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Solutions of the two-level problem in terms of biconfluent Heun functions

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Abstract

Five four-parametric classes of quantum mechanical two-level models permitting solutions in terms of the biconfluent Heun function are derived. Three of these classes are generalizations of the well known classes of Landau–Zener, Nikitin and Crothers. It is shown that two other classes describe super- and sublinear and essentially nonlinear level crossings, as well as processes with three crossing points. In particular, these classes include two-level models where the field amplitude is constant and the detuning varies as $\delta_0 t + \delta_2 t^3$ or $\sim t^{1/3}$. For the essentially nonlinear cubic-crossing model, $\delta_t \sim \delta_2 t^3$, the general solution of the two-level problem is shown to be expressed as series of confluent hypergeometric functions.

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(Some figures in this article are in colour only in the electronic version; see `www.iop.org`)

1. Introduction

A natural generalization of the confluent hypergeometric equation is the so-called biconfluent Heun equation (BCHE) [1] which has, as in the case of the confluent hypergeometric equation, two singularities located, respectively, at the origin and infinity: one regular, and the second irregular with a singularity rank higher by unity than that for the confluent hypergeometric equation. (One should distinguish the biconfluent equation from the doubly confluent Heun equation [1].) The canonical form of this equation, designated in the Ince classification [2] as $[0,1,1_4]$, is given by

$$u_{xx} + \frac{1+\alpha-\beta x-2x^2}{x}u_x + \frac{(\gamma-\alpha-2)x - 1/2\,[\delta+(1+\alpha)\beta]}{x}u = 0. \quad (1)$$

However, for our purposes it is convenient to use another form of equation (1) resulting from the replacement $x = sz$ (by analogy with the case of the confluent hypergeometric equation [3]):

$$u_{zz} + \frac{Cz^2 + Az + B}{z} u_z + \frac{Ez + D}{z} u = 0 \tag{2}$$

where we have employed the notations

$$\begin{aligned} &C = -2s^2 \qquad A = -s\beta \qquad B = 1 + \alpha \\ &E = (\gamma - \alpha - 2)s^2 \qquad D = -\tfrac{1}{2}s\,[\delta + (1+\alpha)\beta]\,. \end{aligned} \tag{3}$$

The evident fact that the BCHE passes directly to the confluent hypergeometric equation at $C = E = 0$ demonstrates the close connection of these equations. However, it is remarkable that the BCHE can be transformed into the confluent hypergeometric equation in a quite different manner, namely by the replacement $z \to \sqrt{z}$, if $A = D = 0$ (or $\beta = \delta = 0$), which is easily verified by direct substitution.

Since the well known level crossing models of Landau–Zener [4], Nikitin [5], and Crothers [6] are described by confluent hypergeometric equation, the last observation gives an alternative representation for solutions to these classes of models in terms of biconfluent Heun functions. As we will show below, the last remark, in turn, allows one to describe a total of five classes of models for the two-level problem, each representing different aspects of term crossings (including several nonlinear crossing types) in quantum systems from a given point of view. Such a unified description is all the more important from the theoretical point of view, since a number of other important quantum mechanical problems may be also reduced to the BCHE. Among these problems are, for instance, the radial problem for the harmonic oscillator, and the quantum doubly anharmonic oscillator [1, 7].

We derive five four-parametric classes of two-level models permitting reduction of the initial problem to the biconfluent Heun equation. Three of these classes are generalizations of the well known classes of Landau–Zener, Nikitin and Crothers. We show that two other classes describe super- and sublinear and essentially nonlinear level crossings, as well as processes with three crossing points. In particular, these classes include two-level models with constant field amplitude and the detuning varying as $\delta_0 t + \delta_2 t^3$ or $\sim t^{1/3}$. For the essentially nonlinear cubic-crossing model, $\delta_t \sim \delta_2 t^3$, we construct the general solution of the two-level problem as series of confluent hypergeometric functions.

