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2010 J. Phys. A: Math. Theor. 43 145203

(http://iopscience.iop.org/1751-8121/43/14/145203)

IOP PUBLISHING JOURNAL OF PHYSICS A: MATHEMATICAL AND THEORETICAL

J. Phys. A: Math. Theor. **43** (2010) 145203 (11pp) doi:10.1088/1751-8113/43/14/145203

The Stokes multiplier for the Landau–Zener model

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Received 18 October 2009, in final form 8 February 2010
Published 16 March 2010
Online at stacks.iop.org/JPhysA/43/145203

Abstract

A new method is presented for calculating the Stokes multiplier for the Landau–Zener model. This method is based on the coupled wave integral equations suggested by Hinton. The calculations are reduced to the matching of the solution of the third-order recursion relation to the asymptotic Birkhoff set. An analytical application of the method is given for the perturbation theory limit at the energy equal to zero.

PACS numbers: 03.65.Nk, 03.65.Vf, 34.10.+x

1. Introduction

The Landau–Zener model is certainly the most known quantum model of two interacting states. A pioneering approach to this problem, presented in the early papers [1, 2], has been subsequently elaborated in the frame of the semiclassical approximation by matching of the classical and the quantum regions [3–6].

The semiclassical level of description is based on a time-dependent approach, leading to a well-studied biconfluent hypergeometric equation (the parabolic cylinder equation). The full quantum–mechanical problem reduces to a triconfluent Heun equation, whose solutions are still not sufficiently known. In the momentum representation, the quantum equations are transformed into the semiclassical ones by the expansion of the equations in the neighborhood of the classical correspondence of momentum and energy. Thus, the threshold domain, which is the most important in physics, is not covered by the time-dependent approach basically.

A full quantum description of the systems with linear potentials has been given rather recently in [7, 8]. In this description, the probability of transitions is related to the Stokes multiplier, which determines the change of asymptotic expansions as a Stokes line is crossed. In [9], Hinton presents the method for calculating the Stokes multipliers for a definite class of linear second-order ordinary differential equations. The method is based on the integral form of equations and includes calculations of Thomé asymptotic series [10]. The Stokes multipliers are obtained in the form of convergent infinite series, which comprises the coefficients of two distinct recurrences.

To calculate the Stokes multiplier for the Landau–Zener model, the authors of [7, 8] have considered the Schrödinger equation with the fourth degree polynomial potential. In physics, the analogous equation is analyzed in connection with the quartic oscillator problem [11–13]. In mathematics, it is known as a triconfluent Heun equation [14, 15].

The triconfluent Heun equation does not belong to the class of equations discussed by Hinton. The Stokes multipliers for the Landau–Zener problem have been calculated in [7, 8] by generalizing the coupled wave integral equation method. Applying this approach, the authors of [8] have found that the procedure for the Stokes multiplier calculation is highly cumbersome and the results are not transparent for analytical analysis. As a consequence, to treat the new physical result, they have used the modifications of semiclassical approximation [16].

In this paper, we are intended to construct a compact method for calculating the Stokes multiplier for the standard Landau–Zener model, which could be convenient for numerical calculations and analytical approximations.

The paper is organized as follows. Section 2 contains the formulation of the problem in the p-representation. In section 3, we obtain the Stokes multiplier as the limit of the expression, which includes the Thomé coefficients. This limit is calculated in section 4 by matching the Thomé coefficients to the Birkhoff solutions [17]. The S-matrix and perturbation approximation in the recurrence method frame are presented in section 5. The conclusion summarizes the results and outlines the future prospects.

