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**QUANTUM TWO-STATE LEVEL-CROSSING MODELS  
IN TERMS OF THE HEUN FUNCTIONS**

by

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## INTRODUCTION

The two-state approximation is a widely known key approach intensively applied to study quantum non-adiabatic transitions in a number of important physical systems for many decades, already starting from early years of quantum mechanics [1-4]. This is a relatively simple, yet, useful and powerful approximation used to gather a basic insight of physical processes, to reveal the qualitative characteristics and underlying mechanisms [1-41]. Besides, numerous are the cases when the approximation provides also highly accurate quantitative description. The approximation basically assumes that the evolution of a physical system due to an interaction effectively consists in mixing of just two of quantum levels of the system; the change of others being negligible because of specific conditions considered.

In the canonical Landau-Zener-Majorana-Stückelberg formulation [1-4] the time-dependent version of the semiclassical quantum two-state problem is written as a system of coupled first-order differential equations for probability amplitudes of two states of a quantum system driven by an external field (time-dependent Schrödinger equations) [1-9]. The field is characterized by two real functions, the amplitude and the phase, composing a complex-valued function of a real argument, time. The analytic models of the time-dependent two-state problem of this form have been applied for studying of a number of important physical phenomena in many branches of contemporary physics, chemistry and engineering ranging from the theory of light-matter interaction, non-linear optics, surface physics to nanophysics, neutrino oscillations, cosmology, nuclear reactions, etc. The occurrences of the problem are too numerous to be listed here.

Among analytic models, of particular interest are the *level-crossing* ones. It is well appreciated, already for a long time starting from the pioneering works by Landau, Zener, Majorana, and Stückelberg [1-4], that the level-crossing presents a key approach for the theory of non-adiabatic transitions in quantum systems. Such models, both time-dependent and time-independent, have been widely applied in the context of many physical and chemical phenomena. Apart from the earlier theory of magnetic resonance [1-4], some representative examples include the theory of atomic and molecular collisions [5,6], the general theory of quantum transitions [7], coherent atomic excitation [8] and controlling diverse quantum structures using laser radiation [9], laser cooling and trapping [10] using mechanical action of light [11], atom optics [12], theory of chemical reactions [13-15], quantum mechanical tunneling effects in inorganic, organic, and complex systems in biology [16-18], quantum phase transitions [19-22], quantum information [23,24], Bose-Einstein condensation [25-27], atom lasers [28-29], cold atom association in degenerate quantum gases [30-34], nanophysics [35-38], neutrino oscillations [39-41], etc.

The analytic models of the two-, three- and generally few-state problems developed in the past make use the (generalized) hypergeometric functions or their particular cases (see, e.g., [8-9,42-66] and references therein). In finding the solutions in terms of the Gauss hypergeometric and the Kummer confluent hypergeometric functions [42-56] as well as in terms of the Clausen [57-64] and Goursat [65,66] generalized hypergeometric functions [67-68], it has been recognized that the set of all solvable cases can be divided into independent classes each containing infinite number of members generated by a corresponding basic integrable model [48-66]. The basic solvable models are defined by a pair of functions the first of which is referred to as the amplitude-modulation and the second one as the detuning-modulation function. The actual field-configuration, that is the pair of the real functions defining the real physical field (the Rabi frequency and the frequency detuning as far as the quantum optical terminology is used) by means of application of a (generally complex-valued) transformation of the independent variable [52-55].

In the present work, we apply this general property of the solvable models of the time-dependent Schrödinger equations to derive solutions of the two-state problem in terms of the five Heun functions - the general Heun function [69] and its four confluent forms [70-72]. The general Heun function is a solution of a second order linear differential equation which is the most general ordinary linear second-order Fuchsian differential equation having four regular singular points [69-72]. The special functions emerging from this equation as well as from its four confluent forms are currently widely faced in fundamental and applied physics, mathematics and engineering. These functions generalize all the functions of the hypergeometric class, as well as the Lamé, Mathieu, spheroidal-wave and many other known special functions, and for this reason they are believed to become a part of the standard set of special functions in the near future.

Currently, the Heun equations are encountered in so many branches of classical and non-classical physics ranging from non-Newtonian liquid mechanics, rheology, surface physics, polymer physics, atomic and nuclear physics to general gravity, astronomy and cosmology, e.g., the dislocation theory and mass-step problem in quantum mechanics, time-dependent few-state models in quantum optics, quantum two-center problem in molecular physics, surface polaritons, lattice systems in statistical mechanics, theory of black holes, etc., that it is difficult to give a classification of all relevant problems (see, e.g., [73,74] and references therein).

Due to extremely rich structure of the Heun functions, the analytic developments based on them promise interesting and important new applications in many branches of contemporary physics and mathematics, and, as already mentioned above, the special functions emerging from the solutions of the Heun equations are supposed to gradually compose an important component of the next generation of standard tools of mathematical physics.

However, despite the considerable effort devoted to the mathematical properties of the Heun equations, they are still much less studied than their predecessors, first of all, the relatives of the hypergeometric class. A major reason for the slow progress in the development of the theory of the Heun equations is that the series solutions (either in terms of powers or in terms of the functions of hypergeometric class) are governed by at least three-term recurrence relations between successive coefficients of expansions [69-72], instead of two-term ones appearing in the hypergeometric case [72]. For this reason, it was commonly thought that the expansion coefficients are no longer determined explicitly.

Nevertheless, it has recently been shown that for the *general* and *single-confluent* Heun equations there exist infinitely many particular choices of the involved parameters for which the recurrence relations for power-series expansions of solutions become two-term. In these cases the solutions can be explicitly written either as a linear combination of a finite number of the (ordinary or confluent) hypergeometric functions or, alternatively, in terms of a single (ordinary or confluent) generalized hypergeometric function. Another result recently reported is that if the solutions of the general and single-confluent Heun equations are expanded in terms of the appropriate functions of the hypergeometric class, there also exist infinitely many particular choices of the involved parameters for which the governing three-term recurrence relations for expansion coefficients become two-term. We note that in all these cases of two-term reductions, the expansion coefficients are explicitly written in terms of the Euler gamma functions. Besides, we have recently constructed expansions of the solutions of the *bi-confluent* Heun equation in terms of the Hermite functions.

Discussing the conditions for deriving finite-sum closed-form solutions by means of termination of the mentioned series, it can be shown that the termination occurs if a regular singularity of the bi-confluent Heun equation is *apparent* and the *accessory* parameter obeys a polynomial equation. We apply these results to derive some particular two-state models for which the problem is solved in terms of special mathematical functions simpler than the Heun functions, that is, we identify some particular models for which the involved Heun functions are expressed in terms of the familiar functions of the hypergeometric class.

The main objectives of this research are:

1. to identify and classify the optical field-configurations (referred to as two-state models) for which the semiclassical time-dependent two-state problem can be solved in terms of the five Heun functions,
2. to identify the level-crossing field-configurations within the set of quantum two-state models solvable in terms of the Heun functions,

3. to construct explicit finite-sum closed-form solutions of the general, single- and bi-confluent Heun equations in terms of simpler special functions, and to identify the two-state Heun models for which the solution of the problem is written as an irreducible combination of functions of the hypergeometric class,
4. to extend the knowledge gained on the exact or conditionally solvability of the two-state problem in terms of the Heun functions to non-relativistic and relativistic wave equations.

It should be noted that the basic set of analytic models of the two-state problem has been developed in the past by solving the time-dependent Schrödinger equations in terms of special functions of the hypergeometric class. Here, we show that much more models are derived when expressing the solution of the problem in terms of the functions of the Heun class. Since the Heun functions represent direct generalizations of the hypergeometric functions, the solutions in terms of the latter functions generalize all hypergeometric cases.

A major result we report is that there exist in total 61 infinite classes of two-state models solvable in terms of the five Heun functions. More specifically, we have shown that there exist thirty-five classes for which the problem can be solved in terms of the general Heun functions [75], fifteen classes solvable in terms of the single-confluent Heun functions have previously been derived in [76], and we have obtained five classes solvable in terms of the double-confluent Heun functions [77], five other classes in terms of the bi-confluent Heun functions [77], and a class in terms of the tri-confluent Heun functions [77].

Another set of our results consists of the expansions of the solutions of the general, single-confluent, and bi-confluent Heun equations in terms of incomplete Beta [78], Kummer confluent hypergeometric [79], and non-integer order Hermite functions [80]. The conditions for termination of these series, in order to produce finite-sum closed-form solutions, are discussed in detail.

A third set of our results comes out if the developed series expansions are applied to identify the particular cases for which the Heun functions involved in the solutions of the presented two-state models can be written as such linear combinations of the functions of the hypergeometric class that cannot be reduced to the one-term ansatz involving only one hypergeometric function. In this way, many new level-crossing models are derived. These results are presented in [81-83].

Finally, a fourth set of results is achieved by applying the above approaches to non-relativistic and relativistic wave equations in order to derive new energy-independent quantum-mechanical potentials for the Schrödinger equation that are solved in terms of the functions of the hypergeometric class [80,84], and to reveal the nine potentials for which the stationary Klein-Gordon equation can be solved in terms of the confluent Heun functions [85].



Based on these results, the key observations of this research are:

1. There exist 61 infinite classes of the quantum time-dependent two-state problem solvable in terms of general, single-confluent and multi-confluent Heun functions.
2. The infinite classes of two-state models solvable in terms of the Heun functions contain numerous models that describe one, two or infinite number of (periodically occurring) level-crossings of the resonance. Different examples of such models are presented.
3. It is possible to construct solutions of the Heun equations as infinite series in terms of the functions of the hypergeometric class of a different structure. Several examples of such series expansions are presented.
4. The analytic solutions of the two-state problem can be projected on the relativistic and non-relativistic wave-equations to derive new solutions of these equations.

The detailed results obtained are as follows.

In **Chapter 1**, following our work [75], we derive 35 five-parametric classes of the quantum time-dependent two-state models solvable in terms of the general Heun functions. Each of the classes is defined by a pair of generating functions the first of which is referred to as the amplitude- and the second one as the detuning-modulation function. The classes suggest numerous families of specific field configurations with different physical properties generated by appropriate choices of the transformation of the independent variable, real or complex. There are many families of models with constant detuning or constant amplitude, numerous classes of chirped pulses of controllable amplitude and/or detuning, families of models with double or multiple (periodic) crossings, periodic amplitude modulation field configurations, etc.

The detuning modulation function is the same for all the derived classes. This function involves four arbitrary parameters, that is, two more than the previously known hypergeometric classes. These parameters in general are complex and should be chosen so that the resultant detuning is real for the applied (arbitrary) complex-valued transformation of the independent variable. The generalization of the detuning modulation function to the four-parametric case is the most notable extension since many useful properties of the two-state models described by the Heun equation are due to namely the additional parameters involved in this function. Many of the derived amplitude modulation functions present different generalizations of the known hypergeometric models. In several cases the generalization is achieved by multiplying the amplitude modulation function of the corresponding prototype hypergeometric class by an extra factor including an additional parameter. Finally, many classes suggest amplitude modulation functions having forms not discussed previously.

We present several families of constant-detuning field configurations generated by a real transformation of the independent variable. The members of these families are symmetric or asymmetric two-peak finite-area pulses with controllable distance between the peaks and controllable amplitude of each of the peaks. We show that the edge shapes, the distance between the peaks as well as the amplitude of the peaks are controlled almost independently, by different parameters. We identify the parameters controlling each of the mentioned features and discuss other basic properties of pulse shapes. We show that the pulse edges may become step-wise functions and determine the positions of the limiting vertical-wall edges. We show that the pulse width is controlled by only two of the involved parameters. For some values of these parameters, the pulse width diverges and for some other values the pulses become infinitely narrow. We show that the effect of the two mentioned parameters is almost similar, that is, both parameters are able to independently produce pulses of almost the same shape and width. We determine the conditions for generation of pulses of almost indistinguishable shape and width, and present several such examples.

Finally, we present a constant-amplitude periodic level-crossing model and several families of constant-detuning field configurations generated by complex transformations of the variable.

Next, following our work [81], we present a specific constant-amplitude periodic level-crossing model of the semiclassical quantum time-dependent two-state problem that belongs to a general Heun class of field configurations. The exact analytic solution for the probability amplitude, generally written for this class in terms of the general Heun functions, in this specific case admits series expansion in terms of the incomplete Beta functions [78]. Terminating this series results in an infinite hierarchy of finite-sum closed-form solutions each standing for a particular two-state model, which generally is only *conditionally* integrable in the sense that for these field configurations the amplitude and phase modulation functions are not varied independently. However, there exists at least one exception when the model is *unconditionally* integrable, that is the Rabi frequency and the detuning of the driving optical field are controlled independently. This is a constant-amplitude periodic level-crossing model, for which the detuning in a limit becomes a Dirac delta-comb configuration with variable frequency of the level-crossings. We derive the exact solution for this model, determine the Floquet exponents and study the population dynamics in the system for various regions of the input parameters.

In **Chapter 2**, we present the fifteen classes of the two-state models for which the solution of the problem is written in terms of the single-confluent Heun functions (these classes have been derived in [76]).

Next, following our work [79], we examine the series expansions of the solutions of the single-confluent Heun equation in terms of different sets of confluent hypergeometric functions. First, we construct several expansions in terms of three distinct Kummer (regular) functions. We show that the successive coefficients of the expansions in general obey three-term recurrence relations defining double-sided infinite series; however, four-term and two-term relations are also possible for particular choices of the involved parameters. The conditions for left- and/or right-hand side termination of the series are discussed in detail.

Furthermore, using the recurrence relations obeyed by the Tricomi (irregular) confluent hypergeometric functions, we construct one more confluent hypergeometric expansion of the solutions of the single-confluent Heun equation.

Next, we show that there exist infinitely many nontrivial choices of parameters of the single-confluent Heun equation for which the three-term recurrence relations governing the expansions of the solutions in terms of the confluent hypergeometric functions are reduced to two-term ones. In such cases the expansion coefficients are explicitly calculated in terms of the Euler gamma functions.

It should be noted that the finite-sum reductions of series solutions of the linear second-order ordinary differential equations in terms of special functions provide a major set of known closed-form analytic solutions of various linear differential equations encountered in contemporary physics research. A general observation concerning such reductions is that, if the special functions of the hypergeometric class are applied as expansion functions, owing to the linear relations between any three contiguous hypergeometric functions, a terminating series can be reduced to a linear combination with generally rational coefficients of just two expansion functions. We stress that this combination is *irreducible* to a form containing only one special function. Due to this observation, one can directly apply a *two-term ansatz* for solving linear ordinary differential equations in terms of hypergeometric functions.

Finally, following our work [83], we apply the above-presented expansions to the fifteen classes of the Heun two-state models. As a result, one obtains a presumably infinite set of solvable models which in general are *conditionally* integrable (besides, in many cases these models describe *dissipative* processes). Among this set, we identify the only new member, which is *exactly* integrable in that the involved parameters are varied independently. This is a three-parametric constant-amplitude level-crossing model. The model presents a field-configuration describing an *asymmetric-in-time* level-crossing process for which the laser field detuning modulation function is given in terms of the Lambert-W function. The general solution of the problem for this model is written as a linear combination, with arbitrary constant coefficients, of two fundamental solutions

each of which presents an irreducible linear combination of two confluent hypergeometric functions. We present the detailed derivation of the fundamental solutions and analyze the behavior of the system in the laser field given by the specific configuration under consideration. We note that each of the fundamental solutions has an alternative representation in terms of a single Goursat generalized confluent hypergeometric function.

In **Chapter 3**, following our work [77], we derive five classes of quantum time-dependent two-state models solvable in terms of the double-confluent Heun functions, five other classes solvable in terms of the bi-confluent Heun functions, and a class solvable in terms of the tri-confluent Heun functions. These classes generalize all the known families of two- or three-parametric models solvable in terms of the confluent hypergeometric functions to more general four-parametric classes involving three-parametric detuning modulation functions. The particular models derived describe different non-linear (parabolic, cubic, sinh, cosh, etc.) level-sweeping or level-glancing processes, double- or triple-level-crossing processes, as well as periodically repeated resonance-glancing or resonance-crossing processes. Finally, we show that more classes can be derived using the equations obeyed by certain functions involving the derivatives of the confluent Heun functions. We present an example of such a class for each of the three discussed confluent Heun equations.

Next, following our work [80], we construct an expansion of the solutions of the bi-confluent Heun equation in terms of the non-integer order Hermite functions of a shifted and scaled argument. The series is shown to be governed by a three-term recurrence relation between successive coefficients of the expansion. We examine the restrictions that are imposed on the involved parameters in order that the series terminates thus resulting in closed-form finite-sum solutions of the bi-confluent Heun equation. We show that the termination is possible if a regular singularity of the bi-confluent Heun equation is an integer and the accessory parameter obeys a polynomial equation.

Finally, we apply the constructed expansion to discuss the exact and conditionally integrable bi-confluent-Heun models of the two-state problem solvable in terms of the Hermite functions. Examining the termination conditions for the Hermite-function expansion we have presented in the previous section, we show that there exist only four exactly solvable models all of which are three-parametric. The first three of these cases reproduce the known Landau-Zener, Nikitin and Crothers-Hughes models, while the fourth one presents a new result. We thus introduce a new unconditionally solvable model for the quantum semiclassical time-dependent two-state problem. This is a constant-amplitude level-crossing field-configuration for which the detuning modulation function behaves as

the inverse square root at the origin and tends to a constant at the infinity. We present the detailed derivation of the model and construct the explicit general solution of the problem through a fundamental solution written as an irreducible linear combination of two non-integer order Hermite functions of a shifted and scaled argument.

In **Chapter 4**, we consider some applications of the approaches developed in previous chapters to non-relativistic Schrödinger and relativistic Klein-Gordon wave equations.

First, following our work [84], we introduce the third *five-parametric* ordinary hypergeometric energy-independent quantum-mechanical potential for the Schrödinger equation, after the Eckart and Pöschl-Teller potentials, which is proportional to an arbitrary variable parameter and has a shape that is independent of that parameter. Depending on an involved parameter, the potential presents either a short-range singular well (which behaves as inverse square root at the origin and vanishes exponentially at infinity) or a smooth asymmetric step-barrier (with variable height and steepness). The general solution of the Schrödinger equation for this potential, which is a member of a general Heun family of potentials, is written through fundamental solutions each of which presents an irreducible linear combination of two Gauss ordinary hypergeometric functions  ${}_2F_1$ .

Next, following our work [80], we consider a physical application of the closed-form solutions of the bi-confluent Heun functions in terms of the Hermite functions discussed in the previous chapter. We present the five six-parametric potentials for which the general solution of the one-dimensional Schrödinger equation is written in terms of the bi-confluent Heun functions and further identify a particular conditionally integrable potential for which the involved bi-confluent Heun function admits a four-term finite-sum expansion in terms of the Hermite functions. This is an infinite well defined on a half-axis. We present the explicit solution of the one-dimensional Schrödinger equation for this potential and discuss the bound states supported by the potential. We derive the exact equation for the energy spectrum and construct an accurate approximation for the bound-state energy levels.

Finally, following our work [85], we present in total fifteen potentials for which the stationary Klein-Gordon equation is solvable in terms of the confluent Heun functions. Because of the symmetry of the confluent Heun equation with respect to the transposition of its regular singularities, only nine of the potentials are independent. Four of these independent potentials are five-parametric. One of them possesses a four-parametric ordinary hypergeometric sub-potential, another one possesses a four-parametric confluent hypergeometric sub-potential, and one potential possesses four-parametric sub-potentials of both hypergeometric types. The fourth five-parametric

potential has a three-parametric confluent hypergeometric sub-potential, which is, however, only conditionally integrable. The remaining five independent Heun potentials are four-parametric and have solutions only in terms of irreducible confluent Heun functions.

The results of this research have been presented in 9 research papers published during the last 6 years (2014-2019):

1. T.A. Ishkhanyan and A.M. Ishkhanyan, "Expansions of the solutions to the confluent Heun equation in terms of the Kummer confluent hypergeometric functions", *AIP Advances* **4**, 087132 (2014).
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3. A.M. Ishkhanyan, T.A. Shahverdyan, T.A. Ishkhanyan, "Thirty five classes of solutions of the quantum time-dependent two-state problem in terms of the general Heun functions", *Eur. Phys. J. D* **69**, 10 (2015).
4. T.A. Shahverdyan, T.A. Ishkhanyan, A.E. Grigoryan, A.M. Ishkhanyan, "Analytic solutions of the quantum two-state problem in terms of the double, bi- and tri-confluent Heun functions", *J. Contemp. Physics (Armenian Ac. Sci.)* **50**(3), 211-226 (2015).
5. A.S. Tarloyan, T.A. Ishkhanyan, and A.M. Ishkhanyan, "Four five-parametric and five four-parametric independent confluent Heun potentials for the stationary Klein-Gordon equation", *Ann. Phys. (Berlin)* **528**, 264-271 (2016).
6. T.A. Ishkhanyan and A.M. Ishkhanyan, "Solutions of the bi-confluent Heun equation in terms of the Hermite functions", *Ann. Phys.* **383**, 79-91 (2017).
7. G. Saget, A.M. Ishkhanyan, C. Leroy, and T.A. Ishkhanyan, "Two-state model of a general Heun class with periodic level-crossings", *J. Contemp. Physics (Armenian Ac. Sci.)* **52**(4), 324-334 (2017).
8. T.A. Ishkhanyan and A.M. Ishkhanyan, "The third five-parametric hypergeometric quantum-mechanical potential", *Advances in High Energy Physics* **2018**, 2769597 (2018).
9. T.A. Ishkhanyan, "A Lambert-W exactly solvable level-crossing confluent hypergeometric two-state model", *J. Contemp. Physics (Armenian Ac. Sci.)* **54**(1), 17-26 (2019).

## Chapter 1

### SOLUTIONS OF THE TWO-STATE PROBLEM IN TERMS OF THE GENERAL HEUN FUNCTIONS

#### 1.1 Thirty five classes of solutions of the quantum time-dependent two-state problem in terms of the general Heun functions

The two-state system is the simplest non-trivial quantum system that can be treated analytically and it is a rather good approximation for many real quantum systems in nature. Examples of such systems arise in a number of phenomena of contemporary physics, chemistry, engineering, etc. In the present research we consider the quantum non-adiabatic transitions between levels during the interaction of external optical fields with the matter, when only a transition between two of the levels of a generally multi-state system is nearly resonant with the external driving field. So, we discuss the dynamics of just two quantum levels, i.e., the quantum two-state problem, assuming the effect of the field on other levels to be negligible as they are far off the resonance.

In the present chapter, following our work [75], we discuss the solutions of the semiclassical two-state problem in terms of the general Heun function [69]. This function is the solution of a second order linear differential equation having four regular singular points in the complex  $z$ -plane. This equation, the general Heun equation, directly generalizes the Gauss hypergeometric equation [70-72], and for this reason, it is routinely encountered in contemporary physics and mathematics research. It contains a large number of important advanced special cases, in particular, the Lamé equation is the most studied one which is of considerable importance in mathematical physics. The occurrences of the general Heun equation in classical and non-classical physics cover such fields as the wave mechanics, surface physics, polymer physics, condensed state physics, particle physics, general gravity, astronomy, cosmology, and many others (see, e.g., [73] and references therein).

It has previously been discussed the reduction of the two-state problem to the confluent Heun equation and it was found fifteen four-parametric classes of solvable models [76]. We have shown that the general Heun equation suggests much wider set of choices [75]. Namely, we have derived 35 five-parametric classes of solvable models which generalize all previously known integrable cases to more general classes and suggest many new families of solvable field configurations [75]. The most notable feature of this generalization is due to the extension of the *detuning modulation* function to a four-parametric family suggesting many useful features. Besides, some of the derived *amplitude modulation* functions present different types of generalizations of the

known hypergeometric ones, while many other classes suggest amplitude modulation functions having forms not discussed before. Finally, the derived classes also generalize the very few cases when the problem was treated using the general Heun equation [55,86,87].

Numerous specific field configurations with different physical properties can be generated by appropriate transformation of the independent variable, real or complex. Below we present several examples corresponding to the *constant detuning* case generated by *real* functions  $z(t)$ . Other such constant detuning configurations can be suggested by complex transformation, e.g., having the form  $z = (1 + iy(t))/2$ . Actually there are many other possible field configurations. For instance, there are numerous models with constant amplitude (in contrast to the case of constant detuning pulses), a variety of generally asymmetric chirped pulses of controllable amplitude and frequency detuning variation, symmetric or asymmetric models with double or multiple (periodic) crossings of the resonance, double or multiple level-glancing models, periodic amplitude modulation and bi-chromatic field configurations, etc. The examples are too many. Here we present only some of the families of constant detuning pulses generated by real functions  $z(t)$  leaving the discussion of other possible field configurations for a separate consideration.

Discussing the constant-detuning field configurations we show that, for ten classes, the members of such families are two-peak finite-area pulses with controllable distance between the peaks and controllable amplitude of each of the peaks. Notably, the distance between the peaks, the amplitude of the peaks as well as the shapes of the pulse edges are controlled almost independently, by different input parameters. We identify the parameters standing for each of these features and discuss the basic properties of pulse shapes. We mention some examples of field configurations of particular physical interest and discuss their general properties. In particular, we show that the pulse edges may be step-wise and determine the positions of the limiting vertical-wall edges. We show that the pulse width is controlled by only two of the involved parameters. However, we show that the effect of these parameters is rather similar, that is, both parameters are able to independently produce pulses almost of the same shape and width. We determine the conditions for generation of pulses of almost indistinguishable shape and width, and present a number of such examples. Finally, we show that pulses with arbitrary width can be produced. The cases of infinitely wide and infinitely narrow pulses are identified explicitly.

### **1.1.1 Reduction of the two-state problem to the general Heun equation**

The semiclassical time-dependent two-state problem is written as a system of coupled first-order differential equations for probability amplitudes  $a_1(t)$  and  $a_2(t)$  of given two states of a



quantum system driven by an external field with amplitude modulation  $U(t) > 0$ , and phase modulation  $\delta(t)$ :

$$i \frac{da_1}{dt} = U e^{-i\delta} a_2, \quad i \frac{da_2}{dt} = U e^{+i\delta} a_1. \quad (1)$$

This system is equivalent to the following linear second-order ordinary differential equation:

$$a_{2tt}(t) + \left( -i\delta_t - \frac{U_t}{U} \right) a_{2t}(t) + U^2 a_2(t) = 0, \quad (2)$$

where and hereafter the alphabetical index denotes differentiation with respect to corresponding variable.

A useful property of solvable models of the two-state problem is that if the function  $a_2^*(z)$  is a solution of this equation rewritten for an auxiliary argument  $z$  for some functions  $U^*(z)$ ,  $\delta^*(z)$  then the function  $a_2(t) = a_2^*(z(t))$  is the solution of Eq. (2) for the field-configuration defined as

$$U(t) = U^*(z) \frac{dz}{dt}, \quad \delta_t(t) = \delta_z^*(z) \frac{dz}{dt} \quad (3)$$

for arbitrary complex-valued function  $z(t)$  [52-55]. We refer to the functions  $U^*(z)$  and  $\delta_z^*(z)$  as the amplitude- and detuning-modulation functions, respectively, and to the pair  $\{U^*, \delta_z^*\}$  as basic integrable model.

Transformation of variables  $z = z(t)$ ,  $a_2 = \varphi(z) u(z)$  together with (3) reduces equation (2) to the following equation for the new dependent variable  $u(z)$ :

$$u_{zz} + \left( 2 \frac{\varphi_z}{\varphi} - i\delta_z^* - \frac{U_z^*}{U^*} \right) u_z + \left( \frac{\varphi_{zz}}{\varphi} + \left( -i\delta_z^* - \frac{U_z^*}{U^*} \right) \frac{\varphi_z}{\varphi} + U^{*2} \right) u = 0. \quad (4)$$

This equation is the general Heun equation [69]

$$u_{zz} + \left( \frac{\gamma}{z} + \frac{\delta}{z-1} + \frac{\varepsilon}{z-a} \right) u_z + \frac{\alpha\beta z - q}{z(z-1)(z-a)} u = 0 \quad (5)$$

with the Fuchsian condition  $1 + \alpha + \beta = \gamma + \delta + \varepsilon$ , if

$$\frac{\gamma}{z} + \frac{\delta}{z-1} + \frac{\varepsilon}{z-a} = 2 \frac{\varphi_z}{\varphi} - i\delta_z^* - \frac{U_z^*}{U^*} \quad (6)$$

and

$$\frac{\alpha\beta z - q}{z(z-1)(z-a)} = \frac{\varphi_{zz}}{\varphi} + \left( -i\delta_z^* - \frac{U_z^*}{U^*} \right) \frac{\varphi_z}{\varphi} + U^{*2}. \quad (7)$$

Searching for solutions of equations (6), (7) in the form

$$\varphi = z^{\alpha_1} (z-1)^{\alpha_2} (z-a)^{\alpha_3}, \quad (8)$$

$$U^* = U_0^* z^{k_1} (z-1)^{k_2} (z-a)^{k_3}, \quad (9)$$

$$\delta_z^* = \frac{\delta_1}{z} + \frac{\delta_2}{z-1} + \frac{\delta_3}{z-a}, \quad (10)$$

where parameters  $\alpha_{1,2,3}$ ,  $U_0^*$ ,  $k_{1,2,3}$  and  $\delta_{1,2,3}$  are supposed to be constants, we multiply equation (7) by  $z^2(z-1)^2(z-a)^2$  and note that then it follows from the obtained equation that the product  $U_0^{*2} z^{2k_1+2} (z-1)^{2k_2+2} (z-a)^{2k_3+2}$  is a polynomial in  $z$  of maximum fourth degree:  $-1 \leq k_{1,2,3} \cup k_1 + k_2 + k_3 \leq -1$ . This leads to 35 possible choices of  $k_{1,2,3}$ . These sets are shown on Fig. 1 by points in 3D-space of parameters  $k_{1,2,3}$ . The corresponding basic models  $U^*(z)$  are explicitly presented in Tables 1-5. Note that since the parameters  $a$ ,  $U_0^*$  and  $\delta_{1,2,3}$  remain arbitrary, all the derived classes are 5-parametric.

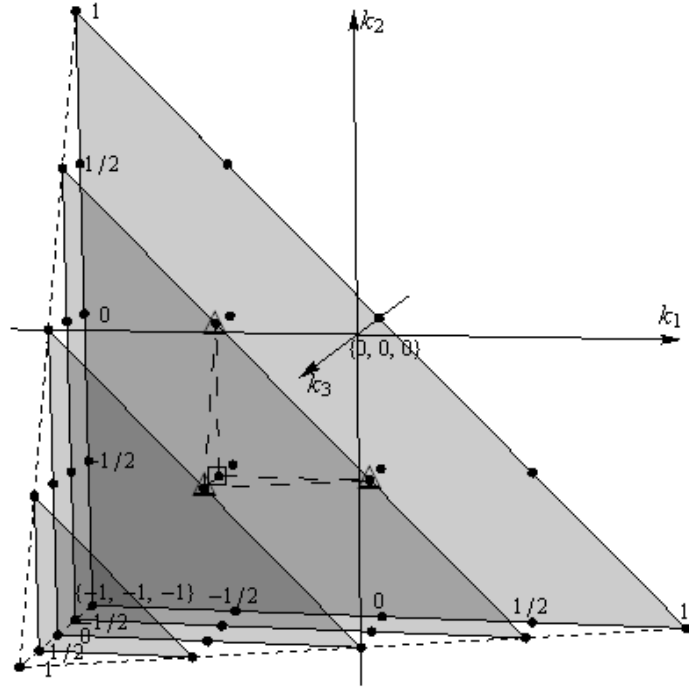


Fig. 1. Thirty five points in the parameter space  $\{k_1, k_2, k_3\}$  defining the 35 classes of 5-parametric models of the two-state problem solvable in terms of the general Heun equation. The four cases for which  $\varphi = 1$  are indicated by three triangles and a square.

### 1.1.2 Thirty five basic integrable models

As it is seen, we have 15 basic models with  $k_3 = -1$  (Table 1) - this is the richest subset of classes. The physical field-configurations  $\{U(t), \delta(t)\}$  generated by the six models closest to the lower left corner generalize the six well known Gauss hypergeometric models (compare with the classes of Table 3), widely discussed in the past by many authors (see, e.g., [8,9], [45-55] and

references therein), by the extra factor  $1/(z-a)$ . Note that along with this extension, an additional generalization comes from extra term  $\delta_3/(z-a)$  in Eq. (10). Other models suggest different extensions of  $U^*(z)$ . Three-parametric subfamilies of field configurations belonging to the classes  $\{k_1, k_2, k_3\} = \{-1/2, k_2, -1\}$  with  $k_2 = -1/2, 0, 1/2$ , for which the solution of the two-state problem is written in terms of the Gauss hypergeometric functions  ${}_2F_1$ , were presented in [55].

$k_2$					$k_3 = -1$
1	$\frac{z-1}{z(z-a)}$				
1/2	$\frac{\sqrt{z-1}}{z(z-a)}$	$\frac{\sqrt{z-1}}{\sqrt{z}(z-a)}$			
0	$\frac{1}{z(z-a)}$	$\frac{1}{\sqrt{z}(z-a)}$	$\frac{1}{z-a}$		
-1/2	$\frac{1}{z\sqrt{z-1}(z-a)}$	$\frac{1}{\sqrt{z(z-1)}(z-a)}$	$\frac{1}{\sqrt{z-1}(z-a)}$	$\frac{\sqrt{z}}{\sqrt{z-1}(z-a)}$	
-1	$\frac{1}{z(z-1)(z-a)}$	$\frac{1}{\sqrt{z}(z-1)(z-a)}$	$\frac{1}{(z-1)(z-a)}$	$\frac{\sqrt{z}}{(z-1)(z-a)}$	$\frac{z}{(z-1)(z-a)}$
	-1	-1/2	0	1/2	1
					$k_1$

Table 1. Fifteen basic models  $U^*/U_0^*$  with  $k_3 = -1$ . The field-configurations  $\{U(t), \delta(t)\}$  generated by the six models closest to the lower left corner generalize the well known six hypergeometric models [53-55] (see Table 3) by the extra factor  $1/(z-a)$  (note that along with this extension, additional generalization comes from the extra term  $\delta_3/(z-a)$  in Eq. (10)). Other models suggest different extensions of  $U^*(z)$ .

The next 10 basic models correspond to the choice  $k_3 = -1/2$  (Table 2). Here again, the six models closest to the lower left corner generalize the hypergeometric models [53-55] (compare with the classes of Table 3), this time, by the extra factor  $1/\sqrt{z-a}$  (note that along with this extension, here also a further generalization comes from the extra term  $\delta_3/(z-a)$  in Eq. (10)), while the four diagonal models are of different structure.

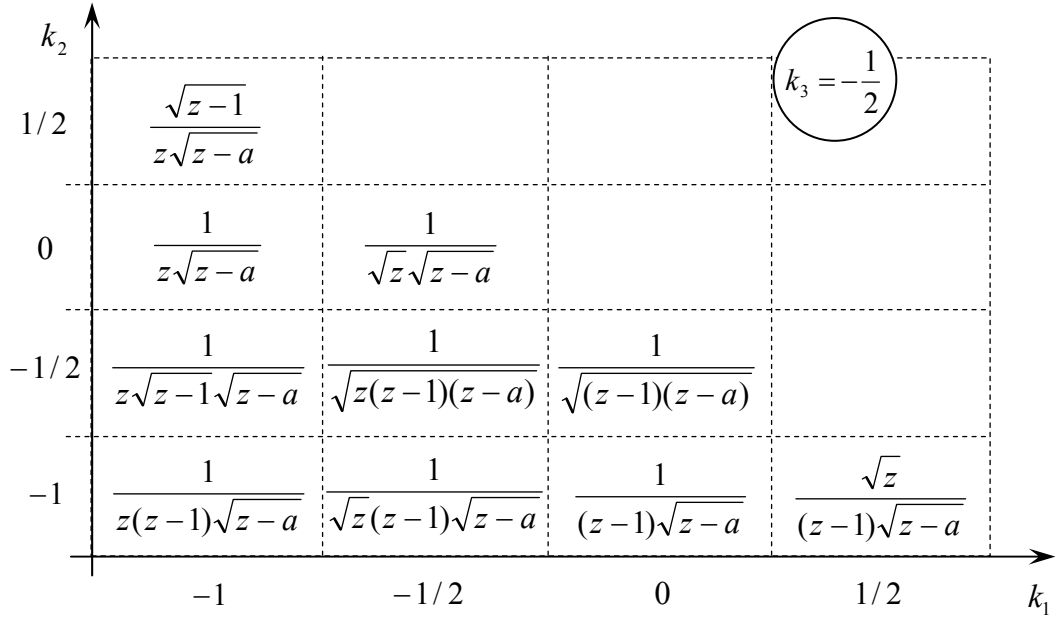


Table 2. Ten basic models  $U^*/U_0^*$  corresponding to  $k_3 = -1/2$ .

Six basic models correspond to  $k_3 = 0$  (Table 3). Though these models are exactly of the same form as the ones solvable in terms of the Gauss hypergeometric equation (see [53-55]), however, due to the additional term  $\delta_3/(z-a)$  in equation (10) for the detuning modulation, the final physical field-configurations  $\{U(t), \delta(t)\}$  generated by these models are more general and include the hypergeometric models as particular cases.

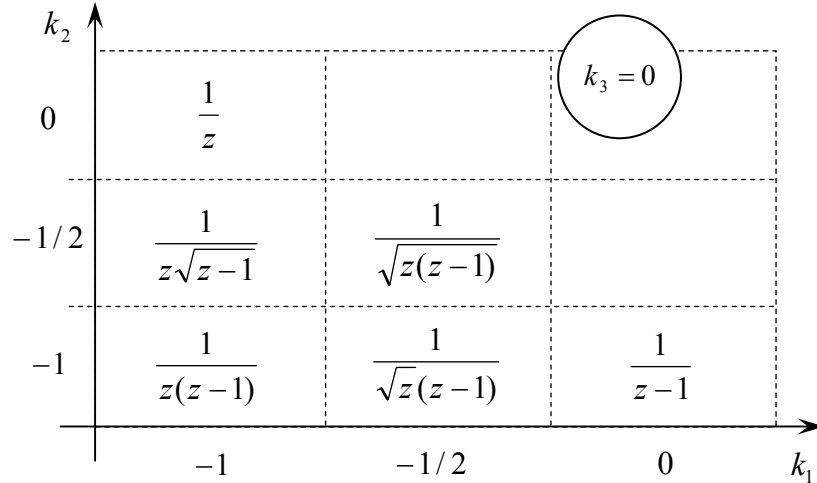


Table 3. Six basic models  $U^*/U_0^*$  corresponding to  $k_3 = 0$ .

Finally, 3 basic models correspond to  $k_3 = 1/2$  (Table 4), and there is only one model in the case  $k_3 = 1$ :  $\{k_1, k_2, k_3\} = \{-1, -1, +1\}$  (Table 5). The three basic models of Table 4 generalize the hypergeometric basic models by the extra factor  $\sqrt{z-a}$ , and the model of Table 5 generalizes the

corresponding hypergeometric model  $U^*/U_0^* = 1/(z(z-1))$  by the factor  $z-a$ . As in the case of all other general Heun models, further generalization for all these classes consists in the term  $\delta_3/(z-a)$  in Eq. (10).

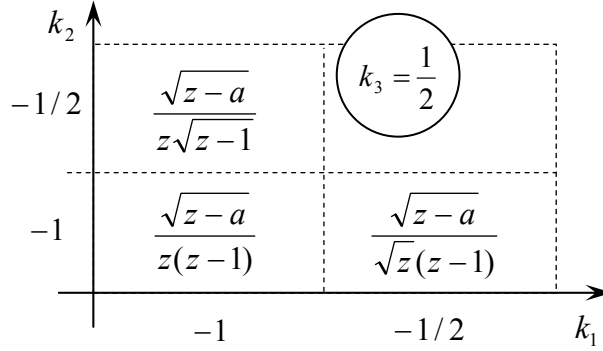


Table 4. Three basic models  $U^*/U_0^*$  corresponding to  $k_3 = 1/2$ . All the three generalize the hypergeometric models by the extra factor  $\sqrt{z-a}$  as well as, as in the case of all other Heun models, further generalization comes from the extra term  $\delta_3/(z-a)$  in Eq. (10).

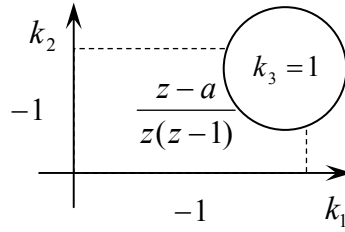


Table 5. The only basic model  $U^*/U_0^*$  corresponding to  $k_3 = 1$ . The generalization of the corresponding hypergeometric model  $U^*/U_0^* = 1/(z(z-1))$  consists in the extra factor  $z-a$  and, furthermore, in the extra term  $\delta_3/(z-a)$  in Eq. (10).

### 1.1.3 Solution of the two-state problem

According to the property (3) of integrable models and Eqs. (9), (10), the physical field-configuration, i.e., the Rabi frequency and the frequency detuning of the laser radiation if quantum optical terminology is applied, are given as

$$U(t) = U_0^* z^{k_1} (z-1)^{k_2} (z-a)^{k_3} \frac{dz}{dt}, \quad (11)$$

$$\delta_i(t) = \left( \frac{\delta_1}{z} + \frac{\delta_2}{z-1} + \frac{\delta_3}{z-a} \right) \frac{dz}{dt}. \quad (12)$$

Note that the parameters  $a$ ,  $U_0^*$ ,  $\delta_{1,2,3}$  are in general *complex* constants which should be chosen so that the functions  $U(t)$  and  $\delta(t)$  are real for given *complex-valued* function  $z(t)$ .

The solution of the initial two-state problem (1) is explicitly written as

$$a_2 = C_0 z^{\alpha_1} (z-1)^{\alpha_2} (z-a)^{\alpha_3} H(a, q; \alpha, \beta; \gamma, \delta; z), \quad C_0 = \text{const}, \quad (13)$$

where  $H(a, q; \alpha, \beta; \gamma, \delta; z)$  is the Heun function satisfying Eq. (5) and  $\alpha_{1,2,3}$  are defined by the following quadratic equations:

$$\begin{aligned} \alpha_1(\alpha_1 + 1 - \gamma) &= \left( z^2 U^{*2} \right) \Big|_{z=0}, \\ \alpha_2(\alpha_2 + 1 - \delta) &= \left( (z-1)^2 U^{*2} \right) \Big|_{z=1}, \\ \alpha_3(\alpha_3 + 1 - \varepsilon) &= \left( (z-a)^2 U^{*2} \right) \Big|_{z=a}. \end{aligned} \quad (14)$$

The Heun function's parameters  $\gamma, \delta, \varepsilon$  and  $q$  are given through the equations

$$\gamma = 2\alpha_1 - i\delta_1 - k_1, \quad \delta = 2\alpha_2 - i\delta_2 - k_2, \quad \varepsilon = 2\alpha_3 - i\delta_3 - k_3, \quad (15)$$

$$q = (\gamma - 2\alpha_1)(\alpha_3 + a\alpha_2) + (a\delta + \varepsilon)\alpha_1 - a \left( zU^{*2} - \alpha_1(\alpha_1 + 1 - \gamma)/z \right) \Big|_{z=0}, \quad (16)$$

and  $\alpha, \beta$  are determined from the Fuchsian condition  $1 + \alpha + \beta = \gamma + \delta + \varepsilon$  together with the following equation

$$\begin{aligned} \alpha\beta &= q + \varepsilon\alpha_2 + \alpha_3(\delta - 2\alpha_2) - (1-a)(2\alpha_1\alpha_2 - \delta\alpha_1 - \gamma\alpha_2) \\ &+ (1-a) \left( (z-1)U^{*2} - \alpha_2(\alpha_2 + 1 - \delta)/(z-1) \right) \Big|_{z=1}. \end{aligned} \quad (17)$$

#### 1.1.4 Series solutions of the general Heun equation

A solution of the general Heun equation can be constructed as a Frobenius series:

$$H(a, q; \alpha, \beta; \gamma, \delta; z) = z^\mu \sum_n c_n z^n. \quad (18)$$

The coefficients of this expansion obey the three-term recurrence relation [70-72]

$$R_n c_n + Q_{n-1} c_{n-1} + P_{n-2} c_{n-2} = 0, \quad (19)$$

where

$$R_n = a(\mu + n)(\mu + n - 1 + \gamma), \quad (20)$$

$$Q_n = -q - (\mu + n) \left( (\mu + n - 1 + \gamma + \delta + \varepsilon)(1 + a) - a\varepsilon - \delta \right), \quad (21)$$

$$P_n = (\mu + n + \alpha)(\mu + n + \beta). \quad (22)$$

For left-hand side termination of the series at  $n = 0$  (i.e.,  $c_0 = 1$  and  $c_{-2} = c_{-1} = 0$ ), should be  $R_0 = 0$ , so that one should choose

$$\mu = 0 \quad \text{or} \quad \mu = 1 - \gamma. \quad (23)$$

The convergence radius of this series is  $\min\{|a|, 1\}$ . The series is right-hand side terminated at some  $n = N$  if  $c_N \neq 0$  and  $c_{N+1} = c_{N+2} = 0$ . Hence, should be  $P_N = 0$ , that is

$$\mu + \alpha = -N \quad \text{or} \quad \mu + \beta = -N, \quad (24)$$

and

$$Q_N c_N + P_{N-1} c_{N-1} = 0. \quad (25)$$

The last equation is a polynomial equation of the order  $N + 1$  for the accessory (spectral) parameter  $q$  having in general  $N + 1$  solutions.

Alternatively, instead of powers, one may apply other expansion functions. For instance, several expansions in terms of the Gauss hypergeometric functions [88-94] and incomplete beta functions [95-98] are known. Using the properties of the derivatives of the solutions of the Heun equation [98-100], expansions in terms of higher transcendental functions, e.g., the Goursat hypergeometric functions or Appell hypergeometric function of two variables, can be constructed [98,101]. The region of convergence in these cases may be other than a circle. Besides, the expansions apply to different combinations of involved parameters, so that they may be useful for applications in different physical situations. We would like to mention here an expansion in terms of the Gauss hypergeometric functions that is convenient for derivation of closed form solutions [93]:

$$u = \sum_n c_n u_n = \sum_n c_n {}_2F_1(\alpha, \beta; \gamma_0 - n; z), \quad (26)$$

where the coefficients of the expansion obey the following three-term recurrence relation:

$$R_n c_n + Q_{n-1} c_{n-1} + P_{n-2} c_{n-2} = 0 \quad (27)$$

with

$$R_n = \frac{a}{\gamma_0 - n} (\gamma - \gamma_0 + n)(\alpha - \gamma_0 + n)(\beta - \gamma_0 + n), \quad (28)$$

$$Q_n = (1-a)(\varepsilon + \gamma - \gamma_0 + n)(\gamma_0 - n - 1) + a(\gamma - \gamma_0 + n)(\alpha + \beta - \gamma_0 + n) + \alpha\beta a - q, \quad (29)$$

$$P_n = (a-1)(\varepsilon + \gamma - \gamma_0 + n)(\gamma_0 - n - 1). \quad (30)$$

The series is terminated from the left-hand side at  $n = 0$  ( $c_0 = 1$ ,  $c_{-2} = c_{-1} = 0$ ) if

$$\gamma_0 = \gamma \quad \text{or} \quad \alpha \quad \text{or} \quad \beta. \quad (31)$$

Furthermore, the series is right-side terminated at some  $n = N$  ( $c_N \neq 0$ ,  $c_{N+1} = c_{N+2} = 0$ ) if  $P_N = 0$ . Since  $\gamma_0$  cannot be a positive integer, we get  $\gamma_0 = \varepsilon + \gamma + N$  or, equivalently,

$$\varepsilon, \varepsilon + \gamma - \alpha \quad \text{or} \quad \varepsilon + \gamma - \beta = -N \quad (32)$$

if  $\gamma_0 = \gamma$  or  $\alpha$  or  $\beta$ , respectively. The second condition for termination of the series,  $Q_N c_N + P_{N-1} c_{N-1} = 0$ , is a polynomial equation of the order  $N + 1$  for the accessory (spectral) parameter  $q$  having in general  $N + 1$  solutions.