2. Five classes of solutions of the two-level problem

According to the method described in detail in [3] (see also [8]), we search for the basic models U^*, δ^* of the two-level problem satisfying the equations

$$\mathrm{i}\delta_z^* - \frac{U_z^*}{U^*} = 2\frac{\varphi_z}{\varphi} + f \qquad U^{*2} = \frac{\varphi_{zz}}{\varphi} + f\frac{\varphi_z}{\varphi} + g \tag{4}$$

where f and g are the coefficients of the initial equation (2). We start from a certain form of the factor φ, which is determined by the structure of f and g, namely

$$\frac{\varphi_z}{\varphi} = \frac{\alpha_1}{z} + \alpha_0 + \alpha_2 z. \tag{5}$$

It is then evident that U^*, δ_z^* should be presented as

$$\frac{U_z^*}{U^*} = \frac{k}{z} \qquad \delta_z^* = \frac{\delta_1}{z} + \delta_0 + \delta_2 z. \tag{6}$$

The substitution of equations (5) and (6) into (4) gives the constraint $k = -1, -1/2, 0, 1/2, 1$; hence, we immediately obtain the relations

$$\begin{aligned} &\alpha_1^2 + \alpha_1(1 + k - \mathrm{i}\delta_1) + Q(0) = 0 \\ &\alpha_2^2 - \mathrm{i}\delta_2\alpha_2 + \frac{Q^{(IV)}(0)}{4!} = 0 \\ &\alpha_0(\mathrm{i}\delta_2 - 2\alpha_2) = \frac{Q^{(III)}(0)}{3!} - \mathrm{i}\delta_0\alpha_2 \end{aligned} \tag{7}$$

where the notation $Q(z) = z^2U^{*2} = z^{2k+2}U_0^{*2}$ is introduced (U_0^* is an arbitrary constant). Simultaneously, the parameters A, B, C, D and E of (2) are uniquely determined by the formulae

$$\begin{aligned} A &= -2\alpha_0 + \mathrm{i}\delta_0 \\ B &= -k - 2\alpha_1 + \mathrm{i}\delta_1 \\ C &= -2\alpha_2 + \mathrm{i}\delta_2 \\ D &= -\left[2\alpha_1\alpha_0 + \alpha_1 A + \alpha_0 B\right] + Q'(0) \\ E &= -\left[\alpha_2 + \alpha_0^2 + 2\alpha_1\alpha_2 + \alpha_1 C + \alpha_0 A + \alpha_2 B\right] + \frac{Q''(0)}{2}. \end{aligned} \tag{8}$$

Relations (7) and (8) thus completely determine the solution of the two-level problems for the five four-parametric classes of models,

$$\begin{aligned} &U(t) = U_0^* z^k \frac{\mathrm{d}z}{\mathrm{d}t} \qquad k = -1, -1/2, 0, 1/2, 1 \\ &\delta_t(t) = \left(\frac{\delta_1}{z} + \delta_0 + \delta_2 z\right)\frac{\mathrm{d}z}{\mathrm{d}t} \end{aligned} \tag{9}$$

(here $z = z(t)$ is an arbitrary function of time one-to-one mapping z to t) in terms of biconfluent Heun functions

$$a_1 = \frac{1}{\varphi(z)} H(A, B, C, D, E; z). \tag{10}$$

By setting $\delta_0 = 0$ and making the replacement $z \to \sqrt{z}$, it is easy to see that classes with $k = -1, 0, 1$ are generalizations of the Landau–Zener, Nikitin and Crothers classes ([4–6], see also [3]). Principally new models are determined by the classes with $k = \pm 1/2$.

Class $k = -1/2$. The amplitude and phase modulation functions explicitly are given as

$$U(t) = \frac{U_0^*}{\sqrt{z}}\frac{\mathrm{d}z}{\mathrm{d}t} \qquad \delta_t = \left(\frac{\delta_1}{z} + \delta_0 + \delta_2 z\right)\frac{\mathrm{d}z}{\mathrm{d}t}. \tag{11}$$

An important member of this family is obtained if we choose $\delta_1 = 0$ and $z = t^2$:

$$U(t) = 2U_0^* = \text{const} \qquad \delta_t(t) = 2(\delta_0 t + \delta_2 t^3) \tag{12}$$

a model that describes superlinear level crossing for $\delta_0\delta_2 > 0$ and sublinear crossing for $\delta_0\delta_2 < 0$ (figure 1). Note that the latter case presents also a threefold level crossing (figure 1). In addition, for $|\delta_2| \gg |\delta_0|$ we have a regime of essentially nonlinear crossing (figure 2), and when $\delta_0 = 0$ this crossing occurs by a purely cubic law $\delta_t = 2\delta_2 t^3$. These types of level crossings have been studied in [8].