2. Formulation of the problem

The Landau–Zener model is defined by the two coupled equations for the components of the wavefunction [5]:

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\chi_1}{\mathrm{d}x^2} - F_1 x\chi_1 - E\chi_1 + V\chi_2 = 0, \tag{1}$$

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\chi_2}{\mathrm{d}x^2} - F_2 x\chi_2 - E\chi_2 + V\chi_1 = 0. \tag{2}$$

The parameters $F_{1,2}$ and V are considered to be positive real. In what follows, we assume

$$F_1 > F_2. \tag{3}$$

Analyzing equations (1) and (2), Nikitin and coauthors in [18] have shown that transformation into the p-representation,

$$\chi_{1,2} = \sqrt{F_{2,1}}\int_{-\mathrm{i}\infty}^{+\mathrm{i}\infty}\exp(px/\hbar)\varphi_{1,2}(p)\mathrm{d}p, \tag{4}$$

leads to the system of two coupled equations of first order:

$$-\left(\frac{p^2}{2m}+E\right)\sqrt{F_2/F_1}\,\varphi_1 + \hbar\sqrt{F_1F_2}\frac{\mathrm{d}\varphi_1}{\mathrm{d}p} + V\varphi_2 = 0, \tag{5}$$

$$-\left(\frac{p^2}{2m}+E\right)\sqrt{F_1/F_2}\,\varphi_2 + \hbar\sqrt{F_1F_2}\frac{\mathrm{d}\varphi_2}{\mathrm{d}p} + V\varphi_1 = 0. \tag{6}$$

With dimensionless variable and parameters

$$z = \frac{V}{\hbar\sqrt{F_1F_2}}\,p, \tag{7}$$

$$F = \frac{\hbar^2\sqrt{F_1F_2}}{2mV^3}\,(F_1 + F_2), \tag{8}$$

$$f = \frac{\hbar^2\sqrt{F_1F_2}}{2mV^3}\,(F_1 - F_2), \tag{9}$$

$$\varepsilon = \frac{mV^2E}{\hbar^2F_1F_2}, \tag{10}$$

the system of equations (5) and (6) looks as follows:

$$-\left(\frac{z^2}{2} + \varepsilon\right)(F - f)\,\varphi_1 + \frac{\mathrm{d}\varphi_1}{\mathrm{d}z} + \varphi_2 = 0, \tag{11}$$

$$-\left(\frac{z^2}{2} + \varepsilon\right)(F + f)\,\varphi_2 + \frac{\mathrm{d}\varphi_2}{\mathrm{d}z} + \varphi_1 = 0. \tag{12}$$

For the new functions,

$$\psi_{1,2} = \exp\left[-(F \mp f)\left(\frac{z^3}{6} + \varepsilon z\right)\right]\varphi_{1,2}, \tag{13}$$

it is converted into the equations

$$\frac{\mathrm{d}\psi_1}{\mathrm{d}z} = -\mathrm{e}^{\Phi}\psi_2, \tag{14}$$

$$\frac{\mathrm{d}\psi_2}{\mathrm{d}z} = -\mathrm{e}^{-\Phi}\psi_1, \tag{15}$$

where

$$\Phi(z) = 2f\left(\frac{z^3}{6} + \varepsilon z\right). \tag{16}$$

We take the solution $[\psi_1,\ \psi_2]$ of the system of equations (14) and (15), which is recessive in the domain $|\arg(z)| < \pi/6$. This solution satisfies the boundary conditions

$$\psi_1(+\infty) = 1, \qquad \psi_2(+\infty) = 0, \tag{17}$$

and the following integral equations:

$$\psi_1(z) = 1 - \int_\infty^z \mathrm{e}^{\Phi(t)}\,\psi_2(t)\,\mathrm{d}t, \tag{18}$$

$$\psi_2(z) = -\int_\infty^z \mathrm{e}^{-\Phi(t)}\,\psi_1(t)\,\mathrm{d}t. \tag{19}$$

