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A Dissipative Conditionally Integrable Two-State Level-Crossing Model Exactly Solvable in Terms of the Bi-Confluent Heun Functions

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Abstract. We present a conditionally integrable level-crossing model for the quantum time-dependent two-state problem involving irreversible losses from the second level. The model is given by an exponentially varying Rabi frequency and a level-crossing detuning that starts from the exact resonance and exponentially diverges at the infinity. The model includes irreversible losses from the second level, while the spontaneous relaxation to the first level is neglected. We derive the exact solution of the two-level problem for this and discuss the dynamics of levels' populations under different regimes of the interaction.

Keywords: Quantum two-state problem; laser excitation; irreversible losses; analytic solutions; bi-confluent Heun equation; Hermite function

1. Introduction

The interaction of real quantum systems with radiation is often approximated by the quantum two-state problem [1-17]. This is a useful approximation which implies that two of system's levels are resonant or nearly resonant with the external driving field, while the remaining levels are far off resonance.

In the present paper we discuss an analytic model of the two-state problem that involves losses from the upper level. The field configuration we consider is given by an exponentially varying Rabi frequency and a level-crossing detuning that starts from the exact resonance and exponentially diverges at the infinity. This model belongs to the bi-confluent Heun class [18,19]. It is a conditionally integrable model in that sense that the amplitude-modulation and detuning-modulation functions, which compose the field configuration, do not vary independently. Applying transformations of both dependent and independent variables, we reduce the time-dependent Schrödinger equations for the two-level system under consideration to the bi-confluent Heun equation which is a second-order ordinary linear differential equation widely encountered in many branches of contemporary physics [20,21].

Further, following the approach of [22,23], we construct the solution of the bi-confluent Heun equation as a series in terms of the Hermite functions [24,25]. We note that these functions have an alternative representation through the Kummer or Tricomi confluent hypergeometric functions. The coefficients of the expansion obey a three-term recurrence relation between successive coefficients. We derive the conditions for both right- and left-hand side termination of the derived series and show that the solution for the particular dissipative that we treat is written as a linear combination of two Hermite functions of a scaled and shifted argument. In general, these are Hermite functions of non-integer order so that they do not reduce to polynomials.

Finally, using the derived solution, we discuss the population dynamics of a dissipative two-state quantum system subject to the optical excitation by a field of the mentioned field configuration. Owing to the explicit analytic form of the solution, we treat both weak and strong interaction regimes.

2. Reduction of the two-state problem to the bi-confluent Heun equation

We consider the semi-classical time-dependent two-state problem with a decaying upper level. Let the probability amplitudes of the ground and excited states be $a_1(t)$ and $b_2(t)$, respectively. If the decay of the excited state is supposed to be to a third state, the equations for the probability amplitudes read [15]

$$i\frac{da_1}{dt} = U(t)\,b_2, \quad i\frac{db_2}{dt} = U(t)\,a_1 + \left(\tilde{\delta}_t(t) - i\Gamma\right)b_2, \tag{1}$$

where the Rabi frequency $U(t)$ and the frequency modulation function $\tilde{\delta}(t)$ (the derivative of this function $\tilde{\delta}_t(t)$ is the detuning of the transition frequency from the field frequency) are arbitrary real functions of time, and the parameter Γ defines the rate of the losses from the upper level.

By change of the variable $b_2 = a_2(t)\,e^{-i\,\delta(t)}$ and further elimination of a_1, system (1) is reduced to the following second-order linear differential equation for $a_2(t)$:

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

where (and hereafter) the lowercase alphabetical index denotes differentiation with respect to the corresponding variable. According to the class property of the integrable models of the two-state problem [26,27], 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

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

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

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

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

This equation is the bi-confluent Heun equation

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

if

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

and

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

Equations (6) and (7) compose an under determined system of two nonlinear equations for three unknown functions, $U^*(z)$, $\delta^*(z)$ and $\varphi(z)$. The general solution of this system is not known. However, many particular solutions can be found starting from specific forms of the involved functions. We here present the known solutions following the approach of [18,19].