Class $k = +1/2$. The amplitude and phase modulation functions now are

$$U(t) = U_0^*\sqrt{z}\frac{\mathrm{d}z}{\mathrm{d}t} \qquad \delta_t(t) = \left(\frac{\delta_1}{z} + \delta_0 + \delta_2 z\right)\frac{\mathrm{d}z}{\mathrm{d}t}. \tag{13}$$

An important member of this family is the model describing another type of essentially nonlinear level crossing, which for $\delta_0 = \delta_1 = 0$ and $z = t^{2/3}$ is derived as

$$U(t) = \tfrac{2}{3}U_0^* \qquad \delta_t(t) = \tfrac{2}{3}\delta_2 t^{1/3}. \tag{14}$$

The plot of the phase modulation function is shown in figure 2.

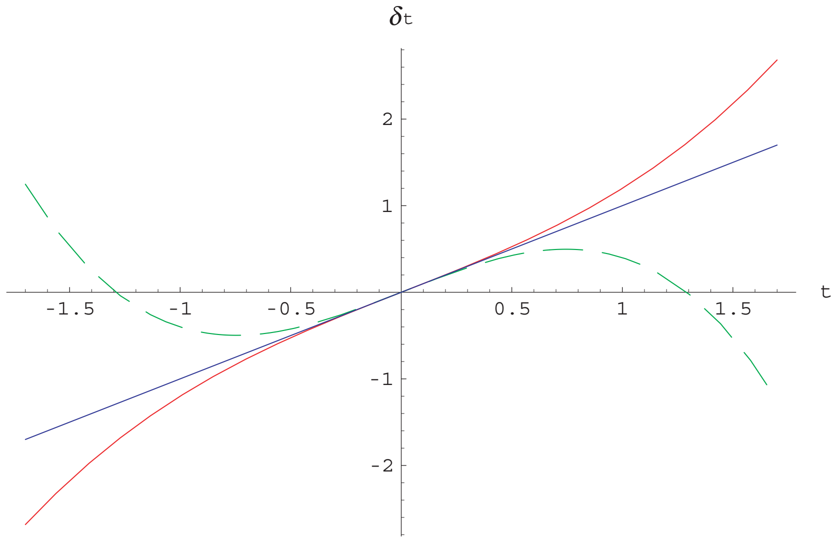

Figure 1. Model $k = -1/2$. The amplitude modulation function is constant. The curves present the phase modulation function at $\delta_0 = 0.5$, $\delta_1 = 0$, $\delta_2 = 0.1$ (superlinear crossing—solid curve) and at $\delta_0 = 0.5$, $\delta_1 = 0$, $\delta_2 = -0.3$ (sublinear crossing—dashed curve). The straight line presents the Landau–Zener model.

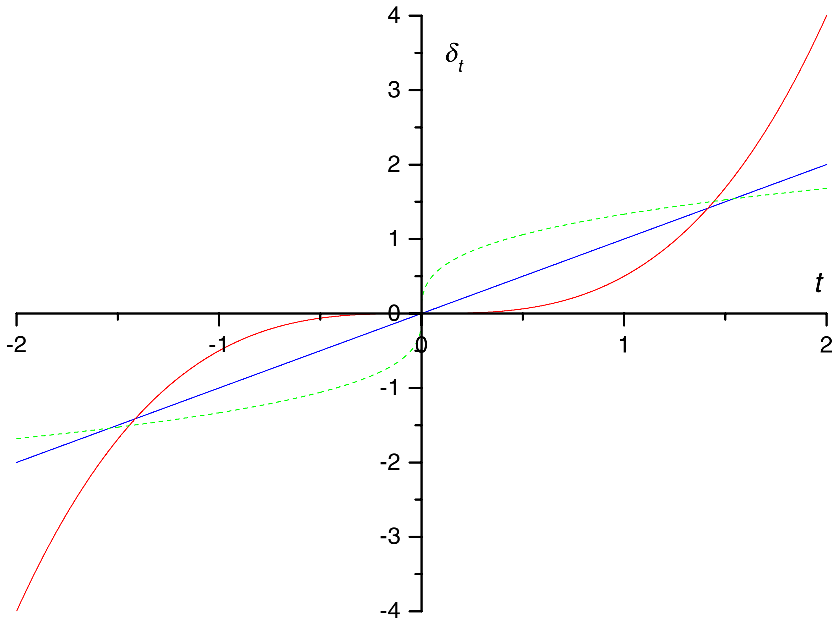

Figure 2. The phase modulation function for model $k = -1/2$ at $\delta_0 = \delta_1 = 0$, $\delta_2 = 0.25$ (essentially nonlinear level crossing—solid curve), and for model $k = +1/2$ at $\delta_0 = \delta_1 = 0$, $\delta_2 = 2$ (another type of the essentially nonlinear level crossing—dotted curve). The straight line presents the Landau–Zener model.

