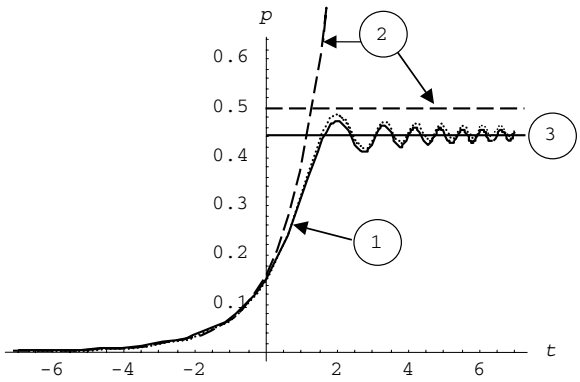

Figure 1. The time evolution of the transition probability, $\lambda = 5$. 1: numerical result (solid line), 2: limit solution (11), (12), 3: final probability (35). The airy-function solution (20) for $t < 2$ and solution (28) for $t > 2$ are shown by the dotted line; in order to distinguish the graphs the approximate solution is raised up.

It should be noted here that this choice of p_0 is not unique. In fact, one may add to the derived equation any other terms of the order of $o(\lambda)$ or less, say, for instance, of the order of $1/\lambda$, without changing the leading asymptotic term.

As was shown in [8], equation (10) admits different particular solutions that can be written in terms of elementary functions. Among these are two trivial ones, $p_0 = 1/2, 1/6$, and several non-trivial solutions. To construct an appropriate initial approximation, one may combine these particular solutions. As a result, we get (see figure 1)

$$p_0(t) = \frac{1}{6} + \frac{2t}{9\lambda}\left(t + \sqrt{t^2 + \frac{3\lambda}{2}}\right), \qquad t < \sqrt{\frac{\lambda}{2}}, \tag{11}$$

$$p_0(t) = \frac{1}{2}, \qquad t > \sqrt{\frac{\lambda}{2}}. \tag{12}$$

This is a rather good approximation almost everywhere (an exception is the point $t = \sqrt{\lambda/2}$, where we encounter discontinuity in derivatives). Indeed, equation (9) now reads

$$f_0''' - \frac{f_0''}{t} + 4t^2 f_0' = -\left\{p_0''' - \frac{p_0''}{t}\right\}. \tag{13}$$

Since the function p_0 given by expression (11) depends on variable $t/\sqrt{\lambda}$ and the right-hand side of equation (13) involves only the second- and third-order derivatives of p_0, it is understood that the inhomogeneous part of the obtained equation is of the order of $1/\lambda$. Note that this term is restricted everywhere excluding the origin. Consequently, the solution of equation (13) is also of the order of $1/\lambda$. Hence, solution (11), (12) provides a rather good forcing function to treat equation (7)—the integral equation for the first approximation function $u(t)$—by Picard's successive approximations (compare with the forcing function $p_0 = \lambda f(t)/4$ of equation (5) which is of the order of λ).

However, here we face another problem, which consists in the fact that, even though the general solution to the homogeneous part of equation (13) is easily found, since it is the equation satisfied by the Fresnel S and C functions, the particular solution to this equation for

a limit function (11) cannot be written analytically. A possible way to overcome this difficulty is to turn to the differential equation for p:

$$p''' - \frac{p''}{t} + 4[t^2 + \lambda(1 - 3p)]p' + \frac{\lambda}{2t}(1 - 8p + 12p^2) = 0. \tag{14}$$

Having proven that limit function (11) is a good initial approximation, we can now linearize this equation, using the same substitution $p = p_0 + u$. As a result, neglecting the (small) nonlinear terms, we get the following linear equation:

$$u_{ttt} - \frac{1}{t}u_{tt} + 4[t^2 + \lambda(1 - 3p_0)]u_t - \frac{4\lambda}{t}(1 - 3p_0 + 3p_{0t}t)u + \left(p_{0ttt} - \frac{1}{t}p_{0tt}\right) = 0. \tag{15}$$

The solution to this equation for the region $t > \sqrt{\lambda/2}$, where $p_0 = 1/2$, is obtained by noting that the substitution $u = C(v - 1/2)$ with arbitrary constant C transforms the equation into that of the *linear* Landau–Zener problem with the parameter $\lambda(1 - 3p_0) = -\lambda/2$ acting as an effective Landau–Zener parameter:

$$v_{ttt} - \frac{1}{t}v_{tt} + 4[t^2 + (-\lambda/2)]v_t + \frac{(-\lambda/2)}{2t}(4 - 8v) = 0. \tag{16}$$

Comparing this linear Landau–Zener equation with equation (14) we see that here the nonlinear terms are of course absent and, additionally, in the last term the summand 1 is changed to 4—this is because of the normalization; in the linear case the second level probability is normalized to unity while in the nonlinear case to 1/2.