The asymptotic expansion of this solution in the domain $-\pi/3 < \arg(z) < 2\pi/3$ is given by

$$\psi_1 = C + R_C + T\Theta(z)\,(D + R_D)\,, \tag{20}$$

$$\psi_2 = A + R_A + T\Theta(z)\,(B + R_B)\,, \tag{21}$$

where T is the Stokes multiplier, the function $\Theta(z)$ is defined as

$$\Theta(z) = \begin{cases} 0, & \arg(z) < \pi/3 \\ 1, & \arg(z) \geqslant \pi/3, \end{cases} \tag{22}$$

and the functions A, B, C and D are the Thomé normal solutions,

$$C = \sum_{0}^{N-1} c_n z^{-n}, \qquad R_C = O(c_N\, z^{-N}), \tag{23}$$

$$A = \mathrm{e}^{-\Phi} \sum_{2}^{N} a_n z^{-n}, \qquad R_A = O(\mathrm{e}^{-\Phi} a_{N+1}\, z^{-N-1}), \tag{24}$$

$$D = \mathrm{e}^{\Phi} \sum_{2}^{N} d_n z^{-n}, \qquad R_D = O(\mathrm{e}^{\Phi} d_{N+1}\, z^{-N-1}), \tag{25}$$

$$B = \sum_{0}^{N-1} b_n z^{-n}, \qquad R_B = O(b_N\, z^{-N}). \tag{26}$$

The positive integer number N is limited by the inequality

$$N \geqslant 2. \tag{27}$$

Asymptotic expansion of the solution in the domain $-2\pi/3 < \arg(z) < \pi/3$ is also given by expressions (20) and (21), where the parameter T is replaced by its complex conjugate and the function $\Theta(z)$ is replaced by the function $\tilde{\Theta}(z)$:

$$\tilde{\Theta}(z) = \begin{cases} 0, & \arg(z) > -\pi/3, \\ 1, & \arg(z) \leqslant -\pi/3. \end{cases} \tag{28}$$

Substituting the expressions for C and A into equations (14) and (15), and using the condition

$$c_0 = 1, \tag{29}$$

which follows from the boundary condition (17), we find

$$c_n = \frac{a_{n+1}}{n}, \qquad n \geqslant 1, \tag{30}$$

$$a_2 = \frac{1}{f}, \qquad a_3 = \frac{a_2}{f}, \qquad a_4 = \frac{a_3}{2f} - 2\varepsilon a_2, \tag{31}$$

$$f a_{n+2} + 2 f \varepsilon a_n + (n-1) a_{n-1} = \frac{a_{n+1}}{n} = c_n, \qquad n \geqslant 3. \tag{32}$$

Analogous calculations for the functions D and B with the condition

$$b_0 = 1, \tag{33}$$

which defines the Stokes multiplier T, lead to the expressions

$$b_n = \frac{d_{n+1}}{n}, \qquad n \geqslant 1, \tag{34}$$

$$d_2 = -\frac{1}{f}, \qquad d_3 = -\frac{d_2}{f}, \qquad d_4 = -\frac{d_3}{2f} - 2\varepsilon d_2, \tag{35}$$

$$-f d_{n+2} - 2 f \varepsilon d_n + (n-1) d_{n-1} = \frac{d_{n+1}}{n} = b_n, \qquad n \geqslant 3. \tag{36}$$

Recursion relations (32) and (36) are formally valid for $n < 3$ if coefficients a_i and d_i with $i < 2$ are considered to be equal to zero while a_{n+1}/n and d_{n+1}/n are replaced by 1 for $n = 0$.

3. The Stokes multiplier representation

Calculating derivatives of Thomé solutions (23)–(26), we find

$$\frac{\mathrm{d}A}{\mathrm{d}z} = -\mathrm{e}^{-\Phi}[C(z) + P(z)], \tag{37}$$

$$\frac{\mathrm{d}D}{\mathrm{d}z} = -\mathrm{e}^{\Phi}[B(z) + \tilde{P}(z)], \tag{38}$$

$$\frac{\mathrm{d}C}{\mathrm{d}z} = -\mathrm{e}^{\Phi} A, \tag{39}$$

$$\frac{\mathrm{d}B}{\mathrm{d}z} = -\mathrm{e}^{-\Phi} D, \tag{40}$$

where

$$P(z) = -f a_{N+1} z^{-N+1} + [2f\varepsilon a_N + (N-1)a_{N-1}]\, z^{-N} + N a_N\, z^{-N-1}, \tag{41}$$

$$\tilde{P}(z) = f d_{N+1} z^{-N+1} + [-2f\varepsilon d_N + (N-1)d_{N-1}]\, z^{-N} + N d_N\, z^{-N-1}. \tag{42}$$