### 1.1.5 Constant detuning models: real $z(t)$

Eqs. (11) and (12) provide a rich variety of field configurations generated by different choices of the transformation  $z(t)$ . Here we restrict ourselves by discussion of the basic case of *constant detuning* field configurations generated by *real* choices of this transformation.

Thus, let the detuning be constant:  $\delta_i(t) = \Delta = \text{const}$ . For a real  $z(t)$ , in order to ensure that the above power series expansion is applicable, let  $z \in (0,1)$  and  $a > 1$ . Then, the families of constant-detuning field configurations are defined parametrically as:

$$t - t_0 = \ln\left(z^{\delta_1/\Delta} (1-z)^{\delta_2/\Delta} (a-z)^{\delta_3/\Delta}\right), \quad (33)$$

$$U(t) = \Delta \frac{U_0^* z^{k_1+1} (z-1)^{k_2+1} (z-a)^{k_3+1}}{(\delta_1 + \delta_2 + \delta_3)z^2 - (\delta_1 + a\delta_1 + a\delta_2 + \delta_3)z + a\delta_1}. \quad (34)$$

To specify the integration constant  $t_0$ , which only defines a nonessential shift in time, we may demand  $z(t=0) = 1/2$ , hence,

$$t_0 = \ln\left(2^{(\delta_1+\delta_2+\delta_3)/\Delta} (2a-1)^{-\delta_3/\Delta}\right). \quad (35)$$

The derived families of pulses include both symmetric and asymmetric members. The pulses may or may not vanish at  $t \rightarrow \pm\infty$ . Among all the families only 10 provide pulses for which the pulse area is finite, i.e. the pulses vanish at infinity. These are the families for which  $k_{1,2} \neq -1$ . The members of the latter families in general are two-peak symmetric or asymmetric pulses with controllable distance between the peaks and controllable amplitude of each of the peaks. We will see that the distance between the peaks as well as the amplitude of the peaks is mainly controlled by the parameters  $a$  and  $\delta_3$ , while the sharpness of the pulse edges is mostly controlled by  $\delta_1$  and  $\delta_2$ . Some representative examples of pulse shapes for different families are shown in Figs. 2-8.

Discussing the general properties of the pulses, it is natural to expect that new properties, compared to the known 6 hypergeometric classes [53-55], should be due to the parameters  $a$  and  $\delta_3$  which are not present in the hypergeometric case. To reveal the role of these parameters, we note that the denominator in the Eq. (34) for  $U(t)$  for  $z \rightarrow 0$  and  $z \rightarrow 1$  tends to  $a\delta_1$  and  $(1-a)\delta_2$ , respectively. Hence, within a fixed class defined by a chosen set of  $k_{1,2,3}$ , for fixed  $a$  and  $\delta_3$ , the behavior of  $U(t)$  for  $t \rightarrow -\infty$  and  $t \rightarrow +\infty$  is controlled by the parameters  $\delta_1$  and  $\delta_2$ , respectively. For the families of pulses, for which  $U(t)$  vanishes at  $t \rightarrow \pm\infty$ , at  $\delta_1 \rightarrow +0$  the left edge of the pulse becomes a step-wise function and for  $\delta_2 \rightarrow -0$  the same happens with the right edge (we consider the case  $z'(t) > 0$ , see the discussion below). In the simultaneous limit  $\delta_{1,2} \rightarrow 0$  we have a pulse with vertical walls. These observations are demonstrated in Fig. 2 where the normalized



( $U_{\max} = 1$ ) pulse shapes for small  $\delta_1$  (left figure) or small  $\delta_2$  (right figure) are shown for the class  $k_{1,2,3} = \{0, 0, -1\}$ .

As it is seen, for the class  $k_{1,2,3} = \{0, 0, -1\}$  the simultaneous limit  $\delta_{1,2} \rightarrow 0$  produces a rectangular box-pulse. For other classes, of course, the pulse shapes are different, see for example Fig. 3. An important common feature, however, is that the width of the pulse is controlled by the parameters  $a$  and  $\delta_3$ . This is demonstrated in Figs. 3 and 4. Note that the pulse width diverges as  $a$  goes to the unity or as  $\delta_3 \rightarrow -\infty$ .

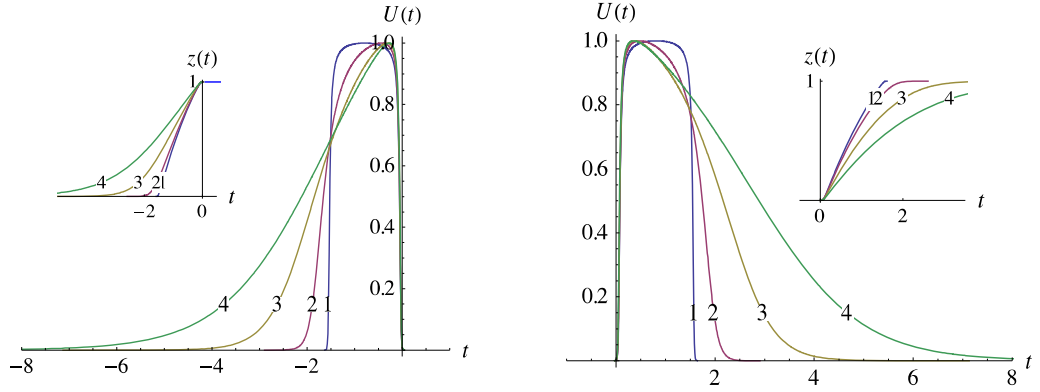


Fig. 2. Class  $k_{1,2,3} = \{0, 0, -1\}$ . Constant detuning case,  $\Delta = 1$ . Normalized ( $U_{\max} = 1$ ) pulse shapes for  $a = 2$ ,  $\delta_3 = -2$ . Graphs in the left figure correspond to  $\delta_1 = 0.01; 0.1; 0.4; 1$  (curves 1, 2, 3, 4, respectively) and small  $\delta_2 = -0.01$ . Right figure's graphs correspond to  $\delta_2 = -0.01; -0.1; -0.4; -1$  (curves 1, 2, 3, 4, respectively) and small  $\delta_1 = 0.01$ .

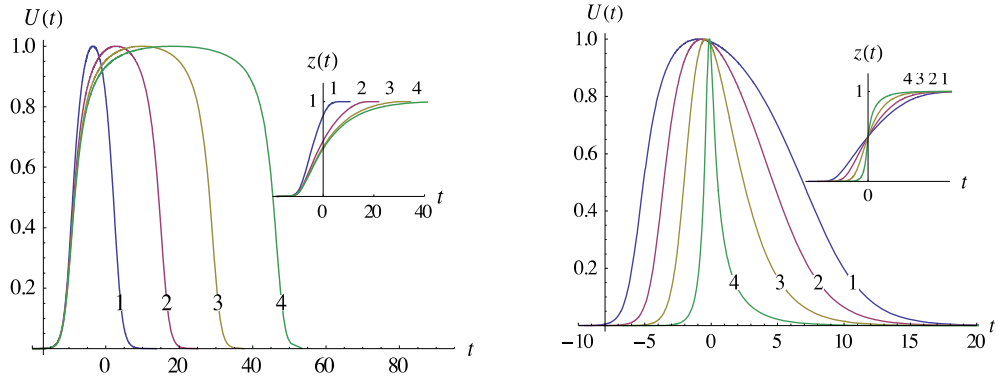
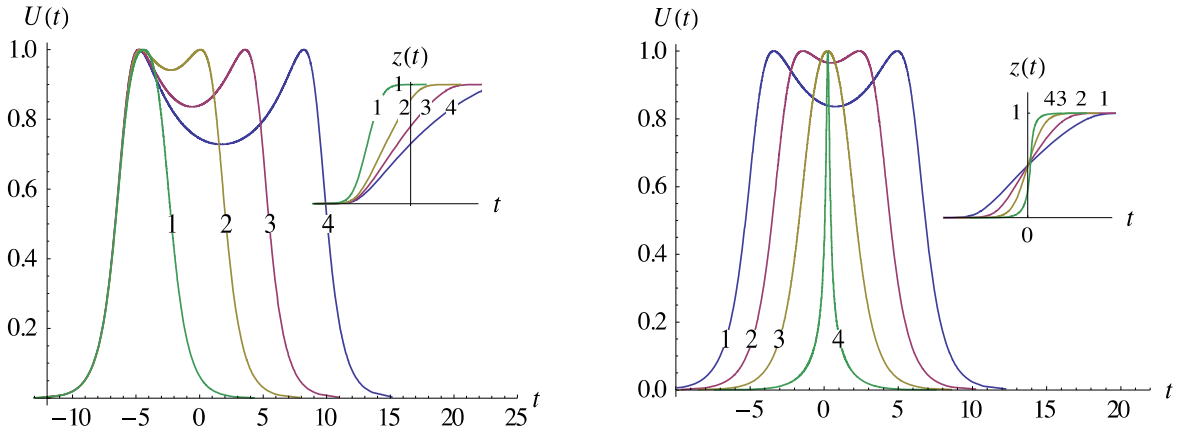
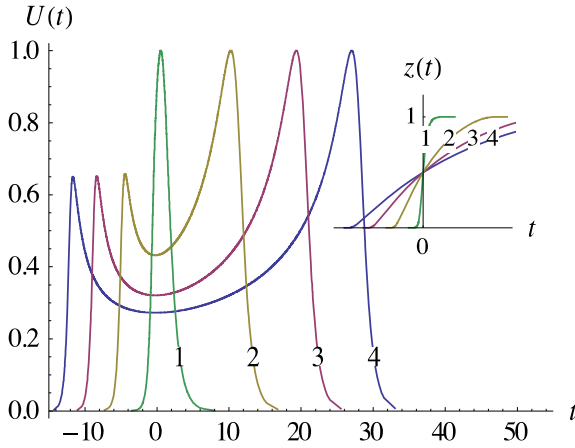


Fig. 3. Class  $k_{1,2,3} = \{0, 0, -1\}$ . Constant detuning case,  $\Delta = 1$ . Normalized ( $U_{\max} = 1$ ) pulse shapes for  $\delta_1 = 1$ ,  $\delta_2 = -1$ . Graphs in the left figure correspond to  $\delta_3 = -10$  and  $a = 2; 1.2; 1.05; 1.01$  (curves 1, 2, 3, 4, respectively). The same pulses are obtained by fixing, e.g.,  $a = 2$  and changing  $\delta_3$ :  $\delta_3 = -10; -26.22; -44.87; -68.85$ . The pulse width diverges as  $a$  goes to the unity or as  $\delta_3 \rightarrow -\infty$ . Graphs in the right figure correspond to  $a = 2$ ,  $\delta_1 = 1/2$ ,  $\delta_2 = -2$  and  $\delta_3 = -10; -5; 0; 5$  (curves 1, 2, 3, 4, respectively). Infinitely narrow pulse is achieved if

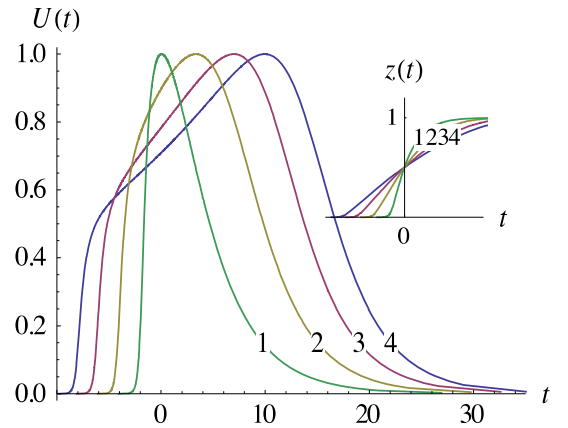
$$\delta_3 = 2\sqrt{2} + 9/2.$$



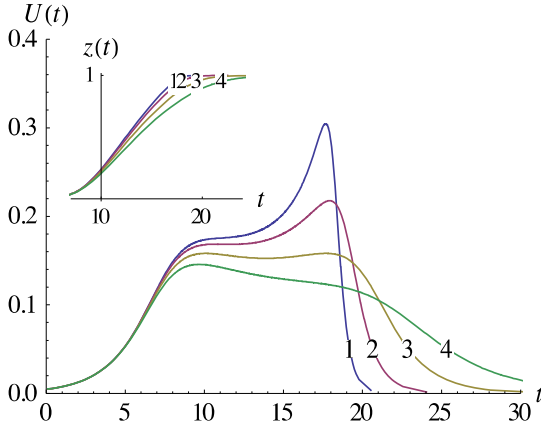
**Fig. 4.** Class  $k_{1,2,3} = -1/2$ . Constant detuning case,  $\Delta = 1$ . Normalized ( $U_{\max} = 1$ ) pulse shapes for  $\delta_1 = 1/2$ ,  $\delta_2 = -1/2$ . Graphs in the left figure correspond to  $\delta_3 = -10$  and  $a = 10; 3; 2; 1.5$  (curves 1, 2, 3, 4, respectively). The pulse width diverges as  $a$  goes to the unity or as  $\delta_3 \rightarrow -\infty$ . The same pulses are produced by fixing an arbitrary chosen  $a$  and varying  $\delta_3$ . For example, for  $a = 2$  the result reads  $\delta_3 = -1.52; -5.85; -10; -15.85$ . On the right figure, curves 1, 2, 3, 4 correspond to  $a = 2$  and  $\delta_3 = -10; -5; -1; 2.1$ , respectively. Infinitely narrow pulse is achieved when  $\delta_3 = 2\sqrt{2} + 3/2$ .



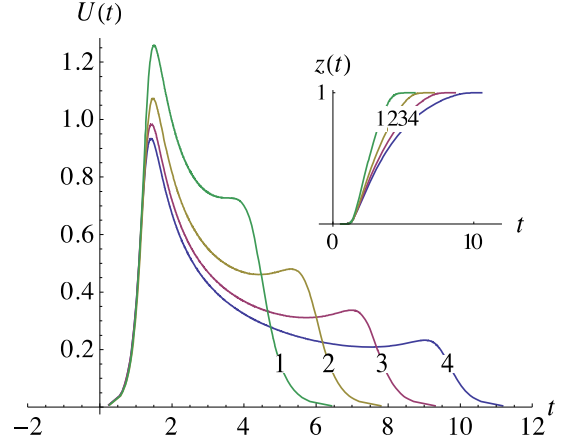
**Fig. 5.** Class  $k_{1,2,3} = \{-1/2, -1/2, -1\}$ . Constant detuning case,  $\Delta = 1$ . Normalized pulse shapes for  $a = 1.2$ ,  $\delta_1 = 1/5$ ,  $\delta_2 = -1/2$  and  $\delta_3 = 0, -7, -14, -20$  (curves 1, 2, 3, 4).



**Fig. 6.** Class  $k_{1,2,3} = \{0, -1/2, -1\}$ . Constant detuning case,  $\Delta = 1$ . Normalized pulse shapes for  $a = 2$ ,  $\delta_1 = 1/5$ ,  $\delta_2 = -2$  and  $\delta_3 = 0, -7, -14, -20$  (curves 1, 2, 3, 4).



**Fig. 7.** Class  $k_{1,2,3} = -1/2$ . Constant detuning case,  $\Delta = 1$ . Pulse shapes for  $U_0^* = -1$ ,  $a = 2$ ,  $\delta_1 = 1$ ,  $\delta_3 = -10$ . Curves 1, 2, 3, 4 correspond to  $\delta_2 = -1/4, -1/2, -1, -1.8$ , respectively.



**Fig. 8.** Class  $k_{1,2,3} = \{-1/2, -1/2, 0\}$ . Constant detuning case,  $\Delta = 1$ . Pulse shapes for  $U_0^* = i$ ,  $\delta_1 = 1/10$ ,  $\delta_2 = -1/5$ ,  $\delta_3 = -3$ . Curves 1, 2, 3, 4 correspond to  $a = 2.1, 1.5, 1.25, 1.12$ , respectively.

Furthermore, it can be checked that the effect of the two parameters  $a$  and  $\delta_3$  is rather similar, namely, in many cases both parameters are able to produce similar pulses with the same width. For instance, it can be shown that for  $\delta_{1,2} \leq 1$  any two pairs  $\{a, \delta_3\}$  and  $\{a_0, \delta_{30}\}$  related by the equation  $\delta_3 / \ln((a-1)/a) = \delta_{30} / \ln((a_0-1)/a_0)$  produce pulses of almost indistinguishable shapes. In the captions of Figs. 3 and 4 several such pairs are presented. Thus, the families (33), (34) allow variation of the edge shapes and pulse width almost independently, using different parameters.

### 1.1.6 Infinitely narrow pulses

Consider now whether infinitely narrow pulses are possible. First, we recall that Eq. (33) defines one-to-one mapping  $t \leftrightarrow z$  if  $z'(t)$  is sign-preserving. Hence, the polynomial

$$P(z) = \delta_1(z-1)(z-a) + \delta_2 z(z-a) + \delta_3 z(z-1), \quad (36)$$

the numerator of the term in brackets before  $z'(t)$  in Eq. (12), should not change its sign on the interval  $z \in (0,1)$ . On the other hand, it follows from Eq. (34) that the pulse should diverge at some point  $z_0$  belonging to this interval in order to become infinitely narrow after being normalized to  $U_{\max} = 1$ . This is achieved if the denominator of the ratio in the right-hand side of Eq. (34) vanishes at  $z_0$ . Since this denominator is the above polynomial  $P(z)$ , we conclude that  $z_0$  is a root of the

equation  $P(z_0) = 0$ . Furthermore, in order the polynomial to be sign-preserving,  $z_0$  should be a multiple root of  $P(z)$ . Hence, the discriminant of the polynomial should be zero. Thus, we get the following conditions for the pulse parameters to produce infinitely narrow pulse:  $D = 0$ ,  $z_0 \in (0,1)$ , where

$$D = (\delta_1 + a\delta_1 + a\delta_2 + \delta_3)^2 - 4a\delta_1(\delta_1 + \delta_2 + \delta_3), \quad (37)$$

$$z_0 = (\delta_1 + a\delta_1 + a\delta_2 + \delta_3)/(2(\delta_1 + \delta_2 + \delta_3)). \quad (38)$$

The equation  $D = 0$  is a quadratic equation with respect to both  $a$  and  $\delta_3$ . However, if considered as an equation for  $a$ , for some set of involved parameters it may have roots not belonging to the supposed variation interval of  $a$ :  $a \in (1, +\infty)$ . In contrary, no restriction is imposed on the variation range of  $\delta_3$ . This is a slight difference between the two considered parameters. Summarizing, we may state that the pulse width may go to zero or a non-zero minimum in both cases: when  $a$  is fixed and  $\delta_3$  is varied and vice versa. The limit of infinitely narrow pulse achieved via variation of  $\delta_3$  is demonstrated in Fig. 3 (right figure) for asymmetric pulses and in Fig. 4 (right figure) for symmetric pulses. Here, the examples of the classes  $k_{1,2,3} = \{0, 0, -1\}$  and  $k_{1,2,3} = -1/2$  are presented, however, the above discussion is general and applies to all the families (33), (34) for which the pulse vanishes at  $t \rightarrow \pm +\infty$ .

### 1.1.7 Vertical edge pulses of controllable width

Next interesting point is how the pulse edge becomes a vertical wall at a limit  $p \rightarrow p_0$  for an involved parameter  $p$ . It is understood that in order this to occur the derivative  $U'(t)$  should diverge for a *fixed* time point  $t_0$  if the limit  $p \rightarrow p_0$  is considered. It can be checked that, in terms of  $z$ ,  $U'(t)$  is a polynomial in  $z$  divided by  $P(z)^3$ , where  $P(z)$  is the quadratic polynomial given by Eq. (36). Hence,  $P(z(t_0))$  should go to zero at the limit  $p \rightarrow p_0$ . This means that  $z(t_0)$  should tend to a *root* of the polynomial  $P(z)$ . However, we recall that  $P(z)$  is sign-preserving on the interval  $z \in (0,1)$  so that it cannot have real roots on this interval. Hence, the only possibility left is that the function  $z(t_0)$  and a root of the polynomial  $P(z)$ ,  $z_1$  or  $z_2$ , as functions of the parameter  $p$ , should simultaneously tend to an endpoint of the segment  $z \in [0,1]$ . If  $z_1 < 0$  and  $z_2 > 1$ , then for the left edge should hold  $z_1(p \rightarrow p_0) = 0 = z(t_0, p \rightarrow p_0)$  and for the right edge should be  $z(t_0, p \rightarrow p_0) = 1 = z_2(p \rightarrow p_0)$ . With these observations, we consider the behavior of the pulse in the vicinity of the points  $z = 0$  and  $z = 1$ .

For  $z \rightarrow 0$ , expanding  $\ln(1-z)$  and  $\ln(a-z)$  in the right-hand side of Eq. (33) in powers of  $z$  and keeping only the constant term we get  $t(z) = t_0 + (\delta_1 \ln(z) + \delta_3 \ln(a))/\Delta$  so that in this approximation  $z(t) = \exp((\Delta t - \Delta t_0 - \delta_3 \ln a)/\delta_1)$ . This function, however, leads to a pulse which diverges at the time point  $t_1 = t_0 + \delta_3 \ln(a)/\Delta$ .

A much better approximation is achieved using the next, linear-in- $z$ , term in the expansion of mentioned two logarithms:

$$t(z) = t_0 + (\delta_1 \ln(z) + \delta_3 \ln(a) - (\delta_2 + \delta_3/a)z)/\Delta. \quad (39)$$

The solution of this equation is given by the Lambert  $W$  function [102,103]:

$$z(t) = -\frac{a\delta_1}{a\delta_2 + \delta_3} W\left(-\frac{a\delta_2 + \delta_3}{\delta_1} e^{\frac{(t-t_0)\Delta - (\delta_1 + \delta_3)\ln a}{\delta_1}}\right). \quad (40)$$

This is a good approximation that leads to an accurate description of the pulse shape near its left edge for all the variation range of the involved parameters (see Fig. 9). For small  $\delta_1$  it describes a jump with the width proportional to  $\delta_1$ . We then conclude, from this solution, that the pulse edge becomes a vertical wall at the limit  $\delta_1 \rightarrow 0$  and the position of the wall is

$$t_1 = t_0 + \delta_3 \ln a / \Delta. \quad (41)$$

In the similar way, expanding now the logarithms  $\ln(z)$  and  $\ln(a-z)$  in the right-hand side of Eq. (33) in powers of  $1-z$  and taking the constant and linear-in- $z$  terms we get an accurate description for the right edge in terms of another Lambert- $W$  function. From this solution we get that this time the wall is formed at the limit  $\delta_2 \rightarrow 0$  and its position is

$$t_2 = t_0 + \delta_3 \ln(a-1)/\Delta. \quad (42)$$

Thus, in the simultaneous limit  $\delta_{1,2} \rightarrow 0$  the pulse width is given as

$$d = t_2 - t_1 = \delta_3 \ln((a-1)/a)/\Delta. \quad (43)$$

This formula shows that the pulse width is mainly controlled by the parameters  $\{\delta_3, a\}$  and explains the above mentioned condition of having almost indistinguishable pulses of the same width using different pairs  $\{\delta_3, a\}$ . The comparison of the pulse shape provided by the approximation (40) as well as the divergent solution generated by the simple exponential approximation for  $z(t)$  with the exact pulse shape is shown on Fig. 9. It is seen, that in the limit  $\delta_1 \rightarrow 0$  the divergent solution accurately determines the position of the wall.

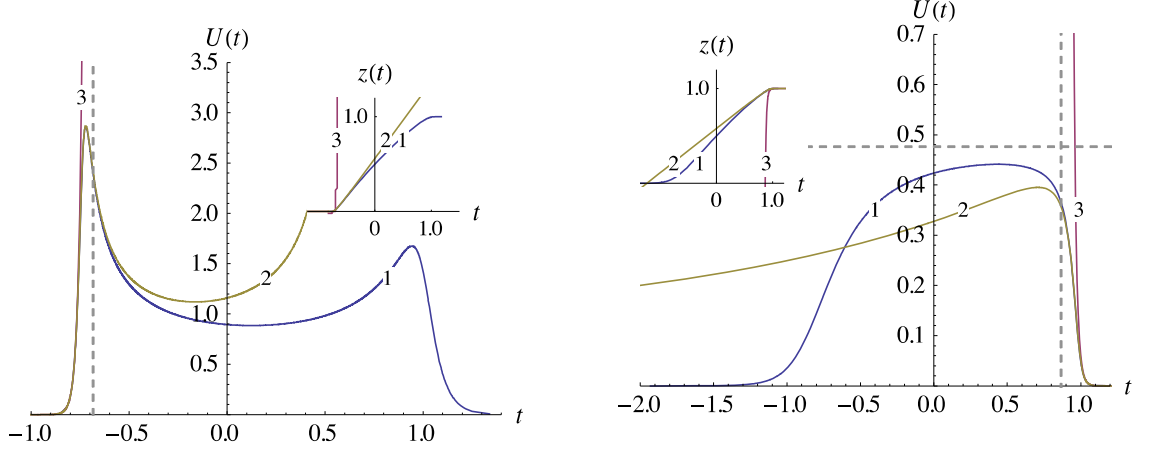


Fig. 9. Constant detuning case,  $\Delta = 1$ . Exact pulse shapes (curves 1) compared with those given by approximation (40) (curves 2). The divergent solutions generated by the simple exponential approximation for  $z(t)$  (curves 3) accurately determine the limiting positions of the left and right edges shown by vertical dashed lines. Left graph: class  $k_{1,2,3} = -1/2$ ,  $U_0^* = -1$ ,  $a = 2.5$ ,  $\delta_1 = 0.01$ ,  $\delta_2 = -0.03$ ,  $\delta_3 = -3$ . Right graph: class  $k_{1,2,3} = \{0,0,-1\}$ ,  $U_0^* = -1$ ,  $a = 2$ ,  $\delta_1 = 0.1$ ,  $\delta_2 = -0.02$ ,  $\delta_3 = -2$ . The horizontal dashed line defines the height of the limiting box pulse.

### 1.1.8 Complex-valued transformation $z(t)$

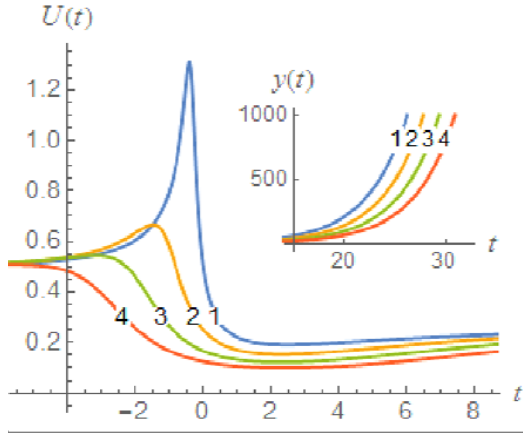
A different set of pulses is generated by Eqs. (11),(12) if a *complex-valued* transformation  $z = x(t) + iy(t)$  is applied. Consider, for instance, constant-detuning field configurations achieved by the substitution  $z = (1 + iy(t))/2$ . It follows from Eq. (11) that real amplitude-modulation functions are generated by this transformation if  $k_1 = k_2$ . Only 9 classes out of 35 satisfy this condition:  $k_{1,2} = -1$ ,  $k_3 = \{-1, -1/2, 0, 1/2, 1\}$ ;  $k_{1,2} = -1/2$ ,  $k_3 = \{-1, -1/2, 0\}$ ; and  $k_{1,2} = 0$ ,  $k_3 = -1$ .

The corresponding pulse shapes are given parametrically as

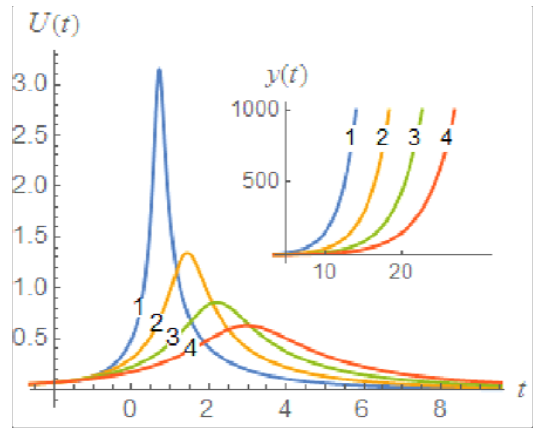
$$t = \lambda_1 \ln(1 + y^2) + 2\lambda_2 \arctan(y) + \lambda_3 \ln\left(\frac{a_0 - y}{a_0}\right), \quad (44)$$

$$U(t) = \frac{U_0(1 + y^2)^{k_1+1}(y - a_0)^{k_3+1}}{2(y - a_0)(\lambda_2 + \lambda_1 y) + \lambda_3(1 + y^2)}, \quad (45)$$

where without loss of generality we have supposed  $y(0) = 0$  and introduced real parameters  $a_0$ ,  $\lambda_{1,2,3}$  and  $U_0$ :  $a = (1 + ia_0)/2$ ,  $\delta_{1,2}/\Delta = \lambda_1 \mp i\lambda_2$ ,  $\delta_3/\Delta = \lambda_3$ ,  $U_0^* = (-2i)^{1+2k_1+k_3} U_0$ . It can be seen from Eq. (44) that if  $a_0 > 0$ , then  $y(t) \in (-\infty, a_0)$  and if  $a_0 < 0$ , then  $y(t) \in (a_0, +\infty)$ . For definiteness, we consider the case  $a_0 < 0$ . Then, at an appropriate choice of the remaining parameters, Eqs. (44)-(45) define asymmetric pulse shapes shown in Figs. 10,11.



**Fig. 10.** Class  $k_{1,2,3} = \{0, 0, -1\}$ . Constant detuning case,  $\Delta = 1$ . Pulse shapes for  $U_0^* = 1$ ,  $a_0 = -2$ ,  $\delta_1 = 1, 1-i/2, 1-i, 1-3i/2$  (curves 1, 2, 3, 4),  $\delta_2 = \overline{\delta_1}$  and  $\delta_3 = 2$ .



**Fig. 11.** Class  $k_{1,2,3} = \{-1, -1, 0\}$ . Constant detuning case,  $\Delta = 1$ . Pulse shapes for  $U_0^* = i$ ,  $a_0 = -0.2$ ,  $\delta_1 = 1/2 + i$ ,  $\delta_2 = \overline{\delta_1} = 1/2 - i$  and  $\delta_3 = 1.2, 1.7, 2.2, 2.7$  (curves 1, 2, 3, 4).

Note that the pulses of the subfamilies  $k_{1,2} = -1$ ,  $k_3 = \{-1, 1\}$ ;  $k_{1,2} = -1/2$ ,  $k_3 = \{-1, 0\}$ ;  $k_{1,2} = 0$ ,  $k_3 = -1$  do not vanish at  $t \rightarrow \pm\infty$ , while the remaining 4 subfamilies,  $\{k_{1,2} = -1$ ,  $k_3 = \{-1/2, 0, 1/2\}\}$  and  $k_{1,2,3} = -1/2$ , suggest bell-shaped asymmetric pulses vanishing at infinity. The limits  $U(t = -\infty) = U(y \rightarrow a_0 + 0)$  and  $U(t = +\infty) = U(y \rightarrow +\infty)$  are listed in [Table 6](#).

$k_{1,2,3}$	$U(t = -\infty)$	$U(t = +\infty)$
$\{-1, -1, -1\}$	$U_0 / (\lambda_3 (1 + a_0^2))$	0
$\{-1, -1, -1/2\}$	0	0
$\{-1, -1, 0\}$	0	0
$\{-1, -1, 1/2\}$	0	0
$\{-1, -1, 1\}$	0	$U_0 / (2\lambda_1 + \lambda_3)$
$\{-1/2, -1/2, -1\}$	$U_0 / (\lambda_3 \sqrt{1 + a_0^2})$	0
$\{-1/2, -1/2, -1/2\}$	0	0
$\{-1/2, -1/2, 0\}$	0	$-U_0 / (2\lambda_1 + \lambda_3)$
$\{0, 0, -1\}$	$U_0 / \lambda_3$	$U_0 / (2\lambda_1 + \lambda_3)$

**Table 6.** The limits  $U(t = \pm\infty)$  for nine classes producing real pulses by the complex-valued transformation  $z = (1 + iy(t))/2$ . It is supposed that  $\lambda_3 > 0$  and  $2\lambda_1 + \lambda_3 > 0$ .

We conclude by noting that other complex-valued transformations leading to real physical field configurations can be suggested. For instance, one may apply the transformation  $z(t) = \sqrt{a} \exp(i\Delta t)$ .  $\mathcal{F} = -\sqrt{a} \text{Exp}[i\Delta t]$  With the parameters chosen as

$$U_0^* = i^{-1-2k_3} U_0 / \Delta, \quad \delta_1 = -i, \quad \delta_2 = \delta_3 = 0, \quad (46)$$

the classes  $k_{1,2,3} = \{-1/2, -1/2, -1/2\}$  and  $k_{1,2,3} = \{0, -1, -1\}$  then result in periodic amplitude modulations. The corresponding field configurations (see Fig. 12) are given as

$$U(t) = \frac{U_0}{(1 + a - 2\sqrt{a} \cos(\Delta t))^{-k_3}}, \quad \delta_i(t) = \Delta. \quad (47)$$

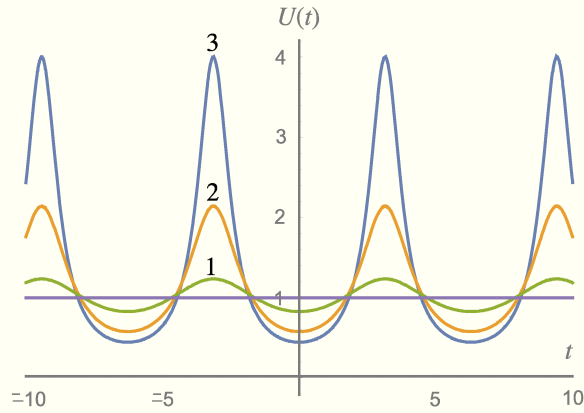


Fig. 12. Class  $k_{1,2,3} = \{0, -1, -1\}$ . Constant-detuning case,  $\delta_i(t) = \Delta = \text{const}$ . Periodic amplitude modulation generated by the complex-valued transformation  $z(t) = \sqrt{a} \exp(i\Delta t)$ :  $U_0^* = iU_0 / \Delta$ ,  $\delta_1 = -i$ ,  $\delta_2 = \delta_3 = 0$ ,  $\Delta = 1$ ,  $U_0 = 1$ ,  $a = 0.01, 0.1, 0.25$  (curves 1, 2, 3).

### 1.1.9 Discussion

Thus, we have derived 35 five-parametric classes of two-state models solvable in terms of the general Heun function. The classes are defined by two generating functions which are referred to as the amplitude- and detuning-modulation functions. The actual field configurations, that is, the Rabi frequency and the detuning, are then generated applying a real or complex-valued transformation of the independent variable. Many of the derived classes present generalizations of the six known 3-parametric hypergeometric classes for which the solution of the two-state problem is written in terms of the Gauss hypergeometric function. In several cases the generalization is achieved by multiplying the amplitude modulation function of the corresponding prototype hypergeometric class by an extra factor including an additional parameter. In all these cases as well as in the cases when the amplitude modulation function is not modified compared with the



hypergeometric prototype an additional generalization comes due to an extra term in the detuning modulation function. Finally, many classes suggest amplitude modulation functions not discussed before.

The detuning modulation function is the same for all the derived 35 classes. This function involves four arbitrary parameters, that is, two more than the hypergeometric classes. These parameters in general are complex and should be chosen so that the resultant detuning is real for the applied complex-valued transformation of the independent variable. The generalization of the detuning modulation function to the four-parametric case is the most notable extension since many useful properties of the two-state models described by the Heun equation are due to namely the additional parameters involved in this function.

We note that the technique applied for derivation of the presented solvable classes essentially rests on the property (3) [52-55] of the solvable cases of the time-dependent Schrödinger equations (1). This approach assumes two successive steps. The first step consists in identification of the basic solvable models, as listed in above Tables 1-5, by means of transformation of the dependent variable. The transformation of the independent variable is explicitly used only in the second step when the actual field configurations are specified, see Eqs. (11),(12). Unlike this approach, in the most of the cases discussed in literature the stress is done, perhaps by historical reasons, on the transformation of the independent variable. However, a short examination shows that this is a rather restrictive approach which is potent to produce only a very few results. Indeed, suppose  $\varphi = 1$ , i.e.,  $\alpha_{1,2,3} = 0$ , so that the Heun function appears in the final solution (13) without a pre-factor. It then follows from Eqs. (14) that in this case should be  $k_{1,2,3} \neq -1$ . This leads to only 4 classes out of presented 35:  $k_{1,2,3} = \{-1/2, -1/2, 0\}$ ,  $\{-1/2, 0, -1/2\}$ ,  $\{0, -1/2, -1/2\}$  and  $\{-1/2, -1/2, -1/2\}$ . Thus, the conclusion is that the approach based on the property (3) of solvable models is significantly more advanced one. The four mentioned cases with  $\varphi = 1$  are indicated in Fig.1 by three triangles and a square which indicates the last class. Note that the first of these four classes presents a generalization of a class solvable in terms of the Gauss hypergeometric functions [53-55] to a more general type of frequency modulation due to the term proportional to  $\delta_3$  in Eq. (12). Furthermore, the next two classes indicated by triangles are modifications of the first class for the singular points  $\{0, a\}$  and  $\{1, a\}$ , respectively. The most interesting is the case  $k_{1,2,3} = \{-1/2, -1/2, -1/2\}$ , which suggests generalizations of both detuning- and amplitude-modulation functions as compared with its hypergeometric prototype. This case was treated in [86,87], however, the treatment there is restricted to the case  $\delta_3 = 0$ , which, of course, notably weakens the extent of the generalization.

We have determined the parameters of the general Heun function involved in the final solution of the initial two-state problem and have presented the power series expansion of this function. Furthermore, we have mentioned a particular series expansion of the general Heun function in terms of the Gauss hypergeometric functions that is convenient for derivation of particular closed form finite sum solutions.

Discussing the constant detuning case, we have presented several particular families of pulses generated by real transformation of the independent variable. These families include both symmetric and asymmetric members. Among all the families only ten provide finite area pulses, that is, pulses that vanish at infinity. The members of these families are in general symmetric or asymmetric two-peak pulses with controllable distance between the peaks and controllable amplitude of each of the peaks. We have shown that the edge shapes, the distance between the peaks as well as the amplitude of the peaks are controlled almost independently, by different parameters. We have identified the parameters controlling each of the mentioned features and have discussed other basic properties of pulse shapes.

We have shown that the pulse edges may become step-wise functions and determined the positions of the limiting vertical-wall edges. We have shown that the pulse width is then controlled by only two of the involved parameters. For some values of these parameters the pulse width diverges and for some other values the pulses become infinitely narrow. We have shown that the effect of the two mentioned parameters is almost similar, that is, both parameters are able to independently produce pulses with almost the same shape and width. We have determined the conditions for generation of pulses of almost indistinguishable shape and width, and have presented several such examples.

The derived classes provide a rich variety of field configurations generated by different real or complex choices of the independent variable transformation. For instance, apart from the above families of constant detuning pulses obtained by real  $z(t)$ , many other such constant detuning families are suggested by a complex transformation of the form  $z = (1 + iy(t))/2$  or  $z(t) = \sqrt{a} \exp(i\Delta t)$ . Examples with variable detuning include numerous models with constant amplitude of the field, several configurations with periodic modulation of the amplitude, a large variety of families of chirped pulses, level-glancing models and models describing double or periodic level-crossings. Notably, the classes also suggest models describing excitation of a two-level atom by bi-chromatic laser fields. This is not the whole list, there are several other possibilities.

We would like to conclude by a brief note concerning possible applications of above models. First, we mention the appreciable richness of the set of the Heun models as compared with

the hypergeometric set (the number of the Heun models prevails by an order of the magnitude). Second, the Heun models suggest a variety of distinct features not present in the hypergeometric ancestors (e.g., double- and multiple level-crossings, two-peak pulses, etc.). For this reason, one may foresee many applications in quantum and atom optics, e.g., in quantum engineering via manipulation of quantum structures with prescribed properties [104,105] by laser pulses, in the theory of chemical reactions including cold atom association in quantum gases, etc., however, it is difficult if not impossible to list all possibilities.

We would like to mention here just a useful point of mathematical character. In several cases the application of the presented Heun models may be advantageous for general considerations (this may be the case even if the qualitative behavior of the pulses is close to those discussed using hypergeometric models). This is because in several cases the models allow closed form solutions based on series expansions of the involved Heun functions. An example supporting this observation is the solution of the two-state problem for the constant-amplitude field configuration describing a periodic level-crossing process that we present in the next section. It is readily checked that the parameters of the general Heun function involved in the final solution in this case all are real and such that allow a series expansion in terms of the incomplete Beta-functions [78]. For a certain infinite (countable) set of parameters this series is terminated thus resulting in closed-form finite-sum solutions. We intend to discuss several other applications of these solutions in our future research.

### **1.2 A periodic level-crossing two-state model of a general Heun class**

The specific model we consider in this section presents a constant-amplitude periodic phase-modulation field configuration, which may be level-crossing, level glancing or non-crossing. We note that though the level-crossing is a key paradigm of the theory of quantum non-adiabatic transitions [7,8], only a few analytic models describing such processes are known [1-4,42,46,50]. Besides, these are only single-crossing models, and to the best of our knowledge no exactly solvable models of periodic crossings of the resonance are known.

The model we discuss in the present section presents a constant-amplitude periodic level-crossing model belonging to one of the thirty-five general Heun classes of field configurations [75]. In the particular case at hand the general Heun function involved in the solution of the two-state problem admits a series expansion in terms of the incomplete Beta functions. The coefficients of the expansion obey a three-term recurrence relation which allows termination of the series. We show that the conditions for simultaneous left- and right-hand side terminations generally lead to *conditionally* integrable models for which the amplitude- and detuning-modulation functions are not

varied independently. However, there exists a particular *unconditionally* integrable model. This is a constant-amplitude periodic level-crossing model for which the detuning modulation function for a large parameter is effectively a Dirac delta-comb threaded on a carrier frequency. Notably, the exact solution of the problem for this particular model is eventually written in terms of elementary functions. This solution explicitly indicates the Floquet exponents expressed through the generalized Rabi frequency for the carrier frequency of the associated constant-detuning field. Using the derived solution, we explore the non-adiabatic dynamics of the two-state system subject to excitation by a driving optical field of the mentioned configuration.

### 1.2.1 A constant-amplitude level-crossing general Heun model of the two-state problem

The two-state model that we introduce belongs to the general Heun class with  $k_{1,2,3} = (-1, 0, 0)$ . The model is given through the equations (11)-(12) with the complex-valued transformation of the independent variable taken as  $z(t) = \sqrt{a} e^{i\Delta(t-t_0)}$  [75]. With the choice of the parameters of the amplitude and detuning modulation functions as

$$\begin{aligned} U_0^* &= -i \frac{U_0}{\Delta}, \\ \delta_1 &= -i \frac{\Delta_1}{\Delta}, \quad \delta_2 = -\delta_3 = i \frac{\Delta_2}{\Delta}, \end{aligned} \quad (48)$$

we get a constant-amplitude field configuration with periodic modulation of the detuning:

$$\begin{aligned} U(t) &= U_0, \\ \delta_i(t) &= \Delta_1 + \frac{(1-a)\Delta_2}{1+a-2\sqrt{a}\cos(\Delta(t-t_0))}, \end{aligned} \quad (49)$$

where  $U_0, a, \Delta_1, \Delta_2$  and  $\Delta, t_0$  are arbitrary real input parameters,  $a > 0$ . Different particular values of these input parameters produce both level-crossing and non-crossing detuning modulations, as well as level-glancing configurations (figure 13). Since the detuning is a  $T = 2\pi / \Delta$ -periodic function of time, the level-glancing occurs if the condition for resonance  $\delta_i(t) = 0$  is achieved at an extremum of the function  $\cos(\Delta t)$ , that is if  $t = t_0$  or  $t = t_0 + \pi / \Delta$ .

$$\text{This is the case if} \quad \frac{\Delta_1}{\Delta_2} = \frac{\sqrt{a} + 1}{\sqrt{a} - 1} \quad (50)$$

or

$$\frac{\Delta_1}{\Delta_2} = \frac{\sqrt{a} - 1}{\sqrt{a} + 1}. \quad (51)$$

The level-glancing subfamily achieved by the second choice is shown in figure 14.

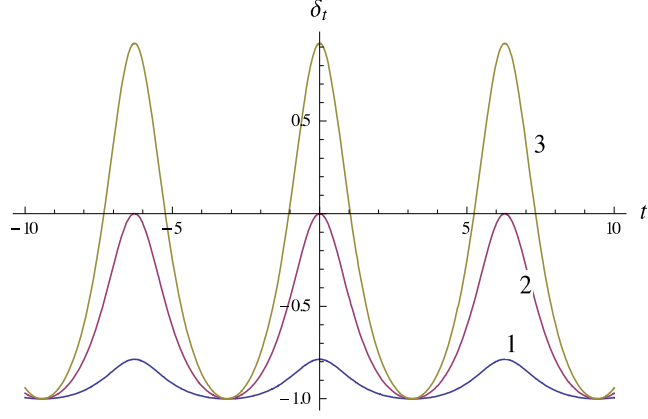


Fig.13. Detuning modulation function (49) for  $a=16$  and  $\Delta_1 = -1 + 3\Delta_2 / 5$ .  
 $\Delta_2 = -0.2, -15/16, -1.8$  for curves 1, 2, 3, respectively,  $\Delta=1, t_0=0$ .