In the region $t < \sqrt{\lambda/2}$, the exact solution to equation (15), however, is not known. For this reason, we turn to asymptotic methods.

We start by noting that in the region $0 \leqslant t \leqslant \sqrt{\lambda/2}$ we encounter several difficulties. First, as it is immediately seen from equation (14), we have a singularity at the point $t = 0$. It is this singularity that stands for the non-adiabatic transition in the systems governed by initial equations (1). Second, a different zeroth-order approximation should be used for the vicinity of the point $t = \sqrt{\lambda/2}$. In addition, one should also note that the point $t = \sqrt{\lambda/2}$ is a turning point for the linearized equation (15), since the term $t^2 + \lambda(1 - 3p_0)$ vanishes at this point. In the linear case, it is this turning point that is responsible for starting oscillations in the region $t > \sqrt{\lambda/2}$ after a non-oscillatory pre-evolution at $t < \sqrt{\lambda/2}$. However, in the nonlinear case under consideration, the role of this turning point is significantly altered because of the nonlinear terms involved. In consequence, the evolution in the neighbourhood of the critical point occurs in more complicated way, and the transition between oscillatory and non-oscillatory regimes becomes more abrupt.

Nevertheless, we will now show that it is possible to construct a *single* uniformly valid approximation for the whole region $-\infty < t < \sqrt{\lambda/2} + \sqrt{1/\lambda}$ including the neighbourhoods of the most significant points, $t = 0$ and $t = \sqrt{\lambda/2}$.

For this purpose, consider the following factorization of the exact equation for $u(t)$:

$$\left(\frac{\mathrm{d}}{\mathrm{d}t} - \frac{1}{t}\right)(u'' + 4[t^2 + \lambda(1 - 3p_0)]u + p_0'' - 6\lambda u^2) - 4tu = 0. \tag{17}$$

Note further that, in the region $0 < t < \sqrt{\lambda/2}$, the function $p_0(t)$ can be approximated as

$$p_0 = \frac{1}{3}\left(\frac{1}{2} + \frac{t}{\sqrt{2\lambda}} + \frac{t^2}{\lambda}\right) + \cdots, \tag{18}$$

whence $4[t^2 + \lambda(1 - 3p_0)] \approx 2\lambda(1 - t/\sqrt{\lambda/2})$ and $p_0'' \approx 2/(3\lambda) = \text{const}$. As is then immediately seen, if u becomes of the order of $1/\lambda$ the term $-6\lambda u^2$ becomes of the same order as p_0'' while the last term remains small under $t \leqslant \sqrt{\lambda/2}$. Therefore, for a moment, we

neglect the last term in equation (17), thus decreasing the order of the differential equation, and further treat the nonlinear term $-6\lambda u^2$ as a perturbation. A straightforward way to do this is to replace u^2 by a constant that can be afterwards adjusted by substituting the resulting solution into equation (13) for the forcing function $f(t)$ and further demanding the inhomogeneous term to be $o(1/\lambda)$, i.e., cancelling all the terms of the order of $1/\lambda$. Note that in doing the last step, we also account for the term $-4tu$ that has been neglected for a while. As appears from the aforesaid, the described technique is a variant of the strained parameters method [11] (we alter constant $2/(3\lambda)$ which originates from p_0'') that, evidently, apart from the nonlinearity, correctly accounts for all other significant peculiarities of the exact initial equation (14) such as the singularity at the origin, the turning point at $t = \sqrt{\lambda/2}$ and all terms with derivatives.