Using equations (37)–(40), we substitute asymptotic expansions (20) and (21) into integral equations (18) and (19). Then, equation (18) leads to a trivial identity. Equation (19) reduces to the following form:

$$\begin{aligned} &T\Theta(z) + O(\mathrm{e}^{-\Phi} a_{N+1} z^{-N-1}) + O(c_N I_N) \\ &\qquad = f a_{N+1} I_{N-1} - [2f\varepsilon a_N + (N-1)a_{N-1}]\, I_N - N a_N I_{N+1}, \end{aligned} \tag{43}$$

where

$$I_n = \int_z^{\infty} \mathrm{e}^{-\Phi(t)}\, t^{-n} \mathrm{d}t. \tag{44}$$

In the domain $|\arg(z)| < \pi/3$, at $z \to \infty$, this integral is estimated as

$$I_n = O\left(\frac{1}{f}\mathrm{e}^{-\Phi}\, z^{-n-2}\right). \tag{45}$$

At $\arg(z) > \pi/3$, it can be represented in the form

$$I_n = \frac{1}{3}\oint_{L_1+L_2} \mathrm{e}^{-fy/3}\,\frac{\exp(-2f\varepsilon y^{1/3})}{y^{(n+2)/3}}\mathrm{d}y, \tag{46}$$

where the contour L_1 is the straight line from $y = z^3$ to $y = +\infty\exp(2\mathrm{i}\pi)$ and the contour L_2 is going from $y = +\infty\exp(2\mathrm{i}\pi)$ to $y = +\infty$ circumventing the singular point $y = 0$ in the negative direction. At $z \to \infty$, the behavior of the first integral in equation (46) is given by estimation (45):

$$\oint_{L_1} \mathrm{e}^{-fy/3}\,\frac{\exp(-2f\varepsilon y^{1/3})}{y^{(n+2)/3}}\mathrm{d}y = O\left(\frac{1}{f}\mathrm{e}^{-\Phi}\, z^{-n-2}\right). \tag{47}$$

Then, introducing the notation

$$t_n = \frac{1}{3}\oint_{L_2} \mathrm{e}^{-fy/3}\,\frac{\exp(-2f\varepsilon y^{1/3})}{y^{(n+2)/3}}\mathrm{d}y, \tag{48}$$

we get for the domain $\arg(z) < 2\pi/3$

$$I_n = O\left(\frac{1}{f}\mathrm{e}^{-\Phi}\, z^{-n-2}\right) + t_n\,\Theta(z). \tag{49}$$

Substitution of this equation into equation (43) results in

$$\Theta(z)\,[T_N + O\,(c_N t_N) - T] = O(\mathrm{e}^{-\Phi} a_{N+1}\, z^{-N-1}), \tag{50}$$

where

$$T_N = f a_{N+1} t_{N-1} - [2f\varepsilon a_N + (N-1)a_{N-1}]\, t_N - N a_N t_{N+1}. \tag{51}$$

From equation (50), we get

$$T = T_N + O\,(c_N t_N)\,. \tag{52}$$

Taking into account

$$\lim_{N\to\infty} \frac{O\,(c_N t_N)}{a_{N+1} t_{N-1}} = 0, \tag{53}$$

we finally obtain the basic expression for the Stokes multiplier T,

$$T = \lim_{N\to\infty} T_N. \tag{54}$$

The alternative form of the Stokes multiplier can be obtained using the properties of the integral t_n (equation (48)). Calculating this integral by part, we get the recursion relation

$$f\, t_n + 2f\varepsilon\, t_{n+2} + (n+2)\, t_{n+3} = 0. \tag{55}$$

Application of this result to definition (51) of the parameter T_N together with the recursion relation (32) results in the equality

$$T_{N+1} = T_N + c_N t_N, \tag{56}$$

where $N \geqslant 2$.