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

$$\varphi = z^{\alpha_1} e^{\alpha_0 z + \alpha_2 z^2/2}\ , \tag{8}$$

$$U^* = U_0^* z^k, \tag{9}$$

$$\delta_z^* = \frac{\delta_1}{z} + \delta_0 + \delta_2 z\,, \tag{10}$$

leads to 5 possible cases of integer or half-integer k, obeying the inequalities $0 \le 2k+2 \le 4$ [18,19]. Hence, according to equations (3), the actual field configuration is given as

$$U(t) = U_0^* z^k \frac{dz}{dt}\,, \tag{11}$$

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

with $k = -1, -1/2, 0, 1/2, 1$ [18]. The parameters U_0^* and $\delta_{0,1,2}$ 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 initial two-state problem is explicitly written as [19]

$$b_2 = z^{\alpha_1} e^{\alpha_0 z + \alpha_2 z^2/2}\, e^{i\delta(t)}\, H_B(\gamma, \delta, \varepsilon; \alpha, q; z)\,, \tag{13}$$

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

$$\gamma = 2\alpha_1 - i\delta_1 - k\,, \quad \delta = 2\alpha_0 - i\delta_0\,, \quad \varepsilon = 2\alpha_2 - i\delta_2 \tag{14}$$

$$\alpha = \alpha_0(\alpha_0 - i\delta_0) + \alpha_1(2\alpha_2 - i\delta_2) + \alpha_2(1 - k - i\delta_1) + Q''(0)/2\,, \tag{15}$$

$$q = \alpha_0(k + i\delta_1) - \alpha_1(2\alpha_0 - i\delta_0) - Q'(0) \tag{16}$$

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

$$\alpha_0\varepsilon - i\alpha_2\delta_0 + Q'''(0)/3! = 0\,, \tag{17}$$

$$\alpha_1^2 - \alpha_1(1 + k + i\delta_1) + Q(0) = 0\,, \tag{18}$$

$$\alpha_2^2 - i\alpha_2\delta_2 + Q^{(4)}(0)/4! = 0\,. \tag{19}$$

3. Series solutions of the bi-confluent Heun equation in terms of the Hermite functions

Following the lines of [28] we present the expansion of the solution of the bi-confluent Heun equation (5) in terms of the Hermite functions of a shifted and scaled argument:

$$u = \sum_n c_n u_n\,, \quad u_n = H_{\alpha_0+n}\left(s_0(z+z_0)\right), \tag{20}$$

where α_0, s_0 and z_0 are complex constants. The involved Hermite functions satisfy the following second-order linear differential equation:

$$\frac{d^2 u_n}{dz^2} - 2s_0^2(z+z_0)\frac{du_n}{dz} + 2s_0^2\alpha_n u_n = 0\,, \quad \alpha_n = \alpha_0 + n\,. \tag{21}$$

Substituting equations (20) and (21) into equation (5) and multiplying the result by z we get

$$\sum_n c_n\left[\left(\gamma + z(\delta + \varepsilon z) + 2s_0^2 z(z+z_0)\right)u_n' + \left(\alpha z - q - 2s_0^2\alpha_n z\right)u_n\right] = 0\,. \tag{22}$$

By putting $s_0 = \pm\sqrt{-\varepsilon/2}$ and $z_0 = \delta/\varepsilon$, the terms proportional to zu_n' and z^2u_n' are cancelled so that using the recurrence identities

$$u_n' = 2s_0\alpha_n u_{n-1}\,, \quad s_0(z+z_0)u_n = \alpha_n u_{n-1} + u_{n+1}/2\,, \tag{23}$$

we arrive at a three-term recurrence relation for coefficients c_n:

$$R_n c_n + Q_{n-1}c_{n-1} + P_{n-2}\,c_{n-2} = 0\,, \tag{24}$$

where

$$R_n = \frac{\sqrt{2}}{\sqrt{-\varepsilon}}(\alpha_0 + n)\left(\alpha + (\alpha_0 + n - \gamma)\varepsilon\right), \tag{25}$$

$$Q_n = \mp \frac{\alpha\,\delta + (q + (\alpha_0 + n)\,\delta)\varepsilon}{\varepsilon}\,, \tag{26}$$

$$P_n = \frac{\alpha + (\alpha_0 + n)\,\varepsilon}{\sqrt{-2\varepsilon}}\,. \tag{27}$$