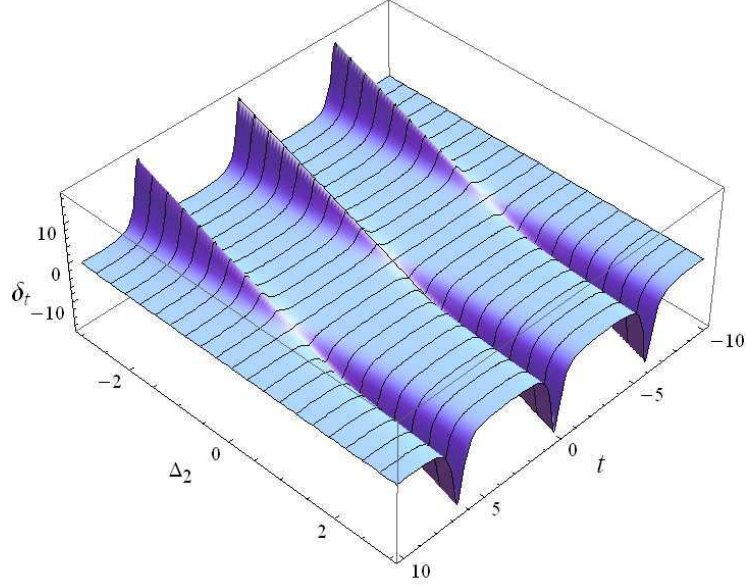


Fig.14. A level-glancing sub-family of the detuning modulation function (49):

$$\Delta_1 = (\sqrt{a} - 1) / (\sqrt{a} + 1) \Delta_2, \quad a = 2 \quad (\Delta = 1, t_0 = 0).$$

The solution of the two-state problem is explicitly written as

$$a_2 = C_0 z^{\alpha_1} (z-1)^{\alpha_2} (z-a)^{\alpha_3} H_G(a, q; \alpha, \beta; \gamma, \delta; z), \quad (52)$$

where  $C_0$  is an arbitrary constant, the parameters  $\gamma, \delta, \varepsilon, \alpha, \beta, q$  of the general Heun function  $H_G$  are determined through the equations (15)-(17) as (without loss of generality we put  $\Delta = 1$ )

$$(\gamma, \delta, \varepsilon, \alpha, \beta, q) = \left( 1 \pm \sqrt{4U_0^2 + \Delta_1^2}, \Delta_2, -\Delta_2, 0, \pm \sqrt{4U_0^2 + \Delta_1^2}, (a-1)\Delta_2\alpha_1 \right), \quad (53)$$

and the pre-factor parameters  $\alpha_{1,2,3}$  are given as

$$\alpha_1 = \frac{\Delta_1}{2} \pm \sqrt{U_0^2 + \frac{\Delta_1^2}{4}}, \quad \alpha_{2,3} = 0. \quad (54)$$

We note that the plus and minus signs in the expression of  $\alpha_1$  produce two independent fundamental solutions.

The general Heun function is a rather complicated mathematical object the theory of which is currently poorly developed. However, during the past years a progress was recorded due to the extension of the approach suggested by Svartholm [88] and Erdélyi [90]. Several new series expansions of the general Heun function have been constructed in terms of simpler special functions such as the incomplete Beta function, the Gauss hypergeometric function, the Appell generalized hypergeometric function of two variables [78,94,106]. Below we use a specific expansion of the general Heun function which is applicable if a characteristic exponent of the singularity at infinity is zero [78].

### 1.2.2 Series solutions of the Heun equation in terms of the incomplete Beta functions

As it is seen from equation (53), for the field configuration (49) a characteristic exponent of the regular singularity of the general Heun equation at infinity is zero:  $\alpha = 0$ . It has been shown in [78] that the Heun function then permits a series expansion in terms of the incomplete Beta functions:

$$u = \sum_n c_n u_n, \quad u_n = B_z(\gamma_n, \delta_n). \quad (55)$$

This expansion is developed as follows. The involved Beta functions satisfy the following second-order linear differential equation:

$$\frac{d^2 u_n}{dz^2} + \left( \frac{1-\gamma_n}{z} + \frac{1-\delta_n}{z-1} \right) \frac{du_n}{dz} = 0. \quad (56)$$

We note that this is a particular specialization of the Gauss hypergeometric equation for which at least one of the characteristic exponents is zero as it is the case for the Heun equation for the field configuration (49). If we now put  $\delta_n = 1 - \delta$  for all  $n$ , we will then make the characteristic exponents coincide at the singular point  $z=1$  as well. Then, the strategy is to achieve the correct behavior of function (55) at the remaining singularities  $z=0$  and  $z=a$  by adjusting the parameters  $\gamma_n$  and the coefficients  $c_n$  of the sum. This is done by substitution of equations (55) and (56) into the general Heun equation, and then, using the recurrence relations between the involved Beta-functions, grouping the terms proportional to a particular  $u_n$  and finally requiring all the resultant

summands of thereby regrouped sum to vanish. After some algebra we arrive at a three-term recurrence relation for successive coefficients:

$$R_n c_n + Q_{n-1} c_{n-1} + P_{n-2} c_{n-2} = 0, \quad (57)$$

where

$$R_n = a(\gamma - 1 + \gamma_n)(\gamma_n - 1), \quad (58)$$

$$Q_n = -a(\gamma - 2 + \gamma_n)(\gamma_n + \delta_n - 2) - ((\gamma - 2 + \gamma_n) + \varepsilon(\gamma_n - 1)) - q, \quad (59)$$

$$P_n = (\gamma_n + \delta_n - 2)((\gamma - 3 + \gamma_n) + \varepsilon). \quad (60)$$

Assuming  $\gamma_{n\pm 1} = \gamma_n \pm 1$ , for the left-hand side termination of the series at  $n = 0$  it should hold  $R_0 = 0$ , so that  $\gamma_0 = 1 - \gamma$  or  $\gamma_0 = 1$ . The choice  $\gamma_0 = 1$  does not work since then  $u_{-1} = B(z, 0, \delta_n)$  which is not defined, so the condition for the left-hand side termination is

$$\gamma_0 = 1 - \gamma. \quad (61)$$

We note that this means that the characteristic exponents of equation (55) at the singular point  $z = 0$  for the first term of the expansion with  $n = 0$ , that is for the term  $u_0 = B_z(\gamma_0, \delta)$ , are also the same as those for the Heun equation.

Thus, we finally have the expansion

$$u = \sum_{n=0}^{\infty} c_n B_z(1 - \gamma + n, 1 - \delta) \quad (62)$$

with the coefficients of the recurrence relation (57) being simplified as

$$R_n = an(n - \gamma) \quad (63)$$

$$Q_n = -an(n + 1 - \gamma - \delta) - (n + \varepsilon)(n + 1 - \gamma) - q, \quad (64)$$

$$P_n = (n + 2 - \gamma - \delta)(n + \varepsilon). \quad (65)$$

The series (62) terminates from the right-hand side and thus generates a closed-form finite-sum solution if two successive coefficients, say  $c_{N+1}$  and  $c_{N+2}$ , vanish for some  $N = 0, 1, 2, \dots$ . Equation  $c_{N+2} = 0$  is satisfied if  $P_N = 0$ . This is equivalent to the condition

$$\varepsilon = -N, \quad N = 0, 1, 2, \dots \quad (66)$$

or

$$\gamma + \delta - 2 = +N, \quad N = 0, 1, 2, \dots, \quad (67)$$

while the equation  $c_{N+1} = 0$  (this equation is referred to as the  $q$ -equation) leads to a polynomial equation of the degree  $N + 1$  for the accessory parameter  $q$  thus imposing a restriction on this parameter.

### 1.2.3 Conditionally and unconditionally integrable sub-models

Having expanded the general Heun function into series in terms of the incomplete Beta-functions and further established the conditions for termination of the constructed series, we now consider if the solution of the two-state problem for the field configuration (49) can be written through a linear combination of a finite number of incomplete Beta functions. So we inspect if the termination conditions are satisfied for the parameters of the general Heun function given by equation (53). It is then found out that for real input parameters  $U_0, a, \Delta_1, \Delta_2$  the termination is not achieved if equation (67) is applied. For the alternative condition  $\varepsilon = -N$  given by equation (66), however, the answer is positive for all non-negative integers  $N = 0, 1, 2, 3, \dots$ . For  $N = 0$  and  $N = 1$  we get the trivial constant-detuning Rabi model. However, starting from  $N = 2$ , the results become non-trivial. It is then understood that we thereby derive an infinite hierarchy of particular sub-models for which the solution of the two-state problem is given by a linear combination of a finite number of incomplete Beta functions. Consider these cases in more detail.

To meet the termination condition  $\varepsilon = -N$  suggested by equation (66), we put  $\Delta_2 = N$  (see equation (53)) with a non-negative integer  $N = 0, 1, 2, \dots$ . This reduces the number of variable input parameters of the field configuration (49) to three (we omit the time scaling and shifting parameters  $\Delta$  and  $t_0$ ). The second termination condition  $c_{N+1} = 0$  will of course further decrease the number of the independent parameters by imposing a relation between the remaining parameters  $U_0, \Delta_1$  and  $a$ . If this is a relation involving only the detuning parameters  $\Delta_1$  and  $a$ , then we have an *unconditionally* integrable model for which the frequency detuning and the Rabi frequency are independent. Otherwise, if the relation links the detuning parameters with the Rabi frequency  $U_0$ , the model is called *conditionally* integrable. The result is that for  $N = 2$  we have an unconditionally integrable model (this model is presented in the next section), while for  $N = 3$  the model is proved to be conditionally integrable. It is expected that for all higher orders  $N > 3$  the models are also conditionally integrable. To give an explicit example of such models, here is the field configuration for the case  $N = 3$ :

$$U = U_0, \quad \delta_t = \Delta_1 + \frac{9 - 3\sqrt{3}R - 9\Delta_1}{(\sqrt{3} - R)R + 3(\Delta_1 - 1)\Delta_1 + \sqrt{1 - \frac{6}{3 + \sqrt{3}R - 3\Delta_1}}(R^2 - 3(\Delta_1 - 1)^2)\cos(t)}, \quad (68)$$

where

$$R = \pm\sqrt{U_0^2 + \Delta_1^2 - 1}. \quad (69)$$



### 1.2.4 An unconditionally integrable sub-model

Consider the case  $N = 2$ , i.e. when the general Heun function involved in solution (52) is represented as a sum of three incomplete Beta functions. We have  $\Delta_2 = 2$  and the equation  $c_{N+1} = 0$  in terms of the input physical parameters of the problem  $U_0, \Delta_1$  and  $a$  (we assume  $\Delta = 1$ ) is reduced to

$$U_0^2 (a-1)^2 (a(\Delta_1 - 1) - \Delta_1 - 1) = 0. \quad (70)$$

Since  $U_0 \neq 0$  and  $a \neq 1$ , this equation relates the parameters  $a$  and  $\Delta_1$ :

$$a = \frac{\Delta_1 + 1}{\Delta_1 - 1}, \quad (71)$$

thus generating an *unconditionally* solvable 2-parametric two-state model:

$$U(t) = U_0 = \text{const}, \quad \delta_i(t) = \Delta_1 - \frac{2}{\Delta_1 - \sqrt{\Delta_1^2 - 1} \cos(t)}. \quad (72)$$

We note that since the detuning should be real, the model is applicable for  $|\Delta_1| > 1$ .

The 3D-plot of the detuning modulation function (72) depending on the parameter  $\Delta_1$  is shown in figure 15. The plot of this function for several particular values of  $\Delta_1$  depicted in figure 16 shows that with increasing  $\Delta_1$  the extremum of the detuning approaches  $\Delta_1$ , so that for large  $\Delta_1$  the detuning modulation function effectively becomes a periodic Dirac delta-comb threaded on the line  $\delta_i(t) = \Delta_1$ .

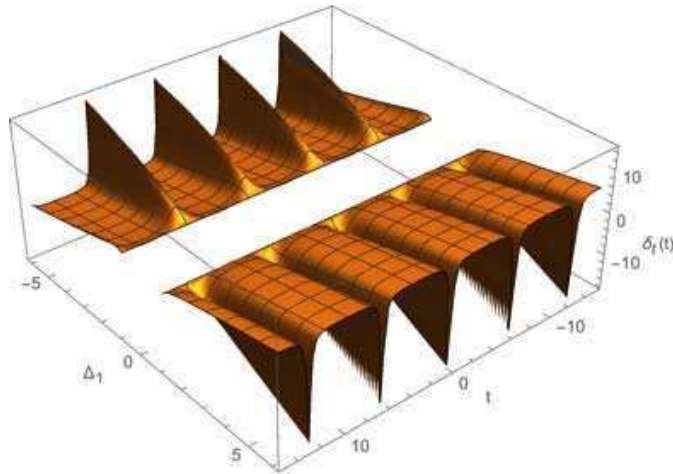


Fig. 15. Exactly integrable constant-amplitude periodic-crossing model (72): 3D-plot of the detuning  $\delta_i(t)$ .

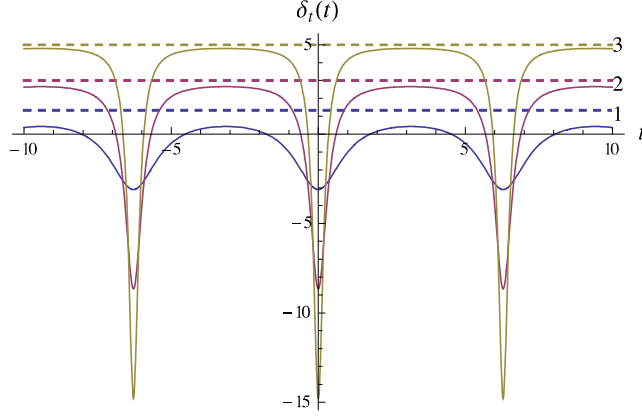


Fig. 16. Exactly integrable constant-amplitude periodic-crossing model (72): solid lines present the frequency modulation and the dashed lines indicate the corresponding parameter  $\Delta_1$  ( $= 4/3, 3, 5$  for curves 1, 2, 3, respectively).

The general Heun function involved in solution (52) presents a linear combination with constant coefficients of three Beta functions:

$$H_G = B_z(R, -1) + \frac{2\Delta_1(1-R)}{(\Delta_1+1)R} B_z(R+1, -1) + \frac{(\Delta_1-1)(R-1)}{(\Delta_1+1)(R+1)} B_z(R+2, -1), \quad (73)$$

where we have introduced the notation  $R = \sqrt{4U_0^2 + \Delta_1^2} > 0$ . Using the recurrence relation between consecutive neighbors

$$B_z(c, b) = \frac{z^c}{c} (1-z)^b + \frac{(b+c)}{c} B_z(c+1, b), \quad (74)$$

the sum in equation (73) is readily reduced to include just one Beta function. It is further checked that the coefficient of the term proportional to this beta function is zero so that the sum is finally simplified to a quasi-polynomial:

$$H_G = z^R \frac{(z-1)(1+R\Delta_1) - (z+1)(R+\Delta_1)}{R(R+1)(\Delta_1+1)(z-1)}, \quad (75)$$

The resultant solution of the two-state problem for  $N = 2$  is eventually written as

$$a_2 = C_0 z^{\frac{\Delta_1+R}{2}} \left( (R-1)(\Delta_1-1) + \frac{2(R+\Delta_1)}{1-z} \right), \quad (76)$$

where  $C_0$  is a constant that is defined from the initial conditions and

$$z(t) = \sqrt{\frac{\Delta_1+1}{\Delta_1-1}} e^{i(t-t_0)}. \quad (77)$$

We note that by changing  $R$  to  $-R$  we get the second independent solution of the problem.

Equation (76) shows that the *Floquet exponent* [107,108] for this solution is  $i\lambda_2$  with

$$\lambda_2 = (\Delta_1 + R) / 2 > 0. \quad (78)$$

This is immediately understood by noting that  $z^{(\Delta_1+R)/2} = e^{i\lambda_2 t}$  while the term in brackets is  $T = 2\pi / \Delta$ -periodic like the coefficients of equation (2) are for the field configuration (72). By changing  $R$  to  $-R$  we get that the Floquet exponent for the second independent solution is  $i\lambda_1$  with

$$\lambda_1 = (\Delta_1 - R) / 2 < 0. \quad (79)$$

Finally, we note that  $\lambda_{1,2}$  are the quasi-energies of the system for the constant field configuration  $(U, \delta_t) = (U_0, \Delta_1)$ . We conclude the discussion of the derived solution by examining the dynamics of the population of the second level described by equation (76). This dynamics is shown in figure 17. We note that since  $1/(1-z)$  is the sum of the geometric progression with common ratio  $z$ :

$$\frac{1}{1-z} = \sum_{n=0}^{\infty} z^n, \quad (80)$$

and  $R + \Delta_1 \neq 0$  for a non-zero interaction, it is understood that the time evolution of the excited level always involves all the harmonics of the driving field's frequency.

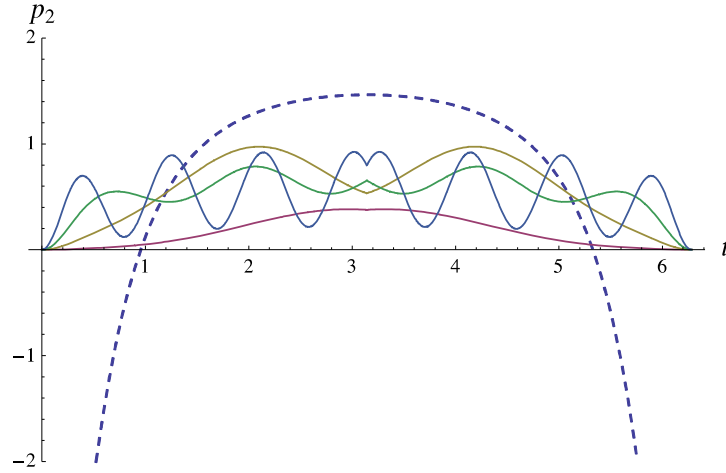


Fig. 17. The dynamics of the population  $p_1 = |a_2|^2$  of the excited level given by equation (76) for  $U_0 = 0.3, 1, 2, 3.5$ . Dashed line presents the detuning ( $\Delta_1 = 2, \Delta = 1, t_0 = 0$ ).

### 1.4.5 Discussion

Thus, we have presented an analytic model of a quantum semiclassical time-dependent two-state problem belonging to the general Heun class. This is a constant-amplitude periodic level-crossing field configuration for which the general Heun function involved in the solution of the

time-dependent Schrödinger equations can be expanded as a convergent series in terms of the incomplete Beta functions. The expansion is possible owing to the condition that a characteristic exponent of the general Heun equation for the regular singular point at infinity is zero. The coefficients of the expansion obey a three-term recurrence relation between the successive coefficients of the expansion that allows termination of the series.

Applying the termination, we have presented two constant amplitude periodic resonance crossing field configurations for which the solution is written in closed form as a finite sum of incomplete Beta functions. One of the models is an unconditionally integrable model and the other is a conditionally integrable one. For the unconditionally integrable model we have written down the explicit solution of the problem and have discussed the behavior of the system subject to excitation by corresponding field configuration. Notably, the solution in this case is finally simplified to an elementary function (quasi-polynomial). This function explicitly indicates the associated Floquet exponents, that is the spectrum of the quasi-energies.

We would like to conclude this chapter by the following remark. The formulation of the semiclassical two-state problem defined by equations (1) assumes that there is no *dissipation*. This is manifested by the motion integral

$$|a_1|^2 + |a_2|^2 = \text{const}. \quad (81)$$

However, the dissipation (irreversible losses) is always available in any real physical system. It is known that in general the losses are not described by a system of time-dependent Schrödinger equations: more advanced mathematical description via density matrix technique is needed [8]. However, in the case of only longitudinal relaxation it is possible to describe the system via time-dependent Schrödinger equations (1) if some additional terms standing for losses are phenomenologically added [8]. For instance, if one neglects the spontaneous relaxation of the system from the excited to the ground state (e.g., if the irreversible losses are assumed to be such that the population is dissipated to a third state of the system) the effective two-state dynamics is described by the following modified pair of equations [8-9]:

$$i \frac{da_1}{dt} = U(t) b_2. \quad (82)$$

$$i \frac{db_2}{dt} = U(t) a_1 + (\Delta(t) - i\Gamma) b_2. \quad (83)$$

Here, like in the case of the lossless two-state problem (1),  $a_1(t)$  and  $b_2(t)$  are the probability amplitudes of the ground and excited states (we again mention that without loss of generality we consider only the excited state being lossy). The pair of *real* functions  $U(t), \Delta(t)$  stands for the

amplitude and detuning modulations, while the parameter  $\Gamma$  defines the rate of a decay process: the dissipation occurring from the excited state to a third state out of the effective two-state system under consideration. It is immediately understood that if constant, the term  $-i\Gamma$  in equation (83) defines an *exponential* decay process. (We note in brackets that, though under the most of real experimental conditions the decay is indeed exponential, however, in general the decay rate  $\Gamma$  is not necessarily fixed to a constant:  $\Gamma$  may be some real function of time).

Applying the simple transformation  $b_2 = a_2(t)e^{-i\omega(t)}$  with

$$\omega_t(t) = \Delta(t) - i\Gamma, \quad (84)$$

the system (82),(83) is rewritten in the exactly same form as (1) and by further elimination of the probability amplitude  $a_1$ , the resulting system is reduced to the equation (2) for  $a_2(t)$  :

$$\frac{d^2 a_2}{dt^2} + \left( -i\omega_t - \frac{U_t}{U} \right) \frac{da_2}{dt} + U^2 a_2 = 0. \quad (85)$$

where instead of  $\delta_t$  we now have  $\omega_t$ .

Given the expression (84) for  $\omega_t$ , one immediately observes that the presented infinite classes of two-state models solvable in terms of the Heun functions are potent to generate dissipative two-state models if the final detuning function  $\delta_t$  in (12) involves an *imaginary* constant term,  $-i\Gamma$ . Recalling formula (12) for  $\delta_t$ , it is readily understood that such a term can always be generated by a proper choice of transformation  $z(t)$ . For instance, like in Section 1.2 of the present chapter, consider the class  $k_{1,2,3} = (-1, 0, 0)$  with the transformation of the independent variable  $z(t) = \sqrt{a} e^{i\Delta_0(t-t_0)}$  in (11),(12). Taking the same

$$U_0^* = -i \frac{U_0}{\Delta_0}, \quad (86)$$

$$\delta_2 = -\delta_3 = i \frac{\Delta_2}{\Delta_0} \quad (87)$$

with real  $U_0, \Delta_2, \Delta_0$ , but choosing  $\delta_1$  as

$$\delta_1 = -\frac{i\Delta_1 + \Gamma}{\Delta_0}, \quad (88)$$

we obtain the following *dissipative* analogue of the same constant-amplitude periodic level crossing two-state model (49):

$$U(t) = U_0, \quad (89)$$

$$\omega_t(t) \equiv \Delta(t) - i\Gamma = \Delta_1 + \frac{(1-a)\Delta_2}{1+a-2\sqrt{a}\cos(\Delta_0(t-t_0))} - i\Gamma.$$

Another dissipative configuration is achieved if one applies the real-valued transformation  $z(t) = -e^t$  in (11),(12) for the same class  $k_{1,2,3} = (-1, 0, 0)$  :

$$U(t) = U_0^*,$$

$$\omega_t(t) = \delta_1 + \frac{\delta_2}{1+e^{-t}} + \frac{\delta_3}{1+ae^{-t}}, \quad (90)$$

where  $\delta_1 = \Delta_1 - i\Gamma$  and the other involved parameters are real. This constant-amplitude dissipative field configuration provides interaction processes with one or two resonance crossings (asymmetric-in-time), level-glancing process, as well as a process of interaction without resonance crossing. The detuning function  $\Delta(t)$  for this configuration is presented on figure 18.

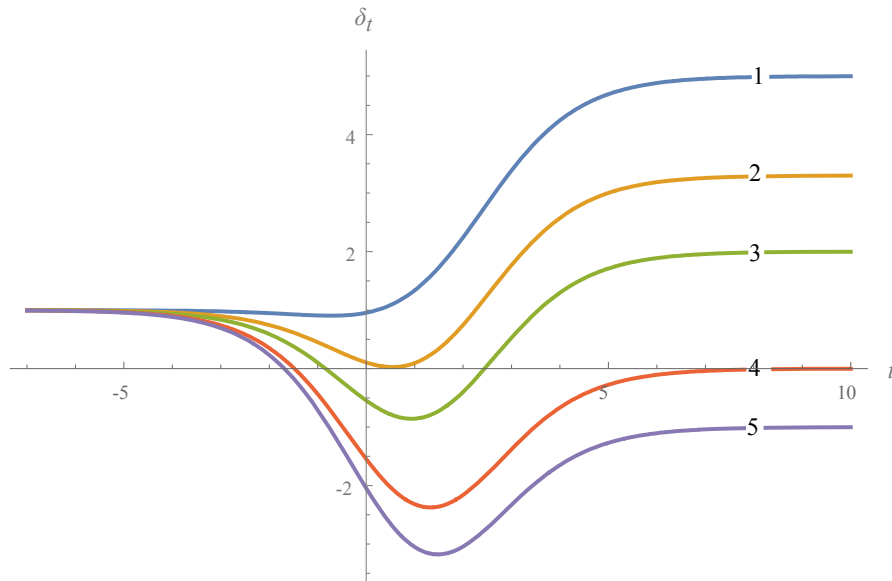


Fig. 18. Detuning modulation function  $\Delta(t)$  for the field configuration given by equation (90) for  $a = 10$ ,  $\Delta_1 = 1$ ,  $\delta_3 = 5$ .  $\delta_2 = -1, -27/10, -4, -6, -7$  for curves 1, 2, 3, 4, 5 respectively.

As regards the cases when the general Heun function involved in the solution is expressed in terms of simpler functions, the additional restrictions, imposed on the field parameters in order to achieve such a simplification, the resulting field-configurations in these cases are conditionally integrable. Several such configurations are presented in the next chapter.

## Chapter 2

### SOLUTIONS OF THE TWO-STATE PROBLEM IN TERMS OF THE SINGLE-CONFLUENT HEUN FUNCTIONS

The solutions of the semiclassical time-dependent two-state models in terms of the single-confluent Heun functions have been discussed in [76]. It has been shown that there exist in total fifteen infinite classes of such solutions [76]. These classes extend over all the families of three- and two-parametric models solvable in terms of the ordinary or confluent hypergeometric functions to more general four-parametric classes involving three-parametric detuning modulation functions [76]. Analyzing the physical field configurations for the general case of variable Rabi frequency and frequency detuning, it has been shown that the most notable features of the models provided by the fifteen classes are due to an extra constant term in the detuning modulation function [76]. Due to this term the classes suggest numerous symmetric or asymmetric chirped pulses and a variety of models with two crossings of the frequency resonance [76]. The latter models are generated by both real and complex transformations of the independent variable [76]. In general, the resulting detuning functions are asymmetric, the asymmetry being controlled by the parameters of the detuning modulation function [76]. Let us present the very classes and the corresponding solutions of the title two-state problem.

#### 2.1 Fifteen classes of models solvable in terms of the single-confluent Heun function

Following the lines of [76], let us briefly outline the derivation lines leading to the mentioned fifteen classes of the solutions of the time-dependent two-state problem in terms of the single-confluent Heun functions. First, we recall that the semiclassical time-dependent two-state problem is equivalent to the linear second-order ordinary differential equation

$$a_{2t} + \left( -i\delta_t - \frac{U_t}{U} \right) a_{2t} + U^2 a_2 = 0. \quad (1)$$

Next, we recall that according to the class property of integrable models of the two-state problem if the function  $a_2^*(z)$  is a solution of this equation rewritten for an auxiliary argument  $z$  for some functions  $U^*(z)$ ,  $\delta^*(z)$  then the function  $a_2(t) = a_2^*(z(t))$  is the solution of equation (2) for the field-configuration defined as

$$U(t) = U^*(z) \frac{dz}{dt}, \quad (2)$$

$$\delta_t(t) = \delta_z^*(z) \frac{dz}{dt} \quad (3)$$

for arbitrary complex-valued function  $z(t)$ . The pair of functions  $U^*(z)$  and  $\delta^*(z)$  is referred to as a basic integrable model.

As already stated in the previous chapter, the transformation of the independent variable  $a_2 = \varphi(z) u(z)$  together with (2),(3) reduces equation (1) to the following equation for the new dependent variable  $u(z)$ :

$$u_{zz} + \left( 2 \frac{\varphi_z}{\varphi} - i \delta_z^* - \frac{U_z^*}{U^*} \right) u_z + \left( \frac{\varphi_{zz}}{\varphi} + \left( -i \delta_z^* - \frac{U_z^*}{U^*} \right) \frac{\varphi_z}{\varphi} + U^{*2} \right) u = 0. \quad (4)$$

This equation becomes the single-confluent Heun equation [70-72]

$$u_{zz} + \left( \frac{\gamma}{z} + \frac{\delta}{z-1} + \varepsilon \right) u_z + \frac{\alpha z - q}{z(z-1)} u = 0, \quad (5)$$

if

$$2 \frac{\varphi_z}{\varphi} - i \delta_z^* - \frac{U_z^*}{U^*} = \frac{\gamma}{z} + \frac{\delta}{z-1} + \varepsilon \quad (6)$$

and

$$\frac{\varphi_{zz}}{\varphi} + \left( -i \delta_z^* - \frac{U_z^*}{U^*} \right) \frac{\varphi_z}{\varphi} + U^{*2} = \frac{\alpha z - q}{z(z-1)}. \quad (7)$$

Equations (6) and (7) present an over-determined system of two nonlinear equations for three unknown functions,  $U^*(z)$ ,  $\delta^*(z)$  and  $\varphi(z)$ . The general solution of this system is currently not known. However, a large list of useful particular solutions can be derived starting from certain specific forms of the involved functions [76].

If one searches for solutions of system (6),(7) applying the ansatz

$$\varphi = e^{\alpha_0 z} z^{\alpha_1} (z-1)^{\alpha_2}, \quad (8)$$

$$U^* = U_0^* z^{k_1} (z-1)^{k_2}, \quad (9)$$

$$\delta_z^* = \delta_0 + \frac{\delta_1}{z} + \frac{\delta_2}{z-1}, \quad (10)$$

he then reveals that the exponents  $k_{1,2}$  should be integers or half-integers satisfying the inequalities  $-1 \leq k_{1,2}$  and  $k_1 + k_2 \leq 0$ . These inequalities lead to fifteen choices of admissible pairs  $k_{1,2}$ . These pairs are shown in Figure 1 by points in the two-dimensional space of the exponent parameters  $k_{1,2}$  [76].



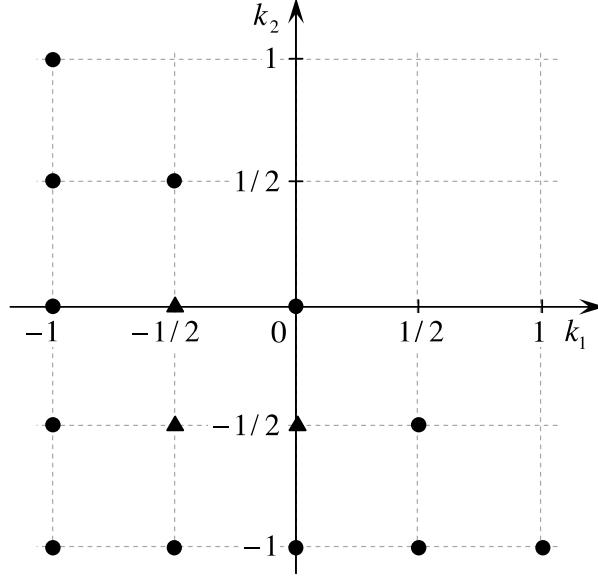


Fig. 1. Fifteen admissible choices for  $k_{1,2}$  [76].

For readers' convenience, we here reproduce the fifteen *basic* models corresponding to these fifteen choices of  $k_{1,2}$  in Table 1 [76]. Owing to the class property of the integrable models of the two-state problem, the actual field configurations are given as

$$U(t) = U_0^* z^{k_1} (z-1)^{k_2} \frac{dz}{dt}, \quad (11)$$

$$\delta_t(t) = \left( \delta_0 + \frac{\delta_1}{z} + \frac{\delta_2}{z-1} \right) \frac{dz}{dt}. \quad (12)$$

Here the independent variable transformation  $z(t)$  can be complex-valued and the involved parameters  $U_0^*$ ,  $\delta_{0,1,2}$  can be complex. They should be chosen so that the resulting field-configuration functions  $U(t)$  and  $\delta(t)$  are real for chosen complex-valued transformation  $z(t)$ . We note that all the listed fifteen classes are in general four-parametric.

We conclude this section by noting that it has been shown that some of the presented classes possess such *three*-parametric subclasses of field configurations for which the title two-state problem is solvable in terms of the Gauss ordinary or the Kummer confluent hypergeometric functions. Finally, we note that some basic models allow *two*-parametric subclasses of both ordinary and confluent hypergeometric types.

$k_2$					
1	$\frac{z-1}{z}$				
1/2	$\frac{\sqrt{z-1}}{z}$	$\sqrt{\frac{z-1}{z}}$			
0	$\frac{1}{z}$ ${}_2F_1$	$\frac{1}{\sqrt{z}}$ ${}_1F_1$	1	${}_1F_1$	
-1/2	$\frac{1}{z\sqrt{z-1}}$ ${}_2F_1$	$\frac{1}{\sqrt{z(z-1)}}$ ${}_2F_1$	$\frac{1}{\sqrt{z-1}}$ ${}_1F_1$	$\sqrt{\frac{z}{z-1}}$	
-1	$\frac{1}{z(z-1)}$ ${}_2F_1$	$\frac{1}{\sqrt{z(z-1)}}$ ${}_2F_1$	$\frac{1}{z-1}$ ${}_1F_1$	$\frac{\sqrt{z}}{z-1}$	$\frac{z}{z-1}$
	-1	-1/2	0	1/2	1
	$k_1$				

**Table 1.** Fifteen basic models of amplitude modulation function  $U^*$  for which the two-state problem is solved in terms of the single-confluent Heun functions. The models that include 3-parametric subclasses solvable in terms of hypergeometric and confluent hypergeometric functions are indicated by " ${}_2F_1$ " and " ${}_1F_1$ ", respectively [76].

### 2.1.1 Solution of the two-state problem for single-confluent Heun models

The solution of the initial two-state problem is explicitly written as [76]

$$a_2 = e^{\alpha_0 z} z^{\alpha_1} (z-1)^{\alpha_2} H_C(\gamma, \delta, \varepsilon; \alpha, q; z), \quad (13)$$

where the parameters  $\gamma, \delta, \varepsilon, \alpha, q$  of the single-confluent Heun function are given as

$$\gamma = 2\alpha_1 - i\delta_1 - k_1, \quad \delta = 2\alpha_2 - i\delta_2 - k_2, \quad \varepsilon = 2\alpha_0 - i\delta_0, \quad (14)$$

$$\alpha = -i\delta_0(\alpha_1 + \alpha_2 - \alpha_0) + \alpha_0(\gamma + \delta - \varepsilon) + Q^{(3)}(0)/6, \quad (15)$$

$$q = \alpha_0(\alpha_0 - i\delta_0 - k_1 - i\delta_1) + \alpha_2(1 - \alpha_2 + k_1 + i\delta_1 + k_2 + i\delta_2) + \alpha_1(1 - \gamma - \delta + \varepsilon + \alpha_1) - Q''(0)/2 - Q'''(0)/6 \quad (16)$$

with 
$$Q(z) = U_0^{*2} z^{2k_1+2} (z-1)^{2k_2+2} \quad (17)$$

and 
$$\alpha_0^2 - i\alpha_0\delta_0 = -Q^{(4)}(1)/4!, \quad (18)$$

$$\alpha_1^2 - \alpha_1(1 + k_1 + i\delta_1) = -Q(0), \quad (19)$$

$$\alpha_2^2 - \alpha_2(1 + k_2 + i\delta_2) = -Q(1). \quad (20)$$

## 2.2 Expansions of the solutions of the single-confluent Heun equation in terms of the Kummer confluent hypergeometric functions

Expansions of the solutions of the single-confluent Heun equation [70-72] in terms of mathematical functions other than powers have been discussed by many authors (see, e.g., [70,91,96,109-114]). The Gauss hypergeometric functions [70,91,109], Kummer and Tricomi confluent hypergeometric functions [110-112], Coulomb wave functions [112-113], Bessel and Hankel functions [114], incomplete Beta functions [96], and other standard special functions have been applied as expansion functions. Using the properties of the derivatives of the solutions of the Heun equation [98-101], it is possible to construct expansions in terms of higher transcendental functions, e.g., the Goursat generalized hypergeometric functions [101] and the Appell generalized hypergeometric functions of two variables of the first kind [106].

Here we discuss, following our work [79], several expansions in terms of the Kummer confluent hypergeometric functions (confluent hypergeometric functions of the first kind) starting from the differential equation and the recurrence relations the latter functions obey for chosen forms of the dependence on the summation variable. In general, the coefficients of the expansions obey three-term recurrence relations; however, for one of the discussed forms of involved confluent hypergeometric functions a four-term recurrence relation is also possible. Besides, for a specific choice of the involved parameters a different two-term recurrence relation is obtained. As a result, the expansion coefficients in this case are explicitly calculated in terms of the Gamma functions. Since the forms of used Kummer confluent hypergeometric functions differ from those applied in previous discussions the conditions for termination of the presented expansions refer to different choices of the involved parameters.

The single-confluent Heun equation is a second order linear differential equation having regular singularities at  $z = 0$  and  $1$ , and an irregular singularity of rank 1 at  $z = \infty$ . We adopt here the following form of this equation [72]:

$$u'' + \left( \frac{\gamma}{z} + \frac{\delta}{z-1} + \varepsilon \right) u' + \frac{\alpha z - q}{z(z-1)} u = 0, \quad (21)$$

which slightly differs from that adopted in [70] since the parameters  $\varepsilon$  and  $\alpha$  are here assumed to be independent. This is a useful convention for practical applications since in this form the equation includes the Whittaker-Ince limit [115] of the single-confluent Heun equation as a particular case achieved by the simple choice  $\varepsilon = 0$ . Note, however, that the expansions presented below do not apply to this limit. The corresponding expansions in terms of the Kummer and Tricomi functions for this case are discussed in [116].

We search for expansions of the solutions of equation (21) in the form

$$u = \sum_n a_n u_n, \quad (22)$$

$$u_n = {}_1F_1(\alpha_n; \gamma_n; s_0 z), \quad (23)$$

where  ${}_1F_1(\alpha_n; \gamma_n; s_0 z)$  is the Kummer confluent hypergeometric function (confluent hypergeometric function of the first kind). Functions  $u_n$  obey the confluent hypergeometric differential equation

$$u_n'' + \left( \frac{\gamma_n}{z} - s_0 \right) u_n' - \frac{\alpha_n s_0}{z} u_n = 0. \quad (24)$$

Substitution of equations (23) and (24) into equation (21) gives

$$\sum_n a_n \left[ \left( \frac{\gamma - \gamma_n}{z} + \frac{\delta}{z-1} + \varepsilon + s_0 \right) u_n' + \frac{(\alpha + \alpha_n s_0)z - (q + \alpha_n s_0)}{z(z-1)} u_n \right] = 0 \quad (25)$$

$$\text{or} \quad \sum_n a_n \left[ ((\varepsilon + s_0)z(z-1) + (\gamma - \gamma_n)(z-1) + \delta z) u_n' + ((\alpha + \alpha_n s_0)z - (q + \alpha_n s_0)) u_n \right] = 0. \quad (26)$$

To proceed further, we need recurrence relations between the involved confluent hypergeometric functions. We discuss here three different sets of such relations applying to the Kummer confluent hypergeometric functions of the form  ${}_1F_1(\alpha_0 + n; \gamma_0 + n; s_0 z)$ ,  ${}_1F_1(\alpha_0 + n; \gamma_0; s_0 z)$  and  ${}_1F_1(\alpha_0; \gamma_0 + n; s_0 z)$ , respectively. Consider these cases separately.

### 2.2.1 Expansions in terms of the Kummer functions ${}_1F_1(\alpha_0 + n; \gamma_0 + n; s_0 z)$

Let  $\alpha_n = \alpha_0 + n$ ,  $\gamma_n = \gamma_0 + n$ , where  $n$  is an integer:  $u_n = {}_1F_1(\alpha_0 + n; \gamma_0 + n; s_0 z)$ .

The starting recurrence relation is simply the differentiation rule for the Kummer confluent hypergeometric functions:

$$u_n' = s_0 \frac{\alpha_n}{\gamma_n} u_{n+1}. \quad (27)$$

A further observation here is that in this case  $z^2 u_n'$ ,  $z u_n'$  and  $z u_n$  are not expressed as a linear combination of functions  $u_n$ . If we then demand the coefficients of these terms to be equal to zero, we reveal that should be  $s_0 = -\varepsilon$  and, furthermore,  $\alpha_n = \alpha / \varepsilon$ ,  $\gamma_n = \gamma + \delta$  for any  $n$ , that is the parameters  $\alpha_n$ ,  $\gamma_n$  should not depend on  $n$ . Thus, this contradiction leads to the conclusion that in this way no expansion can be constructed.

However, there is another possibility. Indeed, put  $s_0 = -\varepsilon$  (thereby canceling the term proportional to  $z^2$ ) and further demand

$$\begin{aligned}
(\alpha + \alpha_n s_0)z - (q + \alpha_n s_0) &= f(n, z), \\
(\gamma - \gamma_n)(z - 1) + \delta z &= Af(n + 1, z),
\end{aligned} \tag{28}$$

where  $A$  is a constant and  $f(n, z)$  is a linear function of  $n$ . It is then easily shown that this is possible only if  $A = 1/\varepsilon$  and

$$\gamma_0 = 1 + \alpha_0 + \gamma + \delta - \alpha/\varepsilon, \tag{29}$$

$$q = \alpha - \delta\varepsilon. \tag{30}$$

equation (26) is then written as:

$$\sum_n a_n \left( -f(n + 1, z) \frac{\alpha_n}{\gamma_n} u_{n+1} + f(n, z) u_n \right) = 0. \tag{31}$$

This gives a simple two-term recurrence relation for the coefficients of the expansion (23):

$$a_n - \frac{\alpha_{n-1}}{\gamma_{n-1}} a_{n-1} = 0, \tag{32}$$

whence

$$u = \sum_n a_n \cdot {}_1F_1(\alpha_0 + n; \gamma_0 + n; -\varepsilon z), \tag{33}$$

$$a_n = \frac{(\alpha_0)_n}{(\gamma_0)_n}, \tag{34}$$

where  $(\alpha_0)_n$  is the Pochhammer symbol:  $(\alpha_0)_n = \alpha_0(\alpha_0 + 1)\dots(\alpha_0 + n - 1)$ . In general, the derived recurrence relation defines a double-sided infinite series. The series is applicable if  $\varepsilon \neq 0$  and  $\gamma_0$  is not zero or a negative integer. It is right-hand side terminated if  $\alpha_0 = 0$  or  $\alpha_0 = -N$  for some positive integer  $N$ . Choosing  $\alpha_0 = 0$  and changing  $n \rightarrow -n$  we arrive at the following expansion for  $q = \alpha - \delta\varepsilon$ :

$$u = \sum_{n=0}^{\infty} \frac{(1 - \gamma_0)_n}{n!} \cdot {}_1F_1(-n; \gamma_0 - n; -\varepsilon z), \tag{35}$$

$$\gamma_0 = 1 + \gamma + \delta - \alpha/\varepsilon. \tag{36}$$

However, the above development can be essentially extended to avoid the additional restriction (30) imposed on the parameters of the single-confluent Heun equation (21). This is achieved by noting that the following recurrence relation holds

$$z(u'_n - s_0 u_n) = (\gamma_n - 1)(u_{n-1} - u_n). \tag{37}$$

Indeed, again put  $s_0 = -\varepsilon$  and demand [compare with equation (28)]

$$\alpha + \alpha_n s_0 = -s_0 [(\gamma - \gamma_n) + \delta], \tag{38}$$

which is fulfilled if

$$\alpha_0 = \gamma_0 - \gamma - \delta + \alpha/\varepsilon. \tag{39}$$

Equation (26) is then rewritten as

$$\sum_n a_n [((\gamma - \gamma_n) + \delta)z(u'_n - s_0 u_n) - (\gamma - \gamma_n)u'_n - (q + \alpha_n s_0)u_n] = 0, \quad (40)$$

so that by virtue of above recurrence relations we have

$$\sum_n a_n \left[ ((\gamma - \gamma_n) + \delta)(\gamma_n - 1)(u_{n-1} - u_n) - (\gamma - \gamma_n)s_0 \frac{\alpha_n}{\gamma_n} u_{n+1} - (q + \alpha_n s_0)u_n \right] = 0. \quad (41)$$

The recurrence relation for the coefficients of the expansion (23) now becomes three-term:

$$R_n a_n + Q_{n-1} a_{n-1} + P_{n-2} a_{n-2} = 0, \quad (42)$$

where

$$R_n = (\gamma + \delta - \gamma_n)(\gamma_n - 1), \quad (43)$$

$$Q_n = -R_n + \varepsilon \alpha_n - q, \quad (44)$$

$$P_n = \varepsilon \frac{\alpha_n}{\gamma_n} (\gamma - \gamma_n). \quad (45)$$

For left-hand side termination of the series at  $n = 0$  should be  $R_0 = 0$ . This is the case if

$$\gamma_0 = \gamma + \delta \quad (\Rightarrow \alpha_0 = \alpha / \varepsilon) \quad (46)$$

( $\gamma_0 = 1$  is forbidden because of division by zero:  $P_1 \sim 1/\gamma_{-1}$ ,  $\gamma_{-1} = 0$ ). Thus, finally, the expansion is explicitly written as

$$u = \sum_{n=0}^{\infty} a_n \cdot {}_1F_1((\alpha / \varepsilon) + n; \gamma + \delta + n; -\varepsilon z) \quad (47)$$

and the coefficients of the recurrence relation (42) are explicitly given as

$$R_n = -n(\gamma + \delta + n - 1), \quad (48)$$

$$Q_n = n(\gamma + \delta + n - 1) + (\varepsilon n + \alpha) - q, \quad (49)$$

$$P_n = -\frac{(\delta + n)(\varepsilon n + \alpha)}{\gamma + \delta + n}. \quad (50)$$

Obviously, this expansion is applicable if  $\varepsilon \neq 0$  and  $\gamma + \delta$  is not a negative integer. A concluding remark is that the second independent solution of equation (21) can be constructed in a similar way after applying the transformation  $z \rightarrow 1 - z$ , which preserves the form of the single-confluent Heun equation.