It follows from equation (56) that

$$T = T_2 + \sum_{n=2}^{\infty} c_n t_n. \tag{57}$$

The parameter T_2 can be found using definition (51) and recurrence (55):

$$T_2 = c_0 t_0 + c_1 t_1. \tag{58}$$

Finally, we obtain the Stokes multiplier T in the following form:

$$T = \sum_{n=0}^{\infty} c_n t_n. \tag{59}$$

Particularly, from this it follows that

$$T = \lim_{N\to\infty} \int_{+\infty\,\mathrm{e}^{2\mathrm{i}\pi/3}}^{+\infty} \mathrm{e}^{-\Phi(t)} C(t)\,\mathrm{d}t. \tag{60}$$

This expression has the evident interpretation. As follows from equations (21), (24) and (26), the value of the function ψ_2 at $z = +\infty\,\mathrm{e}^{2\mathrm{i}\pi/3}$ is equal to T. Then, equation (60) reads: the value of the function ψ_2 at $z = +\infty\,\mathrm{e}^{2\mathrm{i}\pi/3}$ can be calculated using the approximate Thomé normal solution C in the integrand of equation (19).

4. Matching to the Birkhoff set

In this section, we calculate the limit in equation (54). To this end, we must find the asymptotic behavior of the integral t_n, which is given by equation (48), and match the solution of recurrence (32) to the Birkhoff asymptotic set.

The asymptotic form of the integral t_n is given by the saddle point method. The saddle points are the roots of the equation

$$y + \frac{n+2}{f} + 2\varepsilon y^{1/3} = 0. \tag{61}$$

At large n, this equation can be solved taking into account that the term $2\varepsilon y^{1/3}$ is a small perturbation. Three roots of equation (61) are found to have the phases close to $-\pi$, $+\pi$ and 3π. When moving along the contour L_2, the phase of the variable y is changed between 0 and $+2\pi$. As a result, only one saddle point contributes to the integral, namely, the point which has the phase close to $+\pi$. Calculating the contribution of this point, we finally obtain

$$t_n = \sqrt{\frac{2\pi}{3f}} \exp\left[-\frac{n+1/2}{3} \ln\frac{n}{f} + \frac{n}{3} - \frac{\mathrm{i}\pi(n+1/2)}{3} - 2f\varepsilon\, \mathrm{e}^{\mathrm{i}\pi/3}\left(\frac{n}{f}\right)^{1/3} \right]. \tag{62}$$

The asymptotic form of the coefficients a_n in the Thomé normal solution A, equation (24), is the linear combination of the Birkhoff asymptotes fitted to the solution of the recursion relation (32), which is defined by the initial conditions (31). Three asymptotic Birkhoff solutions can be found by fitting the coefficients in the Birkhoff series. However, we calculate the asymptotic solutions directly from the recursion relation. This strategy is preferable for the matching process when the detailed asymptotic behavior is significant.

At large n, we take

$$a_n = \exp(S_n), \tag{63}$$

and we use the Taylor expansion

$$S_{n+k} = S_n + S'k + \tfrac{1}{2}S''k^2 + \cdots \tag{64}$$

In the first approximation, at large n, the recurrence (32) can be reduced as follows:

$$f a_{n+3} + n a_n = 0. \tag{65}$$

This results in three branches of S_n:

$$S' = \frac{1}{3}\ln\frac{n}{f} + \mathrm{i}\varphi, \qquad \varphi = -\frac{\pi}{3}, \frac{\pi}{3}, \pi. \tag{66}$$

Then, the second derivative, S'', is equal to

$$S'' = \frac{1}{3n}. \tag{67}$$

In the next approximation, we must take into account the second derivative of S in the first term of the recursion relation (32). Using the notation

$$q = \exp(S'), \tag{68}$$

we rewrite this relation in the form

$$f\left(1 + \frac{3}{2n}\right)q^3 - \frac{q^2}{n} + 2f\varepsilon q + n = O\left(\frac{1}{n^{2/3}}\right). \tag{69}$$