Here 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 $n = 0$ it should hold $R_0 = 0$ so that $\alpha_0 = 0$ or $\alpha_0 = \gamma - \alpha/\varepsilon$. The choice $\alpha_0 = 0$ leads to polynomial solutions, hence, in order to get a more advanced series we put $\alpha_0 = \gamma - \alpha/\varepsilon$. The final expansion is then written as

$$u = \sum_{n=0}^{\infty} c_n H_{n+\gamma-\alpha/\varepsilon}\left(\pm\sqrt{-\varepsilon/2}\,(z + \delta/\varepsilon)\right). \tag{28}$$

The series terminates from the right-hand side if two successive coefficients, say c_{N+1} and c_{N+2}, vanish for some $N = 0,1,2,\ldots$. Equation $c_{N+2} = 0$ is satisfied if $P_N = 0$. This is equivalent to the condition $\gamma = -N$. Since ε should be non-zero, the equation $c_{N+1} = 0$ leads to a polynomial equation of the degree $N+1$ for the accessory parameter q, which is referred to as q-equation. We will now see that this equation is satisfied for the particular dissipative two-level problem that we consider.

4. A conditionally integrable two-state model

For a given field configuration (11)-(12) with input parameters U_0^* and $\delta_{0,1,2}$, the parameters of the bi-confluent Heun function and those of the pre-factor $\varphi(z)$ involved in the solution (13) are calculated through the equations (14)-(19). According to the expansion presented in the previous section, in order that the bi-confluent Heun function be written as a finite-sum linear combination of the Hermite functions, the parameters of the bi-confluent Heun function should necessarily satisfy the condition $\gamma = -N$ with a non-negative integer N and the corresponding q-equation. Obviously, the latter equations cannot be satisfied for arbitrary parameters U_0^* and $\delta_{0,1,2}$ involved in the field configuration (11)-(12). The necessary conditions for termination of the series (28) are satisfied only for some special sets of U_0^* and $\delta_{0,1,2}$. It turns out that in many cases these allowed sets are such that some parameters of the field configuration are expressed through other parameters. Since then the amplitude- and detuning-modulation functions do not vary independently, in these cases we meet *conditionally* integrable two-state models.

We now present an example of such a conditionally integrable two-state model. We consider the case of two-term termination of the series (28), so that the solution of the initial two-state problem is written as a sum of two Hermite functions. In this case

$$\gamma = -1 \tag{29}$$

and the q-equation is a second-degree polynomial equation [28]:

$$q^2 - \delta q + \alpha = 0\,. \tag{30}$$

Consider the class with $k = 1/2$. For this case equations (29), (30) lead to the only possible value for the parameter δ_1:

$$\delta_1 = -i/2\,. \tag{31}$$

The field amplitude- and detuning-modulation functions (11), (12) then become

$$U(t) = U_0^* \sqrt{z(t)}\,\frac{dz(t)}{dt}\,, \tag{32}$$

$$\delta_t(t) = \left(-\frac{i}{2z} + \delta_0 + z\delta_2\right)\frac{dz(t)}{dt}. \tag{33}$$

As an independent variable transformation we now take the real-valued function $z = \exp(2\Gamma t)$ and arrive at the following three-parametric level-crossing field configuration:

$$U(t) = U_0 e^{3t}, \tag{34}$$

$$\delta_t(t) = \tilde{\delta}_t(t) - i\Gamma = 2\left(\delta_0 e^{2t} + \delta_2 e^{4t}\right) - i. \tag{35}$$

where U_0, δ_0 and δ_2 are arbitrary real parameters. We have here put $U_0 = 2U_0^*$ and $\Gamma = 1$. The last condition implies that hereafter all the involved parameters are supposed dimensionless. Equations (34), (35) define a field configuration with a detuning-modulation function $\tilde{\delta}_t(t)$ describing an asymmetric-in-time level-crossing process. The field configuration is presented in Fig. 1.