The series (47) is terminated if  $a_{N+1} = 0$  and  $a_{N+2} = 0$  for some non-negative integer  $N$ . The first condition is fulfilled if  $Q_N a_N + P_{N-1} a_{N-1} = 0$ , while for a non-zero  $a_N$  the second condition results in the equation  $P_N = 0$ , i.e.,

$$\alpha / \varepsilon = -N \quad \text{or} \quad \delta = -N. \quad (51)$$

The equation  $a_{N+1} = 0$  (or, equivalently,  $Q_N a_N + P_{N-1} a_{N-1} = 0$ ) then presents a polynomial equation of the degree  $N + 1$  for the accessory parameter  $q$ , defining, in general,  $N + 1$  values of  $q$  for which the termination of the series occurs. Note, finally, that in the case  $\alpha/\varepsilon = -N$  the resulting solution (47) is a polynomial in  $z$ .

### 2.2.2 Expansions in terms of the Kummer functions ${}_1F_1(\alpha_0 + n; \gamma_0; s_0 z)$

$\alpha_n = \alpha_0 + n, \gamma_n = \gamma_0 = \text{const}$ , where  $n$  is an integer:  $u_n = {}_1F_1(\alpha_0 + n; \gamma_0; s_0 z)$ .

In this case we have the following recurrence relations

$$z u'_n = \alpha_n (u_{n+1} - u_n), \quad (52)$$

$$s_0 z u_n = (\alpha_n - \gamma_0) u_{n-1} + (\gamma_0 - 2\alpha_n) u_n + \alpha_n u_{n+1}. \quad (53)$$

Combining these equations we also have

$$s_0 z^2 u'_n = \alpha_n (s_0 z u_{n+1} - s_0 z u_n) = \alpha_n ((\alpha_n + 1) u_{n+2} + (\gamma_0 - 3\alpha_n - 2) u_{n+1} + (3\alpha_n - 2\gamma_0 + 1) u_n + (\gamma_0 - \alpha_n) u_{n-1}). \quad (54)$$

equation (26) is rewritten as follows

$$\sum_n a_n \left[ (z^2 (\varepsilon + s_0) + z(-\varepsilon - s_0 + \delta + \gamma - \gamma_0) + \gamma_0 - \gamma) u'_n + ((\alpha + \alpha_n s_0) z - (q + \alpha_n s_0)) u_n \right] = 0. \quad (55)$$

Since  $u'_n$  is not expressed as a linear combination of functions  $u_n$ , we demand  $\gamma_0 - \gamma = 0$ . Now, substituting equations (52), (53) and (54) into equation (55) we obtain a four-term recurrence relation for coefficients  $a_n$ :

$$R_n a_n + Q_{n-1} a_{n-1} + P_{n-2} a_{n-2} + S_{n-3} a_{n-3} = 0, \quad (56)$$

where

$$R_n = (\alpha_n - \gamma)(\alpha_n \varepsilon - \alpha), \quad (57)$$

$$Q_n = (\alpha_n \varepsilon - \alpha)(\gamma - 2\alpha_n) - s_0 (\alpha_n (\varepsilon - \delta) - q) + \alpha_n (\gamma - 1 - \alpha_n)(s_0 + \varepsilon), \quad (58)$$

$$P_n = \alpha_n ((\alpha_n + \delta) \varepsilon - \alpha + (2\alpha_n + 2 - \gamma - \delta - \varepsilon)(\varepsilon + s_0) + (\varepsilon + s_0)^2). \quad (59)$$

$$S_n = -\alpha_n (1 + \alpha_n)(s_0 + \varepsilon). \quad (60)$$

Note that here  $s_0$  is a free parameter that can be chosen as convenient.

If we put  $s_0 = -\varepsilon$  (thereby removing the  $z^2$ -dependence in the coefficient of  $u'_n$  in equation (55)) then the four-term recurrence relation becomes 3-term:

$$R_n a_n + Q_{n-1} a_{n-1} + P_{n-2} a_{n-2} = 0, \quad (61)$$

where

$$R_n = (\alpha_n - \gamma)(\alpha_n - \alpha/\varepsilon), \quad (62)$$

$$Q_n = (\alpha_n - \alpha/\varepsilon)(\gamma - 2\alpha_n) + \alpha_n (\varepsilon - \delta) - q, \quad (63)$$

$$P_n = \alpha_n (\alpha_n + \delta - \alpha / \varepsilon). \quad (64)$$

The initial conditions for left-hand side termination of the derived series at  $n = 0$  are  $a_{-2} = a_{-1} = 0$ . It then follows that should be  $R_0 = 0$ . This is the case only if  $\alpha_0 = \alpha / \varepsilon$  or  $\alpha_0 = \gamma$ . Then, the final expansion is explicitly written as

$$u = \sum_{n=0}^{\infty} a_n \cdot {}_1F_1(\alpha_0 + n; \gamma; -\varepsilon z) \quad (65)$$

and the coefficients of the recurrence relation (61) take the form

$$R_n = (n + \alpha_0 - \gamma)(n + \alpha_0 - \alpha / \varepsilon), \quad (66)$$

$$Q_n = (\gamma - 2(n + \alpha_0))(n + \alpha_0 - \alpha / \varepsilon) + (n + \alpha_0)(\varepsilon - \delta) - q, \quad (67)$$

$$P_n = (n + \alpha_0)(n + \alpha_0 + \delta - \alpha / \varepsilon). \quad (68)$$

This expansion is applicable if  $\varepsilon \neq 0$  and  $\gamma$  is not a negative integer.

The series is right-hand side terminated at some  $n = N$  if  $a_N \neq 0$  and  $a_{N+1} = a_{N+2} = 0$ . Then, should be  $P_N = 0$ . If  $\alpha_0 = \alpha / \varepsilon$ , this condition is satisfied if

$$\alpha / \varepsilon = -N \quad \text{or} \quad \delta = -N. \quad (69)$$

If  $\alpha_0 = \gamma$ , the only possibility, since  $\gamma$  should not be a negative integer, is

$$\gamma + \delta - \alpha / \varepsilon = -N. \quad (70)$$

Again, for each of these cases there exist  $N + 1$  values of  $q$  for which the termination occurs. These values are determined from the equation  $a_{N+1} = 0$  (or, equivalently,  $Q_N a_N + P_{N-1} a_{N-1} = 0$ ).

### 2.2.3 Expansions in terms of the Kummer functions ${}_1F_1(\alpha_0; \gamma_0 + n; s_0 z)$

Let  $\alpha_n = \alpha_0$ ,  $\gamma_n = \gamma_0 + n$ , where  $n$  is an integer, so that

$$u_n = {}_1F_1(\alpha_0; \gamma_0 + n; s_0 z). \quad (71)$$

In this case the following recurrence relations are known:

$$z u'_n = (\gamma_n - 1)(u_{n-1} - u_n), \quad (72)$$

$$u'_n = s_0 \left( u_n - \left( 1 - \frac{\alpha_0}{\gamma_n} \right) u_{n+1} \right). \quad (73)$$

Since in this case  $z^2 u'_n$ , and  $z u_n$  are not expressed as a linear combination of functions  $u_n$  we demand the coefficients of these terms in equation (26) to be equal to zero. It is seen that should be  $s_0 = -\varepsilon$  and

$$\alpha_0 = \alpha / \varepsilon. \quad (74)$$

Hence, equation (26) is rewritten as



$$\sum_n a_n [(\gamma - \gamma_n + \delta)z + (\gamma_n - \gamma)]u'_n + (\alpha - q)u_n = 0. \quad (75)$$

Substituting equations (72) and (73) into equation (75) we obtain the following recurrence relation

$$R_n a_n + Q_{n-1} a_{n-1} + P_{n-2} a_{n-2} = 0, \quad (76)$$

where

$$R_n = (\gamma + \delta - \gamma_n)(\gamma_n - 1), \quad (77)$$

$$Q_n = (\gamma + \delta - \gamma_n)(1 - \gamma_n) + \varepsilon(\gamma - \gamma_n) + \alpha - q, \quad (78)$$

$$P_n = (\gamma_n - \gamma)(\varepsilon - \alpha / \gamma_n). \quad (79)$$

For left-hand side termination of the derived series at  $n = 0$  should be  $R_0 = 0$ . This is the case only if

$$\gamma_0 = \gamma + \delta \quad (80)$$

( $\gamma_0 = 1$  is forbidden because of division by zero:  $P_1 \sim 1/\gamma_{-1}$ ,  $\gamma_{-1} = 0$ ). Thus, the expansion is finally written as

$$u = \sum_{n=0}^{\infty} a_n \cdot F_1(\alpha / \varepsilon; \gamma + \delta + n; -\varepsilon z) \quad (81)$$

and the coefficients of the recurrence relation (76) are explicitly given as

$$R_n = -n(\gamma + \delta + n - 1), \quad (82)$$

$$Q_n = n(\gamma + \delta + n - 1) - \varepsilon(\delta + n) + \alpha - q, \quad (83)$$

$$P_n = (\delta + n) \left( \varepsilon - \frac{\alpha}{\gamma + \delta + n} \right). \quad (84)$$

This expansion is applicable if  $\alpha \neq 0$ ,  $\varepsilon \neq 0$  and  $\gamma + \delta$  is not a negative integer. If the series is right-hand side terminated for a non-negative integer  $N$  then  $P_N = 0$ . This is the case if

$$\gamma + \delta - \alpha / \varepsilon = -N \quad (85)$$

or

$$\delta = -N. \quad (86)$$

The termination occurs for  $N + 1$  values of the accessory parameter  $q$  defined from the equation  $a_{N+1} = 0$ .

#### 2.2.4 Expansions in terms of the Tricomi functions $U(\alpha_n; \gamma_n; s_0 z)$

In this subsection we construct expansions of the solutions of the single-confluent Heun equation (21) in the form

$$u = \sum_n a_n u_n, \quad (87)$$

where the function

$$u_n = U(\alpha_n; \gamma_n; s_0 z) \quad (88)$$

is the Tricomi *irregular* confluent hypergeometric function (confluent hypergeometric function of the second kind). The functions  $u_n$  obey the same confluent hypergeometric differential equation as above equation (24):

$$u_n'' + \left( \frac{\gamma_n}{z} - s_0 \right) u_n' - \frac{\alpha_n s_0}{z} u_n = 0. \quad (89)$$

Hence, the substitution of equations (87)-(89) into the single-confluent Heun equation gives

$$\sum_n a_n [((\varepsilon + s_0)z(z-1) + (\gamma - \gamma_n)(z-1) + \delta z)u_n' + ((\alpha + \alpha_n s_0)z - (q + \alpha_n s_0))u_n] = 0. \quad (90)$$

To proceed further, we again need recurrence relations between the involved confluent hypergeometric functions. Considering three different sets of Tricomi functions of the form  $U(\alpha_0 + n; \gamma_0 + n; s_0 z)$ ,  $U(\alpha_0 + n; \gamma_0; s_0 z)$  and  $U(\alpha_0; \gamma_0 + n; s_0 z)$ , we reveal that the first two choices do not satisfy such recurrence relations that lead to consistent expansions. Only the third choice works. We thus consider this case.

Let  $\alpha_n = \alpha_0$ ,  $\gamma_n = \gamma_0 + n$ , where  $n$  is an integer, so that

$$u_n = U(\alpha_0; \gamma_0 + n; s_0 z). \quad (91)$$

For these functions the following recurrence relations are known:

$$z u_n' = (1 - \gamma_n) u_n + (\gamma_n - 1 - \alpha_0) u_{n-1}, \quad (92)$$

$$u_n' = s_0 (u_n - u_{n+1}). \quad (93)$$

Since in this case  $z^2 u_n'$ , and  $z u_n$  are not expressed as a linear combination of functions  $u_n$  we demand the coefficients of these terms to be equal to zero in equation (90). It is seen that then should be  $s_0 = -\varepsilon$  and

$$\alpha_0 = \alpha / \varepsilon. \quad (94)$$

Hence, equation (90) is rewritten as

$$\sum_n a_n [(\gamma - \gamma_n + \delta)z + (\gamma_n - \gamma)] u_n' + (\alpha - q) u_n = 0. \quad (95)$$

Substituting equations (92) and (93) into this equation we obtain the following three-term recurrence relation:

$$R_n a_n + Q_{n-1} a_{n-1} + P_{n-2} a_{n-2} = 0, \quad (96)$$

where

$$R_n = (\gamma + \delta - \gamma_n)(\gamma_n - 1 - \alpha / \varepsilon), \quad (97)$$

$$Q_n = (\gamma + \delta - \gamma_n)(1 - \gamma_n) + \varepsilon(\gamma - \gamma_n) + \alpha - q, \quad (98)$$

$$P_n = (\gamma_n - \gamma)\varepsilon. \quad (99)$$

For left-side termination of the derived series at  $n = 0$  should be  $R_0 = 0$ . This is the case only if  $\gamma_0 = \gamma + \delta$  ( $\gamma_0 = 1$  is forbidden because of division by zero:  $P_1 \sim 1/\gamma_{-1}$ ,  $\gamma_{-1} = 0$ ). Thus, the expansion is finally written as

$$u = \sum_{n=0}^{\infty} a_n U(\alpha/\varepsilon; \gamma + \delta + n; -\varepsilon z) \quad (100)$$

and the coefficients of the recurrence relation (96) are explicitly given as

$$R_n = -n(\gamma + \delta + n - 1 - \alpha/\varepsilon), \quad (101)$$

$$Q_n = n(\gamma + \delta + n - 1) - \varepsilon(\delta + n) + \alpha - q, \quad (102)$$

$$P_n = (\delta + n)\varepsilon. \quad (103)$$

This expansion applies if  $\alpha \neq 0$  and  $\varepsilon \neq 0$ . If the series is right-hand side terminated for some non-negative integer  $N$  then  $P_N = 0$ . This is the case only if

$$\delta = -N. \quad (104)$$

The termination occurs for  $N + 1$  values of the accessory parameter  $q$  derived from the equation  $a_{N+1} = 0$ .

### 2.2.5 Discussion

Thus, using different recurrence relations obeyed by the Kummer (*regular*) confluent hypergeometric functions, we have constructed several confluent hypergeometric expansions of the solutions of the single-confluent Heun equation. In addition, we have constructed on more expansion in terms of the Tricomi (*irregular*) confluent hypergeometric functions. The forms of the dependence of the used confluent hypergeometric functions on the summation variable differ from that applied in previous discussions.

A major set of physical problems where the presented expansions can be applied is encountered in quantum physics (see, e.g., [70-74] and references therein). For instance, in particle physics, there are many potentials for which the stationary Schrödinger equation is reduced to the single-confluent Heun equation (see, e.g., [117,118]). Similarly, in atomic, molecular and optical physics, as it was shown in [76] (see also the above section 2.1), there are many electromagnetic field configurations for which the time-dependent Schrödinger equations for the probability amplitudes of a driven quantum few-state system can be reduced to the single-confluent Heun equation [52,76].

A known example of application of the above-presented expansions to physical problems is the recent derivation of finite-sum closed-form solutions of the quantum two-state problem for an

atom excited by a time-dependent laser field of Lorentzian shape and variable detuning providing double crossings of the frequency resonance [76]. This field configuration is defined as

$$U(t) = \frac{U_0}{1+t^2}, \quad \frac{d\delta}{dt} = \Delta_0 + \frac{\Delta_1}{1+t^2}, \quad (105)$$

and the solution of the two-state problem for this model is given as [76]

$$a_2 = z^{\alpha_1} (z-1)^{-\alpha_1} H_C(1+R, 1-R, -2\Delta_0; 0, -(R+\Delta_1/2)\Delta_0; z), \quad (106)$$

where

$$z = (1+it)/2, \quad (107)$$

$$\alpha_1 = (\Delta_1 + 2R)/4, \quad (108)$$

and

$$R = \sqrt{U_0^2 + \Delta_1^2}/4 \quad (109)$$

is the effective Rabi frequency. It is readily seen that the above series (65)-(68) may terminate if

$$\delta = 1 - R = -N \quad (110)$$

(i.e. if the effective Rabi frequency is a natural number:  $R=1,2,\dots$ ) thus resulting in closed form exact solutions. The second termination condition then defines a relation between  $\Delta_0$  and  $\Delta_1$  for which the termination actually occurs. Interestingly, the particular sets of the involved parameters for which these closed form solutions are obtained define curves in the 3D-space of the involved physical parameters belonging to the complete return spectrum of the two-state quantum system [76]. This is readily verified using the counterpart expansion of the single-confluent Heun function in terms of the Tricomi confluent hypergeometric functions (100) with coefficients defined by equations (101)-(103) (see also [119]).

In a section below, following our work [82], we present one more application. This time, we treat a constant amplitude level-crossing model, for which the detuning modulation function is given in terms of the Lambert-W function [102,103]. We will see that the general solution is written through fundamental solutions each of which is an irreducible linear combination of two confluent hypergeometric functions.

### 2.3 Two-term reductions of three-term recurrence relations for expansion coefficients

In the present section, we show that for the above-presented expansions of the single-confluent Heun functions in terms of the confluent hypergeometric functions there exist infinitely many particular non-trivial choices of parameters for which the recurrence relations reduce to two-term ones so that the expansion coefficients are explicitly written in terms of the Euler gamma functions.

Consider, for instance, the expansion (47):

$$u = \sum_{n=0}^{\infty} c_n \cdot {}_1F_1(\alpha / \varepsilon + n; \gamma + \delta + n; -\varepsilon z), \quad (111)$$

governed by three-term recurrence relation (48)-(50):

$$R_n c_n + Q_{n-1} c_{n-1} + P_{n-2} c_{n-2} = 0, \quad (112)$$

where

$$R_n = -n(\gamma + \delta + n - 1), \quad (113)$$

$$Q_n = -q + \alpha + (\gamma + \delta + \varepsilon + n - 1)n, \quad (114)$$

$$P_n = -\frac{(\delta + n)(\varepsilon n + \alpha)}{\gamma + \delta + n}. \quad (115)$$

The assertion is that this recurrence admits two-term reductions for infinitely many choices of the involved parameters. These reductions are achieved by the following two-term recurrence relation obeyed by the coefficients of the generalized hypergeometric series [67,68]:

$$c_n = \left( \frac{1 \prod_{k=1}^{N+2} (a_k - 1 + n)}{n \prod_{k=1}^{N+1} (b_k - 1 + n)} \right) c_{n-1}. \quad (116)$$

Choosing

$$a_1, \dots, a_N, a_{N+1}, a_{N+2} = 1 + e_1, \dots, 1 + e_N, \alpha / \varepsilon, \delta, \quad (117)$$

$$b_1, \dots, b_N, b_{N+1} = e_1, \dots, e_N, \gamma + \delta \quad (118)$$

with parameters  $e_1, \dots, e_N$  to be defined later (these parameters cannot be not zero or negative integers), the ratio  $c_n / c_{n-1}$  is explicitly written as

$$\frac{c_n}{c_{n-1}} = \frac{(\alpha / \varepsilon - 1 + n)(\delta - 1 + n)}{(\gamma + \delta - 1 + n)n} \prod_{k=1}^N \frac{e_k + n}{e_k - 1 + n}. \quad (119)$$

The recurrence relation (112) is then rewritten as

$$\begin{aligned} R_n \frac{(\alpha / \varepsilon - 1 + n)(\delta - 1 + n)}{(\gamma + \delta - 1 + n)n} \prod_{k=1}^N \frac{e_k + n}{e_k - 1 + n} + Q_{n-1} + \\ P_{n-2} \frac{(\gamma + \delta - 2 + n)(n-1)}{(\alpha / \varepsilon - 2 + n)(\delta - 2 + n)} \prod_{k=1}^N \frac{e_k - 2 + n}{e_k - 1 + n} = 0. \end{aligned} \quad (120)$$

After a straightforward algebra, this equation is transformed to the following form

$$\begin{aligned} -(\alpha / \varepsilon - 1 + n)(\delta - 1 + n) \prod_{k=1}^N (e_k + n) + \\ + Q_{n-1} \prod_{k=1}^N (e_k - 1 + n) - \varepsilon(n-1) \prod_{k=1}^N (e_k - 2 + n) = 0. \end{aligned} \quad (121)$$

We note that this is a polynomial equation in  $n$ . Importantly, it is of the degree  $N+1$ , not  $N+2$ , because the terms proportional to  $n^{N+2}$  cancel. Thus, we have a polynomial equation of the form

$$\sum_{m=0}^{N+1} A_m(\gamma, \delta, \varepsilon, \alpha, q; e_1, \dots, e_N) n^m = 0. \quad (122)$$

Now, equating to zero the coefficients  $A_m$  of this equation warrants the satisfaction of the three-term recurrence relation (112) for all  $n$ .

We thus have  $N+2$  equations  $A_m = 0$ ,  $m = 0, 1, \dots, N+1$ , of which  $N$  equations serve for determination of the parameters  $e_{1,2,\dots,N}$  and the remaining two impose restrictions on the parameters of the single-confluent Heun equation (5).

One of these restrictions is readily derived by calculating the coefficient  $A_{N+1}$  of the term proportional to  $n^{N+1}$ . As a result, we obtain

$$\gamma = \frac{\alpha}{\varepsilon} + 1 + N. \quad (123)$$

The second restriction imposed on the parameters of the Heun equation is checked to be a polynomial equation of the degree  $N+1$  for the accessory parameter  $q$ .

According to equation (119), the coefficients of expansion (111) are given in terms of the Euler gamma functions as ( $c_0 = 1$ )

$$c_n = \frac{\Gamma(n+\delta)\Gamma\left(n+\frac{\alpha}{\varepsilon}\right)\Gamma\left(\frac{\alpha}{\varepsilon}+\delta+1+N\right)}{n!\Gamma(\delta)\Gamma\left(\frac{\alpha}{\varepsilon}\right)\Gamma\left(n+\frac{\alpha}{\varepsilon}+\delta+1+N\right)} \prod_{k=1}^N \frac{e_k+n}{e_k}, \quad n = 0, 1, 2, \dots \quad (124)$$

The explicit solutions of the recurrence relation (112)-(115) for  $N = 0, 1, 2$  are as follows.

$$N = 0: \quad \gamma = \alpha / \varepsilon + 1, \quad (125)$$

$$q = \alpha(1 - \delta / \varepsilon), \quad (126)$$

$$c_n = \frac{\Gamma(n+\delta)\Gamma\left(n+\frac{\alpha}{\varepsilon}\right)\Gamma\left(\frac{\alpha}{\varepsilon}+\delta+1\right)}{n!\Gamma(\delta)\Gamma\left(\frac{\alpha}{\varepsilon}\right)\Gamma\left(n+\frac{\alpha}{\varepsilon}+\delta+1\right)}. \quad (127)$$

$$N = 1: \quad \gamma = \alpha / \varepsilon + 2, \quad (128)$$

$$q^2 + q\left(\frac{\alpha}{\varepsilon}(1+2\delta) - 2\alpha - \varepsilon + \delta\right) + \frac{\alpha}{\varepsilon}\left(\frac{\alpha}{\varepsilon}(\delta - \varepsilon)(1 + \delta - \varepsilon) + (\delta + \delta^2 - 2\delta\varepsilon + \varepsilon^2)\right) = 0, \quad (129)$$

$$e_1 = q - \alpha + \delta - \varepsilon + \frac{\alpha(1+\delta)}{\varepsilon}, \quad (130)$$

$$c_n = \frac{\Gamma(n+\delta)\Gamma\left(n+\frac{\alpha}{\varepsilon}\right)\Gamma\left(\frac{\alpha}{\varepsilon}+\delta+2\right)}{n!\Gamma(\delta)\Gamma\left(\frac{\alpha}{\varepsilon}\right)\Gamma\left(n+\frac{\alpha}{\varepsilon}+\delta+2\right)} \frac{e_1+n}{e_1}. \quad (131)$$

It immediately follows from equation (119) that the coefficient  $c_n$  may vanish only if  $\alpha/\varepsilon$  or  $\delta$  is zero or a negative integer (we recall that the parameters  $e_1, \dots, e_N$  cannot be zero or negative integers). Since for a non-positive integer  $\alpha/\varepsilon$  the expansion functions  ${}_1F_1$  degenerate to polynomials, the first choice results in a finite-sum polynomial solution. More interesting is the second choice. Here, it is readily checked that for integer  $\delta < -N$  the solution identically vanishes. Consequently, the constructed recurrence results in a non-zero finite-sum expansions of the solutions of the single-confluent Heun equation if

$$-N \leq \delta \leq 0. \quad (132)$$

A concluding observation here is that in these cases expansion (111) reduces to particular cases (because of the additional restriction  $\gamma = \alpha/\varepsilon + 1 + N$ , see equation (123)) of the  ${}_{N+1}F_{1+N}$  solutions of the single-confluent Heun equation that we have recently presented in [82]. These solutions for  $N = 0, 1, 2$  are given as follows.

The solution for  $\delta = 0$  is simply the Kummer function

$$u = {}_1F_1(\alpha/\varepsilon; \gamma; -\varepsilon z), \quad (133)$$

which is obviously achieved by the trivial choice

$$q - \alpha = 0. \quad (134)$$

The solution for  $\delta = -1$  is written in terms of the Goursat function  ${}_2F_2$  [68]. It reads

$$u = {}_2F_2(\alpha/\varepsilon, 1+e_1; \gamma, e_1; -\varepsilon z), \quad (135)$$

where the parameter  $e_1$  is defined as

$$e_1 = \alpha/(q - \alpha) \quad (136)$$

with the accessory parameter obeying the quadratic equation

$$q^2 - (2\alpha + \gamma - 1 + \varepsilon)q + \alpha(\alpha + \gamma + \varepsilon) = 0. \quad (137)$$

The solution for  $\delta = -2$  is given in terms of the Clausen function  ${}_3F_3$  [68]. It reads

$$u = {}_3F_3(\alpha/\varepsilon, 1+e_1, 1+e_2; \gamma, e_1, e_2; -\varepsilon z), \quad (138)$$

where the parameters  $e_{1,2}$  are defined by the equations

$$q = \alpha \frac{(1+e_1)(1+e_2)}{e_1 e_2}, \quad (139)$$

$$1 = \frac{e_1(1+e_1-\gamma)}{(\varepsilon e_1 - \alpha)} \frac{e_2(1+e_2-\gamma)}{(\varepsilon e_2 - \alpha)} \quad (140)$$

and the accessory parameter obeys the cubic equation

$$2(q-\alpha)(\alpha+\varepsilon) + (q-\alpha-2(\gamma-1+\varepsilon))(q^2 - (2\alpha+\gamma-2+\varepsilon)q + \alpha(\alpha+\gamma+\varepsilon)) = 0. \quad (141)$$

We recall that the presented solutions (133),(135),(138) as well as the two-term reduction (124) apply if  $\varepsilon \neq 0$ . However, similar developments can also be constructed for the reduced case  $\varepsilon = 0$  [82]. A geeral result here states that, for any non-positive integer  $\delta = -N$ , the single-confluent Heun equation admits a solution written as

$$u = {}_N F_{1+N}(1+e_1, \dots, 1+e_N; e_1, \dots, e_N, \gamma; -\alpha z). \quad (142)$$

This solution can be derived from a  ${}_{N+1} F_{1+N}$  solution by a limiting procedure. For completeness of the presentation, here are the details of the resulting solutions for  $\delta = 0, 1, 2$ .

The simplest case is the Bessel-function solution for  $\delta = 0$ :

$$u = (\alpha z)^{\frac{1-\gamma}{2}} J_{\gamma-1}(2\sqrt{\alpha z}) = {}_0 F_1(; \gamma; -\alpha z), \quad (143)$$

which is valid for

$$q - \alpha = 0. \quad (144)$$

The solution for  $\delta = -1$  is

$$u = {}_1 F_2(1+e_1; \gamma, e_1; -\alpha z), \quad (145)$$

$$q^2 - (2\alpha + \gamma - 1)q + \alpha(\alpha + \gamma) = 0, \quad (146)$$

where the parameter  $e_1$  is given by equation (134):  $e_1 = \alpha / (q - \alpha)$ .

For  $\delta = -2$  we have the solution

$$u = {}_2 F_3(1+e_1, 1+e_2; \gamma, e_1, e_2; -\alpha z) \quad (147)$$

with the parameters  $e_{1,2}$  obeying the equations (140) with  $\varepsilon = 0$ :

$$q = \alpha \frac{(1+e_1)(1+e_2)}{e_1 e_2}, \quad (148)$$

$$1 = \frac{e_1(1+e_1-\gamma)}{\alpha} \frac{e_2(1+e_2-\gamma)}{\alpha}, \quad (149)$$

and the accessory parameter  $q$  satisfies the cubic equation

$$2(q-\alpha)\alpha + (2+q-\alpha-2\gamma)(q^2 - (2\alpha+\gamma-2)q + \alpha(\alpha+\gamma)) = 0. \quad (150)$$



## 2.4 Exactly and conditionally exactly integrable models generated by termination of series expansions of the single-confluent Heun function

In the present section, we apply the above-presented expansions to derive a new exactly and several conditionally integrable level-crossing models solvable in terms of the Kummer confluent hypergeometric functions.

To do this, we examine the *finite-sum* closed-form solutions of the fifteen single-confluent classes of the Heun two-state models (11),(12). A starting observation is that a major set of such solutions can be derived via termination of the above-presented series expansions of the solutions of the single-confluent Heun equation in terms of the confluent hypergeometric functions. A further point is that the termination conditions, as we have seen above, always impose two restrictions on the parameters of the involved single-confluent Heun function. One of these restrictions is imposed on a characteristic exponent of a (finite or infinite) singularity of the single-confluent Heun equation, while the second one presents a polynomial equation for the accessory parameter of the equation.

It can be shown that the first restriction, that is the one imposed on a characteristic exponent, generally leads to *conditionally integrable* field-configurations for which the involved field-parameters do not vary independently. However, there are *four* remarkable exceptions resulting in *exactly* solvable models. The first three of these cases reproduce the familiar confluent hypergeometric models by Landau-Zener-Majorana-Stückelberg [1-4], Nikitin [42] and Crothers-Hughes [44], while the fourth one is reported very recently in our work [83]. The latter model turns out to be defined in terms of the Lambert-W function, which resolves the equation  $W \exp(W) = z$  [102,103].

To show how the conditionally or exactly integrable field-configurations are constructed and to identify the mentioned exactly solvable Lambert-W model, consider, for example, the expansion of the single-confluent Heun function in terms of the Kummer confluent hypergeometric functions given by equation (47):

$$u = \sum_{n=0}^{\infty} c_n \cdot {}_1F_1((\alpha / \varepsilon) + n; \gamma + \delta + n; -\varepsilon z), \quad (151)$$

the coefficients of which obey the three-term recurrence relation

$$R_n c_n + Q_{n-1} c_{n-1} + P_{n-2} c_{n-2} = 0 \quad (152)$$

with the coefficients given through equations (48)-(50):

$$R_n = -n(\gamma + \delta + n - 1), \quad (153)$$

$$Q_n = n(\gamma + \delta + n - 1) + (\varepsilon n + \alpha) - q, \quad (154)$$

$$P_n = -\frac{(\delta + n)(\varepsilon n + \alpha)}{\gamma + \delta + n}. \quad (155)$$

We know that a condition for termination of this series for some integer  $N = 0, 1, 2, \dots$  is reduced to the equation  $P_N = 0$ . Hence, one should put  $\alpha/\varepsilon = -N$  or  $\delta = -N$ . As it is seen from equation (151), the expansion functions for the first choice are polynomials. To examine the more advanced non-polynomial solutions, we discuss the second choice

$$\delta = -N, \quad (156)$$

which is a restriction imposed on a characteristic exponent of the singularity of the single-confluent Heun equation located at the finite point  $z = 1$ . With this, we now examine the equations for the exponent  $\alpha_2$  of the pre-factor  $\varphi(z)$  of the solution (13), that is the second equation (14) and equation (20):

$$\delta = 2\alpha_2 - i\delta_2 - k_2, \quad (157)$$

$$\alpha_2^2 - \alpha_2(1 + k_2 + i\delta_2) = -Q(1), \quad (158)$$

Excluding  $\alpha_2$ , we have the equation

$$(\delta + k_2 + i\delta_2)(\delta - k_2 - 2 - i\delta_2) = -4Q(1). \quad (159)$$

Examining this equation, we recall that the function  $Q(z)$  depends only on the amplitude parameter  $U_0^*$ :  $Q(z) = U_0^{*2} z^{2k_1+2} (z-1)^{2k_2+2}$ , so that  $Q(1)$  is a function of  $U_0^*$  only. It is then understood that if  $\delta$  is fixed to a constant value, we face an equation for which the left-hand side depends on the detuning parameter  $\delta_2$ , while the right-hand side depends on the amplitude parameter  $U_0^*$ . Thus, in general, the parameters  $\delta_2$  and  $U_0^*$  are not varied independently; the parameters are related by equation (159). This is why the models solvable in terms of linear combinations of the confluent hypergeometric functions are in general conditionally integrable.

A remarkable exception is the case for which both sides of equation (159) identically vanish. In that case, the condition  $Q(1) = 0$  yields  $k_2 \neq -1$ . Besides, from the remaining equation (159) we conclude that the detuning parameter  $\delta_2$  is either a fixed number or should vanish. In the first case one obtains *dissipative* conditionally integrable two-state models (see examples below), while the second case, for which  $\delta_2 = 0$ , leads to *exactly* solvable models. We note that all of these exactly solvable models are utmost *three-parametric* because they may involve only three parameters –  $U_0^*$ ,  $\delta_0$  and  $\delta_1$ .

For exactly solvable models, for which  $\delta_2 = 0 \cup Q(1) = 0$ , equation (159) becomes

$$(\delta + k_2)(\delta - k_2 - 2) = 0. \quad (160)$$

With the restrictions that  $\delta$  is a non-positive integer and  $k_2$  may adopt only four integer or half-integer values:  $k_2 = -1/2, 0, 1/2, 1$  (we recall that  $k_2 \neq -1$ ), we reveal that exactly solvable models are constructed only if  $\delta = k_2 = 0$  or  $\delta = -1 \cup k_2 = 1$ . To have a detailed representation on the corresponding classes, consider these cases separately.

Let  $\delta = 0$  and  $\delta_2 = k_2 = 0$ . From the second equation (14) we have  $\alpha_2 = 0$ . Now, the second condition for termination of the series (151) ( $q$ -equation) for  $\delta = 0$  is

$$q - \alpha = 0. \quad (161)$$

Substituting equations (14)-(20), we then arrive at a restriction imposed solely on the auxiliary function  $Q(z)$ :

$$Q(0) - \frac{Q''(0)}{2} - \frac{Q'''(0)}{3} - \frac{Q^{(4)}(0)}{8} = 0, \quad (162)$$

where, since  $k_2 = 0$ ,

$$Q(z) = U_0^{*2} z^{2k_1+2} (z-1)^2. \quad (163)$$

A brief inspection shows that equation (162) is satisfied only if  $k_1 = -1, -1/2, 0$ . These cases result in the classical models by Nikitin [42], Landau-Zener [1-4] and Crothers-Hughes [44], respectively. According to (11),(12), the physical field-configurations defined by these classes are given as (see also [52])

$$U(t) = U_0^* z^{k_1} \frac{dz}{dt}, \quad (164)$$

$$\delta_t(t) = \left( \delta_0 + \frac{\delta_1}{z} \right) \frac{dz}{dt}. \quad (165)$$

The Nikitin constant-amplitude exponential-crossing model ( $k_1 = -1$ ) is derived by choosing  $z(t) = e^t$  [42]:

$$U = U_0^*, \quad \delta_t(t) = \delta_1 + \delta_0 e^t. \quad (166)$$

The Landau-Zener constant-amplitude linear-crossing model ( $k_1 = -1/2$ ) is derived by putting  $\delta_1 = 0$  and choosing  $z(t) = t^2$  [1-4]:

$$U(t) = 2U_0^*, \quad \delta_t(t) = 2\delta_0 t. \quad (167)$$

Finally, the Crothers-Hughes exponential-amplitude exponential-crossing model ( $k_1 = 0$ ) is derived by choosing  $z(t) = e^t$  [44]:

$$U(t) = U_0^* e^t, \quad \delta_t(t) = \delta_1 + \delta_0 e^t. \quad (168)$$

For completeness of the treatment, we consider also the conditionally integrable models generated by termination of expansion (151) on the first expansion term ( $N = \delta = 0$ ), that is, the models for which the solution of the two-state problem can be written in terms of an ansatz involving only one confluent hypergeometric function. These models are derived by inspection of the termination equations  $\delta = 0$  and  $q - \alpha = 0$  with the assumption that the parameters of the field configuration can be dependent. The results are presented in Table 2.

In the table, the three above-mentioned exactly solvable classes of models are marked by grey background. Five classes lead to conditionally exactly solvable field configurations. Three classes that describe dissipative level-crossing processes are indicated as D.

Finally, we note that the classes No.2,7,11,14 do not permit solutions compatible with the conditions  $\delta = 0$  and  $q - \alpha = 0$ . To this end, it should be said that one may consider counterpart conditions  $\gamma = 0$  and  $q = 0$  too. It can then be checked that these four classes also generate conditionally integrable models similar to the ones presented in Table 2.

Consider now two examples of conditionally integrable models.

Class No. 5:  $k_{1,2} = -1, 1$ . We have the field configuration

$$U(t) = U_0^* \frac{z-1}{z} \frac{dz}{dt}, \quad (169)$$

$$\delta_i(t) = \left( \delta_0 + \frac{\delta_1}{z} + \frac{i}{z-1} \right) \frac{dz}{dt} \quad (170)$$

with arbitrary (real or complex)  $U_0^*$ ,  $\delta_0$  and  $\delta_1$ . This is a conditionally integrable class since the detuning modulation functions contains a parameter fixed to a constant ( $\delta_2 = i$ ).

By choosing the independent variable transformation as

$$z = 1 + e^{-\Gamma t}, \quad (171)$$

we obtain the three-parametric field configuration

$$U(t) = \frac{U_0}{e^{\Gamma t} (1 + e^{\Gamma t})}, \quad (172)$$

$$\delta_i(t) = e^{-\Gamma t} \left( \Delta_0 + \frac{\Delta_1}{1 + e^{-\Gamma t}} \right) - \Gamma i, \quad (173)$$

where we have introduced the notations  $U_0 = -\Gamma U_0^*$  and  $\Delta_{0,1} = -\Gamma \delta_{0,1}$ . If we now decompose the detuning modulation function as  $\delta_i(t) \equiv \Delta(t) - i\Gamma$ , we have a level-crossing process given as

$$U(t) = \frac{U_0}{e^{\Gamma t} (1 + e^{\Gamma t})}, \quad \Delta(t) = e^{-\Gamma t} \left( \Delta_0 + \frac{\Delta_1}{1 + e^{-\Gamma t}} \right). \quad (174)$$

This is a process describing an excitation of a two-state quantum system with *dissipation* from or *gain* to the excited state. Such a system with loss/gain from the excited state is governed by the two-state equations [8,9]

$$i \frac{da_1}{dt} = U(t) b_2, \quad (175)$$

$$i \frac{db_2}{dt} = U(t) a_1 + (\Delta(t) - i\Gamma) b_2, \quad (176)$$

where the real parameter  $\Gamma$  stands for the loss/gain rate. Positive  $\Gamma > 0$  resembles to a dissipative system, while negative  $\Gamma < 0$  stands for a system with gain. We conclude the discussion of this model by noting that in order to eliminate the dependence of  $U(t)$  and  $\Delta(t)$  on  $\Gamma$ , one may put  $\Gamma = 1$  for a dissipative case and  $\Gamma = -1$  for a case with gain. Physically, the condition  $|\Gamma| = 1$  can be achieved by choosing a proper time-scale.

Class No. 6:  $k_{1,2} = -1/2, -1$ . We have the conditionally integrable field-configuration

$$U(t) = \frac{U_0^*}{\sqrt{z(z-1)}} \frac{dz}{dt}, \quad (177)$$

$$\delta_t(t) = \left( \delta_0 - \frac{\delta_0 + \delta_2/2}{z} + \frac{\delta_2}{z-1} \right) \frac{dz}{dt}, \quad (178)$$

where

$$\delta_2 = \sqrt{-1 - 4U_0^2}. \quad (179)$$

By choosing the independent variable transformation as

$$z = -e^t, \quad (180)$$

we obtain the two-parametric field configuration

$$U(t) = U_0 \operatorname{sech}(t/2), \quad (181)$$

$$\delta_t(t) = \Delta_0 (1 + e^t) + \sqrt{4U_0^2 - 1/4} \tanh(t/2), \quad (182)$$

where we have introduced the real parameters  $U_0 = -iU_0^*/2$  and  $\Delta_0 = -\delta_0$ . This is an asymmetric-in-time level-crossing model with a bell-shaped amplitude modulation (see Figure 2). As it is seen, the amplitude modulation function is that of the Rosen-Zener [45] or Demkov-Kunike [46] models. Furthermore, for non-zero  $\Delta_0$  the detuning modulation is rather similar to that of Nikitin [42] or the Crothers-Hughes model [44], while for  $\Delta_0 = 0$  it becomes the detuning function of the Demkov-Kunike model [46]. We conclude this section by noting that the model (177)-(182) have been introduced in [52] and two other conditionally exactly integrable models listed in Table 2 have been presented in [56].

$N$	$k_1, k_2$	$U^* / U_0$	$\delta_z^*(z)$	Conditions resulting from equations $\delta = 0$ and $q = \alpha$	Remark
1	-1, -1	$\frac{1}{z(z-1)}$	$\delta_0 + \frac{\delta_1}{z} + \frac{\delta_2}{z-1}$	$\delta_0 + \delta_1 = -\delta_2$ $\delta_2^2 + 4U_0^{*2} = -1$	Conditionally integrable
2	-1, -1/2	$\frac{1}{z\sqrt{z-1}}$	$\delta_0 + \frac{\delta_1}{z} + \frac{\delta_2}{z-1}$	-- This case does not work --	
3	-1, 0	$\frac{1}{z}$	$\delta_0 + \frac{\delta_1}{z}$	$\delta_2 = 0, \delta_{1,2} - \nabla$	Nikitin [42]
4	-1, 1/2	$\frac{\sqrt{z-1}}{z}$	$\delta_0 + \frac{\delta_1}{z} + \frac{i/2}{z-1}$	$\delta_2 = i/2, \delta_{1,2} - \nabla$	D
5	-1, 1	$\frac{z-1}{z}$	$\delta_0 + \frac{\delta_1}{z} + \frac{i}{z-1}$	$\delta_2 = i, \delta_{1,2} - \nabla$	D
6	-1/2, -1	$\frac{1}{\sqrt{z}(z-1)}$	$\delta_0 + \frac{\delta_1}{z} + \frac{\delta_2}{z-1}$	$\delta_0 + \delta_1 = -\delta_2/2$ $\delta_2^2 + 4U_0^{*2} = -1$	Conditionally integrable
7	-1/2, -1/2	$\frac{1}{\sqrt{z(z-1)}}$	$\delta_0 + \frac{\delta_1}{z} + \frac{\delta_2}{z-1}$	-- This case does not work --	
8	-1/2, 0	$\frac{1}{\sqrt{z}}$	$\delta_0 + \frac{\delta_1}{z}$	$\delta_2 = 0, \delta_{1,2} - \nabla$	Landau-Zener [1-4]
9	-1/2, 1/2	$\sqrt{\frac{z-1}{z}}$	$\delta_0 + \frac{\delta_1}{z} + \frac{i/2}{z-1}$	$\delta_2 = i/2, \delta_{1,2} - \nabla$	D
10	0, -1	$\frac{1}{z-1}$	$\delta_0 + \frac{\delta_1}{z} + \frac{\delta_2}{z-1}$	$\delta_0 + \delta_1 = 0$ $\delta_2^2 + 4U_0^{*2} = -1$	Conditionally integrable
11	0, -1/2	$\frac{1}{\sqrt{z-1}}$	$\delta_0 + \frac{\delta_1}{z} + \frac{\delta_2}{z-1}$	-- This case does not work --	
12	0, 0	1	$\delta_0 + \frac{\delta_1}{z}$	$\delta_2 = 0, \delta_{1,2} - \nabla$	Crothers-Hughes [44]
13	1/2, -1	$\frac{\sqrt{z}}{z-1}$	$\delta_0 + \frac{\delta_1}{z} + \frac{\delta_2}{z-1}$	$\delta_0 + \delta_1 = \delta_2/2$ $\delta_2^2 + 4U_0^{*2} = -1$	Conditionally integrable
14	1/2, -1/2	$\sqrt{\frac{z}{z-1}}$	$\delta_0 + \frac{\delta_1}{z} + \frac{\delta_2}{z-1}$	-- This case does not work --	
15	1, -1	$\frac{z}{z-1}$	$\delta_0 + \frac{\delta_1}{z} + \frac{\delta_2}{z-1}$	$\delta_0 + \delta_1 = \delta_2$ $\delta_2^2 + 4U_0^{*2} = -1$	Conditionally integrable

**Table 2.** Two-state models of the single-confluent Heun class, which are solvable through a one-term ansatz involving one confluent hypergeometric function. The three exactly solvable classes by Nikitin, Landau-Zener and Crothers-Hughes are marked by grey background. The classes defining dissipative level-crossing models are indicated in the last column as D.

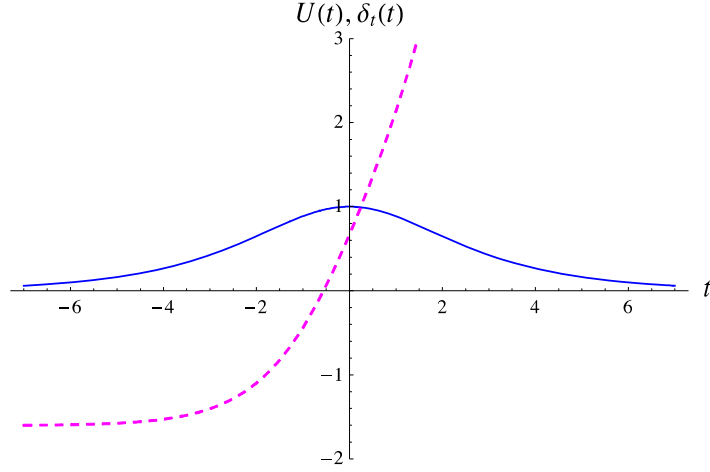


Fig. 2. The two-parametric asymmetric level-crossing model (181),(182) for Rabi frequency with  $U_0 = 1$  (solid line) and detuning with  $\Delta_0 = 1/3$  (dashed line).

### 2.5 A Lambert-W exactly solvable level-crossing confluent hypergeometric two-state model

Consider now the case when the series expansion, in terms of the Kummer confluent hypergeometric functions, of the single-confluent Heun function involved in the solution (13) of the two-state problem is terminated on the second term, that is when  $\delta = -1$ . As we have seen above, for exactly solvable models should be  $\delta_2 = 0$  and  $k_2 = 1$ . With this, from the second equation (14), we again have  $\alpha_2 = 0$ . Now, for  $\delta = -1$ , the second condition for termination of series (151) ( $q$ -equation) is given as (137):

$$q^2 - q(2\alpha - 1 + \gamma + \varepsilon) + \alpha(\alpha + \gamma + \varepsilon) = 0. \quad (183)$$

Substituting equations (14)-(20), it is readily checked that this equation is satisfied only if  $k_1 = -1$ . Thus we conclude that there is only one exactly solvable configuration.