Thus, neglecting the term $-4tu$ and replacing $p_0'' - 6\lambda u^2$ by a constant, say B, we easily integrate equation (17) once and arrive at an *inhomogeneous* Airy equation [10]

$$u'' + 2\lambda(1 - t/\sqrt{\lambda/2})u + B + C_0 t = 0, \qquad C_0 = \text{const}. \tag{19}$$

The general solution to this equation is written as

$$u_{t\leqslant\sqrt{\lambda/2}} = \frac{C_0}{2\sqrt{2\lambda}} + A_1\mathrm{Ai}(\tau) + A_2\mathrm{Bi}(\tau) + u_0(\tau), \qquad \tau = \lambda^{1/6}(\sqrt{2}t - \sqrt{\lambda}). \tag{20}$$

$$u_0 = \frac{(B + C_0\sqrt{\lambda/2})\tau^2}{4\lambda^{1/3}}[{}_0F_1(;2/3;\tau^3/9){}_1F_2(2/3;4/3,5/3;\tau^3/9) - 2\,{}_0F_1(;4/3;\tau^3/9){}_1F_2(1/3;2/3,4/3;\tau^3/9)], \tag{21}$$

where Ai and Bi are the Airy functions. Substituting this solution into equation (13) and cancelling the terms of the order of $1/\lambda$, we get

$$B = \frac{2/9}{\lambda} + \frac{\ln(\lambda)}{\lambda^2}, \qquad C_0 = \frac{1}{\lambda} - \frac{\sqrt{3}\ln(\lambda)}{\lambda^2} \tag{22}$$

and further find the constants $A_{1,2}$ from the initial conditions (note that for $\lambda \gg 1$ we have $A_1 \approx 0$ and A_2 is defined from the equation $u_{t\leqslant\sqrt{\lambda/2}}(0) = -2/(9\lambda^2) + 1/(6\lambda^3)$).

This is a fairly good approximation (see figure 1, note that in order to distinguish the graphs the approximate solution is raised up). For integral equation (7), formulae (20)–(22) provide a forcing function that is of the order of $1/\lambda^2$ in the whole region $t \leqslant \sqrt{\lambda/2}$ even for $\lambda \approx 1$. This gives good first-order approximation for the whole region $t \in (-\infty, \sqrt{\lambda/2})$ and for all $\lambda \geqslant 1$ (the relative error being everywhere of the order of 10^{-3} or less).

The last step is now to calculate the final transition probability at $t \to +\infty$. Using formulae (20)–(22), we get that the maximum of $p(t)$ is achieved approximately at the point $t_m\sqrt{\lambda/2} + \sqrt{1/\lambda}$, the initial conditions for the solution valid for region $t \geqslant t_m$ being at this point given as

$$u(t_m) = -\frac{1}{12\lambda}, \qquad u'(t_m) = 0, \qquad u''(t_m) = -\frac{2}{3}\sqrt{\frac{2}{\lambda}}. \tag{23}$$

The matching procedure is rather cumbersome. In order to facilitate this procedure, it is convenient to separate off a fundamental solution of equation (16) that is *non-oscillatory* in the region $t > \sqrt{\lambda/2}$. This *unique* solution is given in terms of the solution to the linear Landau–Zener problem with the parameter $-\lambda/2$ standing instead of λ and with argument $-t$ instead of t:

$$y_1(t) = 1 - 2p_{\mathrm{LZ}}(-\lambda/2, -t). \tag{24}$$

It is not difficult to see that this solution plays a distinguished role, since it alone can be used to construct an appropriate initial approximation. Next, as two other fundamental solutions,

we choose the following functions:

$$y_2(t) = (1 - 2p_{\mathrm{LZ}}(-\lambda/2, +t))\,/(-1 + 2\,\mathrm{e}^{\pi\lambda/2}), \tag{25}$$

$$y_3(t) = t\,\mathrm{Im}[{}_1F_1(\mathrm{i}\lambda/8;\,1/2;\,-\mathrm{i}\delta_0 t^2)\,{}_1F_1(1/2 - \mathrm{i}\lambda/8;\,3/2;\,\mathrm{i}\delta_0 t^2)]/F_{3\infty}, \tag{26}$$

$$F_{3\infty} = \frac{\pi\,\mathrm{e}^{\pi\lambda/8}}{2}\mathrm{Im}\left(\frac{(-1)^{1/4}}{\Gamma(1/2 - \mathrm{i}\pi\lambda/8)\Gamma(1 + \mathrm{i}\pi\lambda/8)}\right). \tag{27}$$

Note that the chosen functions y_1, y_2 and y_3 are normalized to unity at $t \to +\infty$.