The crossing of the resonance occurs at the time point

$$t_0 = \ln(-\delta_0/\delta_2)/2. \tag{36}$$

We note that in the vicinity of the resonance crossing point the behavior of the detuning is approximately modeled by the linear crossing law of the Landau-Zener type:

$$\delta_t = \frac{4\delta_0^2}{\delta_2} t + O(t^2), \tag{37}$$

so that the resonance crossing rate is mostly defined by the combined parameter δ_0^2/δ_2.

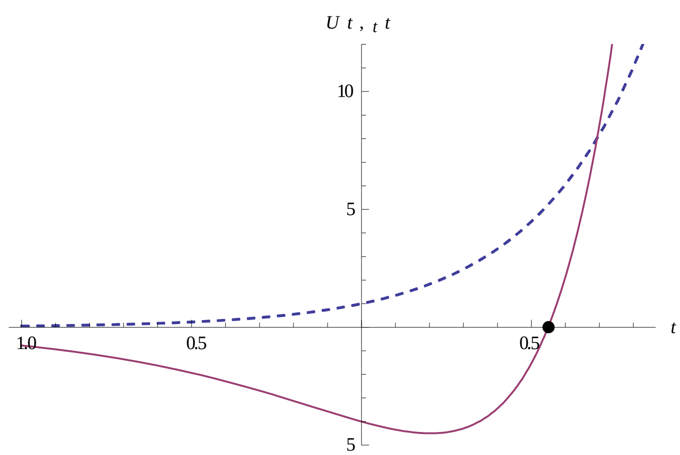

Fig. 1. Conditionally integrable dissipative two-state level-crossing model (34)-(35). The dashed line is the Rabi frequency ($U_0 = 1$) and the solid line stands for the detuning ($\delta_2 = 1$, $\delta_0 = -3$). The filled circle indicates the level-crossing time point $t_0 = \ln(-\delta_0/\delta_2)/2$.

5. The population dynamics of the dissipative two-state system

According to the expansion (28), a fundamental solution of the initial two-state problem (1) is written through a linear combination of two Hermite functions:

$$b_2^F(t) = z^{\alpha_1} e^{\alpha_0 z + \alpha_2 z^2/2}\, e^{i\delta(t)} \left(c_0 H_{\alpha/\varepsilon - 1}(y) + c_1 H_{\alpha/\varepsilon}(y)\right), \tag{38}$$

where

$$y = s\sqrt{\frac{-\varepsilon}{2}}\left(z + \frac{\delta}{\varepsilon}\right), \quad z(t) = e^{2\Gamma t}. \tag{39}$$

The expansion coefficients $c_{0,1}$ are conveniently written through the parameters of the bi-confluent Heun function, which are readily calculated through the amplitude and detuning modulation functions' parameters and an auxiliary parameter $s=\pm 1$. The result reads

$$c_0 = 1, \quad c_1 = s\sqrt{\frac{-\varepsilon}{2}}\left(\frac{\delta - q}{\alpha}\right). \tag{40}$$

We note that $s=+1$ and $s=-1$ produce linearly independent fundamental solutions. This is readily verified by checking the Wronskian of the two solutions. Hence, the linear combination of these fundamental solutions

$$b_2(t) = C_1 b_2^F\Big|_{s\to+1} + C_2 b_2^F\Big|_{s\to-1}. \tag{41}$$

with arbitrary constant coefficients $C_{1,2}$ presents the general solution of the problem.