This is the class No. 5 ( $k_{1,2} = -1, 1$ ) with  $\delta_2 = 0$ . The field configuration is given as

$$U(t) = U_0^* \frac{z-1}{z} \frac{dz}{dt}, \quad (184)$$

$$\delta_i(t) = \left( \delta_0 + \frac{\delta_1}{z} \right) \frac{dz}{dt} \quad (185)$$

with arbitrary (real or complex)  $U_0^*$ ,  $\delta_0$  and  $\delta_1$ . It follows from equation (184) that the *constant-amplitude* member of this class is defined by the equation

$$\int \frac{z-1}{z} dz = -\frac{t}{\sigma} + C_0, \quad (186)$$

where the parameters  $\sigma$  and  $C_0$  stand for the time scale and integration constant, respectively, and the sign minus on the right-hand side is chosen for convenience. By choosing  $C_0 = t_0 / \sigma + i\pi$ , the integration results in the transformation

$$z(t) = -W\left(e^{(t-t_0)/\sigma}\right), \quad (187)$$

where  $W$  is the Lambert-W function which is an elementary function that resolves the equation  $z = We^z$  [102,103]. Thus, we arrive at the exactly solvable field configuration

$$U(t) = U_0, \quad \Delta(t) = \Delta_R + \frac{\Delta_L - \Delta_R}{1 + W(e^{(t-t_0)/\sigma})}, \quad (188)$$

where we have put  $U_0^* = -U_0\sigma$ ,  $\delta_0 = -\Delta_R\sigma$  and  $\delta_1 = \Delta_L\sigma$ . This is a model describing an asymmetric-in-time level-crossing process (see Figure 3). It should be stressed that this asymmetry is what differs this model from the well-known Demkov-Kunike one [46]. The detuning starts from  $\delta_i(t) = \Delta_L$  at  $t = -\infty$  and ends with  $\delta_i(t) = \Delta_R$  at  $t = +\infty$ .

It is readily checked that in order to adjust the resonance-crossing time-point to  $t = 0$ , one should choose

$$t_0 = \sigma \left( \frac{\Delta_L}{\Delta_R} + \ln \left( -\frac{\Delta_R}{\Delta_L} \right) \right). \quad (189)$$

We recall that a fundamental solution of the single-confluent Heun equation for  $\delta = -1$  and accessory parameter satisfying equation (183) is explicitly written as [79,82]

$$H_c = {}_1F_1\left(\frac{\alpha}{\varepsilon}; \gamma - 1; -\varepsilon z\right) + \frac{q - q\gamma + \alpha\gamma}{(\gamma - 1)(q - \alpha - \varepsilon)} {}_1F_1\left(\frac{\alpha}{\varepsilon} + 1; \gamma; -\varepsilon z\right). \quad (190)$$

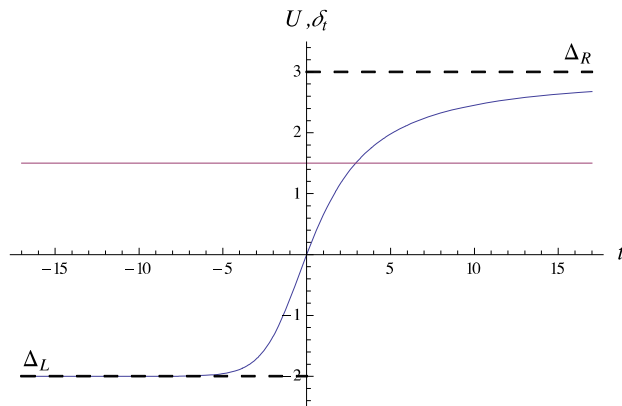


Fig. 3. The Lambert-W exactly solvable level-crossing confluent hypergeometric two-state model (188) for  $U_0 = 1.5$ ,  $\Delta_L = -2$ ,  $\Delta_R = 3$ ,  $\sigma = 1$ .



Alternatively, this solution can be written in a more compact form in terms of the Goursat generalized confluent hypergeometric function  ${}_2F_2$  as [82]

$$H_c = {}_2F_2\left(\frac{\alpha}{\varepsilon}, \frac{q}{q-\alpha}; \gamma, \frac{\alpha}{q-\alpha}; -\varepsilon z\right). \quad (191)$$

With this, a fundamental solution of the two-state problem for models (184),(185), according to (13), is written in terms of the Kummer confluent hypergeometric functions as ( $\alpha_2 = 0$ )

$$a_2 = e^{\alpha_0 z} z^{\alpha_1} H_c(\gamma, \delta, \varepsilon; \alpha, q; z). \quad (192)$$

To discuss the behavior of the presented solution, it is convenient to rewrite the general solution of the two-state problem it in the following equivalent form:

$$a_2 = z^{i\sigma\lambda_L} e^{-i\sigma\lambda_R z} \left( F + A \frac{dF}{dz} \right), \quad (193)$$

$$F(z) = C_1 \cdot {}_1F_1(a; c; -\varepsilon z) + C_2 z^{1-c} {}_1F_1(a+1-c; 2-c; -\varepsilon z), \quad (194)$$

where  $C_{1,2}$  are arbitrary constants,

$$(a, c, \varepsilon) = \left( \frac{i\sigma(2U_0^2 + \Delta_R\lambda_L + (\Delta_L - 2\lambda_L)\lambda_R)}{\Delta_R - 2\lambda_R}, i\sigma(2\lambda_L - \Delta_L), i\sigma(\Delta_R - 2\lambda_R) \right), \quad (195)$$

and

$$A = \frac{2U_0^2 + (\Delta_L + \Delta_R - 2\lambda_L)\lambda_L}{a(\Delta_R - \lambda_L - \lambda_R)(\Delta_R - 2\lambda_R)}. \quad (196)$$

Here  $\lambda_{L,R}$  are the *quasi-energies* for  $t \rightarrow \infty$ :

$$\lambda_L = \frac{1}{2} \left( \Delta_L \pm \sqrt{\Delta_L^2 + 4U_0^2} \right), \quad (197)$$

$$\lambda_R = \frac{1}{2} \left( \Delta_R \pm \sqrt{\Delta_R^2 + 4U_0^2} \right). \quad (198)$$

We note that any combination of signs for  $\lambda_{L,R}$  is applicable, each producing an independent fundamental solution. For definiteness, we choose *minus* sign for both quasi-energies.

Consider next the asymptotes of  $a_2(t)$  at  $t \rightarrow \infty$ . To do this, we examine the behavior of the transformation  $z(t)$  at infinity. Using the properties of the Lambert-W function [72], one readily finds the following asymptotes (see Figure 4):

$$z|_{t \rightarrow -\infty} \sim -e^{(t-t_0)/\sigma}, \quad (199)$$

$$z|_{t \rightarrow +\infty} \sim -\frac{t-t_0}{\sigma} + \left( 1 - \frac{\sigma}{t-t_0} \right) \ln \left( \frac{t-t_0}{\sigma} \right). \quad (200)$$

As it is seen, the asymptote at  $t \rightarrow -\infty$  is exponential, while the asymptote at  $t \rightarrow +\infty$  becomes linear at large times.

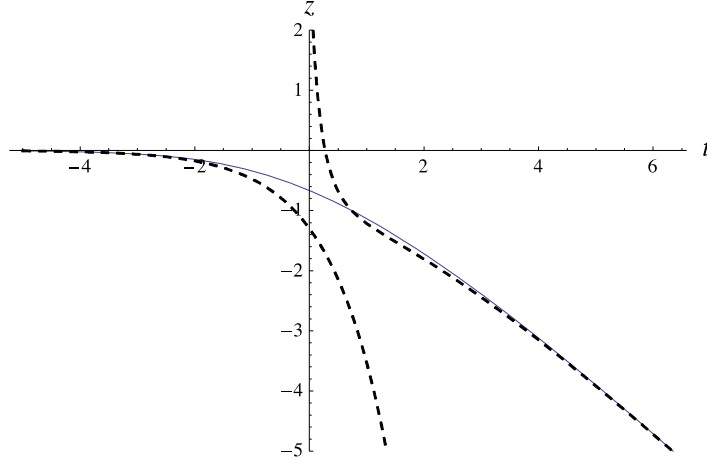


Fig. 4. Transformation (187) (solid line) together with asymptotes (199) and (200) (dashed lines),  $\sigma = 1$ .

Next, using the standard asymptotes for the Kummer functions [72], we have

$$a_2|_{t \rightarrow -\infty} \approx C_1 \left(1 - \frac{aA\varepsilon}{c}\right) e^{i\lambda_{1L}(t-t_0+i\pi\sigma)} + C_2 A(1-c) e^{i\lambda_{2L}(t-t_0+i\pi\sigma)} \quad (201)$$

where

$$\lambda_{1L} = \frac{1}{2} \left( \Delta_L - \sqrt{\Delta_L^2 + 4U_0^2} \right), \quad (202)$$

$$\lambda_{2L} = \frac{1}{2} \left( \Delta_L + \sqrt{\Delta_L^2 + 4U_0^2} \right). \quad (203)$$

For the initial condition that the system starts at  $t \rightarrow -\infty$  from the *first* quasi-energy state with the quasi-energy  $\lambda_{1L}$  we have  $C_2 = 0$  so that

$$a_2|_{t \rightarrow -\infty} \sim C_1 \left(1 - \frac{aA\varepsilon}{c}\right) e^{i\lambda_{1L}t}, \quad (204)$$

$$a_1|_{t \rightarrow -\infty} = \frac{ia'_2}{Ue^{-i\Delta_L t}} \Big|_{t \rightarrow -\infty} \sim \frac{i\lambda_{1L}}{U_0} C_1 \left(1 - \frac{aA\varepsilon}{c}\right) e^{i(\Delta_L + \lambda_{1L})t}. \quad (205)$$

The normalization condition  $|a_1|^2 + |a_2|^2 = 1$  then gives

$$|C_1|^2 = \frac{c^2 e^{2\pi\lambda_{1L}U_0^2}}{(c - aA\varepsilon)^2 (U_0^2 + \lambda_{1L}^2)}. \quad (206)$$

Now, to reveal the behavior of the system at the end of the interaction at  $t \rightarrow +\infty$ , we apply the asymptote (200) to derive

$$a_2|_{t \rightarrow +\infty} \approx C_1 \left( -\frac{t\varepsilon}{\sigma} \right)^{-a} \left( -\frac{t}{\sigma} \right)^{i\sigma\lambda_{1L}} \left( \frac{t}{\sigma} \right)^{-i\sigma\lambda_{1R}} \times \left( \frac{\Gamma(c)}{\Gamma(c-a)} e^{i\lambda_{1R}(t-t_0)} + (1-A\varepsilon)(-\varepsilon)^a \varepsilon^{a-c} \left( \frac{t}{\sigma} \right)^{2a-c-\varepsilon} \frac{\Gamma(c)}{\Gamma(a)} e^{i\lambda_{2R}(t-t_0)} \right), \quad (207)$$

where

$$\lambda_{1R} = \frac{1}{2} \left( \Delta_R - \sqrt{\Delta_R^2 + 4U_0^2} \right), \quad (208)$$

$$\lambda_{2R} = \frac{1}{2} \left( \Delta_R + \sqrt{\Delta_R^2 + 4U_0^2} \right). \quad (209)$$

The expressions for the probability of staying at the first quasi-energy state or for transition to the second quasi-energy state are rather cumbersome; we omit these.

## Chapter 3

### LEVEL-CROSSING TWO-STATE MODELS IN TERMS OF THE DOUBLE-, BI- AND TRI-CONFLUENT HEUN FUNCTIONS

#### 3.1 Analytic solutions of the quantum two-state problem in terms of the double-, bi- and tri-confluent Heun functions

In the present chapter, we discuss the solutions of the semiclassical time-dependent two-state problem in terms of the double-, bi- and tri-confluent Heun functions [70-72]. These are members of the Heun class of mathematical functions, which generalize many of the familiar special functions including the hypergeometric, Airy, Bessel, Mathieu functions, etc. In Chapters 1 and 2 we have discussed the reduction of the two-state problem to the general and confluent Heun equations. It was shown that there exist, respectively, thirty-five five-parametric [75] and fifteen four-parametric [76] classes of models allowing solutions in terms of these functions. Earlier, the bi-confluent Heun equation was used to extend the models solvable in terms of the confluent hypergeometric functions to five four-parametric classes of models solvable in terms of the bi-confluent Heun functions [120].

As it was already mentioned above, the approach we apply to find the field configurations for which the two-state problem is reduced to an equation having known analytic solution is based on the following general property of the solvable models. Consider the time-dependent Schrödinger equations defining the semiclassical time-dependent two-state problem. This is a system of coupled first-order differential equations for the probability amplitudes of the involved two quantum states  $a_{1,2}(t)$  containing two arbitrary real functions of time,  $U(t)$  and  $\delta(t)$ :

$$i \frac{da_1}{dt} = U e^{-i\delta} a_2, \quad i \frac{da_2}{dt} = U e^{+i\delta} a_1. \quad (1)$$

It is then checked that if the functions  $a_{1,2}^*(z)$  solve this system rewritten for an auxiliary argument  $z$  for some functions  $U^*(z)$  and  $\delta^*(z)$ , then the functions  $a_{1,2}(t) = a_{1,2}^*(z(t))$  solve the system (1) for the field-configuration defined as

$$U(t) = U^*(z) \frac{dz}{dt}, \quad \delta(t) = \delta_z^*(z) \frac{dz}{dt} \quad (2)$$

for arbitrary complex-valued function  $z(t)$  [52-55]. The pair of functions  $U^*(z)$  and  $\delta_z^*(z)$  is conventionally referred to as basic integrable model.

This property allows one to group all the solvable models into separate classes, each of which includes the models that are derived from the same amplitude- and detuning-modulation

functions  $U^*(z)$  and  $\delta_z^*(z)$  via transformations (2). Then, the search for the whole variety of models solvable in terms of a particular special function is reduced to the identification of the independent pairs  $\{U^*, \delta_z^*\}$ , referred to as the basic integrable models, for which the solution of the two-state problem is written in terms of this special function.

Here we consider the double-, bi-, and tri-confluent Heun functions, which are solutions of particular confluent modifications of the general Heun equation [69] arising by means of coalescence of some of its singular points [70-72]. The three equations under consideration can be written in the following form:

$$P(z)u_{zz} + (\gamma + \delta z + \varepsilon z^2)u_z + (\alpha z - q)u = 0, \quad (3)$$

where

$$P(z) = z^2, z, 1 \quad (4)$$

for the double-, bi- and tri-confluent Heun equations, respectively.

Let us recall the technique to find two-state models for which the Schrödinger equations (1) are reduced to a target equation (i.e., in this case the double-, bi- and tri-confluent Heun equations (3)). Consider the differential equation for  $a_2$  derived from system (1) by elimination of  $a_1$ :

$$\frac{d^2 a_2}{dt^2} + \left( -i\delta_t - \frac{U_t}{U} \right) \frac{da_2}{dt} + U^2 a_2 = 0. \quad (5)$$

The transformation of the dependent variable  $a_2 = \varphi(z)u(z)$  together with (2) reduces Eq. (5) to the following equation for the new dependent variable  $u(z)$ :

$$u_{zz} + \left( 2\frac{\varphi_z}{\varphi} - i\delta_z^* - \frac{U_z^*}{U^*} \right) u_z + \left( \frac{\varphi_{zz}}{\varphi} + \left( -i\delta_z^* - \frac{U_z^*}{U^*} \right) \frac{\varphi_z}{\varphi} + U^{*2} \right) u = 0, \quad (6)$$

where and hereafter the lowercase Latin index denotes differentiation with respect to the corresponding variable. This equation becomes one of the discussed three types of confluent Heun equations (3) if

$$2\frac{\varphi_z}{\varphi} - i\delta_z^* - \frac{U_z^*}{U^*} = \frac{\gamma + \delta z + \varepsilon z^2}{P(z)} \quad (7)$$

and

$$\frac{\varphi_{zz}}{\varphi} + \left( -i\delta_z^* - \frac{U_z^*}{U^*} \right) \frac{\varphi_z}{\varphi} + U^{*2} = \frac{\alpha z - q}{P(z)}. \quad (8)$$

Though this is an underdetermined system of two nonlinear equations for three unknown functions,  $U^*(z)$ ,  $\delta^*(z)$  and  $\varphi(z)$ , the general solution of which is not known, however, many particular solutions can be found starting from an ansatz, which is guessed by inspecting the structure of the right-hand sides of equations (7) and (8).

This approach has previously been applied to generalize the known models solvable in terms of the hypergeometric functions to six infinite three-parametric classes [53,55], as well as to generalize the models solvable in terms of the confluent hypergeometric functions to three infinite three-parametric classes [52]. In Chapter 1, we have discussed the solvability of the two-state problem in terms of the general Heun functions [75] and in Chapter 2 we have presented the solutions of the two-state problem in terms of the confluent Heun functions [76]. Thirty-five five-parametric and fifteen four-parametric classes of models allowing solutions in terms of these functions have been derived, a useful feature of which is the extension of the previously known detuning modulation functions - two-parametric at most - to functions involving more parameters. In the case of constant detuning this leads to two-peak symmetric or asymmetric pulses with controllable width [76], and, in the general case of variable detuning, it provides a variety of level-crossing models including symmetric and asymmetric models of non-linear sweeping through the resonance [121,122], level-glancing configurations [123-125], processes with two resonance-crossing time points [125] and multiple (periodically repeated) crossing models [126-130].

Here we follow the steps applied in [52-55,76,120] and derive five four-parametric basic models solvable in terms of the double-confluent Heun functions, five more such models solvable in terms of the bi-confluent Heun functions, and a model solvable in terms of the tri-confluent Heun functions. These models generalize all the known two- and three-parametric basic models solvable in terms of the confluent hypergeometric functions to more general four-parametric ones involving three-parametric detuning modulation functions. A subsequent transformation of the independent variable is further applied to generate different families of real field configurations with real Rabi frequency  $U(t)$  and detuning  $\delta(t)$ . The derived models describe different non-linear-in-time (parabolic, cubic, sinh, cosh, etc.) level-sweeping and level-glancing, as well as double, triple and periodically repeated resonance-crossing processes.

### 3.1.1 Two-state models solvable in terms of the double-confluent Heun functions

The double-confluent Heun equation is written as [70-72]

$$\frac{d^2u}{dz^2} + \left( \frac{\gamma}{z^2} + \frac{\delta}{z} + \varepsilon \right) \frac{du}{dz} + \frac{\alpha z - q}{z^2} u = 0. \quad (9)$$

Accordingly, equations (7) and (8) are written as:

$$\frac{\gamma}{z^2} + \frac{\delta}{z} + \varepsilon = 2 \frac{\varphi_z}{\varphi} - i \delta_z^* - \frac{U_z^*}{U^*}, \quad (10)$$

$$\frac{\alpha z - q}{z^2} = \frac{\varphi_{zz}}{\varphi} + \left( -i \delta_z^* - \frac{U_z^*}{U^*} \right) \frac{\varphi_z}{\varphi} + U^{*2}. \quad (11)$$

Examination of the structures of these equations suggests searching for their particular solutions in the following form:

$$\frac{\varphi_z}{\varphi} = \frac{\alpha_2}{z^2} + \frac{\alpha_1}{z} + \alpha_0 \Leftrightarrow \varphi = z^{\alpha_1} e^{\alpha_0 z - \frac{\alpha_2}{z}}, \quad (12)$$

$$\frac{U_z^*}{U^*} = \frac{k}{z} \Leftrightarrow U^* = U_0^* z^k, \quad (13)$$

$$\delta_z^* = \frac{\delta_2}{z^2} + \frac{\delta_1}{z} + \delta_0. \quad (14)$$

Multiplying now Eq. (11) by  $z^4$  we get that, for arbitrary  $\delta_{0,1,2}$ , the product  $U_0^{*2} z^{2k+4}$  should be a polynomial in  $z$  of the fourth degree at most. Hence,  $k$  is an integer or half-integer obeying the inequalities  $0 \leq 2k + 4 \leq 4$ . This leads to five admissible cases of  $k$ , namely,  $k = -2, -3/2, -1, -1/2, 0$ , generating five respective classes of two-state models solvable in terms of the double-confluent Heun function. The amplitude modulation functions for these classes are given as

$$\frac{U^*}{U_0^*} = \frac{1}{z^2}, \quad \frac{1}{z\sqrt{z}}, \quad \frac{1}{z}, \quad \frac{1}{\sqrt{z}}, \quad 1. \quad (15)$$

According to equations (2), the actual field configurations, for which the solution of the two-state problem is written in terms of the double-confluent Heun function, are given as

$$U(t) = U_0^* z^k \frac{dz}{dt}, \quad (16)$$

$$\delta_t(t) = \left( \frac{\delta_2}{z^2} + \frac{\delta_1}{z} + \delta_0 \right) \frac{dz}{dt}, \quad (17)$$

where  $k = -2, -3/2, -1, -1/2, 0$  and the parameters  $U_0^*$ ,  $\delta_{0,1,2}$  are complex constants which should be chosen so that the functions  $U(t)$  and  $\delta(t)$  are real for the chosen complex-valued  $z(t)$ . Since these parameters are arbitrary, all the derived classes are 4-parametric in general.

The solution of the two-state problem (1) is explicitly written as

$$a_2 = z^{\alpha_1} e^{\alpha_0 z - \frac{\alpha_2}{z}} H_D(\gamma, \delta, \varepsilon; \alpha, q; z), \quad (18)$$

where the parameters of the double-confluent Heun function  $\gamma, \delta, \varepsilon, \alpha, q$  are given as

$$\gamma = 2\alpha_2 - i\delta_2, \quad \delta = 2\alpha_1 - i\delta_1 - k, \quad \varepsilon = 2\alpha_0 - i\delta_0, \quad (19)$$

$$\alpha = \alpha_1 \varepsilon - \alpha_0(k + i\delta_1) + Q'''(0)/6, \quad (20)$$

$$q = \alpha_1(1 + k + i\delta_1 - \alpha_1) - \alpha_2 \varepsilon + i\alpha_0 \delta_2 - Q''(0)/2 \quad (21)$$

with

$$Q(z) = U_0^{*2} z^{2k+4} \quad (22)$$

$$\alpha_0^2 - i\alpha_0\delta_0 + Q^{(4)}(0)/4! = 0, \quad (23)$$

$$\alpha_1\gamma - \alpha_2(2+k+i\delta_1) + Q'(0) = 0, \quad (24)$$

$$\alpha_2^2 - i\alpha_2\delta_2 + Q(0) = 0. \quad (25)$$

Formal power-series expansions of the double-confluent Heun function  $H_D$  are constructed using the substitution [70-72]:

$$H_D(\gamma, \delta, \varepsilon; \alpha, q; z) = e^{\nu_0 z - \nu_1/z} z^\mu \sum c_n z^n. \quad (26)$$

However, the convergence radius of such a series is zero. Nevertheless, these expansions present asymptotic series that can be useful in both theoretical developments and practical applications [70-72]. For instance, if terminated, the series yield finite-sum closed-form exact solutions (quasi-polynomials).

The coefficients of the series (26) generally obey a five-term recurrence relation. However, the relation reduces to a three-term one if  $\nu_1 = 0$  or  $-\gamma$  and  $\nu_0 = 0$  or  $-\varepsilon$ . For the simplest choice  $\nu_0 = \nu_1 = 0$ , the result is

$$R_n c_n + Q_{n-1} c_{n-1} + P_{n-2} c_{n-2} = 0 \quad (27)$$

with

$$R_n = \gamma(n + \mu), \quad (28)$$

$$Q_n = (n + \mu)(n + \mu + \delta - 1) - q, \quad (29)$$

$$P_n = \alpha + \varepsilon(n + \mu). \quad (30)$$

If  $\gamma \neq 0$ , the series is left-hand side terminated if  $\mu = 0$ . It is then right-hand side terminated at some  $n = N$  ( $N = 1, 2, 3, \dots$ ) if  $\alpha + \varepsilon N = 0$  and  $c_{N+1} = 0$ . The last equation is a  $(N + 1)$ -th- order polynomial equation for the parameter  $q$ .

To present examples of field configurations generated by the basic models (14),(15) through equations (16),(17), we consider the transformations  $z(t) = e^t$  and  $z(t) = e^{it}$ .

With  $z(t) = e^t$  and  $U_0^* = U_0$ , we have the families

$$U(t) = U_0 e^{(k+1)t}, \quad \delta_t(t) = \delta_0 e^t + \delta_1 + \delta_2 e^{-t}, \quad (31)$$

for which the detuning varies in such a way that the field frequency may cross the resonance  $\delta_t = 0$  up to two times. For the class  $k = -1$  the amplitude of the field is constant.

If  $\delta_2 = \delta_0$ , the field configuration for  $k = -1$  is specified as

$$U(t) = U_0, \quad \delta_t(t) = \delta_1 + 2\delta_0 \cosh(t). \quad (32)$$

Here, non-crossing, level glancing and double crossing processes are possible depending on the parameters  $\delta_{0,1}$  (Figure 1). Level glancing takes place if  $\delta_1 = -2\delta_0$ .



If  $\delta_2 = -\delta_0$ , we have the following field configuration for  $k = -1$ :

$$U(t) = U_0, \quad \delta_t(t) = \delta_1 + 2\delta_0 \sinh(t), \quad (33)$$

which provides only one resonance crossing (Figure 2). For nonzero  $\delta_1$  the crossing is asymmetric in time, while if  $\delta_1 = 0$ , this is a symmetric quasi-linear-in-time level-crossing:  $\delta_t \sim 2\delta_0 t$  at  $t \rightarrow 0$  (if the terminology of [121] is used, this is an example of super-linear crossing since at  $t \rightarrow \infty$  the detuning diverges faster than the linear Landau-Zener detuning).

A solution of the two-state problem (1) for the configuration (31) corresponding to the choice  $\alpha_{0,1,2} = 0$  ( $\varphi(z) = 1$ ) is written as

$$a_2 = H_D(-i\delta_2, 1 - i\delta_1, -i\delta_0; 0, -U_0^2; e^t). \quad (34)$$

The second independent solution is written using a different triad  $\alpha_{0,1,2}$  (see (23)-(25)).

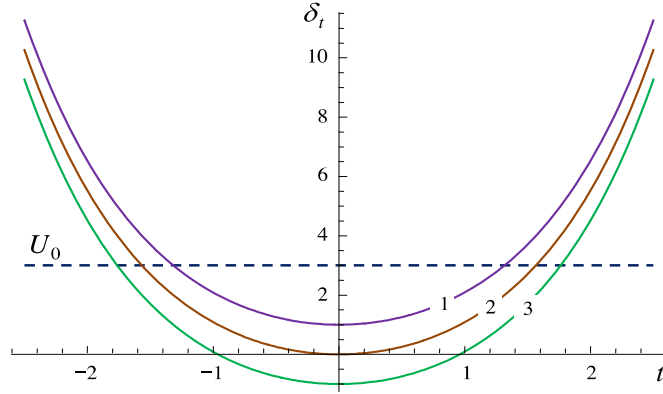


Fig. 1. Double-confluent Heun class  $k = -1$ ,  $z(t) = e^t$ ,  $U_0 = 3$ . Detunings corresponding to  $\delta_2 = \delta_0 = 1$  and  $\delta_1 = -1; -2; -3$  (curves 1, 2, 3, respectively).

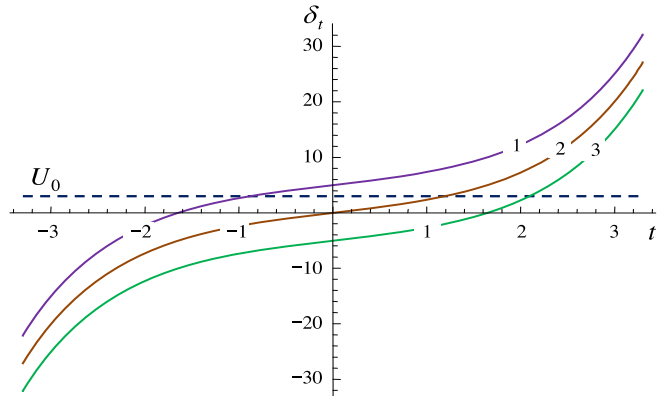


Fig. 2. Double-confluent Heun class  $k = -1$ ,  $z(t) = e^t$ ,  $U_0 = 3$ . Detunings corresponding to  $\delta_2 = -\delta_0 = -1$  and  $\delta_1 = 5; 0; -5$  (curves 1, 2, 3, respectively).

A different level crossing model is obtained by the transformation  $z(t) = e^{i(t-t_0)}$  ( $t_0 = \text{const}$ ). Again, considering the class  $k = -1$  and choosing  $U_0^* = -iU_0$ ,  $\delta_0 = \delta_2 = -i\Delta_2/2$  and  $\delta_1 = -i\Delta_1$  we obtain the following field configuration

$$U(t) = U_0, \quad \delta_i(t) = \Delta_1 + \Delta_2 \cos(t - t_0), \quad (35)$$

which provides periodically repeated level-glancing or resonance crossing processes (Figure 3). For this case, a solution of the two-state problem corresponding to the choice  $\alpha_{0,1,2} = 0$  is explicitly written as

$$a_2 = H_D(-\Delta_2/2, 1 - \Delta_1, -\Delta_2/2; 0, U_0^2; e^{i(t-t_0)}). \quad (36)$$

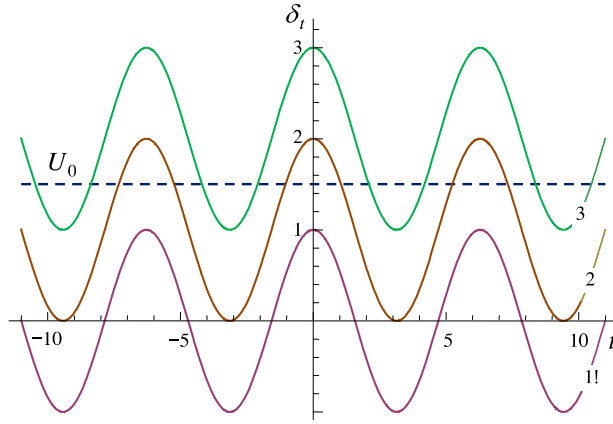


Fig. 3. Double-confluent Heun class  $k = -1$ ,  $z(t) = e^{i(t-t_0)}$ ,  $U_0 = 1.5$ . Detunings corresponding to  $t_0 = 0$ ,  $\Delta_2 = 1$  and  $\Delta_1 = 0; 1; 2$  (curves 1, 2, 3, respectively).

### 3.1.2 Two-state models solvable in terms of the bi-confluent Heun functions

The bi-confluent Heun equation is written as

$$\frac{d^2 u}{dz^2} + \left( \frac{\gamma}{z} + \delta + \varepsilon z \right) \frac{du}{dz} + \frac{\alpha z - q}{z} u = 0. \quad (37)$$

Hence, the equations (7) and (8) in this case are written as:

$$\frac{\gamma}{z} + \delta + \varepsilon z = 2 \frac{\varphi_z}{\varphi} - i \delta_z^* - \frac{U_z^*}{U^*}, \quad (38)$$

$$\frac{\alpha z - q}{z} = \frac{\varphi_{zz}}{\varphi} + \left( -i \delta_z^* - \frac{U_z^*}{U^*} \right) \frac{\varphi_z}{\varphi} + U^{*2}. \quad (39)$$

We search for solutions of these equations in the following form:

$$\frac{\varphi_z}{\varphi} = \frac{\alpha_1}{z} + \alpha_0 + \alpha_2 z \Leftrightarrow \varphi = z^{\alpha_1} e^{\alpha_0 z + \frac{\alpha_2}{2} z^2}, \quad (40)$$

$$\frac{U_z^*}{U^*} = \frac{k}{z} \Leftrightarrow U^* = U_0^* z^k, \quad (41)$$

$$\delta_z^* = \frac{\delta_1}{z} + \delta_0 + \delta_2 z. \quad (42)$$

Multiplying Eq. (39) by  $z^2$  we get that, for arbitrary  $\delta_{0,1,2}$ , the product  $U_0^{*2} z^{2k+2}$  should be a polynomial in  $z$  of the fourth degree at most. Hence,  $k$  is an integer or half-integer obeying the inequalities  $0 \leq 2k+2 \leq 4$ . This leads to five admissible cases of  $k$ , namely,  $k = -1, -1/2, 0, 1/2, 1$ , generating five classes of two-state models solvable in terms of the bi-confluent Heun functions. The amplitude modulation functions for these classes are

$$\frac{U^*}{U_0^*} = \frac{1}{z}, \quad \frac{1}{\sqrt{z}}, \quad 1, \quad \sqrt{z}, \quad z. \quad (43)$$

Thus, the field configurations, for which the solution of the two-state problem is written in terms of the bi-confluent Heun functions, are given as [120]

$$U(t) = U_0^* z^k \frac{dz}{dt}, \quad (44)$$

$$\delta_t(t) = \left( \frac{\delta_1}{z} + \delta_0 + \delta_2 z \right) \frac{dz}{dt} \quad (45)$$

with  $k = -1, -1/2, 0, 1/2, 1$ , and  $U_0^*, \delta_{0,1,2}$  being complex constants which should be chosen so that the functions  $U(t)$  and  $\delta(t)$  are real for the chosen complex-valued  $z(t)$ . Since these parameters are arbitrary, the classes are four-parametric.

The solution of the initial two-state problem (1) is explicitly written as

$$a_2 = z^{\alpha_1} e^{\alpha_0 z + \frac{\alpha_2}{2} z^2} H_B(\gamma, \delta, \varepsilon; \alpha, q; z), \quad (46)$$

where the parameters of the bi-confluent Heun function  $\gamma, \delta, \varepsilon, \alpha, q$  are given as

$$\gamma = 2\alpha_1 - i\delta_1 - k, \quad \delta = 2\alpha_0 - i\delta_0, \quad \varepsilon = 2\alpha_2 - i\delta_2 \quad (47)$$

$$\alpha = \alpha_0(\alpha_0 - i\delta_0) + \alpha_1(2\alpha_2 - i\delta_2) + \alpha_2(1 - k - i\delta_1) + Q''(0)/2, \quad (48)$$

$$q = \alpha_0(k + i\delta_1) - \alpha_1(2\alpha_0 - i\delta_0) - Q'(0) \quad (49)$$

with  $Q(z) = U_0^{*2} z^{2k+2}$  and

$$\alpha_0 \varepsilon - i\alpha_2 \delta_0 + Q'''(0)/3! = 0, \quad (50)$$

$$\alpha_1^2 - \alpha_1(1 + k + i\delta_1) + Q(0) = 0, \quad (51)$$

$$\alpha_2^2 - i\alpha_2 \delta_2 + Q^{(4)}(0)/4! = 0. \quad (52)$$

The origin is a regular singular point of Eq. (37). Hence, the equation permits of a Frobenius power-series solution:

$$u = z^\mu \sum_{n=0}^{\infty} c_n z^n. \quad (53)$$

Substitution of Eq. (53) into Eq. (37) gives the following recurrence relation for the coefficients of the expansion:

$$R_n c_n + Q_{n-1} c_{n-1} + P_{n-2} c_{n-2} = 0, \quad (54)$$

where

$$R_n = (n + \mu)(n + \mu - 1 + \gamma), \quad (55)$$

$$Q_n = \delta(n + \mu) - q, \quad (56)$$

$$P_n = \alpha + \varepsilon(n + \mu), \quad (57)$$

where one should put  $\mu = 0$  or  $\mu = 1 - \gamma$ .

Unlike the above power series for the double-confluent Heun equation, this series is convergent everywhere in the complex  $z$ -plane. The series is right-hand side terminated at some  $n = N = 1, 2, 3, \dots$ , thus producing finite-sum polynomial solutions, if  $\alpha + \varepsilon(N + \mu) = 0$  and  $c_{N+1} = 0$ . The latter equation is a  $(N + 1)$ th-order polynomial equation for  $q$ .

The classes (44),(45) include all the known confluent-hypergeometric level-crossing models. For instance, by setting  $\delta_0 = 0$  and making the replacement  $z \rightarrow \sqrt{z}$ , it is verified that the classes with  $k = -1, 0, 1$  become the classes by Landau-Zener-Majorana-Stückelberg [1-4], Nikitin [6,42] and Crothers-Hughes [44], respectively.

In addition, the derived classes suggest several other interesting level-crossing models. One example is provided by the class  $k = -1/2$ . With specifications  $U_0^* = U_0/2$ ,  $\delta_0 = \Delta_1/2$ ,  $\delta_1 = 0$ ,  $\delta_2 = \Delta_2/2$  and transformation  $z(t) = t^2$ , we have a non-linear-in-time level-crossing model, namely, a constant-amplitude cubic-crossing model providing one or three crossings of the resonance (Figure 4):

$$U(t) = U_0, \quad \delta_t(t) = \Delta_1 t + \Delta_2 t^3. \quad (58)$$

A solution of the two-state problem for this model corresponding to the choice  $\alpha_{1,2,3} = 0$  (see equations (50)-(52)) is written as

$$a_2 = H_B \left( \frac{1}{2}, -\frac{i\Delta_1}{2}, -\frac{i\Delta_2}{2}; 0, -\frac{U_0^2}{4}; t^2 \right). \quad (59)$$

Another class,  $k = +1/2$  with specifications  $U_0^* = 3U_0/2$ ,  $\delta_0 = \delta_1 = 0$ ,  $\delta_2 = 3\Delta_2/2$  and transformation  $z(t) = t^{2/3}$ , presents an example of a constant-amplitude level-crossing model with infinitely fast sweeping through the resonance (Figure 5):

$$U(t) = U_0, \quad \delta_t(t) = \Delta_2 t^{1/3}. \quad (60)$$

A solution of the two-state problem for this model is written as (here we take  $\alpha_{1,2} = 0$ )

$$a_2 = e^{\delta t^{2/3}/2} H_B \left( -\frac{1}{2}, \delta, -\frac{3i\Delta_2}{2}, \frac{\delta^2}{4}, \frac{\delta}{4}, t^{2/3} \right), \quad (61)$$

where  $\delta = -3iU_0^2/\Delta_2$ , and we assume  $t > 0$ .

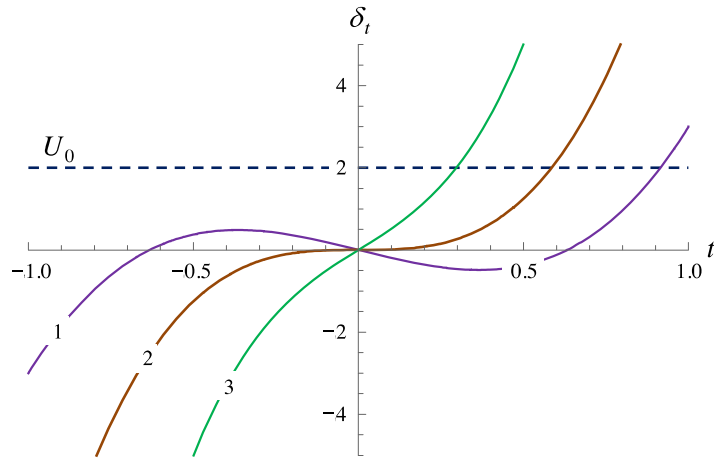


Fig. 4. Bi-confluent Heun class  $k = -1/2$ ,  $z(t) = t^2$ ,  $U_0 = 2$ . Detunings corresponding to  $(\Delta_1, \Delta_2) = (-2, 5); (0, 10); (5, 20)$  (curves 1, 2, 3, respectively).

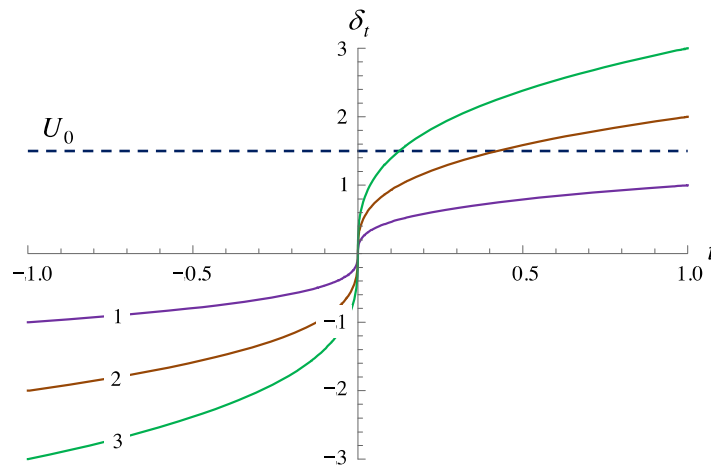


Fig. 5. Bi-confluent Heun class  $k = +1/2$ ,  $z(t) = t^{2/3}$ ,  $U_0 = 1.5$ . Detunings corresponding to  $\Delta_2 = 1; 2; 3$  (curves 1, 2, 3, respectively).

### 3.1.3 Two-state models solvable in terms of the tri-confluent Heun functions

The tri-confluent Heun equation is written as

$$\frac{d^2u}{dz^2} + (\gamma + \delta z + \varepsilon z^2) \frac{du}{dz} + (\alpha z - q)u = 0. \quad (62)$$

Respectively, equations (7) and (8) take the form:

$$\gamma + \delta z + \varepsilon z^2 = 2 \frac{\varphi_z}{\varphi} - i\delta_z^* - \frac{U_z^*}{U^*}, \quad (63)$$

$$\alpha z - q = \frac{\varphi_{zz}}{\varphi} + \left( -i\delta_z^* - \frac{U_z^*}{U^*} \right) \frac{\varphi_z}{\varphi} + U^{*2}. \quad (64)$$

Inspecting the structure of Eq. (63), we search for solutions of these equations in the form:

$$\frac{\varphi_z}{\varphi} = \alpha_0 + \alpha_1 z + \alpha_2 z^2, \quad (65)$$

$$\delta_z^* = \delta_0 + \delta_1 z + \delta_2 z^2, \quad (66)$$

$$\frac{U_z^*}{U^*} = k_0 + k_1 z + k_2 z^2. \quad (67)$$

The second equation then immediately shows that there is only one choice:  $k_{1,2,3} = 0$ , so that

$U^* = U_0^* = \text{const}$ . This defines a four-parametric class with field configuration given as

$$U(t) = U_0^* \frac{dz}{dt}, \quad (68)$$

$$\delta_t(t) = (\delta_0 + \delta_1 z + \delta_2 z^2) \frac{dz}{dt}. \quad (69)$$

The solution of the initial two-state problem for this class is written as

$$a_2 = e^{\alpha_0 z + \frac{\alpha_1}{2} z^2 + \frac{\alpha_2}{3} z^3} H_T(\gamma, \delta, \varepsilon; \alpha, q; z), \quad (70)$$

where the involved parameters are given as

$$\alpha_{1,2,3} = (0, 0, 0), \quad (71)$$

$$(\gamma, \delta, \varepsilon, \alpha, q) = (-i\delta_0, -i\delta_1, -i\delta_2, 0, -U_0^{*2}), \quad (72)$$

or

$$\alpha_{1,2,3} = (i\delta_0, i\delta_1, i\delta_2), \quad (73)$$

$$(\gamma, \delta, \varepsilon, \alpha, q) = (i\delta_0, i\delta_1, i\delta_2, 2i\delta_2, -U_0^{*2} - i\delta_1), \quad (74)$$

The tri-confluent Heun equation (62) has only one singular point. This is an irregular singularity of rank 3, located at  $z = \infty$ . Since the origin is an ordinary point, the equation permits of a power-series solution of the form:

$$u = z^\mu \sum_{n=0}^{\infty} c_n z^n, \quad (75)$$

which is convergent everywhere. However, this time the recurrence relation for the coefficients of the expansion generally involves four terms:

$$S_n c_n + R_{n-1} c_{n-1} + Q_{n-2} c_{n-2} + P_{n-3} c_{n-3} = 0, \quad (76)$$

where

$$S_n = (n + \mu)(n + \mu - 1), \quad (77)$$

$$R_n = \gamma(n + \mu), \quad (78)$$

$$Q_n = \delta(n + \mu) - q, \quad P_n = \alpha + \varepsilon(n + \mu). \quad (79)$$

Here, in order to have a consistent series, from two characteristic exponents,  $\mu = 0, 1$ , one should take the greater one,  $\mu = 1$  (the other one leads to a logarithmic solution). The series is right-hand side terminated at some  $n = N = 1, 2, 3, \dots$  if  $\alpha + \varepsilon(N + \mu) = 0$  and the parameters of the equation meet the conditions  $c_{N+1} = c_{N+2} = 0$ .

Concerning the point that the recurrence relation (76) involves four terms, the following remark is appropriate. As compared with the confluent hypergeometric classes, the field configuration (69) provides an extension only if  $\delta_2 \neq 0$ , which implies that  $\varepsilon \neq 0$  (since  $\varepsilon = \pm i\delta_2$ , see equations (72),(74)). However, in the case of non-zero  $\varepsilon$  one always may achieve  $\gamma = 0$  by shifting the origin:  $z \rightarrow z - z_0$ . Since then  $R_n = 0$  vanishes for all  $n$ , we see that one can always reduce the recurrence relation (76) to one involving only three terms, however, non-successive.

Applying the transformation  $z = \Delta(t - t_1)$  and using the specifications

$$U_0^* = \frac{U_0}{\Delta}, \quad (80)$$

$$\delta_0 = 0, \quad \delta_1 = \frac{t_1 - t_2}{\Delta}, \quad \delta_2 = \frac{1}{\Delta^2} \quad (81)$$

we get a field configuration with constant amplitude and parabolic detuning (Figure 6):

$$U(t) = U_0, \quad (82)$$

$$\delta_t(t) = \Delta(t - t_1)(t - t_2). \quad (83)$$

This is a non-crossing model (if  $t_{1,2}$  have non-zero imaginary parts) or double-crossing model (if  $t_{1,2}$  are real and not zero simultaneously), and it is a level-glancing model if  $t_1 = t_2 = 0$ .

A solution of the two-state problem for this model corresponding to  $\alpha_{1,2,3} = 0$  is

$$a_2 = H_T \left( 0, -\frac{i(t_1 - t_2)}{\Delta}, -\frac{i}{\Delta^2}; 0, -\frac{U_0^2}{\Delta^2}; \Delta(t - t_1) \right). \quad (84)$$

The second independent solution is given by Eq. (70) using the second set of the parameters given by Eq. (74).

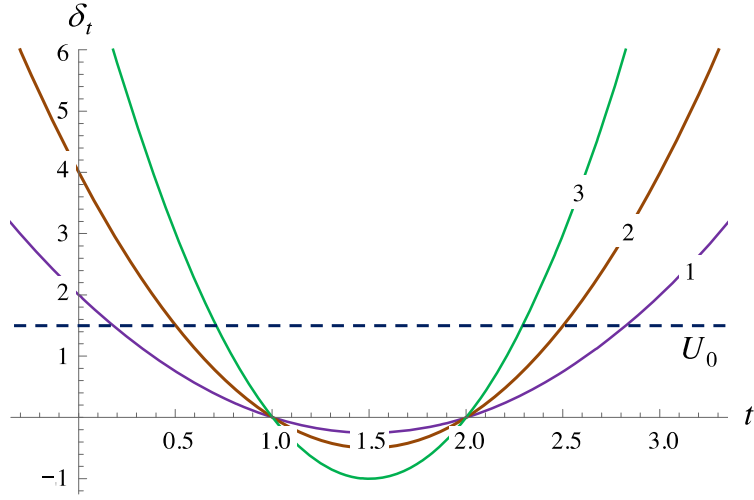


Fig. 6. Tri-confluent Heun class,  $z = \Delta(t - t_1)$ ,  $U_0 = 1.5$ .