The solution of this equation can be obtained using the perturbation technique and the first approximation given above. Finally, we get three branches

$$S_n = -\frac{1}{2}\ln n + \frac{n}{3}\ln\frac{n}{f} - \frac{n}{3} + \mathrm{i}\varphi n + 2f\varepsilon\,\mathrm{e}^{\mathrm{i}\varphi}\left(\frac{n}{f}\right)^{1/3} + \frac{\mathrm{e}^{2\mathrm{i}\varphi}}{f}\left(1+\frac{(2f\varepsilon)^2}{6}\right)\left(\frac{f}{n}\right)^{1/3} + O\left(\frac{1}{n^{2/3}}\right). \tag{70}$$

These three branches define three Birkhoff solutions (63).

The recurrence (32) with the real initial conditions (31) has the real solution. Therefore, at $\varepsilon \neq 0$, the asymptotic behavior of the coefficients a_n can be expressed as a proper real linear combination of two maximal Birkhoff solutions:

$$a_n = P\exp\left[-\frac{1}{2}\ln n + \frac{n}{3}\ln\frac{n}{f} - \frac{n}{3} + f\varepsilon\left(\frac{n}{f}\right)^{1/3}\right] \times \cos\left[\frac{\pi n}{3} + f\varepsilon\sqrt{3}\left(\frac{n}{f}\right)^{1/3} + \eta\right], \tag{71}$$

where P and η are the real functions of the parameters f and ε.

Now, using definitions (54) and (51), and asymptotic expressions (62) and (71), the Stokes multiplier T is obtained in the nice form,

$$T = \mathrm{i}P\sqrt{\frac{3\pi}{2}}\mathrm{e}^{\mathrm{i}\eta}. \tag{72}$$

The expression for the Stokes multiplier T in equation (72) is the main result of this work. Two parameters, P and η, are given by the asymptotic values of the amplitude and the phase of the solution of recurrence (32), respectively. On the other hand, as follows from the form of the S-matrix (see below), these two parameters have evident physical meaning. The parameter P defines the probability of nonadiabatic transitions and the phase η can be considered as an accurate analytical generalization of the semiclassical Stückelberg phase. For practical applications, these two parameters can be easily calculated numerically.

5. The S-matrix in terms of the Stokes multipliers

The Stokes multiplier T defines the basic characteristic of the Landau–Zener problem—the S-matrix, which connects the amplitudes of incoming and outgoing waves in the general solution of basic equations (1) and (2). The general solution can be found as a linear combination of two independent solutions. The first of them, $\left[\chi_1^{(1)}(x), \chi_2^{(1)}(x)\right]$, is defined by the solution $\left[\psi_1^{(1)}(z), \psi_2^{(1)}(z)\right]$ of the integral equations (18) and (19). Using the symmetry properties of differential equations (14) and (15), the second independent solution in z-representation can be written in the form

$$\psi_1^{(2)}(z) = \psi_2^{(1)}(-z), \qquad \psi_2^{(2)}(z) = -\psi_1^{(1)}(-z). \tag{73}$$

For calculating the integrals in equation (4) for amplitudes $\chi_{1,2}(x)$ at large x, we use the method of steepest descent. In the vicinities of the saddle points, we replace the accurate solutions, $\left[\psi_1^{(1)}, \psi_2^{(1)}\right]$ and $\left[\psi_1^{(2)}, \psi_2^{(2)}\right]$, by their asymptotic expansions at $z \to \infty$. As a result, the asymptotic behavior of two independent solutions in x-representation is found as

$$\begin{aligned} \chi_1^{(1)} &= \frac{c}{\sqrt{P_1}}\left[\exp\left(\frac{\mathrm{i}}{\hbar}S_1 - \frac{\mathrm{i}\pi}{4}\right) + \exp\left(-\frac{\mathrm{i}}{\hbar}S_1 + \frac{\mathrm{i}\pi}{4}\right)\right], \\ \chi_2^{(1)} &= \frac{c}{\sqrt{P_2}}\left[T\exp\left(\frac{\mathrm{i}}{\hbar}S_2 - \frac{\mathrm{i}\pi}{4}\right) + T^*\exp\left(-\frac{\mathrm{i}}{\hbar}S_2 + \frac{\mathrm{i}\pi}{4}\right)\right], \end{aligned} \tag{74}$$