Thus, the solution to the problem in the region $t > \sqrt{\lambda/2}$ can be rewritten as

$$p_{t>\sqrt{\lambda/2}} = \tfrac{1}{2} + C_1(1 - 2p_{\mathrm{LZ}}(-\lambda/2, -t)) + C_2 y_2 + C_3 y_3. \tag{28}$$

Now, the last two of the three conditions for matching this solution with $p_0 + u_{t\leqslant\sqrt{\lambda/2}}$ give

$$C_2 + C_3 = 0. \tag{29}$$

Since the fundamental solutions $y_{1,2,3}$ are normalized to unity, this relation indicates that only the non-oscillatory solution y_1 contributes to the final transition probability, y_2 and y_3 thus only standing for gradually vanishing oscillations around y_1.

Further, the equation for determining the coefficient C_1 of solution (28) is explicitly written as

$$\frac{1}{2} + C_1(1 - 2p_{\mathrm{LZ}}(-\lambda/2, -t = -\sqrt{\lambda/2})) = \frac{1}{2} + \left(\frac{C_0}{2\sqrt{2}\lambda} + A_1\mathrm{Ai}(0) + A_2\mathrm{Bi}(0)\right), \tag{30}$$

whence we have

$$C_1 = \left(\frac{C_0}{2\sqrt{2}\lambda} + \frac{A_1/\sqrt{3} + A_2}{3^{1/6}\Gamma(2/3)}\right)\Big/(1 - 2p_{\mathrm{LZ}}(-\lambda/2, -t = -\sqrt{\lambda/2})). \tag{31}$$

Since $y_1(t \to +\infty) = 1$, we finally arrive at the following principal result:

$$p(+\infty) = \tfrac{1}{2} + C_1. \tag{32}$$

This expression is the desired formula for the final transition probability. It can be checked that this formula provides the final transition probability with a relative error less than 10^{-2} for all $\lambda \geqslant 1$. For sufficiently large $\lambda(\lambda \geqslant 4)$ the formulae are highly simplified since then $A_1 \approx 0$ and A_2 is explicitly written as

$$A_2 = \frac{1}{\mathrm{Bi}(-\lambda^{2/3})}\left(-\frac{2}{9\lambda^2} - \frac{C_0}{2\sqrt{2}\lambda} - \lambda\frac{(B + C_0\sqrt{\lambda/2})}{4}\left[{}_0F_1\left(;\,\frac{2}{3};\,\frac{-\lambda^2}{9}\right){}_1F_2\left(\frac{2}{3};\,\frac{4}{3},\,\frac{5}{3};\,\frac{-\lambda^2}{9}\right)\right.\right.$$
$$\left.\left. - 2\,{}_0F_1\left(;\,\frac{4}{3};\,\frac{-\lambda^2}{9}\right){}_1F_2\left(\frac{1}{3};\,\frac{2}{3},\,\frac{4}{3};\,\frac{-\lambda^2}{9}\right)\right]\right). \tag{33}$$

Passing now to the asymptotes of involved hypergeometric functions, using standard expansions [10], we get that the leading terms of the involved expressions are, respectively, of the following orders:

$$\left(\frac{C_0}{2\sqrt{2}\lambda} + \frac{A_1/\sqrt{3} + A_2}{3^{1/6}\Gamma(2/3)}\right) \sim -\frac{1}{2\lambda}, \qquad (1 - 2p_{\mathrm{LZ}}(-\lambda/2, -t = -\sqrt{\lambda/2})) \sim \frac{3\pi}{4}, \tag{34}$$

so that equation (32) reads

$$p(+\infty) \approx \frac{1}{2} - \frac{2/(3\pi)}{\lambda}. \tag{35}$$

Thus, we have established an interesting result: in the strong coupling limit, the final probability for non-transition to the molecular state is in the leading order of approximation

inversely proportional to the Landau–Zener parameter [12] (in contrast to the linear two-state case when the dependence is exponential [9]). In other words, the non-transition probability is a linear function of the resonance crossing rate. Interestingly, such a linear dependence on the resonance sweep rate was recently shown to be also the case for degenerate gases of fermionic atoms subject to coupling via adiabatic passage through a Feshbach resonance [13, 14]. We would like to note in conclusion that more accurate examination of formula (31) slightly corrects the proportionality coefficient $2/(3\pi) \approx 0.2122$ in equation (35) to 0.2214.

Acknowledgments

This work was supported by the International Science and Technology Center (grant A-1241) and by a grant-in-aid for Scientific Research on Specially Promoted Project no 15002011 from the Ministry of Education, Culture, Sports, Science, and Technology of Japan. AI thanks the Institute for Molecular Science, Okazaki National Research Institutes (Japan), where this research has been accomplished, for kind hospitality.

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