Detunings corresponding to  $t_1 = 1$ ,  $t_2 = 2$  and  $\Delta = 1; 2; 4$  (curves 1, 2, 3, respectively).

### 3.1.4 Other classes solvable in terms of the Heun functions

The above classes do not cover all the field configurations, for which the solution of the two-state problem is written in terms of the Heun functions. Several other classes can be derived, e.g., if one considers the equations obeyed by the derivatives of the Heun functions. This is because the latter functions generally do not belong to the Heun class, but obey more complicated equations generally involving one more regular singular point [131-133].

Consider, for instance, the tri-confluent Heun equation (62). It is readily shown that the weighted first derivative of its solution  $v(z) = e^{\gamma z} u_z$  obeys the equation

$$v_{zz} + \left( -\gamma + \delta z + \varepsilon z^2 - \frac{1}{z - z_0} \right) v_z + \frac{\Pi(z)}{z - z_0} v = 0, \quad (85)$$

where  $z_0 = q/\alpha$  and  $\Pi(z)$  is the cubic polynomial

$$\Pi(z) = -\gamma \varepsilon z^3 + (\alpha + \varepsilon - \gamma \delta + z_0 \gamma \varepsilon) z^2 + z_0 (\gamma \delta - 2\alpha - 2\varepsilon) z + z_0 (q - \delta). \quad (86)$$

It is seen that for non-zero  $\alpha$  this equation has an additional regular singularity located at the point  $z = z_0$ . If  $q = 0$  (note that in the case of non-zero  $\alpha$  one always may achieve this by shifting the origin) and additionally  $\alpha + \varepsilon = \gamma \delta$ , the equation is simplified to

$$v_{zz} + \left( -\gamma + \delta z + \varepsilon z^2 - \frac{1}{z} \right) v_z - \gamma \varepsilon z^2 v = 0. \quad (87)$$



Comparing now this equation with Eq. (5) rewritten for the variable  $z$  :

$$\frac{d^2 a_2^*}{dz^2} + \left( -i\delta_z^* - \frac{U_z^*}{U^*} \right) \frac{da_2^*}{dz} + U^{*2} a_2^* = 0, \quad (88)$$

we see that  $a_2^*(z) = v(z)$  if

$$\delta_z^* = \delta_0 + \delta_1 z + \delta_2 z^2, \quad U^* = U_0^* z, \quad (89)$$

and

$$\gamma = i\delta_0, \quad \delta = -i\delta_1, \quad \varepsilon = -i\delta_2, \quad U_0^{*2} = -\gamma\varepsilon. \quad (90)$$

Hence, according to the property (2), the solution of the two-state problem (1) for the class of models given as (compare with Eq. (69))

$$U(t) = U_0^* z \frac{dz}{dt}, \quad \delta_t(t) = (\delta_0 + \delta_1 z + \delta_2 z^2) \frac{dz}{dt} \quad (91)$$

with arbitrary (complex-valued) function  $z(t)$  is written in terms of the derivative of a tri-confluent Heun function (we recall that  $q = 0$  and  $\alpha + \varepsilon = \gamma\delta$ ):

$$a_2 = e^{i\delta_0 z} \frac{d}{dz} H_T(i\delta_0, -i\delta_1, -i\delta_2; i\delta_2 + \delta_0\delta_1; 0; z). \quad (92)$$

However, not all parameters here are independent. The last Eq. (90) imposes the constraint  $U_0^{*2} = -\delta_0\delta_2$ . Thus, the class (91) is three-parametric.

Similar classes are readily derived using the derivatives of the bi-confluent and double confluent Heun functions. For instance, the function  $v = z^\sigma u_z$ , where  $u(z)$  is a solution of the bi-confluent Heun equation (37), obeys the equation

$$v_{zz} + \left( \frac{\gamma + 1 - 2\sigma}{z} + \delta + \varepsilon z - \frac{1}{z - z_0} \right) v_z + \frac{(\alpha + \varepsilon - \varepsilon\sigma)(z - z_0)^2}{z^2} v = 0, \quad (93)$$

where  $z_0 = q/\alpha$ ,  $\sigma = \gamma + \delta z_0 + \varepsilon z_0^2$  and  $(\alpha + \varepsilon)z_0 = (\delta + 2\varepsilon z_0)\sigma$ . Comparing this equation with Eq. (88) we immediately find the class

$$U(t) = U_0^* \frac{z - z_0}{z} \frac{dz}{dt}, \quad \delta_t(t) = \left( \frac{\delta_1}{z} + \delta_0 + \delta_2 z \right) \frac{dz}{dt}, \quad (94)$$

for which the solution of the two-state problem is written as

$$a_2 = z^\sigma \frac{d}{dz} H_B(-i\delta_1 + 2\sigma, -i\delta_0, -i\delta_2; \alpha; \alpha z_0; z) \quad (95)$$

with  $\sigma = i(\delta_1 + \delta_0 z_0 + \delta_2 z_0^2)$ ,  $\alpha = i\delta_2(1 - 2\sigma) - i\delta_0\sigma/z_0$ ,  $U_0^{*2} = \alpha + \varepsilon - \varepsilon\sigma$ . (96)

Here,  $\delta_{0,1,2}$  and  $z_0$  are arbitrary real parameters, hence, this is a four-parametric class.

Constant-amplitude family of field configurations is achieved by the transformation

$$z(t) = -z_0 W(-e^{-t/z_0} / z_0), \quad (97)$$

where  $W$  is the Lambert- $W$  (product log) function [102,103]. A corresponding family of chirped detunings is shown in Figure 7.

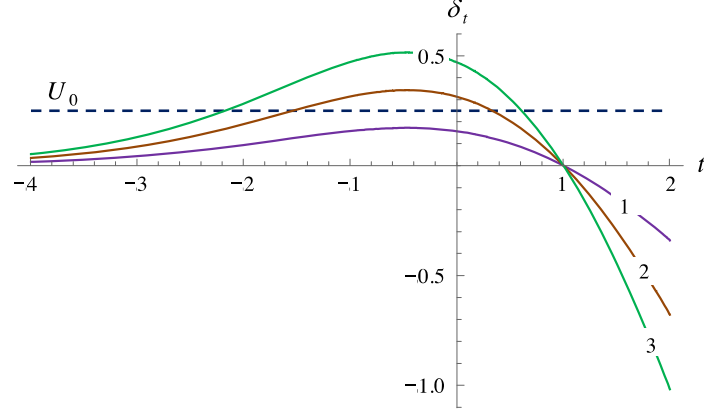


Fig. 7. Bi-confluent Heun class (94). Constant-amplitude family with  $z_0 = -1$ :  $z = W(e^t)$ ,  $\delta_1 = 0$ ,  $\delta_2 = -\delta_0$ .  $\delta_0 = 1$ ; 2; 3 (curves 1, 2, 3, respectively).

Similarly, the function  $v = e^{-\sigma/z} u_z$  with  $u(z)$  being a solution of the double-confluent Heun equation (9) with  $\alpha = -\varepsilon$  and  $q = \delta/2$  obeys the equation

$$v_{zz} + \left( \frac{\gamma - 2\sigma}{z^2} + \frac{\delta + 2}{z} + \varepsilon - \frac{1}{z - z_0} \right) v_z - \frac{\varepsilon \sigma (z - z_0)^2}{z^4} v = 0, \quad (98)$$

where  $z_0 = q/\alpha$  and  $\sigma = \gamma - \delta^2/(4\varepsilon)$ . Comparing this equation with Eq. (88) we immediately find the three-parametric class

$$U(t) = U_0^* \frac{z - z_0}{z^2} \frac{dz}{dt}, \quad \delta_t(t) = \left( \frac{\delta_2}{z^2} + \frac{\delta_1}{z} + \delta_0 \right) \frac{dz}{dt} \quad (99)$$

with  $U_0^{*2} = -\varepsilon\sigma$ , for which the solution of the two-state problem is written as

$$a_2 = e^{-\sigma/z} \frac{d}{dz} H_D(-i\delta_2 + 2\sigma, -i\delta_1, -i\delta_0; i\delta_0; -i\delta_1/2; z). \quad (100)$$

Because of the constraint  $U_0^{*2} = -\varepsilon\sigma$ , this is a three-parametric class. The constant-amplitude family is now achieved by the transformation (compare with Eq. (97))

$$z(t) = -\frac{z_0}{W(-z_0 e^{-t})} \quad (101)$$

with  $z_0 = -\delta_1 / (2\delta_0)$ . A one-parametric family of constant-amplitude field configurations describing asymmetricly chirped detunings is shown in Figure 8. Of course, other families, e.g., describing constant-detuning pulses, can be constructed by an appropriate choice of the transformation  $z(t)$  and the involved parameters.

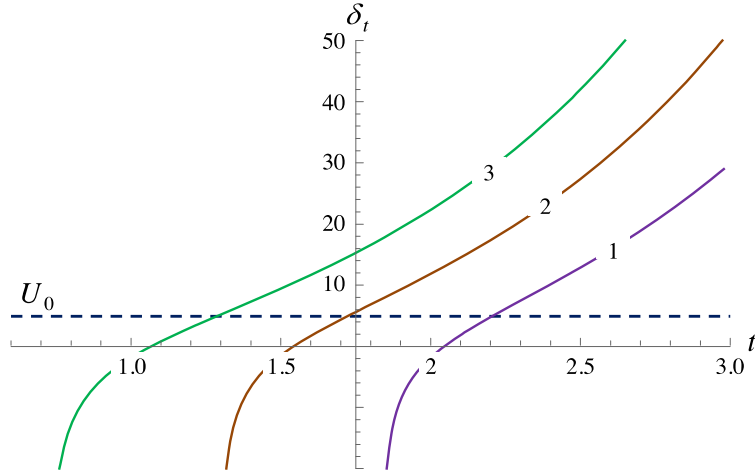


Fig. 8. Double-confluent Heun class (99). Constant-amplitude family with  $z(t) = -z_0 / W(-z_0 e^{-t})$ ,

$$z_0 = -\delta_1 / (2\delta_0), \quad \delta_1 = -2\sqrt{25 - \delta_0^2}, \quad \delta_2 = -\delta_0.$$

Detunings corresponding to  $\delta_0 = 2; 3; 4$  (curves 1, 2, 3, respectively).

### 3.1.5 Discussion

Thus, we have presented five classes of quantum time-dependent two-state models solvable in terms of the double-confluent Heun functions, five other classes solvable in terms of the bi-confluent Heun functions, and a class solvable in terms of the tri-confluent Heun functions. All the derived classes are four-parametric. In the case of constant-amplitude field configuration, the models describe different non-linear (parabolic, cubic, sinh, cosh, etc.) level-sweeping or level-glancing, double- or triple-level-crossing processes. Models describing periodically repeated resonance-glancing or resonance-crossing are also possible.

We have indicated that many other classes can be derived using equations obeyed by certain functions involving the derivatives of the Heun functions. We have presented an example of such a class for each of the three confluent Heun equations. It should be noted that one cannot construct similar additional classes if the hypergeometric equations alone are considered. This is because the derivatives of the hypergeometric functions are again hypergeometric functions, while the derivatives of the Heun functions, as already was said above, generally do not belong to the Heun

class, but obey more complicated equations generally involving one more regular singular point [97-99,131-133].

The Heun functions used are solutions of corresponding confluent modifications of the general Heun equation, derived due to coalescence of some of its singular points. For some values of the involved parameters, each of these three equations is reduced to the confluent hypergeometric equation either directly or by a transformation of the dependent or independent variable. The above classes then reproduce the three known three-parametric classes solvable in terms of the confluent hypergeometric functions [52].

For instance, the double-confluent Heun equation is directly reduced to the confluent hypergeometric equation if  $\gamma = q = 0$ . We then note that in this case the system (19)-(25) becomes over-determined and permits of a solution only for the classes  $k = -1, -1/2, 0$ . Similarly, the bi-confluent Heun equation is directly reduced to the confluent hypergeometric equation if  $\varepsilon = \alpha = 0$ . In this case the system (47)-(52) becomes over-determined and it is readily checked that the solution exists only for the classes with  $k = -1, -1/2, 0$ . In both cases we have  $\alpha_2 = \delta_2 = 0$ , so that these classes exactly reproduce the three three-parametric confluent hypergeometric classes [52].

However, the tri-confluent Heun equation is not directly reduced to the confluent hypergeometric equation. If  $\varepsilon = 0$ , one needs a transformation of both independent and dependent variables, while if  $\varepsilon \neq 0$  and  $\gamma = \delta = 0$  the cubic transformation of the independent variable  $z \rightarrow -\varepsilon(z - z_0)^3 / 3$  will suffice. It is then checked that the tri-confluent class (69) in each of these cases reproduces a confluent hypergeometric class (e.g., obviously, in the case  $\gamma = \varepsilon = \alpha = 0$  we immediately have the Landau-Zener model). Another example of reproducing the confluent hypergeometric classes was mentioned above for the bi-confluent Heun equation, achieved by the change  $z \rightarrow \sqrt{z}$ . The latter case is of particular interest since in this case the reproduction is achieved within the classes with  $k = -1, 0, 1$ . Hence, in addition to the classes  $k = -1, -1/2, 0$ , the bi-confluent class  $k = +1$  also includes a confluent hypergeometric subclass. Finally, it can be checked that this is the case for all other classes. Then, the conclusion is that all the presented double-, bi- and tri-confluent classes of two-state models, each in its own manner, present different generalizations of the prototype confluent hypergeometric families of models.

We would like to conclude by a brief discussion of the solutions of the multi-confluent Heun equations. These are complicated functions, the theory of which still needs development. We have presented above the basic power-series solutions of the considered confluent Heun equations. However, in practical applications, especially, if non-linear extensions are discussed [26,30-34], one may need more advanced techniques. In this case, one may try expansions in terms of functions

other than mere powers, e.g., in terms of familiar special functions such as the Kummer and Tricomi confluent hypergeometric functions [70-72,79,110,111,114], Bessel functions [111,116], Gauss hypergeometric functions [70-72,116], Coulomb wave functions [109,112,113], incomplete Gamma- and Beta-functions [96-98], etc. Expansions in terms of higher transcendental functions [67,68], e.g., in terms of the Goursat and the Appell generalized hypergeometric functions, are also possible [101,106,134]. In several cases these expansions may provide exact finite-sum solutions.

### 3.2 Solutions of the bi-confluent Heun equation in terms of the Hermite functions

The bi-confluent Heun equation is widely encountered in contemporary physics and mathematics research [70-72,117,118]. For example, in nuclear and atomic physics this equation frequently appears in studying the motion of quantum particles in one-, two- or three-dimensional confinement potentials [70]. The double-well quartic and sextic anharmonic oscillator potentials and the special class of singular confinement potentials consisting of a combination of Coulomb, linear and harmonic potentials are well-known examples of this class of potentials [135,136]. The recent examples include the inverse square root potential [137] and its conditionally exactly integrable generalization [138], applications to quantum chemistry [139], quantum dots [140], and, as presented above, quantum two-state systems [77].

Due to its wide appearance in theoretical physics, mathematical properties of the bi-confluent Heun equation have been studied by many authors (see, e.g., [70-72,133,141-153]). In particular, the power-series solutions near the regular singularity at the origin and in the neighborhood of the irregular singularity at the infinity [145,146], the continued fraction technique [147] and the Hill determinant approach [148] for a class of confinement potentials have been discussed in detail. Among the recent developments one may mention the following results. In [133,149] relations between the linear equations of the (deformed) Heun class and the six Painlevé nonlinear equations have been established via an anti-quantization procedure. In [150] the factorization of the confluent Heun equations is re-examined. In [151]  $k$ -summability is used to obtain new integral formulas for the solutions near the infinity and in [152] integral representations for a fundamental system of solutions to the bi-confluent Heun equation are derived using the properties of the Meijer  $G$ -functions. Integral equations for special functions of the Heun class are discussed in [153].

However, despite the large number of articles treating the bi-confluent Heun equation, the theory of this equation certainly needs further development. A particular observation appropriate in this instance is that the solutions are mostly constructed through power-series expansions and, as a

consequence, the applications are mostly based on the polynomial reductions. However, the recent developments such as the exact solution of the Schrödinger equation for the inverse square root potential in terms of the Hermite functions of non-integer order [137], which are not polynomials (nor quasi-polynomials), suggests that the extension to the non-polynomial cases is an interesting and important challenge, as stated in [139]. Presumably, some useful properties of the solutions of the bi-confluent Heun equation may be revealed if expanding the solutions in terms of more advanced mathematical functions rather than powers.

In the next section we make a step in this direction by constructing an expansion of the solutions of the bi-confluent Heun equation in terms of the Hermite functions. Being inspired by the two-term Hermite-function solutions constructed in [137,138], as expansion functions we apply a set of non-integer order Hermite functions of a shifted and scaled argument. As a result, we derive an expansion governed by a three-term recurrence relation between the successive coefficients of the expansion. Notably, under some restrictions imposed on the involved parameters the constructed series is terminated and thus closed-form finite-sum solutions of the bi-confluent Heun equation in terms of the Hermite functions are derived. This is a main result of the next section.

Another result is the general solution of the one-dimensional stationary Schrödinger equation for a bi-confluent-Heun potential in terms of the Hermite functions that are not reduced to quasi-polynomials. The treatment is based on the constructed expansion and applies the described termination technique. This result demonstrates that the expansions of the Heun functions in terms of advanced special functions rather than simple powers suggest a quite productive approach. We note that a similar message follows from the recently reported results for a single-confluent-Heun [154] and a general-Heun [155] potentials.

Below we apply the constructed expansion to derive a new exactly solvable constant-amplitude level-crossing model for the quantum time-dependent two-state problem (for this model the frequency detuning behaves as the inverse square root at the coordinate origin and becomes constant at the infinity). For this model, the solution of the problem is written as an irreducible linear combination of two Hermite functions. Furthermore, in the next chapter, we present another representative example of application of the presented expansion by considering the bi-confluent Heun potentials for the one-dimensional stationary Schrödinger equation [117,119,156]. Our analysis indicates that there presumably exists an infinite number of conditionally exactly solvable potentials the solution for which is written as a linear combination of a finite number of generally non-integer order Hermite functions of shifted and scaled argument. This list of potentials starts with the classical harmonic oscillator potential (plus the potential of the uniform field) [157] and the two conditionally integrable potentials by Stillinger [158]. For these potentials, the solution is given

by a single Hermite function. The next in the list are the two Exton potentials [159] for which the solution presents an irreducible linear combination of two Hermite functions. Remarkable particular cases of the first Exton potential are the inverse square root potential [137] and the two super-symmetric partner potentials presented by Lopez-Ortega [160].

### 3.2.1 Series expansions in terms of the Hermite functions

The bi-confluent Heun equation is a second-order ordinary linear differential equation, which has one regular singularity and an irregular singularity of rank 2 [70-72]. Conventionally, the regular singularity is put in the origin and the irregular one is located at the infinity. This is a confluent form of the general Heun equation derived via coalescence of its two finite regular singularities with the one located at the infinity [70-72].

Though the bi-confluent Heun equation involves only four irreducible parameters [70-72], for the sake of simplicity and generality we adopt here the following five-parametric form of this equation:

$$\frac{d^2u}{dz^2} + \left( \frac{\gamma}{z} + \delta + \varepsilon z \right) \frac{du}{dz} + \frac{\alpha z - q}{z} u = 0, \quad (102)$$

where  $\gamma, \delta, \varepsilon, \alpha, q$  are arbitrary complex parameters. The advantage of this form is that the different canonical forms of the bi-confluent Heun equation as well as its limiting cases applied in the standard reference literature [70-72] and in numerous applications [77,117,118,133,135-140,141-149,150-153] are readily derived from this form by simple specifications of the involved parameters.

Based on the experience gained in solving the Schrödinger equation for the three-parametric inverse square root potential [137] and its four-parametric conditionally exactly solvable generalization [138], we consider the following expansion of the solution of the bi-confluent Heun equation (102) in terms of the Hermite functions of a shifted and scaled argument:

$$u = \sum_n c_n u_n, \quad (103)$$

$$u_n = H_{\alpha_0+n}(s_0(z+z_0)), \quad (104)$$

where  $\alpha_0, s_0$  and  $z_0$  are complex constants to be defined afterwards. We note that in general the index parameter  $\alpha_0$  is not an integer so that the expansion functions are not reduced to quasi-polynomials.

The Hermite functions satisfy the following second-order linear differential equation:

$$\frac{d^2u_n}{dz^2} - 2s_0^2(z+z_0) \frac{du_n}{dz} + 2s_0^2 \alpha_n u_n = 0, \quad \alpha_n = \alpha_0 + n. \quad (105)$$

Substituting (104) and (105) into equation (102) and multiplying the result by  $z$  we obtain

$$\sum_n c_n \left[ (\gamma + z(\delta + \varepsilon z) + 2s_0^2 z(z + z_0)) u'_n + (\alpha z - q - 2s_0^2 \alpha_n z) u_n \right] = 0. \quad (106)$$

This equation is considerably simplified if we put  $2s_0^2 = -\varepsilon$  and  $2s_0^2 z_0 = -\delta$ , that is

$$s_0 = \pm \sqrt{-\varepsilon/2}, \quad z_0 = \delta/\varepsilon. \quad (107)$$

This choice cancels the terms proportional to  $z u'_n$  and  $z^2 u'_n$  so that using the recurrence identities

$$u'_n = 2s_0 \alpha_n u_{n-1} \quad (108)$$

and

$$s_0(z + z_0)u_n = \alpha_n u_{n-1} + u_{n+1}/2, \quad (109)$$

we straightforwardly arrive at a three-term recurrence relation for coefficients  $c_n$ :

$$R_n c_n + Q_{n-1} c_{n-1} + P_{n-2} c_{n-2} = 0 \quad (110)$$

with

$$R_n = \frac{\sqrt{2}}{\sqrt{-\varepsilon}} (\alpha_0 + n) (\alpha + (\alpha_0 + n - \gamma) \varepsilon), \quad (111)$$

$$Q_n = \frac{\alpha \delta + (q + (\alpha_0 + n) \delta) \varepsilon}{\varepsilon}, \quad (112)$$

$$P_n = \frac{\alpha + (\alpha_0 + n) \varepsilon}{\sqrt{-2\varepsilon}}, \quad (113)$$

where the signs  $\mp$  in the equation for  $Q_n$  refer to the choices  $s_0 = \pm \sqrt{-\varepsilon/2}$ , respectively.

For the left-hand side termination of the series at  $n=0$ , applying the initial conditions  $c_{-2} = c_{-1} = 0$ ,  $c_0 \neq 0$ , we get  $R_0 = 0$ . This condition is satisfied if  $\alpha_0 = 0$  or  $\alpha_0 = \gamma - \alpha/\varepsilon$ . The first choice  $\alpha_0 = 0$  leads to the known polynomial solutions [70], hence, we discuss the second choice  $\alpha_0 = \gamma - \alpha/\varepsilon$  which is applicable for non-zero  $\varepsilon$ . The summation index  $n$  in expansion (104) then runs from zero to infinity and thus the final expansion is written as

$$u = \sum_{n=0}^{\infty} c_n H_{n+\gamma-\alpha/\varepsilon} \left( \pm \sqrt{-\varepsilon/2} (z + \delta/\varepsilon) \right). \quad (114)$$

We note that by choosing here different signs for the argument of the involved Hermite functions we get in general different independent solutions of the bi-confluent Heun equation (102) under consideration. Hence, by taking a linear combination, with arbitrary constant coefficients, of the two expansions corresponding to the plus and minus signs, we get an expansion for the general solution of equation (102).



### 3.2.2 Termination conditions

The developed series may terminate from the right-hand side thus resulting in closed-form finite-sum solutions. This happens if two successive coefficients vanish for some  $n = N = 0, 1, 2, \dots$ , i.e., if  $c_{N+1} = c_{N+2} = 0$  while  $c_N \neq 0$ . From equation  $c_{N+2} = 0$  we find that the termination is possible if  $P_N = 0$ . This condition is satisfied if  $\gamma = -N$ . Since  $\varepsilon$  is non-zero, the remaining equation  $c_{N+1} = 0$  then presents a polynomial equation of the degree  $N+1$  for the accessory parameter  $q$  (we refer to this equation as  $q$ -equation), which defines, in general,  $N+1$  values of  $q$  for which the termination of the series occurs. To be specific, here are these equations for  $N = 0, 1$  and 2:

$$\gamma = 0: \quad q = 0. \quad (115)$$

$$\gamma = -1: \quad q^2 - \delta q + \alpha = 0. \quad (116)$$

$$\gamma = -2: \quad q^3 - 3\delta q^2 + 2(\delta^2 + \varepsilon + 2\alpha)q - 4\alpha\delta = 0. \quad (117)$$

There are many physical situations when these equations are satisfied for a particular problem at hand. To demonstrate this, we apply the developed series to the two-level problem (see below section 3.3) and to the one-dimensional stationary Schrodinger equation (Chapter 4 of this thesis).

### 3.2.3 Discussion

Thus, we have constructed an expansion of the general solution of the bi-confluent Heun equation in terms of the Hermite functions of a shifted and scaled argument. The expansion functions are in general of non-integer order so that they in general are not quasi-polynomials. The expansion applies for arbitrary sets of the involved parameters (with the proviso  $\varepsilon \neq 0$ ). The coefficients of the expansion obey a three-term recurrence relation between the successive coefficients. We have shown that the constructed series may terminate thus resulting in closed-form solutions of the bi-confluent Heun equation involving a finite number of the Hermite functions. The restrictions imposed on the involved parameters in order that the series allow termination are: i) the characteristic (Frobenius) exponent  $\mu = 1 - \gamma$  of the regular singularity in the origin  $z = 0$  should be a positive integer (this is achieved if  $\gamma = -N$  with  $N = 0, 1, 2, \dots$ ) and ii) the accessory parameter  $q$  should obey a polynomial equation of the degree  $N+1$  ( $q$ -equation). The resultant solution of the bi-confluent Heun equation then presents a linear combination of  $N+1$  Hermite functions of a shifted and scaled argument presented above. This is a main result of the present section.

We have presented the explicit  $q$ -equations for the accessory parameter for  $N = 0, 1, 2$ . Furthermore, when discussing a particular application to the one-dimensional Schrödinger equation

in Chapter 4, we will also present the  $q$ -equation for  $N = 3$ . This is a representative example of higher-order termination resulting in a solution written as a linear combination of four Hermite functions.

Taking finally a general look at the presented results, we find that, apart from the very expansion that we have presented, a general message of the present development is that the expansions of the Heun functions in terms of advanced special functions rather than simple powers suggest a quite productive approach. In particular, the expansion of the bi-confluent Heun function in terms of the Hermite functions allows construction of closed-form finite-sum non-polynomial solutions.

It is well understood that the conclusion is general and applies also to other problems such as, e.g., the relativistic evolution governed by the Dirac or the Klein-Gordon equations. Supporting this statement are the applications of the recent expansions of the solutions of the single-confluent Heun equation in terms of the Kummer confluent hypergeometric [79], the incomplete Beta and the Appell generalized hypergeometric [134] functions to the quantum two-state problem [75,76].

Expansions of the solutions of the Heun equations in terms of more advanced functions instead of simple powers have been initiated by Svartholm [88] and Erdélyi [90] who proposed series expansions of the general Heun functions in terms of the Gauss hypergeometric functions. This is a useful extension of the series technique applicable to many other differential equations including those of more general type such as the five *deformed* Heun equations which are the Heun equations with an additional *apparent* singularity [133]. As already stated above, a useful property suggested by these expansions is the possibility to derive finite-sum solutions by means of termination of the series. However, it should be noted that the infinite series themselves are also of notable interest as it is the case of the expansions of the general Heun functions in terms of the incomplete Beta functions applied to the surface plasmon-polariton problem [97]. The general conclusion is then that there is a pronounced need to explore the variety of all possible expansions of the Heun functions in terms of the functions of the hypergeometric class which currently form the most developed and most familiar set of special functions. Because of the enormous number of appearances of the Heun equations in contemporary classical and non-classical science one may envisage many important applications of these expansions.

### 3.3 Inverse square root level-crossing two-state model

In the present section, we discuss the exact and conditionally integrable models of the two-state problem using the above-presented expansion (114) of the solutions of the bi-confluent Heun

equation in terms of the Hermite functions. We introduce an exactly integrable model generated by termination of the expansion on the second term - the inverse square root level-crossing model.

As we have seen in **Section 3.2.2**, the termination of the series (114) imposes two restrictions on the parameters of the involved bi-confluent Heun function (e.g., equations (115)-(117)). One of these restrictions is imposed on a characteristic exponent of the finite singularity of the bi-confluent Heun equation, while the second one presents a polynomial equation for the accessory parameter ( $q$ -equation). As it was in the case of the Kummer-function expansions of the single-confluent Heun function (**Section 2.4**), here also the condition imposed on a characteristic exponent generally leads to conditionally integrable models. However, like in the case of the single-confluent Heun function, there are four remarkable exceptions resulting in exactly solvable models. The first three of these cases again reproduce the known models by Landau-Zener, Nikitin and Crothers-Hughes (see [120]), while the fourth one presents a new result. In this case the detuning function behaves as the inverse square root function at the origin and goes to a constant detuning at infinity.

To present the details, following the lines of **Section 2.4**, we start with the termination condition for series given by equation

$$\gamma = -N, \quad (118)$$

which is a restriction imposed on the characteristic exponent of the singularity of the bi-confluent Heun equation located at the origin  $z = 0$ . With this condition, we examine the equations for the exponent  $\alpha_1$  of the pre-factor  $\varphi(z)$  of the solution (46), that is, the first equation (47) and equation (51):

$$\gamma = 2\alpha_1 - i\delta_1 - k, \quad (119)$$

$$\alpha_1^2 - \alpha_1(1 + k + i\delta_1) + Q(0) = 0, \quad (120)$$

Excluding  $\alpha_1$ , we have the equation

$$(\gamma + k + i\delta_1)(\gamma - k - 2 - i\delta_1) = -4Q(0). \quad (121)$$

The function  $Q(z) = U_0^{*2} z^{2k+2}$  depends only on the amplitude parameter  $U_0^*$ , hence,  $Q(0)$  is a function of  $U_0^*$  only. It is then understood that if  $\gamma$  is a fixed constant, we have an equation for which the left-hand side depends on the detuning parameter  $\delta_1$ , while the right-hand side depends on the amplitude parameter  $U_0^*$ . Thus, in general, the parameters  $\delta_1$  and  $U_0^*$  are not independent, they are related by equation (121). Hence, the models solvable in terms of linear combinations of the Hermite functions of shifted and scaled argument are in general *conditionally* integrable.

Exceptional are the cases for which both sides of equation (121) identically vanish. For these cases, from the condition  $Q(0)=0$ , should be  $k \neq -1$ . Besides, it follows from the remaining equation (121) that the detuning parameter  $\delta_1$  is either a fixed number or should vanish. In the first case one again obtains dissipative conditionally integrable models, while the second case, for which  $\delta_1 = 0$ , leads to *exactly* solvable models.

For the latter models, equation (121) reads

$$(\gamma + k)(\gamma - k - 2) = 0. \quad (122)$$

Since  $\gamma$  is a non-positive integer and  $k$  may adopt only four integer or half-integer values:  $k = -1/2, 0, 1/2, 1$  ( $k \neq -1$ ), we conclude that exactly solvable models are constructed only if  $\gamma = k = 0$  or  $\gamma = -1 \cup k = 1$ . The first case  $\gamma = 0$  is accompanied with the  $q$ -equation  $q = 0$ . This case is not of much interest because then the bi-confluent Heun equation directly reduces to the confluent hypergeometric equation and, as a result, one obtains the three known confluent hypergeometric models by Landau-Zener, Nikitin and Crothers-Hughes (see the details in [120]).

A new result is achieved if one considers the case when the series expansion in terms of the non-integer order Hermite functions of a scaled and shifted argument, of the bi-confluent Heun function involved in the solution (46) of the two-state problem, is terminated on the second term. In this case we have  $\gamma = -1$  and the second condition for termination of series (114) ( $q$ -equation) is given by equation (116):

$$q^2 - \delta q + \alpha = 0. \quad (123)$$

We recall that for exact solvability it additionally should be  $k = 1$  and  $\delta_1 = 0$ . From the first equation (47), we have  $\alpha_1 = 0$ . With this, it is readily checked that the  $q$ -equation is satisfied for all other parameters being arbitrary. Thus, we derive a new *three-parametric* class of exactly solvable bi-confluent-Heun two-state models:

$$U(t) = U_0^* \cdot z \frac{dz}{dt}, \quad \delta_i(t) = (\delta_0 + \delta_2 z) \frac{dz}{dt}. \quad (124)$$

By choosing the transformation of the independent variable as

$$z(t) = \sqrt{t}, \quad (125)$$

we arrive at the *constant-amplitude inverse square root* level-crossing model (Figure 9):

$$U(t) = U_0, \quad (126)$$

$$\delta_i(t) = \Delta_0 + \frac{\Delta_1}{\sqrt{t}}, \quad (127)$$

where we have put  $U_0^* = 2U_0$ ,  $\delta_0 = 2\Delta_1$ ,  $\delta_2 = 2\Delta_0$ .

It is readily checked that the two-state equation (5) for this field configuration admits a fundamental solution involving two Hermite functions written as

$$a_2^F(t) = c_0 e^{\alpha_0 z + \frac{\alpha_2}{2} z^2} (A H_{-\alpha/\varepsilon}(y) + H_{-\alpha/\varepsilon-1}(y)), \quad (128)$$

where

$$A = s \sqrt{\frac{-\varepsilon}{2}} \frac{\delta - q}{\alpha}, \quad y = s \sqrt{\frac{-\varepsilon}{2}} \left( z + \frac{\delta}{\varepsilon} \right), \quad (129)$$

$$\delta, \varepsilon, \alpha, q = 2(\alpha_0 - i\Delta_1), 2(\alpha_2 - i\Delta_0), \alpha_0(\alpha_0 - 2i\Delta_1), \alpha_0, \quad (130)$$

and

$$\alpha_0 = i\Delta_1 \left( 1 - \frac{\Delta_0}{\sqrt{4U_0^2 + \Delta_0^2}} \right), \quad \alpha_2 = i \left( \Delta_0 \sqrt{4U_0^2 + \Delta_0^2} \right). \quad (131)$$

Here the auxiliary parameter  $s$  may adopt values  $s = +1$  or  $s = -1$ . We note that each of these parameters produces a linearly independent fundamental solution. Also, any sign plus or minus is applicable for  $\alpha_{0,2}$ . For definiteness, we choose the *minus* sign for both alphas. Then, the general solution of the problem is written as ( $C_{1,2}$  are arbitrary constants.).

$$a_2(t) = C_1 a_2^F|_{s=-1} + C_2 a_2^F|_{s=+1}. \quad (132)$$

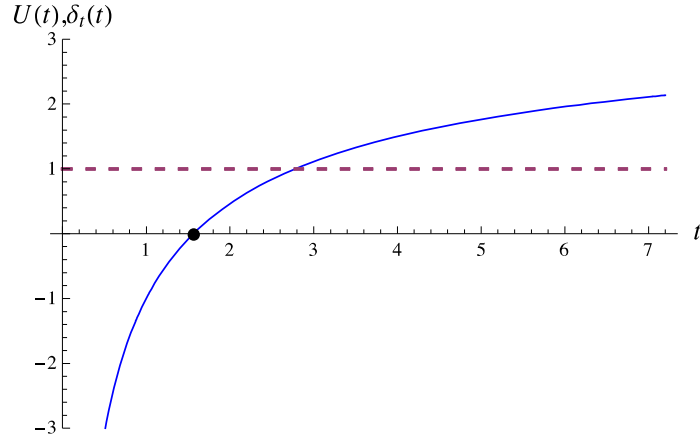


Fig. 9. Two-state level-crossing model (127). The dashed line is the Rabi frequency ( $U_0 = 1$ ) and the solid line present the detuning ( $\Delta_0 = 4, \Delta_1 = -5$ ). The filled circle indicates the level-crossing time point  $t_0 = -\Delta_1^2 / \Delta_0^2$ .

## Chapter 4

### APPLICATIONS TO NON-RELATIVISTIC AND RELATIVISTIC WAVE EQUATIONS

In the present chapter we consider some applications of the basic mathematical approaches developed in the previous chapters to the non-relativistic Schrödinger and relativistic Klein-Gordon-Fock wave equations. We first introduce the third *five-parametric* ordinary hypergeometric energy-independent quantum-mechanical potential for the Schrödinger equation and further derive a particular *conditionally integrable* potential for which the solution of the Schrödinger equation is written as a four-term expansion in terms of the Hermite functions of a scaled and shifted spatial argument. Finally, we present the nine independent potentials for which the stationary Klein-Gordon equation is solvable in terms of the confluent Heun functions. Because of the symmetry of the confluent Heun equation with respect to the transposition of its regular singularities, only nine of the potentials are independent. Four of these potentials are five-parametric and other five are four-parametric.

Methodologically, we follow the route for reduction of the problem to a target second-order ordinary differential equation having rational coefficients first developed for solving the quantum time-dependent two-state problem. The basic approach for construction of exactly integrable energy-independent quantum-mechanical potentials by transforming the dependent and independent variables rests on the observation that, if a potential is proportional to an energy-independent parameter and the potential shape is independent of both energy and that parameter, then the logarithmic derivative  $\rho'(z)/\rho(z)$  of the function  $\rho = z'(x)$ , where  $z = z(x)$  is the coordinate transformation, cannot have poles other than the finite singularities of the target equation. It then follows that the function  $\rho$  should necessarily be of the Manning form  $\rho(z) = \prod_i (z - z_i)^{A_i}$  with  $z_i$  being the finite singularities of the target equation and the exponents  $A_i$  all being integers or half-integers.

The solutions of the Schrödinger equation for both potentials we present is derived via termination of series expansions of the Heun functions in terms of the functions belonging to the hypergeometric class. The general solution of the problem is composed of fundamental solutions each of which can be written as an *irreducible* linear combination of two hypergeometric functions. We note that owing to the contiguous functions relations, this two-term structure of the solution is a general property of all finite-sum hypergeometric reductions of the Heun functions achieved via termination of series solutions.

#### 4.1 The third five-parametric hypergeometric quantum-mechanical potential

The solutions of the Schrödinger equation in terms of special functions for energy-independent potentials which are proportional to an arbitrary variable parameter and have a shape independent of that parameter are very rare [137,154,155,157,161-167] (see the discussion in [156]). It is a common convention to refer to such potentials as *exactly* solvable in order to distinguish them from the *conditionally* integrable ones for which a condition is imposed on the potential parameters such that the shape of the potential is not independent of the potential strength (e.g., a parameter is fixed to a constant or different term-strengths are not varied independently). While there is a relatively large set of potentials of the latter type (see, e.g., [158-160,168-175] for some examples discussed in the past, and [138,176-181] for some recent examples), the list of the known exactly integrable potentials is rather limited even for the potentials of the most flexible *hypergeometric* class. The list of the exactly solvable hypergeometric potentials currently involves only ten items. Six of these potentials are solved in terms of the confluent hypergeometric functions [137,154,157,161-163]. These are the harmonic oscillator [157], Coulomb [161] and Morse [163] classical potentials and the three recently derived potentials, which are the inverse square root [137], the Lambert-W step [154] and Lambert-W singular [164] potentials. The other four exactly integrable potentials which are solved in terms of the Gauss hypergeometric functions are the Eckart [165] and Pöschl-Teller [166] potentials and the two new potentials introduced recently [155,167].

An observation here is that all five classical hypergeometric potentials, both confluent and ordinary, involve *five* arbitrary variable parameters, while all new potentials are four-parametric. In this communication, following our work [84], we show that the two four-parametric ordinary hypergeometric potentials [155,167] are in fact particular cases of a more general five-parametric potential which is solved in terms of the hypergeometric functions. This generalization thus suggests the third five-parametric ordinary hypergeometric quantum-mechanical potential after the ones by Eckart [165] and Pöschl-Teller [166].

The potential we introduce belongs to one of the eleven independent eight-parametric general Heun families [181] (see also [117]). From the mathematical point of view, a peculiarity of the potential is that this is the only known case when the location of a singularity of the equation to which the Schrödinger equation is reduced is not fixed to a particular point but stands for a variable potential-parameter. Precisely, in our case the third finite singularity of the Heun equation, that located at a point  $z = a$  of the complex  $z$ -plane (that is the singularity which is additional if compared with the ordinary hypergeometric equation), is not fixed but is variable – it stands for the fifth free parameter of the potential.

The potential is in general defined parametrically as a pair of functions  $V(z), x(z)$ . However, in several cases the coordinate transformation  $x(z)$  is inverted thus producing explicitly written potentials given as  $V = V(z(x))$  through an elementary function  $z = z(x)$ . All these cases are achieved by fixing the parameter  $a$  to a particular value, hence, all these particular potentials are four-parametric. The mentioned two recently presented four-parametric ordinary hypergeometric potentials [155,167] are just such cases.

The potential we present is either a singular well (which behaves as the inverse square root in the vicinity of the origin and exponentially vanishes at infinity) or a smooth asymmetric step-barrier (with variable height, steepness, and asymmetry). The general solution of the Schrödinger equation for this potential is written through fundamental solutions each of which presents an irreducible linear combination of two ordinary hypergeometric functions  ${}_2F_1$ . The singular version of the potential describes a short-range interaction and for this reason supports only a finite number of bound states. We derive the exact equation for energy spectrum and estimate the number of bound states.

#### 4.1.1 The potential

The potential is given parametrically as

$$V(z) = V_0 + \frac{V_1}{z}, \quad (1)$$

$$x(z) = x_0 + \sigma(a \ln(z-a) - \ln(z-1)), \quad (2)$$

where  $a \neq 0,1$  and  $x_0, \sigma, V_0, V_1$  are arbitrary (real or complex) constants. Rewriting the coordinate transformation as

$$\frac{(z-a)^a}{z-1} = e^{\frac{x-x_0}{\sigma}}, \quad (3)$$

it is seen that for real rational  $a$  the transformation is rewritten as a polynomial equation for  $z$ , hence, in several cases it can be inverted.

Since  $a \neq 0,1$ , the possible simplest case is if the polynomial equation is quadratic. This is achieved for  $a = -1, 1/2, 2$ . It is checked, however, that these three cases lead to four-parametric sub-potentials which are equivalent in the sense that each is derived from another by specifications of the involved parameters. For  $a = -1$  the potential reads [155]:

$$V(x) = V_0 + \frac{V_1}{\sqrt{1 + e^{(x-x_0)/\sigma}}}, \quad (4)$$

where we have changed  $\sigma \rightarrow -\sigma$ .



The next are the cubic polynomial reductions which are achieved in six cases:  $a = -2, -1/2, 1/3, 2/3, 3/2, 3$ . It is again checked, however, that these choices produce only one independent potential. This is the four-parametric potential presented in [167]:

$$V = V_0 + \frac{V_1}{z}, \quad (5)$$

$$z = -1 + \frac{1}{\left(e^{x/(2\sigma)} + \sqrt{1+e^{x/\sigma}}\right)^{2/3} + \left(e^{x/(2\sigma)} + \sqrt{1+e^{x/\sigma}}\right)^{2/3}}, \quad (6)$$

where one should replace  $x$  by  $x - x_0$ . Similar potentials in terms of elementary functions through quartic and quintic reductions of equation (3) are rather cumbersome; we omit those.

For arbitrary real  $a \neq 0, 1$ , assuming  $z \in (0, 1)$  and shifting

$$x_0 \rightarrow x_0 - \sigma a \ln(-a) + i\pi\sigma, \quad (7)$$

the potential (1),(2) presents a singular well. In the vicinity of the origin it behaves as  $x^{-1/2}$ :

$$V|_{x \rightarrow 0} \sim \sqrt{\frac{(a-1)\sigma}{2a}} \frac{V_1}{\sqrt{x}}, \quad (8)$$

and exponentially approaches a constant,  $V_0 + V_1$ , at infinity:

$$V|_{x \rightarrow +\infty} \sim \left(\frac{a-1}{a}\right)^a V_1 e^{-x/\sigma}, \quad (9)$$

The potential and the two asymptotes are shown in Fig. 1.

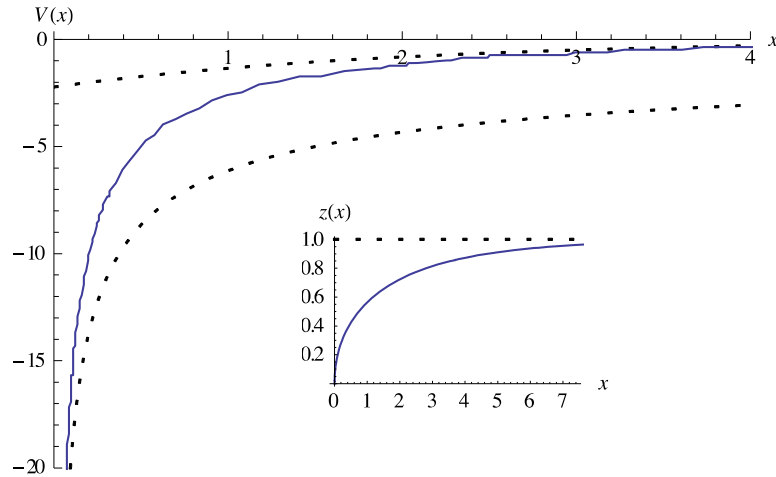


Fig.1. Potential (1), (2) for  $a = -2$  and  $(\sigma, x_0, V_0, V_1) = (2, 0, 5, -5)$ . The inset presents the coordinate transformation  $z(x) \in (0, 1)$  for  $x \in (0, \infty)$ .

A potential of a different type is constructed if one allows the parameterization variable  $z$  to vary within the interval  $z \in (1, \infty)$  for  $a < 1$  or within the interval  $z \in (1, a)$  for  $a > 1$ . This time, shifting (compare with Eq. (7))

$$x_0 \rightarrow x_0 - \sigma a \ln(1 - a), \quad (10)$$

we derive an asymmetric step-barrier the height of which depends on  $V_0$  and  $V_1$ , while the asymmetry and steepness are controlled by the parameters  $a$  and  $\sigma$ . The shape of the potential is shown in Fig. 2 for  $a = -2$  and  $a = 1.25$ . We note that in the limit  $\sigma \rightarrow 0$  the potential turns into the abrupt-step potential and that the sub-family of barriers generated by variation of  $\sigma$  at constant  $V_0$  and  $V_1$  has a  $\sigma$ -independent fixed point located at  $x = x_0$  (marked in Fig. 2 by filled circles).