3. Structure of solutions

The solution of the BCHE in a power series of z can be easily constructed by direct substitution of the series

$$u = z^{\mu} \sum_{n=0}^{\infty} a_n z^n \tag{15}$$

into the initial equation (2) (or (1)) whereby one obtains two values for the exponent $\mu = 0$ and $1 - B$. Under the initial condition $u(0) = 1$, we have $\mu = 0$ and the coefficients of the series obey the three-term recurrence relation

$$\begin{aligned} &a_n n\,[(n-1)+B] + a_{n-1}\,[(n-1)A + D] + a_{n-2}\,[(n-2)C + E] = 0 \qquad n \geqslant 0 \\ &a_{-2} = a_{-1} = 0 \qquad a_0 = 1 \qquad a_1 = -D/B. \end{aligned} \tag{16}$$

It is easy to check that for the parameters (7) and (8) this series is not terminated, i.e. the polynomial solutions are impossible. In addition, though the series (15), (16) converges everywhere, it may be used in calculations only in the vicinity of the origin of coordinates. For large z it is appropriate to use the asymptotic solution, which is easily obtained from equation (2); indeed, for $z \to \infty$ we have

$$u_{zz} + Czu_z \approx 0$$

and therefore

$$u \approx c_1 + c_2 \int_0^z \mathrm{e}^{-\frac{Cz^2}{2}}\,\mathrm{d}z. \tag{17}$$

Note, however, that for one of the physically most interesting cases, for the essentially nonlinear level crossing (12) (at $\delta_0 = 0$)

$$\delta_t(t) = 2\delta_2 t^3 \tag{18}$$

one can construct an exact analytical solution of the problem as a convergent everywhere series in terms of confluent hypergeometric functions. To do this, one should choose the parameters $\alpha_{0,1,2}$ (see (7)) so that the parameter A is zero.

According to [1], this expansion has the form

$$u = \sum_{n=0}^{\infty} \tilde{k}^n y_n(z) \tag{19}$$

where

$$y_n(z) = \frac{4^n \Gamma(2\tilde{c}-1)}{n!\,\Gamma(2\tilde{c}-1+n)} \left(-\frac{C}{2}\right)^{n/2} z^n G_n \cdot {}_2F_2\left(\tilde{a}+\frac{n}{2}, 1; \tilde{c}+\frac{n}{2}, 1+\frac{n}{2}; -\frac{C}{2}z^2\right) \tag{20}$$

$$G_n = \prod_{m=1}^{n} \cdot {}_4F_3\left(\tilde{a}+\frac{m-1}{2}, \tilde{c}+\frac{m-2}{2}, \frac{m}{2}, 1; \tilde{c}+\frac{m-1}{2}, \tilde{a}+\frac{m}{2}, \frac{1+m}{2}; 1\right) \tag{21}$$

and the new parameters $\tilde{a}$, $\tilde{c}$ and $\tilde{k}$ are defined by the relations

$$\tilde{a} = \frac{E}{2C} \qquad \tilde{c} = \frac{B+1}{2} \qquad \tilde{k} = -\frac{D}{4}\sqrt{\frac{-2}{C}}. \tag{22}$$

It is remarkable that for one of the independent solutions we obtain $\tilde{a} = \tilde{c}$, and for the second one $\tilde{a} = 1$. Hence, the generalized hypergeometric function ${}_2F_2$ in equation (20) is reduced in both cases to the familiar confluent hypergeometric function. Besides, the coefficients (21) of the expansion are also simplified in these cases, since the functions ${}_4F_3$ are reduced to ${}_3F_2$. Finally, the general solution of the initial problem is thus expressed in the series of confluent hypergeometric functions.

4. Summary

We have derived five four-parametric classes of solutions of the two-level problem expressed in terms of biconfluent Heun functions. Three of these classes are generalizations of the Landau–Zener, Nikitin and Crothers classes. Two other classes contain models with principally distinctive physical properties. These classes were shown to describe sub- and superlinear processes of level crossing as well as two essentially nonlinear types of crossing and processes with three crossing points. Finally, we have constructed the general solution of the initial two-level problem for the cubic term crossing as a convergent everywhere series in terms of confluent hypergeometric functions.

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