and

$$\chi_1^{(2)} = \frac{c}{\sqrt{P_1}}\left[T^* \exp\left(\frac{\mathrm{i}}{\hbar}S_1 - \frac{\mathrm{i}\pi}{4}\right) + T\exp\left(-\frac{\mathrm{i}}{\hbar}S_1 + \frac{\mathrm{i}\pi}{4}\right)\right],$$
$$\chi_2^{(2)} = -\frac{c}{\sqrt{P_2}}\left[\exp\left(\frac{\mathrm{i}}{\hbar}S_2 - \frac{\mathrm{i}\pi}{4}\right) + \exp\left(-\frac{\mathrm{i}}{\hbar}S_2 + \frac{\mathrm{i}\pi}{4}\right)\right], \tag{75}$$

where

$$c = \mathrm{i}\sqrt{2\pi\hbar m F_1 F_2}, \tag{76}$$

$$P_{1,2} = \sqrt{2m(E + F_{1,2}x)}, \tag{77}$$

$$S_{1,2} = \int^x P_{1,2}(x)\,\mathrm{d}x = \frac{P_{1,2}^3}{3mF_{1,2}}. \tag{78}$$

Consequently, the general solution, $[\chi_1(x), \chi_2(x)]$, at $x \to \infty$ presents the superposition of incoming and outgoing waves:

$$\chi_1 = a_+\frac{1}{\sqrt{P_1}}\exp\left(\frac{\mathrm{i}}{\hbar}S_1 - \mathrm{i}\frac{\pi}{4}\right) + a_-\frac{1}{\sqrt{P_1}}\exp\left(-\frac{\mathrm{i}}{\hbar}S_1 + \mathrm{i}\frac{\pi}{4}\right), \tag{79}$$

$$\chi_2 = b_+\frac{1}{\sqrt{P_2}}\exp\left(\frac{\mathrm{i}}{\hbar}S_2 - \mathrm{i}\frac{\pi}{4}\right) + b_-\frac{1}{\sqrt{P_2}}\exp\left(-\frac{\mathrm{i}}{\hbar}S_2 + \mathrm{i}\frac{\pi}{4}\right). \tag{80}$$

Here the amplitudes of waves are connected by the S-matrix

$$\begin{pmatrix} a_+ \\ b_+ \end{pmatrix} = \mathbf{S}\begin{pmatrix} a_- \\ b_- \end{pmatrix} \tag{81}$$

with

$$\mathbf{S} = \frac{1}{1+|T|^2}\begin{pmatrix} 1+T^{*2}, T - T^* \\ T - T^*, 1 + T^2 \end{pmatrix}. \tag{82}$$

In [8], Nakamura and coauthors have already obtained a similar expression relating the Stokes multipliers and the S-matrix for the Landau–Zener problem. To compare their results with expression (82), we should take into account the differences in the definitions of the amplitudes in p-representation in the present paper and the cited paper. Also, in defining the Stokes multipliers, we used the normal Thomé solutions, while the authors of [8] preferred the standard WKB asymptotes. Given these differences, formula (82) coincides with the expression given in [8].

The procedure for calculating the S-matrix developed in sections 2–5 is applicable for any values of the parameters of the standard Landau–Zener model. In particular, it is effective at the threshold energy, where the Birkhoff limit is reached rather quickly. The method can be generalized to the nonadiabatic tunneling and opposite signs of slopes of potentials. It contains only one recurrence and, therefore, it is much more compact than the method proposed in the pioneering work [8].