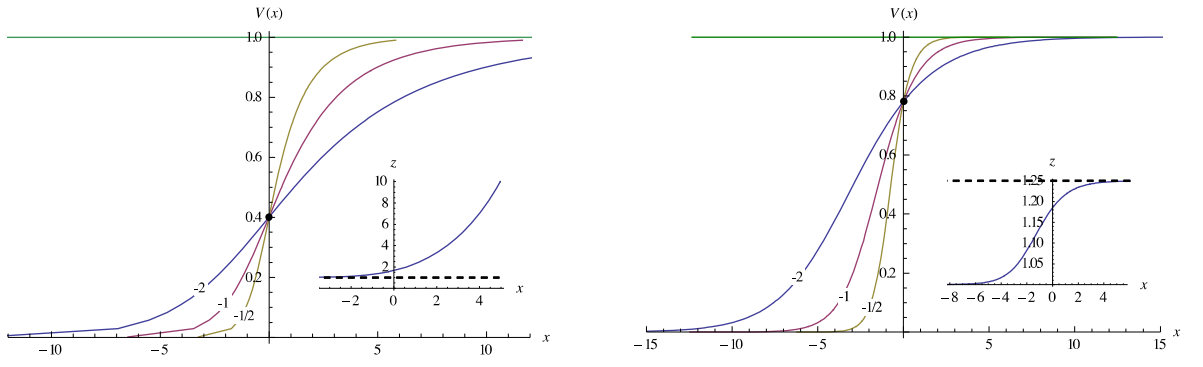


Fig.2. Potential (1),(2) for  $a = -2$  and  $(x_0, V_0, V_1) = (0, 1, -1)$  (left figure) and for  $a = 1.25$  and  $(x_0, V_0, V_1) = (0, 5, -5)$  (right figure);  $\sigma = -2, -1, -1/2$ . The fixed points are marked by filled circles. The insets present the coordinate transformation  $z(x)$  for  $\sigma = -1$ .

#### 4.1.2 Reduction to the general Heun equation

The solution of the one-dimensional Schrödinger equation for potential (1),(2):

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2} (E - V(x))\psi = 0, \quad (11)$$

is constructed via reduction to the general Heun equation in its most general form [70-72]

$$\frac{d^2u}{dz^2} + \left( \frac{\gamma}{z - a_1} + \frac{\delta}{z - a_2} + \frac{\varepsilon}{z - a_3} \right) \frac{du}{dz} + \frac{\alpha\beta z - q}{(z - a_1)(z - a_2)(z - a_3)} u = 0. \quad (12)$$

The details of the technique are presented in [156] and [181]. It has been shown that the energy-independent general-Heun potentials, which are proportional to an arbitrary variable parameter and have shapes which are independent of that parameter, are constructed by the coordinate transformation  $z = z(x)$  of the Manning form [182] given as

$$\frac{dz}{dx} = (z - a_1)^{m_1} (z - a_2)^{m_2} (z - a_3)^{m_3} / \sigma, \quad (13)$$

where  $m_{1,2,3}$  are integers or half-integers and  $\sigma$  is an arbitrary scaling constant. As it is seen, the coordinate transformation is solely defined by the singularities  $a_{1,2,3}$  of the general Heun equation. The canonical form of the Heun equation assumes two of the three finite singularities at 0 and 1, and the third one at a point  $a$ , so that  $a_{1,2,3} = (0, 1, a)$  [70-72]. However, it may be convenient for practical purposes to apply a different specification of the singularities, so for a moment we keep the parameters  $a_{1,2,3}$  unspecified.

The coordinate transformation is followed by the change of the dependent variable

$$\psi = (z - a_1)^{\alpha_1} (z - a_2)^{\alpha_2} (z - a_3)^{\alpha_3} u(z) \quad (14)$$

and application of the ansatz

$$V(z) = \frac{v_0 + v_1 z + v_2 z^2 + v_3 z^3 + v_4 z^4}{(z - a_1)^2 (z - a_2)^2 (z - a_3)^2} \left( \frac{dz}{dx} \right)^2, \quad v_{0,1,2,3,4} = \text{const}. \quad (15)$$

The form of this ansatz and the permissible sets of the parameters  $m_{1,2,3}$  are revealed through the analysis of the behavior of the solution in the vicinity of the finite singularities of the general Heun equation [156]. This is a crucial point which warrants that all the parameters involved in the resulting potentials can be varied independently.

It has been shown that there exist in total thirty-five permissible choices for the coordinate transformation each being defined by a triad  $(m_1, m_2, m_3)$  satisfying the inequalities  $-1 \leq m_{1,2,3} \leq 1$  and  $1 \leq m_1 + m_2 + m_3 \leq 3$  [181]. However, because of the symmetry of the general Heun equation with respect to the transpositions of its singularities, only eleven of the resultant potentials are independent [181]. The potential (1),(2) belongs to the fifth independent family with  $m_{1,2,3} = (1, 1, -1)$  for which from equation (15) we have

$$V(z) = \frac{V_4 + V_3 z + V_2 z^2 + V_1 z^3 + V_0 z^4}{(z - a_3)^4} \quad (16)$$

with arbitrary  $V_{0,1,2,3,4} = \text{const}$ , and, from equation (13),

$$\frac{x - x_0}{\sigma} = \frac{a_1 - a_3}{a_1 - a_2} \ln(z - a_1) + \frac{a_3 - a_2}{a_1 - a_2} \ln(z - a_2). \quad (17)$$

It is now convenient to have a potential which does not explicitly involve the singularities. Hence, we put  $a_3 = 0$  and apply the specification  $a_{1,2,3} = (a, 1, 0)$  to derive the potential

$$V(z) = V_0 + \frac{V_1}{z} + \frac{V_2}{z^2} + \frac{V_3}{z^3} + \frac{V_4}{z^4} \quad (18)$$

with 
$$\frac{x-x_0}{\sigma/(a-1)} = a \ln(z-a) - \ln(z-1). \quad (19)$$

The solution of the Schrödinger equation (11) for this potential is written in terms of the general Heun function  $H_G$  as

$$\psi = (z-a)^{\alpha_1} z^{\alpha_2} (z-1)^{\alpha_3} H_G(a_1, a_2, a_3; q; \alpha, \beta, \gamma, \delta, \varepsilon; z), \quad (20)$$

where the involved parameters  $\alpha, \beta, \gamma, \delta, \varepsilon$  and  $q$  are given through the parameters  $V_{0,1,2,3,4}$  of the potential (18) and the exponents  $\alpha_{1,2,3}$  of the pre-factor by the equations [181]

$$(\gamma, \delta, \varepsilon) = (1+2\alpha_1, 1+2\alpha_2, -1+2\alpha_3), \quad (21)$$

$$1 + \alpha + \beta = \gamma + \delta + \varepsilon, \quad (22)$$

$$\alpha\beta = (\alpha_1 + \alpha_2 + \alpha_3)^2 + 2m\sigma^2 (E - V_0) / \hbar^2, \quad (23)$$

$$q = \frac{2m\sigma^2}{\hbar^2} (V_1 - (1+a)(E - V_0)) + (-\alpha_2^2 + (-1 + \alpha_1 + \alpha_3)(\alpha_1 + \alpha_3)) + a(-\alpha_1^2 + (-1 + \alpha_2 + \alpha_3)(\alpha_2 + \alpha_3)); \quad (24)$$

the exponents  $\alpha_{1,2,3}$  of the pre-factor being defined by the equations

$$\alpha_1^2 = \frac{2m\sigma^2}{a^2(a-1)^2\hbar^2} (V_4 + aV_3 + a^2V_2 + a^3V_1 + a^4(V_0 - E)), \quad (25)$$

$$\alpha_2^2 = -\frac{2m\sigma^2}{(a-1)^2\hbar^2} (E - V_0 - V_1 - V_2 - V_3 - V_4), \quad (26)$$

$$\alpha_3(\alpha_3 - 2) = \frac{2m\sigma^2 V_4}{a^2\hbar^2}. \quad (27)$$

#### 4.1.3 The solution of the Schrödinger equation in terms of the Gauss functions

Having determined the parameters of the Heun equation, the next step is to examine the cases when the general Heun function  $H_G$  is written in terms of the Gauss hypergeometric functions  ${}_2F_1$ . An observation here is that the direct one-term Heun-to-hypergeometric reductions discussed by many authors (see, e.g., [70,71,183-186]) are achieved by such restrictions, imposed on the involved parameters (three or more conditions), which are either not satisfied by the Heun potentials or produce very restrictive potentials. It is checked that the less restrictive reductions reproduce the classical Eckart and Pöschl-Teller potentials, while the other reductions result in conditionally integrable potentials.

More advanced are the finite-sum solutions achieved by termination of the series expansions of the general Heun function in terms of the hypergeometric functions [88-90,92-94]. For such

reductions, only two restrictions are imposed on the involved parameters and, notably, these restrictions are such that in many cases they are satisfied. The solutions for the above-mentioned four-parametric sub-potentials [155,167] have been constructed right in this way. Other examples achieved by termination of the hypergeometric series expansions of the functions of the Heun class include the recently reported inverse square root [137], Lambert-W step [154] and Lambert-W singular [164] potentials.

The series expansions of the general Heun function in terms of the Gauss ordinary hypergeometric functions are governed by three-term recurrence relations for the coefficients of the successive terms of the expansion. A useful particular expansion in terms of the functions of the form  ${}_2F_1(\alpha, \beta; \gamma_0 - n; z)$  which leads to simpler coefficients of the recurrence relation is presented in [94]. If the expansion functions are assumed irreducible to simpler functions, the termination of this series occurs if  $\varepsilon = -N$ ,  $n = 0, 1, 2, \dots$ , and a  $(N + 1)$ -th degree polynomial equation for the accessory parameter  $q$  is satisfied. For  $\varepsilon = 0$  the latter equation is  $q = a\alpha\beta$ , which corresponds to the trivial direct reduction of the general Heun equation to the Gauss hypergeometric equation. This case reproduces the classical Eckart and Pöschl-Teller potentials [181]. For the first nontrivial case  $\varepsilon = -1$  the termination condition for singularities  $a_{1,2,3} = (a, 1, 0)$  takes a particularly simple form:

$$q^2 + q(\gamma - 1 + a(\delta - 1)) + a\alpha\beta = 0. \quad (28)$$

The solution of the Heun equation for a root of this equation is written as [94]

$$u = {}_2F_1\left(\alpha, \beta; \gamma; \frac{a-z}{a-1}\right) + \frac{\gamma-1}{q+a(\delta-1)} \cdot {}_2F_1\left(\alpha, \beta; \gamma-1; \frac{a-z}{a-1}\right), \quad (29)$$

This solution has a representation through Clausen's generalized hypergeometric function  ${}_3F_2$  [187,188].

Consider if the termination condition (28) for  $\varepsilon = -1$  is satisfied for the parameters given by equations (21)-(27). From the last equation (21) we find that for  $\varepsilon = -1$  holds  $\alpha_3 = 0$ . It then follows from Eq. (27) that  $V_4 = 0$ . With this, equation Eq. (28) is reduced to

$$V_2 + V_3 \left( \frac{1+a}{a} - \frac{2m\sigma^2}{a^2\hbar^2} V_3 \right) = 0. \quad (30)$$

This equation generally defines a conditionally integrable potential in that the potential parameters  $V_2$  and  $V_3$  are not varied independently. Alternatively, if the potential parameters are assumed independent, the equation is satisfied only if  $V_2 = V_3 = 0$ . Thus, we put  $V_{2,3,4} = 0$  and potential (18) is reduced to that given by equation (1). Furthermore, since  $\sigma$  is arbitrary, in order for equation (19) to exactly reproduce the coordinate transformation (2), we replace  $\sigma / (1-a) \rightarrow \sigma$ .

With this, the solution of the Schrödinger equation (11) for potential (1) is written as

$$\psi = (z-a)^{\alpha_1} (z-1)^{\alpha_2} \left( {}_2F_1\left(\alpha, \beta; \gamma; \frac{a-z}{a-1}\right) + \frac{2\alpha_1}{a\alpha_2 - \alpha_1} \cdot {}_2F_1\left(\alpha, \beta; \gamma-1; \frac{a-z}{a-1}\right) \right) \quad (31)$$

with

$$(\alpha, \beta, \gamma) = (\alpha_1 + \alpha_2 + \alpha_0, \alpha_1 + \alpha_2 - \alpha_0, 1 + 2\alpha_1), \quad (32)$$

$$\alpha_{0,1,2} = \left( \pm \sqrt{\frac{2m\sigma^2(a-1)^2}{\hbar^2}(V_0 - E)}, \pm \sqrt{\frac{2m\sigma^2 a^2}{\hbar^2}\left(V_0 - E + \frac{V_1}{a}\right)}, \pm \sqrt{\frac{2m\sigma^2}{\hbar^2}(V_0 - E + V_1)} \right). \quad (33)$$

This solution applies for any real or complex set of the involved parameters. Furthermore, we note that any combination for the signs of  $\alpha_{1,2}$  is applicable. Hence, by choosing different combinations, one can construct different independent fundamental solutions. Thus, this solution supports the general solution of the Schrödinger equation.

A final remark is that using the contiguous functions relations for the hypergeometric functions one can replace the second hypergeometric function in Eq. (31) by a linear combination of the first hypergeometric function and its derivative. In this way we arrive at the following representation of the general solution of the Schrödinger equation:

$$\psi = (z-a)^{\alpha_1} (z-1)^{\alpha_2} \left( F + \frac{z-a}{\alpha_1 + a\alpha_2} \frac{dF}{dz} \right), \quad (34)$$

where

$$F = c_1 \cdot {}_2F_1\left(\alpha, \beta; \gamma; \frac{a-z}{a-1}\right) + c_2 \cdot {}_2F_1\left(\alpha, \beta; 1 + \alpha + \beta - \gamma; \frac{z-1}{a-1}\right). \quad (35)$$

#### 4.1.4 Bound states

Consider the bound states supported by the singular version of potential (1),(2), achieved by shifting  $x_0 \rightarrow x_0 - \sigma a \ln(-a) + i\pi\sigma$  in Eq. (2). Since the potential vanishes at infinity exponentially, it is understood that this is a short-range potential. The integral of the function  $xV(x)$  over the semi-axis  $x \in (0, +\infty)$  is finite, hence, according to the general criterion [189-193], the potential supports only a finite number of bound states. These states are derived by demanding the wave function to vanish both at infinity and in the origin (see the discussion in [194]). We recall that for this potential the coordinate transformation maps the interval  $x \in (0, +\infty)$  onto the interval  $z \in (0, 1)$ . Thus, we demand  $\psi(z=0) = \psi(z=1) = 0$ .

The condition  $V(+\infty) = 0$  assumes  $V_0 + V_1 = 0$ , hence,  $\alpha_2$  is real for negative energy. Choosing, for definiteness, the plus signs in Eq. (33), we have  $\alpha_2 > 0$ . Then, examining the equation  $\psi(z=1) = 0$ , we find that

$$\psi|_{z \rightarrow 1} \sim c_1 A_1 (1-z)^{-\alpha_2} + c_2 A_2 (1-z)^{\alpha_2} \quad (36)$$

with some constants  $A_{1,2}$ . Since for positive  $\alpha_2$  the first term diverges, we conclude  $c_1 = 0$ . The condition  $\psi(z=0) = 0$  then gives the following exact equation for the spectrum:

$$S(E) \equiv 1 + \frac{\alpha_1 + a\alpha_2}{2(1-a)\alpha_2} \frac{{}_2F_1\left(\alpha+1, \beta+1; 1+2\alpha_2; \frac{1}{1-a}\right)}{{}_2F_1\left(\alpha, \beta; 2\alpha_2; \frac{1}{1-a}\right)} = 0. \quad (37)$$

The graphical representation of this equation is shown in Fig. 3. The function  $S(E)$  has a finite number of zeros. For the parameters  $m, \hbar, V_0, \sigma, a = 1, 1, 5, 2, -2$  applied in the figure there are just three bound states.

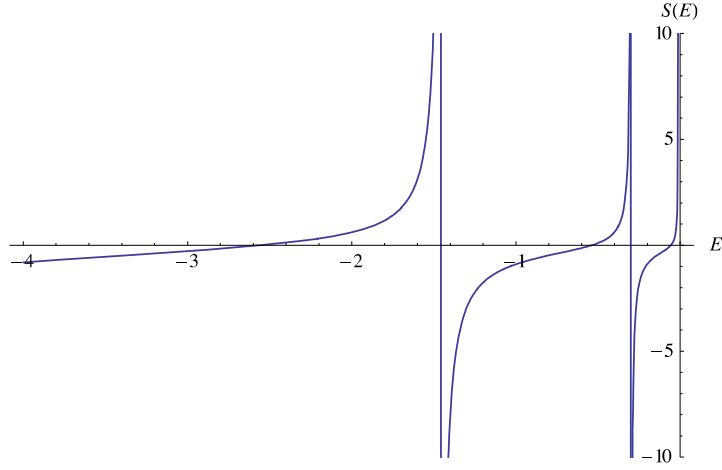


Fig.3. Graphical representation of the spectrum equation (37) for  $m, \hbar, V_0, \sigma, a = 1, 1, 5, 2, -2$ .

According to the general theory, the number of bound states is equal to the number of zeros (not counting  $x=0$ ) of the zero-energy solution, which vanishes at the origin [189-193]. We note that for  $E=0$  the lower parameter of the second hypergeometric function in Eq. (35) vanishes:  $1 + \alpha + \beta - \gamma = 0$ . Hence, a different second independent solution should be applied. This solution is constructed by using the first hypergeometric function with  $\alpha_1$  everywhere replaced by  $-\alpha_1$ . The result is rather cumbersome. It is more conveniently written in terms of the Clausen functions as

$$\begin{aligned} \psi_{E=0} = & c_1 (z-a)^{\alpha_1} {}_3F_2\left(-\sqrt{\frac{a-1}{a}}\alpha_1 + \alpha_1, \sqrt{\frac{a-1}{a}}\alpha_1 + \alpha_1, 1 + \alpha_1; \alpha_1, 1 + 2\alpha_1; \frac{a-z}{a-1}\right) + \\ & c_2 (z-a)^{-\alpha_1} {}_3F_2\left(-\sqrt{\frac{a-1}{a}}\alpha_1 - \alpha_1, \sqrt{\frac{a-1}{a}}\alpha_1 - \alpha_1, 1 - \frac{\alpha_1}{a}; -\frac{\alpha_1}{a}, 1; \frac{z-1}{a-1}\right), \end{aligned} \quad (38)$$

where  $\alpha_1 = \sqrt{2a(a-1)m\sigma^2V_0/\hbar^2}$  and the relation between  $c_1$  and  $c_2$  is readily derived from the condition  $\psi_{E=0}(0) = 0$ . This solution is shown in Fig. 4. It is seen that for parameters  $m, \hbar, V_0, \sigma, a = 1, 1, 5, 2, -2$  used in Fig. 3 the number of zeros (excluded the origin) is indeed 3.

For practical purposes, it is useful to have an estimate for the number of bound states. The absolute upper limit for this number is given by the integral [189,190]

$$I_B = \int_0^{\infty} r |V(x \rightarrow r\hbar/\sqrt{2m})| dr = (1-a) \left( Li_2\left(\frac{1}{1-a}\right) + 2a \coth^{-1}(1-2a)^2 \right) \frac{2m\sigma^2V_0}{\hbar^2}. \quad (39)$$

where  $Li_2$  is Jonquière's polylogarithm function of order 2 [195,196]. Though of general importance, however, in many cases this is a rather overestimating limit. Indeed, for the parameters applied in Fig. 3 it gives  $n \leq I_B \approx 24$ .

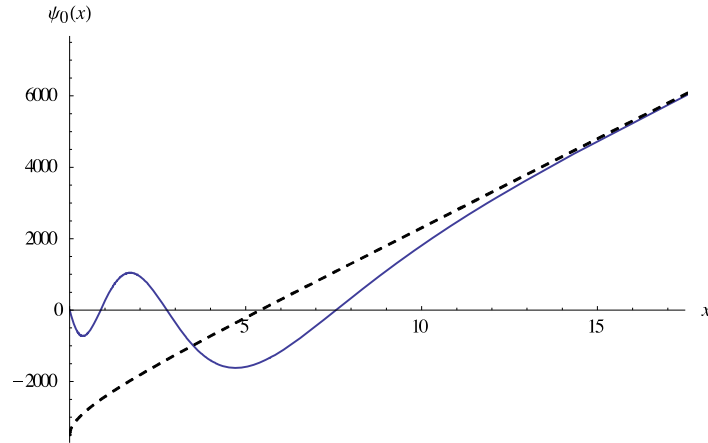


Fig.4. The zero-energy solution for  $m, \hbar, V_0, \sigma, a = 1, 1, 5, 2, -2$ . The dashed line shows the logarithmic asymptote at infinity:  $\psi_0|_{x \rightarrow \infty} \sim A + B \ln(1-z)$ .

More stringent are the estimates by Calogero [191] and Chadan [192] which are specialized for everywhere monotonically non-decreasing attractive central potentials. Calogero's estimate reads  $n \leq I_C$  with [191]

$$I_C = \frac{2/\pi}{\hbar/\sqrt{2m}} \int_0^{\infty} \sqrt{-V(x)} dx = \left( 1 + \left( \sqrt{1-a} - \sqrt{-a} \right)^2 \right) \sqrt{\frac{2m\sigma^2V_0}{\hbar^2}}, \quad (40)$$

We note that  $I_C \approx \sqrt{2I_B}$ . The result by Chadan further tunes the upper limit for the number of bound states to the half of that by Calogero, that is  $n \leq I_C/2$  [192]. For the parameters applied in Fig. 3 this gives  $n \leq 3.48$ , which is, indeed, an accurate estimate. The dependence of the function



$n_c = I_C / 2$  on the parameter  $a$  for  $a \in (-\infty, 0) \cup (1, +\infty)$  is shown in Fig. 5. It is seen that more bound states are available for  $a$  close to zero. The maximum number achieved in the limit  $a \rightarrow 0$  is  $\sqrt{2m\sigma^2 V_0 / \hbar^2}$ , hence, for sufficiently small  $V_0$  or  $\sigma$  such that  $2m\sigma^2 V_0 < \hbar^2$ , bound states are not possible at all.

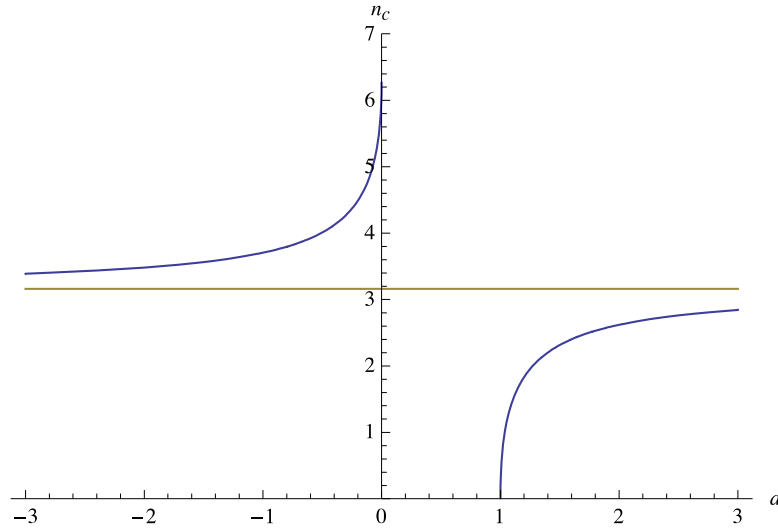


Fig.5. The dependence of Chadan's estimate  $n_c = I_C / 2$  for the number of bound states on the parameter  $a$  ( $m, \hbar, V_0, \sigma = 1, 1, 5, 2$ ).

#### 4.1.5 Discussion

Thus, we have presented the third five-parametric quantum-mechanical potential for which the solution of the Schrödinger equation is written in terms of the Gauss ordinary hypergeometric functions. The potential involves five (generally complex) parameters which are varied independently. Depending on the particular specifications of these parameters, the potential suggests two different appearances. In one version we have a smooth step-barrier with variable height, steepness and asymmetry, while in the other version this is a singular potential-well which behaves as the inverse square root in the vicinity of the origin and exponentially vanishes at infinity.

The potential is in general given parametrically; however, in several cases the involved coordinate transformation allows inversion thus leading to particular potentials which are explicitly written in terms of elementary functions. These reductions are achieved by particular specifications of a parameter standing for the third finite singularity of the general Heun equation. The resultant sub-potentials all are four-parametric (see, e.g., [155,167]). These particular cases are defined by coordinate transformations which are roots of polynomial equations. It turns out that different

polynomial equations of the same degree produce the same potential (with altered parameters). The reason for this is well understood in the case of quadratic equations. In that case the third singularity of the general Heun equation, to which the Schrödinger equation is reduced, is specified as  $a = -1, 1/2$  or  $2$ . We then note that the form-preserving transformations of the independent variable map the four singularities of the Heun equation,  $z = 0, 1, a, \infty$ , onto the points with  $a_1$  adopting one of the six possible values  $a, 1/a, 1-a, 1/(1-a), a/(1-a), (a-1)/a$  [70-72]. It is seen that the triad  $(-1, 1/2, 2)$  is a specific set which remains invariant at form-preserving transformations of the independent variable.

The potential belongs to the general Heun family  $m_{1,2,3} = (1, 1, -1)$ . This family allows several conditionally integrable reductions too [181]. A peculiarity of the exactly integrable potential that we have presented here is that the location of a finite singularity of the general Heun equation is not fixed to a particular point of the complex  $z$ -plane but serves as a variable potential-parameter. In the step-barrier version of the potential, this parameter stands for the asymmetry of the potential.

The solution of the Schrödinger equation is constructed via termination of a series expansion of the general Heun function in terms of the Gauss ordinary hypergeometric functions. The general solution of the problem is composed of fundamental solutions each of which is an *irreducible* combination of two Gauss hypergeometric functions. Several other potentials allowing solutions of this type have been reported recently [137,138,154,155,164,167,177-181]. Further cases involve the solutions for super-symmetric partner potentials much discussed in the past [174,197,198] and for several non-analytic potentials discussed recently [199-201]. One should distinguish these solutions from the case of reducible hypergeometric functions [139,202-204] when the solutions eventually reduce to quasi-polynomials, e.g., discussed in the context of quasi-exactly solvability [202-204]. We stress that owing to the contiguous functions relations [72], the two-term structure of the solution is a general property of all finite-sum hypergeometric reductions of the general Heun functions achieved via termination of series solutions. Finally, it is checked that in our case the linear combination of the involved Gauss functions is expressed through a single generalized hypergeometric function  ${}_3F_2$ .

We have presented the explicit solution of the problem and discussed the bound states supported by the singular version of the potential. We have derived the exact equation for the energy spectrum and estimated the number of bound states. The exact number of bound states is given by the number of zeros of the zero-energy solution which we have also presented.

## 4.2 A bi-confluent Heun potential solvable in terms of the Hermite functions

In the present section, as a representative application of the expansions of the bi-confluent Heun functions in terms of the Hermite-functions, we discuss the reduction of the one-dimensional Schrödinger equation to the bi-confluent Heun equation. It is known that there are five six-parametric potentials for which the general solution of the one-dimensional stationary Schrödinger equation is written in terms of the bi-confluent Heun functions [117,118,156]. We present here the solution for these potentials applying the general approach proposed in [156]. The derivation lines are as follows.

Examining the termination conditions for the series solution, we show that there exists a hierarchy of potentials for which the solution of the Schrödinger equation is written in terms of the Hermite functions. The first potentials of the list are the harmonic oscillator potential [157] and the two Stillinger potentials [158] the solution for which involves just one Hermite function. The next come the first Exton potential [159] (involving the inverse square root potential [137] and its conditionally integrable generalization [138]) and the second Exton potential [159]. The general solution for the latter two Exton potentials involves fundamental solutions each of which presents an irreducible combination of two Hermite functions. To give a representative example of a higher order expansion involving more terms, we here consider the case involving *four* Hermite functions. The corresponding potential is an infinite well defined on a half-axis. We present the four-term explicit solution of the Schrödinger equation for this potential and derive the exact energy-spectrum equation for the bound states that vanish both in the origin and at the infinity. Finally, we construct an accurate approximation for the bound-state energy levels.

### 4.2.1 Bi-confluent Heun potentials for the stationary Schrödinger equation

The one-dimensional stationary Schrödinger equation for a particle of mass  $m$  and energy  $E$  in a potential  $V(x)$  is

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}(E - V(x))\psi = 0. \quad (41)$$

Applying the transformation of the independent variable  $z = z(x)$ , this equation is rewritten for the new argument  $z$  as

$$\frac{d^2\psi}{dz^2} + \frac{\rho_z}{\rho} \frac{d\psi}{dz} + \frac{2m}{\hbar^2} \frac{E - V(z)}{\rho^2} \psi = 0, \quad (42)$$

where  $\rho = dz/dx$ . The further transformation of the dependent variable  $\psi = \varphi(z)u(z)$  reduces this equation to the following equation for the new dependent variable  $u(z)$ :

$$\frac{d^2u}{dz^2} + \left( 2 \frac{\varphi_z}{\varphi} + \frac{\rho_z}{\rho} \right) \frac{du}{dz} + \left( \frac{\varphi_{zz}}{\varphi} + \frac{\rho_z}{\rho} \frac{\varphi_z}{\varphi} + \frac{2m}{\hbar^2} \frac{E - V(z)}{\rho^2} \right) u = 0. \quad (43)$$

This equation is the bi-confluent Heun equation [70-72] if

$$2 \frac{\varphi_z}{\varphi} + \frac{\rho_z}{\rho} = \frac{\gamma}{z} + \delta + \varepsilon z \quad (44)$$

and

$$\frac{\varphi_{zz}}{\varphi} + \frac{\rho_z}{\rho} \frac{\varphi_z}{\varphi} + \frac{2m}{\hbar^2} \frac{E - V(z)}{\rho^2} = \frac{\alpha z - q}{z}. \quad (45)$$

Since the point  $z = 0$  is the only singularity of the bi-confluent Heun equation located in the finite part of the complex  $z$ -plane, according to the approach of [156], in order to identify the potentials that are proportional to an energy-independent parameter and have a shape that is independent of both energy and that parameter, we search for the solutions of equations (44) and (46) applying the transformation

$$\rho = \frac{dz}{dx} = \frac{z^{m_1}}{\sigma} \quad (46)$$

with an integer or half-integer  $m_1$  and arbitrary  $\sigma$ . Resolving equation (44), we then have

$$\varphi = z^{\alpha_0} e^{\alpha_1 z + \alpha_2 z^2}, \quad (47)$$

where the constants  $\alpha_{0,1,2}$  are defined through  $m_1, \sigma$  and the parameters involved in the target bi-confluent Heun equation. Substituting equations (46) and (47) into the remaining equation (45) and multiplying further the equation by  $z^2$ , we note that the last term of the obtained equation, that is  $z^2 (E - V(z)) / \rho^2$ , is a polynomial in  $z$  of at most fourth degree. If the energy  $E$  adopts arbitrary values and the potential is energy-independent, this is possible only if the two summands of this term, the one proportional to  $E$  and the other proportional to  $V(z)$ , independently of each other, are polynomials of at most fourth degree [156]:

$$\frac{z^2}{\rho^2} = r_0 + r_1 z + r_2 z^2 + r_3 z^3 + r_4 z^4, \quad (48)$$

$$V(z) \frac{z^2}{\rho^2} = v_0 + v_1 z + v_2 z^2 + v_3 z^3 + v_4 z^4. \quad (49)$$

Equation (48) together with equation (46) leads to 5 admissible sets of integer or half-integer  $m_1$  defined by the inequalities  $0 \leq 2 - 2m_1 \leq 4$ . Thus,  $m_1 = -1, -1/2, 0, 1/2, 1$ . With these  $m_1$ , equation (49) defines five independent six-parametric bi-confluent Heun potentials first identified by Lemieux and Bose [117]. The potentials are listed in Table 1, where for convenience both  $z$ - and  $x$ -representations of these potentials are presented since the  $z$ -representation is in some cases

more useful for practical calculations while from the physical point of view just the  $x$ -representation matters. Note that the parameters  $x_0$  and  $\sigma$  are not shown in the table; to get the full representation for the potential and the corresponding coordinate transformation, one should everywhere make the replacement  $x \rightarrow (x - x_0) / \sigma$ .

$m_1$	Potential $V(z)$	Coordinate transformation	Explicit potential $V(x)$
-1	$V_0' + \frac{V_1'}{z} + \frac{V_2'}{z^2} + \frac{V_3'}{z^3} + \frac{V_4'}{z^4}$	$z = \sqrt{2x}$	$V_0 + \frac{V_1}{\sqrt{x}} + \frac{V_2}{x} + \frac{V_3}{x^{3/2}} + \frac{V_4}{x^2}$
-1/2	$V_0' + V_1' z + \frac{V_2'}{z} + \frac{V_3'}{z^2} + \frac{V_4'}{z^3}$	$z = (3x/2)^{2/3}$	$V_0 + V_1 x^{2/3} + \frac{V_2}{x^{2/3}} + \frac{V_3}{x^{4/3}} + \frac{V_4}{x^2}$
0	$V_0' + V_1' z + V_2' z^2 + \frac{V_3'}{z} + \frac{V_4'}{z^2}$	$z = x$	$V_0 + V_1 x + V_2 x^2 + \frac{V_3}{x} + \frac{V_4}{x^2}$
1/2	$V_0' + V_1' z + V_2' z^2 + V_3' z^3 + \frac{V_4'}{z}$	$z = x^2 / 4$	$V_0 + V_1 x^2 + V_2 x^4 + V_3 x^6 + \frac{V_4}{x^2}$
1	$V_0' + V_1' z + V_2' z^2 + V_3' z^3 + V_4' z^4$	$z = e^x$	$V_0 + V_1 e^x + V_2 e^{2x} + V_3 e^{3x} + V_4 e^{4x}$

**Table 1.** Five six-parametric bi-confluent Heun potentials ( $V_{0,1,2,3,4}$  are arbitrary constants) together with the corresponding coordinate transformation  $z = z(x)$ .

For these potentials together with corresponding  $m_1$ , collecting the coefficients at powers of  $z$  in equations (44) and (45), we get eight equations which are linear for the parameters  $\gamma, \delta, \varepsilon, \alpha, q$  of the bi-confluent Heun function  $u(z)$  as well as for the parameter  $\alpha_1$  of the pre-factor  $\varphi(z)$ , and are quadratic for the parameters  $\alpha_0$  and  $\alpha_2$ . The solution of the stationary Schrödinger equation (41) for the presented potentials is thus explicitly written in terms of the bi-confluent Heun function as

$$\psi = z^{\alpha_0} e^{\alpha_1 z + \alpha_2 z^2} H_B(\gamma, \delta, \varepsilon; \alpha, q; z) \quad (50)$$

with the involved parameters being given by the equations

$$\gamma = 2\alpha_0 + m_1, \quad \delta = 2\alpha_1, \quad \varepsilon = 4\alpha_2, \quad (51)$$

$$\alpha = \alpha_1^2 + 2\alpha_2(2\alpha_0 + m_1 + 1) + 2m(Er_2 - v_2) / \hbar^2, \quad (52)$$

$$q = -\alpha_1(2\alpha_0 + m_1) - 2m(Er_1 - v_1) / \hbar^2 \quad (53)$$

and 
$$\alpha_0(\alpha_0 + m_1 - 1) + 2m(Er_0 - v_0)/\hbar^2 = 0, \quad (54)$$

$$\alpha_1\alpha_2 + m(Er_3 - v_3)/(2\hbar^2) = 0, \quad (55)$$

$$\alpha_2^2 + m(Er_4 - v_4)/(2\hbar^2) = 0. \quad (56)$$

This fulfills the development. Starting from a particular potential of [Table 1](#), one calculates, through equations (51)-(56), the parameters  $\gamma, \delta, \varepsilon, \alpha, q$  of the bi-confluent Heun function  $H_B$  and the parameters  $\alpha_{0,1,2}$  of the pre-factor  $\varphi(z)$ . We note that for a given potential with corresponding  $m_1$  the auxiliary parameters  $r_{0,1,2,3,4}$  and  $v_{0,1,2,3,4}$  involved in these equations are readily calculated through the definitions (48) and (49). A last remark concerns the factor  $\sigma$  involved in equation (46) and the constant  $x_0$  which comes out from integration of equation (46). It is immediately seen from the form of the presented potentials that, since  $V_{0,1,2,3,4}$  are arbitrary, without loss of the generality one may put  $\sigma = 1$ . As regards  $x_0$ , depending on the particular physical problem at hand, e.g., if a possible non-Hermitian extension is considered, this constant standing for the space origin may be chosen complex.

Thus, we have presented the solution of the Schrödinger equation for the five bi-confluent-Heun Lemieux-Bose potentials. If we now apply the expansion of the bi-confluent Heun function in terms of the Hermite functions that we have presented in the previous Chapter, we may check if the conditions for termination of the series for some  $n = N$  are fulfilled for particular choices of the parameters involved in the potential under consideration. If yes, then we arrive at the solution of the Schrödinger equation for that particular potential written as a sum of a finite number of the Hermite functions:

$$\psi(z) = z^{\alpha_0} e^{\alpha_1 z + \alpha_2 z^2} \sum_{n=0}^N c_n H_{(\gamma-\alpha/\varepsilon)+n} \left( \pm \sqrt{-\frac{\varepsilon}{2}} \left( z + \frac{\delta}{\varepsilon} \right) \right). \quad (57)$$

The inspection shows that there are several cases for which the result of the test is positive. For instance, the termination conditions can be satisfied for  $m_1 = -1/2$ . The results are as follows. For  $N=0$  we get the exactly solvable general harmonic oscillator potential [157] and the two conditionally exactly solvable potentials by Stillinger [158]. The solution of the Schrödinger equation for these potentials involves only one Hermite function. For  $N=1$  we get the inverse square root potential [137] and its conditionally solvable generalization [138]. For these potentials the solution involves two Hermite functions. We note that the pointed generalized conditionally exactly solvable potential was first identified by Exton (Eq. (21) of [159]). We refer to this potential as the first conditionally integrable Exton potential. It is worth mentioning that it involves as

particular cases also the two super-symmetric partner potentials treated by Lopez-Ortega [160] (note that these SUSY partner potentials can also be derived by considering the inverse square root potential as a super-potential). Apart from this first potential by Exton, the case  $N=1$  yields also the second conditionally integrable potential proposed by Exton as well (Eq. (22) of [159]). It is understood that the cases  $N=2,3,\dots$  may result in an infinite sequence of conditionally exactly solvable potentials. As a representative example, we present a higher-order termination with  $N=3$ , i.e. a potential for which the solution of the Schrödinger equation is a linear combination of *four* Hermite functions.

#### 4.2.2 The potential

Let the series solution of the bi-confluent Heun equation terminates at  $N=3$ , that is  $c_3 \neq 0$  and  $c_4 = c_5 = 0$ . For this to be the case should be  $\gamma = -3$  and the accessory parameter  $q$  should satisfy the equation

$$q^4 - 6\delta q^3 + (11\delta^2 + 10\varepsilon + 10\alpha)q^2 - 6\delta(\delta^2 + 3\varepsilon + 5\alpha)q + 9\alpha(2\delta^2 + 2\varepsilon + \alpha) = 0. \quad (58)$$

Let  $m_1 = -1/2$ . By checking the parameters  $\gamma, \delta, \varepsilon, \alpha, q$  obeying equations (51)-(56) for fulfillment of equation (58), we readily get that this is the case for the potential

$$V(x) = \frac{55\hbar^2}{72m x^2} + \frac{V_2}{x^{2/3}} + V_0 + \frac{9mV_2^2}{8\hbar^2} x^{2/3}. \quad (59)$$

Since one can everywhere make the replacement  $x \rightarrow x - x_0$  with an arbitrary  $x_0$  standing for the coordinate origin, this is in general a three-parametric potential. We note that, since this potential involves a fixed parameter ( $55\hbar^2 / (72m)$ ) and the strengths of the terms proportional to  $x^{-2/3}$  and  $x^{2/3}$  do not vary independently, this is a conditionally integrable potential. The shape of the potential is shown in Fig. 6. We note that a reason for the potential to be of interest is that owing to the involved centrifugal-barrier term it models, to a certain extent, the one-dimensional reduction of the three-dimensional Schrödinger problem for the central fractional-power singular potential involving  $r^{-2/3}$  and  $r^{2/3}$  terms used in the past in particle physics phenomenology [205,206].

According to the expansion (57), the fundamental solutions  $\psi_F$  of the Schrödinger equation (41) for this potential are written as a sum of four Hermite functions:

$$\psi_F(z) = z^{-5/4} e^{-y^2/2} (c_0 H_{a-3}(y) + c_1 H_{a-2}(y) + c_2 H_{a-1}(y) + c_3 H_a(y)), \quad (60)$$

where

$$y = \sqrt{-2\alpha_2} \left( \left( \frac{3x}{2} \right)^{2/3} + \frac{\alpha_1}{2\alpha_2} \right). \quad (61)$$

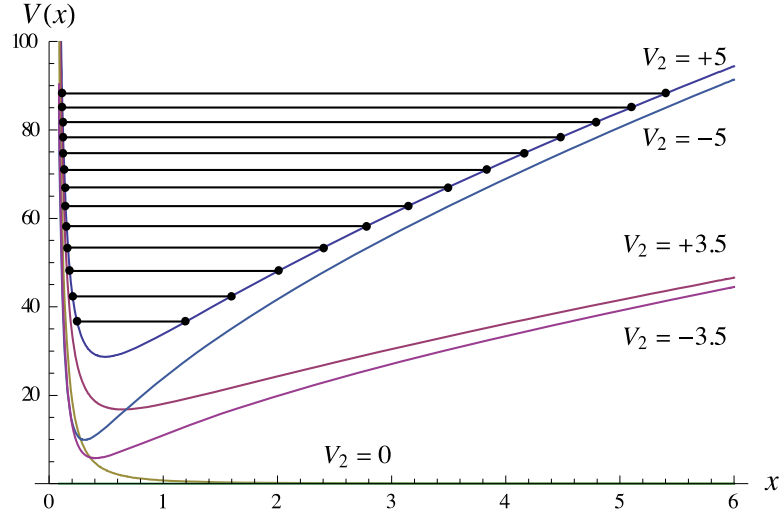


Fig. 6. Potential (59) for  $V_0 = 0$  and  $V_2 = 0, \pm 3.5, \pm 5$  ( $m = \hbar = 1$ ).

The index parameter  $a$  as well as the expansion coefficients  $c_{0,1,2,3}$  are conveniently written through the pre-factor exponents  $\alpha_1$  and  $\alpha_2$  (which are explicitly calculated by equations (54) and (56), respectively) and an auxiliary parameter  $s = \pm 1$ . The result reads

$$a = 1 + s - \frac{\alpha_1^2}{4\alpha_2}, \quad (62)$$

and

$$c_0 = 8\sqrt{-2\alpha_2}a(a-1)(a-2), \quad c_1 = 12\alpha_1a(a-1), \quad (63)$$

$$c_2 = 6\sqrt{-2\alpha_2}a(2a-3-s), \quad c_3 = \alpha_1(2a-1+s). \quad (64)$$

with

$$\alpha_1 = \left(\frac{2}{3}\right)^{2/3} \frac{V_3 - E}{V_2 s}, \quad \alpha_2 = \left(\frac{3}{2}\right)^{2/3} \frac{mV_2 s}{2\hbar^2}. \quad (65)$$

We note that  $s = +1$  and  $s = -1$  produce linearly independent solutions. This is readily verified by checking the Wronskian of the two solutions. Hence, the linear combination of these fundamental solutions

$$\psi(z) = C_1 \psi_F|_{s \rightarrow +1} + C_2 \psi_F|_{s \rightarrow -1} \quad (66)$$

with arbitrary constant coefficients  $C_{1,2}$  presents the general solution of the problem.



### 4.2.3 Bound states

The bound states supported by potential (59) are derived by imposing the boundary conditions of vanishing the wave-function (66) in the origin and at the infinity:  $\psi(0) = 0$  and  $\psi(\infty) = 0$ . The first condition presents a linear relation between the coefficients  $C_{1,2}$ :

$$C_1 \psi_F(x=0)|_{s=+1} + C_2 \psi_F(x=0)|_{s=-1} = 0, \quad (67)$$

while the second condition for the infinity reveals, after some algebra when passing to the large-argument asymptotes of the involved Hermite functions, that  $C_1 = 0$  if  $V_2 > 0$  and  $C_2 = 0$  if  $V_2 < 0$ .

It is then readily seen from equation (67) that for the bound states it holds

$$\psi_F(x=0)|_{s=-\text{sign}(V_2)} = 0. \quad (68)$$

This is the exact equation for the energy spectrum and the bound-state wave functions are given by the first term of the general solution (66) if  $V_2 < 0$  and by the second term if  $V_2 > 0$ . Combining the two cases, we thus have

$$\psi_B(x) = C_N \psi_F(x)|_{s=-\text{sign}(V_2)}, \quad (69)$$

where  $C_N$  is the normalization constant:

$$C_N = \sqrt{\int_0^{+\infty} (\psi_F \psi_F^*)|_{s=-\text{sign}(V_2)} dx}, \quad (70)$$

It turns out that the spectrum equation is considerably simplified when separately considering positive and negative  $V_2$  cases. Indeed, consider, for example, the case  $V_2 < 0$  for which  $s = +1$ . Since the pre-factor  $z^{-5/4} e^{-y^2/2}$  of the fundamental solution  $\psi_F$  does not adopt zeros, equation (68) reduces to

$$(c_0 H_{a-3} + c_1 H_{a-2} + c_2 H_{a-1} + c_3 H_a)|_{y=y_0} = 0, \quad (71)$$

with

$$y_0 \equiv y|_{x=0, s=1} = -\frac{\alpha_1}{\sqrt{-2\alpha_2}} \Big|_{s=1} = -\sqrt{2(a-2)}. \quad (72)$$

Using the recurrence relations between the involved Hermite functions, equation (71) can be rewritten in a two-term form:

$$(A_1 H_{a-1} + A_2 H_a)|_{y=y_0} = 0 \quad (73)$$

with

$$A_1 = 2(a-2)(c_1 y_0 + (a-1)c_2) + c_0(1-a+2y_0^2), \quad (74)$$

$$A_2 = c_0 y_0 + (a-2)c_1 - 2(2-3a+a^2)c_3. \quad (75)$$

Notably, the inspection reveals that for the parameters (62)-(65) with  $s = +1$  the second of the coefficients  $A_{1,2}$  identically vanishes for arbitrary parameters of the potential (59) (with the proviso  $V_2 < 0$ ), i.e.,  $A_2 \equiv 0$ . We then arrive at a remarkably simple eigenvalue equation for the energy spectrum:

$$H_{a-1}\left(-\sqrt{2(a-2)}\right)\Big|_{s=1} = 0, \quad V_2 < 0. \quad (76)$$

Similarly, for a positive  $V_2$  we get

$$H_{a-2}\left(-\sqrt{2a}\right)\Big|_{s=1} = 0, \quad V_2 > 0. \quad (77)$$

It should be stressed that these are exact equations. The first energy levels for the potential parameters  $V_0 = 0$  and  $V_2 = +5$  ( $m = \hbar = 1$ ) are shown in Fig. 6. The corresponding normalized bound-state wave functions are plotted in Fig. 7.