5.1. *Example of the analytical solution in the perturbation theory limit*

The S-matrix (82) can be found analytically in the recurrence method frame at $\varepsilon = 0$, $f \gg 1$. Since the condition $\varepsilon = 0$ is fulfilled, equations (31) and (32) read

$$a_2 = \frac{1}{f}, \qquad a_3 = \frac{a_2}{f} = \frac{1}{f^2}, \qquad a_4 = \frac{a_3}{2f} = \frac{1}{2f^3}, \tag{83}$$

$$f\,a_{n+3} + n\,a_n = \frac{a_{n+2}}{n+1}, \qquad n \geqslant 2. \tag{84}$$

Because of the condition $f \to \infty$, the coefficients a_n with $n \neq 3k+2$, where $k = 0, 1, 2, \ldots,$ can be considered to be equal to zero. Then, the recursion relation for coefficients a_n with

$$n = 3k+2, \qquad k = 1, 2, 3, \ldots, \tag{85}$$

is simplified as follows (cf equation (65)):

$$f\,a_{n+3} + n\,a_n = 0. \tag{86}$$

This recurrence has the solution

$$a_{3k+2} = (-1)^k \frac{3^k \Gamma(k+2/3)}{\Gamma(2/3) f^{k+1}}. \tag{87}$$

At large values of n, $n = 3k+2$, this solution is approximated as

$$a_n = (-1)^k \frac{1}{\Gamma(2/3) f^{k+1}} \sqrt{\frac{2\pi}{n/3}} \exp\left(\frac{n}{3} \ln\frac{n}{3} - \frac{n}{3} + k\,\ln 3\right). \tag{88}$$

To find the coefficient P and the phase η in the expression of equation (72), we match the asymptotic expression in equation (88) with the Birkhoff asymptotic solutions. It should be noted that in the case under consideration ($\varepsilon = 0$), all Birkhoff solutions have the same order, and, therefore, all three solutions must be included in the matching procedure. So, the general form of the asymptotic behavior of the real solution of recurrence (84) is given by (cf equation (71))

$$\begin{aligned} a_n = {} & P f^{-n/3} n^{-1/2} \exp\left(\frac{n}{3}\ln\frac{n}{3} - \frac{n}{3}\right) \cos\left(\frac{\pi n}{3} + \eta\right) \\ & + P_1 (-1)^n f^{-n/3} n^{-1/2} \exp\left(\frac{n}{3}\ln\frac{n}{3} - \frac{n}{3}\right). \end{aligned} \tag{89}$$

This expression must coincide with the expression in equation (88) for $n = 3k+2$, while for the case $n \neq 3k+2$, it must generate zeros. These conditions are satisfied at

$$\eta = -\frac{2\pi}{3}, \tag{90}$$

$$P_1 = \frac{P}{2}, \tag{91}$$

$$P = \sqrt{\frac{2}{\pi}} \frac{\Gamma(1/3)}{3^{2/3} f^{1/3}}. \tag{92}$$

Finally, we get the analytical expression for the Stokes multiplier T,

$$T = \frac{\Gamma(1/3)}{3^{1/6} f^{1/3}} \mathrm{e}^{-\mathrm{i}\pi/6}, \tag{93}$$

and the amplitude of nonadiabatic transition S_{12},

$$S_{12} = -\mathrm{i}\frac{\Gamma(1/3)}{3^{1/6} f^{1/3}}. \tag{94}$$

This result coincides with the result obtained by the perturbation theory approach [19].

6. Conclusion

Formulae (31), (32), (71) and (72) give the compact ansatz to the calculation of the Stokes multiplier for the Landau–Zener problem. It includes the solution of the third-order recursion relation for the Thomé coefficients and asymptotic matching to the Birkhoff set. The matching gives the amplitude and the phase of the Stokes multiplier directly. The form of the *S*-matrix (82) shows that the asymptotic phase of the Thomé coefficients controls the oscillations of nonadiabatic transition amplitude and defines the Stückelberg phase [20] correctly. Particularly, this gives the possibility of formulating the exact quantization condition for the nonadiabatic resonances.

Possibly, the analytical solutions to the Thomé recurrences (see [21]) can be found not only in the perturbation limit [19]. Also, we hope that the approach proposed can be employed for the analysis of the general triconfluent Heun equation, which could result in the exact quantization condition for the levels of the quartic oscillator.

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