Consider now the approximate solution of the eigenvalue equations (76),(77). Note that the indexes and arguments of the Hermite functions  $H_\nu(w)$  involved in these equations belong to the transition layer where  $w \approx \pm\sqrt{2v}$ . An appropriate approximation of the Hermite function for this region is [207]:

$$H_\nu(w) \propto 2^{\frac{1+\nu}{2}} e^{\frac{w^2 - \nu + \nu \ln \nu}{2}} \left(1 - \frac{w^2}{2\nu}\right)^{-1/4} \cos\left(\frac{\pi\nu}{2} - w\sqrt{\frac{\nu}{2} - \frac{w^2}{4}} - \frac{2\nu+1}{2} \arcsin\left(\frac{w}{\sqrt{2\nu}}\right)\right). \quad (78)$$

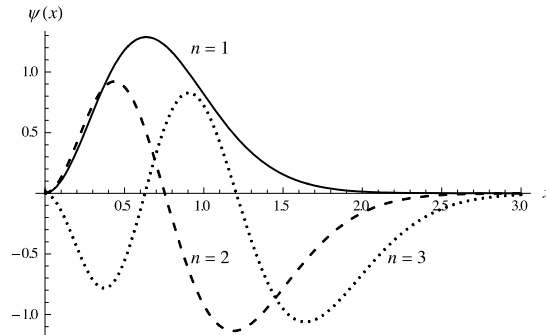


Fig. 7. The first three normalized wave functions for  $V_0 = 0$ ,  $V_2 = +5$  ( $m = \hbar = 1$ ).

This is an accurate approximation that includes an appropriate factor for changing the amplitude and takes into account the uneven spacing of the zeros of the Hermite function. Importantly, the approximation is applicable to the whole admissible variation range  $a > 2$  of the parameter  $a$ , which is the only parameter involved in equations (77) and (78). The approximation for the function  $H_{a-2}(-\sqrt{2a})$  is shown in Fig. 8.

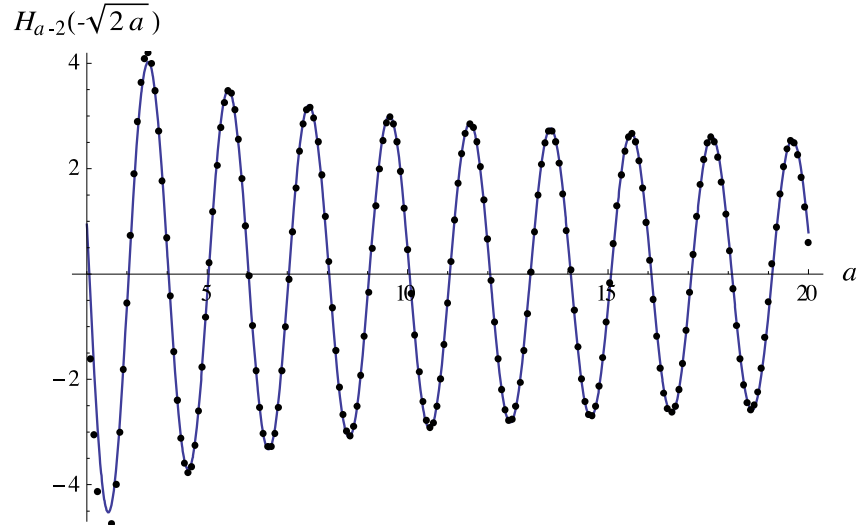


Fig. 8. Approximation (78) (solid line) for function  $H_{a-2}(-\sqrt{2a})$  (points).

Owing to the approximation (78) the spectrum equation is accurately approximated as

$$\frac{\pi v}{2} - w \sqrt{\frac{v}{2} - \frac{w^2}{4}} - \frac{2v+1}{2} \arcsin\left(\frac{w}{\sqrt{2v}}\right) = -\frac{\pi}{2} + \pi n, \quad n = 1, 2, \dots \quad (79)$$

The next step is now to express the parameters  $v = a-1, a-2$  and  $w = -\sqrt{2(a-2)}, -\sqrt{2a}$  through the energy  $E$ , using the definition (62) together with equations (63)-(65), and further make in equation (79) the substitution  $E_n = V_3 + \left(9m|V_2|^3 / (2\hbar^2)\right)^{1/2} f(n)$ , which is readily guessed from the form of the derived expressions. The last step is then to expand  $f(n)$  for large  $n$  into the series in terms of half-integer and integer powers of  $n$ . The resultant expansions for the eigenvalues up to the accuracy of the order of  $O(1/n)$  are given as

$$E_n = V_3 + \sqrt{\frac{9m|V_2|^3}{2\hbar^2}} \left( \sqrt{n+1} - \frac{7}{8\sqrt{n+1}} \right) \quad \text{if } V_2 < 0 \quad (80)$$

and

$$E_n = V_3 + \sqrt{\frac{9m|V_2|^3}{2\hbar^2}} \left( \sqrt{n+1} + \frac{1}{64} \frac{1}{\sqrt{n+1}} \right) \quad \text{if } V_2 > 0. \quad (81)$$

These approximations are compared with the exact energy eigenvalues in Fig. 9. As seen, these are rather accurate results. Precisely, except for the first level, the relative error is less than  $2.5 \times 10^{-3}$  for all  $n \geq 2$  (this is shown in the inset of Fig. 9).

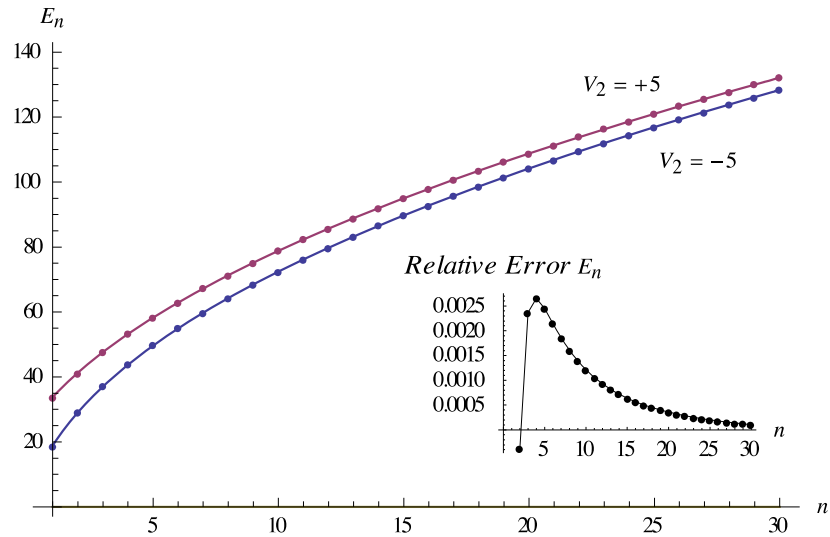


Fig. 9. Approximations (80),(81) (solid lines) versus exact energy levels (points) for  $V_0 = 0$ ,  $V_2 = \pm 5$  ( $m = \hbar = 1$ ). The inset presents the relative error for  $n > 1$ .

#### 4.2.4 Discussion

We have presented the five six-parametric Lemieux-Bose potentials and have constructed the solution of the problem for these potentials in terms of the bi-confluent Heun functions. Further, we have identified a sub-potential for which the involved parameters allow termination of the Hermite-function expansion of the involved bi-confluent Heun function at  $N = 3$ . This is a three-parametric conditionally integrable potential for which the general solution of the Schrödinger equation is written through fundamental solutions each of which presents a linear combination of four Hermite functions.

The derived potential is an infinite well defined on a half-axis. It involves a repulsive centrifugal-barrier core  $\sim x^{-2}$  and fractional-power terms proportional to  $x^{-2/3}$  and  $x^{2/3}$ . The strength of the first term is fixed and those for the latter two terms do not vary independently. This is why it is a conditionally integrable potential.

We have presented the four-term explicit solution of the Schrödinger equation for this potential in terms of the Hermite functions and have discussed the bound states supported by the potential. The exact energy-spectrum for the bound states that vanish both in the origin and at the infinity is defined by the zeros of a Hermite function of a non-integer order. However, the parameters of this Hermite function depend on the sign of the coefficient  $V_2$  of the singular term proportional to  $x^{-2/3}$  (the term  $x^{2/3}$  is always repulsive). It is understood that this is because the case  $V_2 = 0$  is exceptional in that then both fractional-power terms vanish so that in this case the potential is not a well (see Fig. 1).

Finally, we have considered the approximate solution of the eigenvalue equations for both negative and positive  $V_2$ . It is worth mentioning that the parameters of the Hermite functions  $H_\nu(w)$  involved in these equations in both cases belong to the transition layer for which  $w \approx \pm\sqrt{2\nu}$ . Applying a specific asymptotic expansion applicable to the whole variation range of the parameters within this layer, we have derived highly accurate approximations for the bound-state energy levels written as a linear combination of half-integer powers of the quantum number  $n+1$ :  $(n+1)^{1/2}$  and  $(n+1)^{-1/2}$ , for both negative and positive  $V_2$ .

### **4.3 Four five-parametric and five four-parametric independent confluent Heun potentials for the stationary Klein-Gordon equation**

The Klein-Gordon equation [208,209] is a relativistic version of the Schrödinger equation that describes the behavior of spinless particles. The equation has a large range of applications in contemporary physics, including particle physics, astrophysics, cosmology, classical mechanics, etc. (see [208-211] and references therein). For the stationary problems, when the Hamiltonian does not depend on time, particular solutions can be obtained by applying the separation of variables that reduces the problem to the solution of the stationary Klein-Gordon equation. This approach is widely used to treat particles in various external fields or curved space-time using functions of the hypergeometric [212-221] or the Heun [222-227] classes.

In the present section we consider the reduction of the one-dimensional stationary Klein-Gordon equation to the single-confluent Heun equation [70-72]. This equation possesses two regular singular points located at finite points of the complex  $z$ -plane and an irregular singularity of rank 1 at infinity. Owing to such a structure of the singularities, the confluent Heun equation directly incorporates, by simple choices of the involved exponent parameters, the Gauss ordinary hypergeometric and the Kummer confluent hypergeometric equations as well as the algebraic form of the Mathieu equation and several other familiar equations. Because of the richer structure of the singularities, it is clear that the confluent Heun equation is potent to suggest a set of potentials that cannot be treated by the hypergeometric equations in reasonable limits. In the meantime, since the parameters standing for different singularities are clearly separated so that the influence of the each feature originating from a particular singularity is well identified, it is expected that the confluent Heun generalizations will suggest a clear route to follow the details relevant to a particular prototype hypergeometric or Mathieu potential.

We show that, to derive energy-independent potentials that are in addition proportional to an energy-independent continuous parameter and for which the potential shape is independent of the

latter parameter, there exist only 15 permissible choices for the coordinate transformation. Each of these transformations leads to a four- or five-parametric potential solvable in terms of the confluent Heun functions. However, because of the symmetry of the confluent Heun equation with respect to the transposition of its regular singularities, only nine of these potentials are independent. Four of the independent potentials are five-parametric and five others are four-parametric.

The five-parametric Heun potentials all possess hypergeometric sub-potentials while the four-parametric ones do not. One of the five-parametric potentials has a four-parametric sub-potential solvable in terms of the Gauss hypergeometric function, another potential has a four-parametric sub-potential solvable in terms of the Kummer confluent hypergeometric function and there is a potential that possesses four-parametric sub-potentials of both hypergeometric types. Finally, the fourth five-parametric Heun potential possesses a three-parametric confluent hypergeometric sub-potential which is, however, only conditionally integrable in the sense that in this case the potential cannot be presented as being proportional to a parameter and having a shape that is independent of that parameter.

The section is organized as follows. In section 4.3.1 we derive the nine independent potentials and present the solution of the problem for these potentials in terms of the single-confluent Heun functions. In section 4.3.2 we discuss the exactly and conditionally exactly solvable hypergeometric sub-potentials and present a new conditionally exactly solvable potential written in terms of the Lambert W-function. The section is concluded by a brief discussion of the derived results.

### 4.3.1 Confluent Heun potentials for the Klein-Gordon equation

The one-dimensional Klein-Gordon equation for a particle of rest mass  $m$  and energy  $E$  in a scalar potential field  $V(x)$  is written as [208]

$$\frac{d^2\psi}{dx^2} + \frac{1}{\hbar^2 c^2} \left( (E - V(x))^2 - m^2 c^4 \right) \psi = 0. \quad (82)$$

Applying the transformation  $z = z(x)$ , this equation is rewritten for the new argument  $z$  as

$$\psi_{zz} + \frac{\rho_z}{\rho} \psi_z + \frac{1}{\hbar^2 c^2} \frac{(E - V(z))^2 - m^2 c^4}{\rho^2} \psi = 0, \quad (83)$$

where  $\rho = dz / dx$  and the lowercase Latin index denotes differentiation. Further transformation of the dependent variable  $\psi = \varphi(z) u(z)$  reduces this equation to the following one for the new dependent variable  $u(z)$ :

$$u_{zz} + \left( 2 \frac{\varphi_z}{\varphi} + \frac{\rho_z}{\rho} \right) u_z + \left( \frac{\varphi_{zz}}{\varphi} + \frac{\rho_z}{\rho} \frac{\varphi_z}{\varphi} + \frac{1}{\hbar^2 c^2} \frac{(E - V(z))^2 - m^2 c^4}{\rho^2} \right) u = 0. \quad (84)$$

This equation becomes the single-confluent Heun equation [70-72]:

$$u_{zz} + \left( \frac{\gamma}{z} + \frac{\delta}{z-1} + \varepsilon \right) u_z + \frac{\alpha z - q}{z(z-1)} u = 0, \quad (85)$$

if

$$\frac{\gamma}{z} + \frac{\delta}{z-1} + \varepsilon = 2 \frac{\varphi_z}{\varphi} + \frac{\rho_z}{\rho} \quad (86)$$

and

$$\frac{\alpha z - q}{z(z-1)} = \frac{\varphi_{zz}}{\varphi} + \frac{\rho_z}{\rho} \frac{\varphi_z}{\varphi} + \frac{1}{\hbar^2 c^2} \frac{(E - V(z))^2 - m^2 c^4}{\rho^2}. \quad (87)$$

Resolving equation (86) for  $\varphi$ :

$$\varphi = \frac{e^{\varepsilon z/2}}{\sqrt{\rho(z)}} z^{\frac{\gamma}{2}} (z-1)^{\frac{\delta}{2}}, \quad (88)$$

and substituting this into equation (87), we obtain

$$\frac{C_0 + C_1 z + C_2 z^2 + C_3 z^3 + C_4 z^4}{z^2 (z-1)^2} + \left( \frac{\rho_z^2}{4\rho^2} - \frac{\rho_{zz}}{2\rho} \right) + \frac{1}{\hbar^2 c^2} \frac{(E - V(z))^2 - m^2 c^4}{\rho^2} = 0, \quad (89)$$

where the constants  $C_{0,1,2,3,4}$  are defined by the parameters of the confluent Heun equation.

We suppose that the potential is energy-independent and is proportional to an independent parameter  $\mu$ :  $V(x) = \mu f(x)$ , with a potential shape  $f(x)$  that is independent of that parameter:  $f \neq f(\mu)$ . A key observation of [156] for this case is that, for an  $E$ -independent coordinate transformation  $z = z(x)$ , equation (89) can be satisfied only if

$$z'(x) = \rho = z^{m_1} (z-1)^{m_2} / \sigma \quad (90)$$

with integer or half-integer  $m_{1,2}$ .

The lines leading to this conclusion are as follows. Taking the second derivative of equation (89) with respect to  $E$ , we see that

$$\frac{1}{\rho^2} = \frac{r_0 + r_1 z + r_2 z^2 + r_3 z^3 + r_4 z^4}{z^2 (z-1)^2} \equiv \frac{r(z)}{z^2 (z-1)^2}, \quad (91)$$

where  $r_i = (c^2 \hbar^2 / 2) d^2 C_i / dE^2$ . Rewriting now the polynomial  $r(z)$  as  $r(z) = \prod_i (r - s_i)$ , taking

the limit  $E, \mu \rightarrow 0$  and applying the identity

$$\frac{\rho_{zz}}{\rho} = \left( \frac{\rho_z}{\rho} \right)_z + \left( \frac{\rho_z}{\rho} \right)^2, \quad (92)$$

we see that the roots  $s_i$  are 0 or 1 (in other words, one can say that the logarithmic derivative  $\rho_z / \rho$  cannot have poles other than the finite singularities  $z = 0, 1$  of the confluent Heun equation). With this and equation (91), we arrive at equation (90) with integer or half-integer  $m_{1,2}$  and arbitrary  $\sigma$ . Besides, since  $z^2(z-1)^2 / \rho^2 = z^{2-2m_1}(z-1)^{2-2m_2} \sigma^2$  is a polynomial of at most fourth degree, we have the inequalities  $-1 \leq m_{1,2} \leq 1$ ,  $0 \leq m_1 + m_2 \leq 2$ . This leads to 15 possible sets of  $m_{1,2}$  shown in Fig.10. We note that, because of symmetry of the confluent Heun equation with respect to the transposition  $z \leftrightarrow 1-z$ , only nine of these cases are independent. The independent cases are marked in the figure by filled shapes.

The next step is matching the cross-term  $-2EV(z) / \rho^2$  and the term  $V^2(z) / \rho^2$  with the rest in equation (89). Taking the first derivative with respect to  $E$ , we first get

$$z^2(z-1)^2 \frac{V(z)}{\rho^2} = v_0 + v_1 z + v_2 z^2 + v_3 z^3 + v_4 z^4 \equiv v(z), \quad (93)$$

and further taking the limit  $E \rightarrow 0$  find that the parameters  $v_{0,1,2,3,4}$  should be so chosen that

$$z^2(z-1)^2 \frac{V^2(z)}{\rho^2} = z^{2m_1-2}(z-1)^{2m_2-2} v^2(z) / \sigma^2 \equiv w(z) \quad (94)$$

is a polynomial of at most fourth degree. By direct inspection it is then shown that the last requirement is fulfilled only for certain permissible sub-sets of the parameters  $v_{0,1,2,3,4}$ . For the nine independent cases of  $m_{1,2}$  the resultant potentials can be conveniently written in the form presented in Table 2. Four of the independent potentials are five-parametric, while the remaining five potentials are four-parametric ( $V_{0,1,2}, x_0, \sigma$  are arbitrary complex constants). The types of the hypergeometric sub-potentials for the four five-parametric cases possessing such sub-potentials are indicated in the last column of the table.

The solution of the problem is readily written taking the pre-factor  $\phi(z)$  as

$$\phi = e^{\alpha_0 z} z^{\alpha_1} (z-1)^{\alpha_2}. \quad (95)$$

Then, collecting the coefficients at powers of  $z$  in the numerators of equations (86) and (87), we get eight equations which are linear for the five parameters  $\gamma, \delta, \varepsilon, \alpha, q$  of the confluent Heun function  $u(z)$  and are quadratic for the three parameters  $\alpha_{0,1,2}$  of the pre-factor.

Resolving these equations, we finally get that the solution of the stationary Klein-Gordon equation is explicitly written in terms of the confluent Heun function as

$$\psi = e^{\alpha_0 z} z^{\alpha_1} (z-1)^{\alpha_2} H_C(\gamma, \delta, \varepsilon; \alpha, q; z) \quad (96)$$

with the involved parameters being given by the equations



$$\gamma = 2\alpha_1 + m_1, \quad \delta = 2\alpha_2 + m_2, \quad \varepsilon = 2\alpha_0, \quad (97)$$

$$\alpha = \alpha_0 (m_1 + m_2 + 2(\alpha_1 + \alpha_2 - \alpha_0)) + \frac{1}{\hbar^2 c^2} \left( (E^2 - m^2 c^4) r_3 - 2E v_3 + w_3 \right), \quad (98)$$

$$q = \alpha_1 (2 - m_1 - m_2) + (2\alpha_1 + m_1)(\alpha_0 - \alpha_1 - \alpha_2) + \frac{1}{\hbar^2 c^2} \left( (E^2 - m^2 c^4) r_1 - 2E v_1 + w_1 \right). \quad (99)$$

The equations for the exponents  $\alpha_{0,1,2}$  read

$$\alpha_0^2 + \frac{1}{\hbar^2 c^2} \left( (E^2 - m^2 c^4) r_4 - 2E v_4 + w_4 \right) = 0, \quad (100)$$

$$\alpha_1^2 - \alpha_1 (1 - m_1) + \frac{1}{\hbar^2 c^2} \left( (E^2 - m^2 c^4) r(0) - 2E v(0) + w(0) \right) = 0, \quad (101)$$

$$\alpha_2^2 - \alpha_2 (1 - m_2) + \frac{1}{\hbar^2 c^2} \left( (E^2 - m^2 c^4) r(1) - 2E v(1) + w(1) \right) = 0 \quad (102)$$

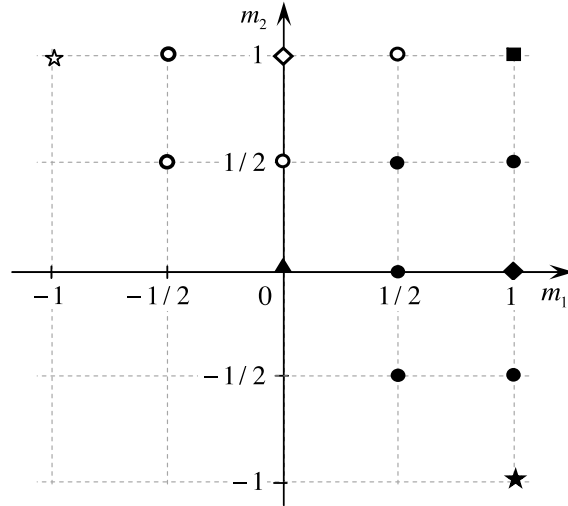
and the auxiliary parameters  $r_{0,1,2,3,4}$ ,  $v_{0,1,2,3,4}$  and  $w_{0,1,2,3,4}$  for each row of [Table 1](#) are readily calculated through the definitions [\(91\)](#), [\(93\)](#) and [\(94\)](#):

$$r(z) = r_0 + r_1 z + r_2 z^2 + r_3 z^3 + r_4 z^4 = z^{2-2m_1} (z-1)^{2-2m_2}, \quad (103)$$

$$v_0 + v_1 z + v_2 z^2 + v_3 z^3 + v_4 z^4 = r(z) V(z), \quad (104)$$

$$w_0 + w_1 z + w_2 z^2 + w_3 z^3 + w_4 z^4 = r(z) V^2(z) \quad (105)$$

The coordinate transformation  $x(z)$  or  $z(x)$  calculated using equation [\(90\)](#) is presented in the third column of [Table 2](#).



[Fig.10](#). Fifteen possible pairs  $m_1, m_2$ . The nine independent cases are marked by filled shapes. The cases possessing ordinary or confluent hypergeometric sub-potentials are marked by squares or triangles, respectively. The rhombs indicate the cases that possess hypergeometric sub-potentials of both types. The asterisks mark the conditionally integrable cases.

N	$m_1, m_2$	Potential $V(z)$	Coordinate transformation $z(x)$ or $x(z)$	Hypergeom. sub-potential
1	0, 0	$V_0 + \frac{V_1}{z} + \frac{V_2}{z-1}$	$z(x) = \frac{x-x_0}{\sigma}$	${}_1F_1$ [161]
2	1/2, -1/2	$V_0 + \frac{V_1}{z-1}$	$x(z) = x_0 + \sigma \left( \sqrt{z(z-1)} - \sinh^{-1} \left( \sqrt{z-1} \right) \right)$	--
3	1/2, 0	$V_0 + \frac{V_1}{z-1}$	$z(x) = \frac{(x-x_0)^2}{4\sigma^2}$	--
4	1/2, 1/2	$V_0 + V_1 z$	$z(x) = \cosh^2 \left( \frac{x-x_0}{2\sigma} \right)$	--
5	1, -1	$V_0 + \frac{V_1}{z-1} + \frac{V_2}{(z-1)^2}$	$x(z) = x_0 + \sigma(z - \log(z))$ Lambert W: $z(x) = -W \left( -e^{-(x-x_0)/\sigma} \right)$	Conditionally solvable: ${}_1F_1$
6	1, -1/2	$V_0 + \frac{V_1}{z-1}$	$x(z) = x_0 + 2\sigma \left( \sqrt{z-1} - \tan^{-1} \left( \sqrt{z-1} \right) \right)$	--
7	1, 0	$V_0 + V_1 z + \frac{V_2}{z-1}$	$z(x) = e^{\frac{x-x_0}{\sigma}}$	${}_1F_1$ [163] ${}_2F_1$ [228,229]
8	1, 1/2	$V_0 + V_1 z$	$z(x) = \sec^2 \left( \frac{x-x_0}{2\sigma} \right)$	--
9	1, 1	$V_0 + V_1 z + V_2 z^2$	$z(x) = \frac{1}{e^{(x-x_0)/\sigma} + 1}$	${}_2F_1$ [230]

**Table 2.** Nine independent potentials.  $V_{0,1,2}$  and  $x_0, \sigma$  are arbitrary (complex) constants.

The derived solution applies to any set of the involved parameters. It should be stressed that the parameters in general may be chosen complex. For example, putting  $x_0 \rightarrow x_0 + i\pi\sigma$ , one may change the sign of the exponents involved in the coordinate transformations in the 7th and 9th rows of [Table 2](#).

### 4.3.2. Hypergeometric sub-potentials

Consider the hypergeometric reductions of the above confluent Heun potentials. We first demand for the parameters of the hypergeometric sub-potentials to be independent of each other. Then, the results are as follows.

The confluent Heun equation is reduced to the Kummer equation if  $\delta = 0 \cup q = \alpha$  or  $\gamma = 0 \cup q = 0$ . Examining these two possibilities through equations (97)-(105), one readily reveals that this is possible only in three cases when  $m_{1,2}$  are integers (half-integer  $m_{1,2}$  lead to constant potentials) obeying the inequality  $0 \leq m_1 + m_2 \leq 1$ . Because of the symmetry with respect to the transposition  $m_1 \leftrightarrow m_2 \cup z \leftrightarrow 1-z$ , the number of the independent cases is reduced to two. These are the Coulomb potential [161] and the exponential potential shown in Table 2, where the numbers in the first column indicate the number of the confluent Heun potential to which the particular hypergeometric sub-potential belongs. The first of the two confluent hypergeometric potentials, the Coulomb potential, has been applied in the past by many authors starting from the early days of quantum mechanics. The second potential can be viewed as a truncated one-term version of the Morse potential [163].

The confluent Heun equation is reduced to the Gauss ordinary hypergeometric equation if  $\varepsilon = \alpha = 0$ . It then follows from Eqs. (97), (98), (100) that in this case  $r_3 = v_3 = w_3 = 0$  and  $r_4 = v_4 = w_4 = 0$ , so that the polynomials  $r(z)$ ,  $v(z)$  and  $w(z)$  are of the second degree. Accordingly,  $m_{1,2}$  obey the inequality  $1 \leq m_1 + m_2 \leq 2$  (see Eq. (103)). Hence, hypergeometric sub-potentials may exist only for the six sets  $m_{1,2}$  close to the upper right-hand corner in Fig.10. Because of the symmetry of the hypergeometric equation with respect to the transposition  $z \leftrightarrow 1-z$ , the number of the independent cases is reduced to four. A closer inspection further reveals that the sets with  $m_1 = 1/2$  or  $m_2 = 1/2$  do not lead to non-constant potentials. Thus, we arrive at two four-parametric potentials presented in Table 3.

The first one is identified as a version of the Hulthén potential [228,229], which presents a one-term four-parametric specification of the two-term five-parametric Eckart potential [165]. The second potential is the Woods-Saxon potential [230], which is again a four-parametric one-term specification of the Eckart potential. We note that the two hypergeometric sub-potentials are transformed into each other by simple change  $x_0 \rightarrow x_0 + i\pi\sigma$ . Thus, there exists only one independent ordinary hypergeometric potential. This potential has been explored in the past by many authors on several occasions (see, e.g., [213-216]).

N	$m_1, m_2$	Potential $V(z)$	Coordinate transformation $z(x)$	Reference
1	0, 0	$V_0 + \frac{V_1}{z}$	$z(x) = \frac{x-x_0}{\sigma}$	${}_1F_1$ Coulomb [161]
7	1, 0	$V_0 + V_1 z$	$z(x) = e^{\frac{x-x_0}{\sigma}}$	${}_1F_1$ Exponential (Morse [163])
7	1, 0	$V_0 + \frac{V_1}{z-1}$	$z(x) = e^{\frac{x-x_0}{\sigma}}$	${}_2F_1$ Hulthén [228,229] (Eckart [165])
9	1, 1	$V_0 + V_1 z$	$z(x) = \frac{1}{e^{(x-x_0)/\sigma} + 1}$	${}_2F_1$ Woods-Saxon [230] (Eckart [165])

**Table 3.** Confluent and ordinary hypergeometric potentials. The two ordinary hypergeometric potentials are transformed into each other by the change  $x_0 \rightarrow x_0 + i\pi\sigma$ .

We would like to conclude this section by noting that if a weaker requirement of *conditional* solvability (that is if a parameter of the potential is fixed to a specific value or if the parameters standing for characteristics of different physical origin are dependent) is examined, there may exist other hypergeometric sub-potentials. An example of this kind of sub-potentials is as follows. Consider the case  $m_{1,2} = (1, -1)$ . It is then readily verified that for

$$V_1 = -\frac{c\hbar}{\sqrt{3}\sigma}, \quad V_2 = -\frac{\sqrt{3}c\hbar}{2\sigma}, \quad (106)$$

that is for the potential

$$V = V_0 - \frac{c\hbar}{\sqrt{3}\sigma} \left( \frac{1}{z-1} + \frac{3/2}{(z-1)^2} \right), \quad z = -W \left( -e^{\frac{x-x_0}{\sigma}} \right) \quad (107)$$

it holds  $\delta = 0$  and  $\alpha = q$  so that the confluent Heun equation (85) is reduced to the scaled Kummer confluent hypergeometric equation. This is a conditionally integrable potential since the interaction strengths  $V_{1,2}$  depend on the space scale  $\sigma$ . More strictly, this potential cannot be presented as  $V = \mu f(z)$  with  $f \neq f(\mu)$ . This three-parametric potential ( $V_0, x_0, \sigma$  are arbitrary) and its counterpart for  $m_{1,2} = (-1, 1)$  are marked in Fig.10 by asterisks.

Choosing  $x_0 = -\sigma$  and

$$V_0 = \frac{c\hbar}{2\sqrt{3}\sigma}, \quad (108)$$

we get a single-parametric potential defined for a positive  $\sigma$  on the positive half-axis  $x > 0$  that has a singularity at the origin and vanishes at infinity (Fig.11):

$$V = V_0 \frac{z(z-4)}{(z-1)^2}, \quad z = -\mathcal{W}\left(-e^{-1-x/\sigma}\right). \quad (109)$$

In the vicinity of the origin the behavior of the potential is Coulomb-like:

$$V|_{x \rightarrow 0} = -\frac{\sqrt{3}c\hbar/4}{x} + O(1), \quad (110)$$

while at infinity the potential vanishes exponentially:

$$V|_{x \rightarrow +\infty} = -\frac{2c\hbar}{\sqrt{3}\sigma} e^{-x/\sigma} + O(e^{-2x/\sigma}). \quad (111)$$

The solution of the Klein-Gordon equation for this potential is explicitly written as

$$\psi = z^{\alpha_1} (1-z)^{1/2} e^{\varepsilon z/2} {}_1F_1(\alpha_1; 1+2\alpha_1; -\varepsilon z) \quad (112)$$

with 
$$\alpha_1 = \pm \frac{\sigma}{c\hbar} \sqrt{m^2 c^4 - E^2}, \quad \varepsilon = \pm \frac{2\sigma}{c\hbar} \sqrt{m^2 c^4 - (E - V_0)^2} \quad (113)$$

and 
$$a = \alpha_1 + \left( \frac{1-\varepsilon}{2} - \frac{2}{3\varepsilon} \right) + \frac{m^2 c^4 - E^2}{3\varepsilon V_0^2} + \frac{E}{\varepsilon V_0}. \quad (114)$$

Here any combination of the signs + or - is applicable for  $\alpha_1$  and  $\varepsilon$ . We note that by choosing different signs we get different independent fundamental solutions.

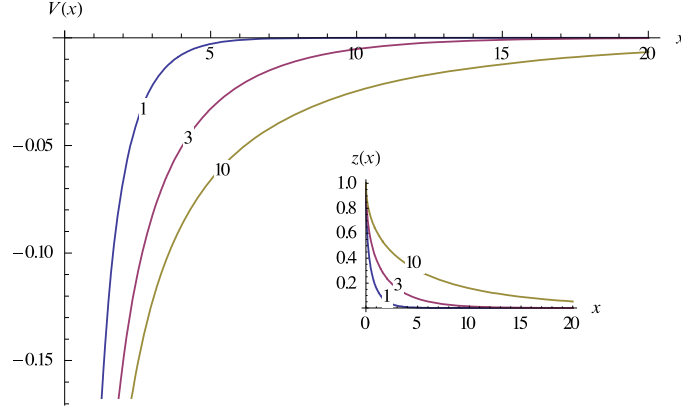


Fig.11. Potential (109) for  $\sigma = 1, 3, 10$  ( $c = \hbar = 1$ ). The inset presents the transformation  $z(x)$ .

#### 4. Discussion

There have been many studies employing reductions of the stationary Klein-Gordon equation to the Heun class of differential equations (for the reductions to the single-confluent Heun equation see, for instance, [222-226] and for a list of sub-cases belonging to the hypergeometric class see [221]). However, to the best of our knowledge, there has not been a general discussion of the solvability of the Klein-Gordon equation in terms of the hypergeometric or more advanced special functions.

In this section we have presented a systematic treatment of this question using the general approach developed in [156,181] for the stationary Schrödinger equation and in [75-77] for the time-dependent quantum two-state problem (see also [52-55]). This is an approach for searching for exactly solvable energy-independent potentials via energy-independent coordinate transformation that is designed for identification of solvable potentials that are proportional to an energy-independent parameter and have a shape that does not depend on that parameter [156]. It should be noted, however, that the technique is also potent to generate conditionally integrable potentials – we have presented an example of this kind of potentials (several other examples are presented in [177-181]).

Discussing the example of the confluent Heun equation which directly incorporates the two hypergeometric equations, we have shown that there exist in total fifteen permissible choices for the coordinate transformation each leading to a four- or five- parametric potential. Because of the symmetry of the single-confluent Heun equation with respect to the transposition  $z \rightarrow 1-z$ , only nine of these potentials are independent. Five of the independent potentials are four-parametric. A peculiarity of these potentials is that they do not possess hypergeometric sub-potentials. Four other independent confluent Heun potentials are five-parametric. These potentials present distinct generalizations of hypergeometric potentials.

Among the independent five-parametric confluent Heun potentials, one potential extends the Coulomb confluent hypergeometric potential [161], another one extends the Hulthén ordinary hypergeometric potential [228,229], and there is a potential that possesses four-parametric sub-potentials of both hypergeometric types (exponential potential, which is a truncated version of the Morse confluent hypergeometric potential [163], and the Woods-Saxon ordinary hypergeometric potential [230]). The fourth five-parametric Heun potential possesses a confluent hypergeometric sub-potential which is a conditionally integrable in the sense that it cannot be presented as being proportional to an energy-independent parameter and having a shape that is independent of that parameter. This is a three-parametric potential explicitly given through a coordinate transformation written in terms of the Lambert- $W$  function [102,103]. The Schrödinger counterpart of this potential has been presented in [164].

We would like to conclude by noting that the applied approach and the lines of the presented analysis are rather general and can be extended to other target equations or to treat other structurally similar problems, for instance, to derive the Heun solutions of the Klein- Gordon equation on manifolds with variable geometry [231] or to identify the potentials for which the Klein-Gordon and other relativistic quantum mechanical wave equations [208] are solvable in terms of the general or multiply-confluent Heun functions.

## Summary and Conclusion

The thesis is devoted to theoretical approaches for resonant optical control of quantum systems having discrete energy spectrum. We consider the manipulation of simplest quantum two-state systems by external optical laser fields when the field is resonant or quasi-resonant for some two of the levels of the system (quantum time-dependent two-state problem). We develop a systematic analytical theory for the quantum two-state dynamics based on the mathematical tools provided by the most advanced at present time special functions - the five functions of the Heun class. The main focus of our study is on the analytic description of physically interesting non-adiabatic evolution of quantum two-state systems subject to excitation by level-crossing field-configurations.

Analytic solutions of physical problems have always been of considerable interest, providing the opportunity of comprehensive analysis of the systems under consideration. However, for the most of contemporary physical problems the analytic solutions are rare because of the lack of appropriate mathematical tools. As regards the quantum two-state problem (one of the simplest quantum problems; even for it the general analytic solution is not known), an observation is that the basic set of analytic models (Landau-Zener, Demkov-Kunike, etc.) has been developed in the past by solving the time-dependent Schrödinger equations in terms of special functions of the hypergeometric class. However, it has recently been shown that there are no more two-state models non-conditionally integrable in terms of the hypergeometric functions and thus the set of possible hypergeometric two-state models is currently exhausted. Furthermore, a peculiarity of hypergeometric models is that they provide utmost one resonance crossing during the interaction process. As known, this is not enough for efficient quantum control: the theory of non-adiabatic transitions indicates that at least two crossings are required to provide efficient control of quantum systems. Hence, more advanced mathematical tools are needed and here is where the Heun functions arise: in this thesis we show that much more models are constructed when expressing the solution of the two-state problem in terms of the Heun functions. Since the Heun functions represent direct generalizations of the hypergeometric functions, the solutions in terms of the Heun functions generalize all hypergeometric cases.

We classify the complete set of the semiclassical time-dependent quantum two-state models solvable in terms of the five advanced special mathematical functions of the Heun class. A major

result we report is that there exist in total 61 infinite classes of two-state models solvable in terms of the Heun functions. More precisely, we have shown that there exist thirty-five classes for which the problem can be solved in terms of the general Heun functions [75], fifteen classes are solvable in terms of the single-confluent Heun functions (these classes have been recently identified by A. Ishkhanyan and A. Grigoryan [76]), and we have shown that there exist five classes solvable in terms of the double-confluent Heun functions [77], five other classes in terms of the bi-confluent Heun functions [77], and a class solvable in terms of the tri-confluent Heun functions [77].

Another set of our results consists of the expansions of the solutions of the general, single-confluent, and bi-confluent Heun equations in terms of the incomplete Beta [78], Kummer confluent hypergeometric [79], and non-integer order Hermite [80] functions. The conditions for termination of these series, in order to produce finite-sum closed-form solutions, are discussed in detail. A remark here is that the general interest in Heun equations and functions arise both from fundamental and computational fields: in parallel to the fundamental research on the properties of solutions of these equations various computational algorithms for numerical calculations of the Heun functions are being developed. Currently, the author of this thesis is working on the project of implementation of the Heun functions into the modern computer algebra system Mathematica.

A third set of our results came out due to the application of the developed series expansions to identify the particular two-state sub-models that describe interesting physical phenomena (such as the periodically repeated or asymmetric-in-time level-crossing processes, etc.) and have exact closed-form solution in terms of simpler mathematical functions [81-83].

The mathematical approaches that are developed in the framework of the present thesis are rather universal and can be applied to explore a wide set of different physical problems. This leads to the fourth set of our results. By applying the developed approaches to non-relativistic and relativistic wave equations, we have derived several new energy-independent quantum-mechanical potentials for the Schrödinger equation that are solved in terms of the functions of the hypergeometric class [80, 84], and have revealed the nine potentials for which the stationary Klein-Gordon equation can be solved in terms of the confluent Heun functions [85]. These results demonstrate the wide applicability of the mathematical tools that we have developed when solving the quantum two-state problem.



Here are the main results of the thesis in detail:

1. We have shown that there exist thirty-five infinite classes of models for which the semiclassical time-dependent two-state problem can be solved in terms of the general Heun functions.
2. We have presented a specific constant-amplitude periodic level-crossing model belonging to a general Heun class of field configurations.
3. We have constructed several series expansions of the general Heun function in terms of the incomplete Beta functions and of the single-confluent Heun function in terms of the Kummer confluent hypergeometric functions.
4. We have introduced an exactly solvable constant-amplitude Lambert-W level-crossing confluent hypergeometric two-state model.
5. We have derived in total eleven infinite classes of the two-state problem solvable in terms of the multi-confluent Heun functions.
6. We have constructed an expansion of the solutions of the bi-confluent Heun equation in terms of the non-integer-order Hermite functions of a shifted and scaled argument.
7. We have introduced the third five-parametric ordinary hypergeometric energy-independent quantum-mechanical potential for the Schrödinger equation, after the Eckart and Pöschl-Teller potentials.
8. We have presented the general solution of the one-dimensional Schrödinger equation for the five independent six-parametric bi-confluent Heun potentials.
9. We have presented in total nine independent potentials for which the stationary Klein-Gordon equation is solvable in terms of the confluent Heun functions.

The thesis thus suggests a set of tools that can be viewed as an advanced theoretical ground for further research on quantum systems dynamics' prediction, analysis and, hence, effective control in real-world experiments.

Many questions are open and have not been considered in the framework of the thesis. First of all, this concerns the particular applications of the derived two-state models of laser-field configurations to concrete physical situations. Next, in the framework of the thesis, we have basically considered only the simplest *lossless* quantum two-state model, while it is well understood that the irreversible losses of different nature are always available in any physical system. Though this question is not explicitly discussed in the thesis, it should be noted the following. All 61 classes of two-state Heun models derived in the thesis generally allow complex parameters. This indicates

that the models may in fact describe the dissipation. We have explicitly demonstrated this in **Chapters 1 and 2** by presenting a few particular two-state Heun models that do describe level-crossing processes with dissipation. Thus, we have shown that it is possible to construct physically realistic and interesting models within these 61 two-state Heun classes. The idealized lossless two-state representations are not imperative for the presented models. Importantly, the dissipative two-state models present shortcuts to the Schrödinger potentials. This is an assertion done in the sense that there is one-to-one mapping between the dissipative two-state models and the real potentials for the Schrödinger equation (e.g., the well known Landau-Zener model is directly transformed, if complex parameters are assumed, to the harmonic oscillator potential). It is also worth mentioning that the dissipative two-state models may open new horizons in the study of non-Hermitian Hamiltonian systems. We intend to study these important topics in our future research.

One more interesting point is the question of the initial conditions. Though all the results presented in the thesis are analytic, and hence, in principle one is able to analyze/predict the behavior of the system under any laser-field configuration from the listed 61 two-state Heun models, it is sometimes difficult to construct the explicit solution which satisfies the prescribed initial conditions. This is because the theory of the Heun functions is still insufficiently developed. As regards the particular cases of exact closed-form solutions written in terms of linear combinations of the hypergeometric functions, the initial conditions for which these solutions are applicable is not discussed in the thesis. This is one more point that we suppose to discuss in the future.

Summarizing, using the tools developed in the current thesis we intend to make the next step in the research on quantum control of few-state systems focusing on the underlying physics. It is understood that the Heun functions and related mathematical developments are merely intermediaries.

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# QUANTUM TWO-STATE LEVEL-CROSSING MODELS IN TERMS OF THE HEUN FUNCTIONS

## Abstract

The thesis is devoted to the fundamental problem of excitation and manipulation of quantum systems, having discrete energy spectrum, via external laser fields. We examine the semiclassical time-dependent quantum two-state problem, when the external electromagnetic field is resonant or quasi-resonant for some two of many levels of the system. The focus of the thesis is on the analytic description of the non-adiabatic evolution of quantum systems subject to excitation by level-crossing field-configurations. In the present thesis we classify the complete set of the semiclassical time-dependent quantum two-state models solvable in terms of the five function of the Heun class.

Main results of the thesis are:

1. In total 61 infinite classes of two-state models (i.e. external laser field configurations) solvable in terms of general and confluent Heun functions are derived.
2. In these infinite classes three original level-crossing submodels are identified: one describes infinite (periodical) crossings of resonance, one describes asymmetric resonance crossing with a finite time of process and the last one describes infinite asymmetric resonance crossing process. The behavior of the two-state quantum system under these field configurations is comprehensively analyzed.
3. Solutions of the Heun equations in terms of incomplete Beta functions, Kummer confluent hypergeometric functions and non-integer-order Hermite functions of a shifted and scaled argument are constructed.
4. Analytic solutions of the quantum two-state problem are projected on the relativistic and non-relativistic wave-equations: new potentials for the Schrödinger and Klein-Gordon equations are derived and solved.

**Keywords:** *laser excitation; quantum two-state problem; level-crossings; Heun functions.*

# MODÈLES QUANTIQUES À DEUX ÉTATS AVEC CROISEMENTS DE NIVEAUX DÉCRITS PAR LES FONCTIONS DE HEUN

## Résumé

La thèse est consacrée au problème fondamental de l'excitation et de la manipulation de systèmes quantiques à spectre d'énergie discret, via des champs lasers externes. Nous examinons le problème semi-classique à deux états quantiques, dépendant du temps, lorsque le champ électromagnétique externe est résonant ou quasi résonant pour deux des nombreux niveaux du système. La thèse est centrée sur la description analytique de l'évolution non adiabatique des systèmes quantiques soumis à une excitation par des configurations de champs avec croisements de niveaux. Dans la présente thèse, nous classifions l'ensemble complet des modèles quantiques à deux états semi-classiques dépendants du temps, qui peuvent être résolus en cinq fonctions de la classe de Heun.

Les principaux résultats de la thèse sont :

1. Au total, 61 classes infinies de modèles à deux états (i.e. les configurations de champ laser externe) solubles en termes de fonctions de Heun générale et confluentes sont dérivées.
2. Dans ces classes infinies, trois sous-modèles originaux avec croisements de niveaux sont identifiés: l'un décrit les croisements infinis de résonance (périodiques), l'autre décrit les croisements de résonance asymétrique avec un temps de processus fini et le dernier décrit les processus de croisements infinis de résonance asymétrique. Le comportement du système quantique à deux états dans ces configurations de champ est analysé de manière exhaustive.
3. Les solutions des équations de Heun en termes de fonctions bêta incomplètes, de fonctions hypergéométriques confluentes de Kummer et de fonctions Hermite d'ordre non entier sont construites.
4. Des solutions analytiques du problème quantique à deux états sont projetées sur les équations d'onde relativistes et non relativistes : de nouveaux potentiels pour les équations de Schrödinger et de Klein-Gordon sont dérivés et résolus.

**Mots clefs :** *excitation laser; système quantique à deux états; croisements de niveaux; fonctions de Heun.*