We consider the situation when the system initially starts from the ground state, that is, we impose the initial conditions

$$a_1(-\infty) = 1, \quad b_2(-\infty) = 0. \tag{42}$$

In Fig. 2 we present the graphs for the probability $p_1 = |a_1(t)|^2$ for the atom to stay on the first level and the probability $p_2 = |b_2(t)|^2$ for the atom to be occupying the excited state during the interaction. As it is clearly seen, for the chosen field parameters the result of the dissipation is the complete removal of the population from both levels. It is understood that this is because the chosen field parameters provide a sufficiently intensive interaction with the field accompanied with a strong decay rate from the excited state. The analysis of the asymptotes of the solution reveals that the physical parameter defining the interaction regime is $\lambda \sim U_0^2/(\delta_0\delta_2)$: The strong interaction regime corresponds to large $\lambda \gg 1$, while the weak interaction regime applies to small $\lambda \ll 1$.

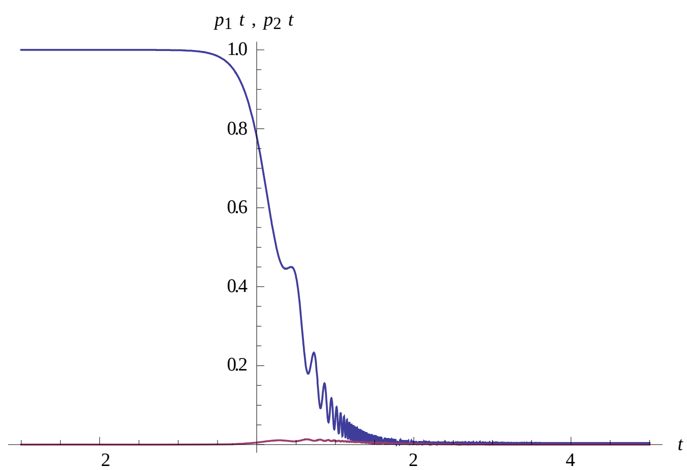

Fig. 2. Probabilities $p_1 = |a_1(t)|^2$ and $p_2 = |b_2(t)|^2$ (blue and orange lines, respectively) for the field configuration parameters $U_0 = 1$, $\delta_0 = -3$, $\delta_2 = 1$.

As the field amplitude increases, the excitation of the atom intensifies, the second level becomes more populated, hence, the losses from the second level become more pronounced (Fig. 3). In contrast, if the field amplitude decreases, the excitation processes slows down, the excited state becomes less populated so that the losses from the second level wash out from the system a lesser population and, as a result, the system may end up with a not depleted population of the ground state (Fig. 4).

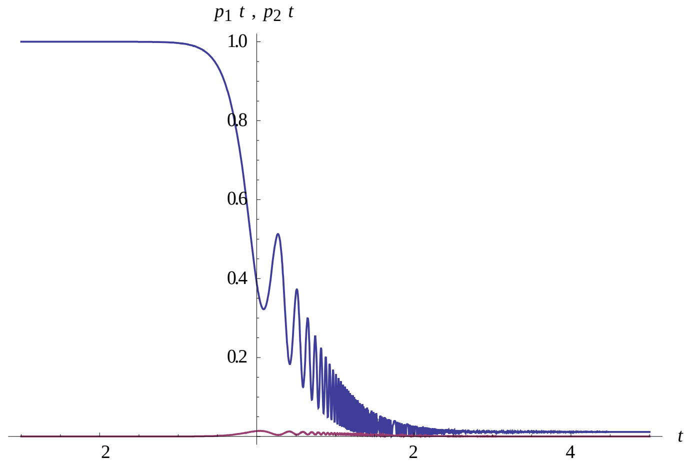

Fig. 3. Occupation probabilities for the ground and excited states (blue and magenta lines, respectively) for the field configuration parameters $U_0 = 2$, $\delta_0 = -3$, $\delta_2 = 1$.

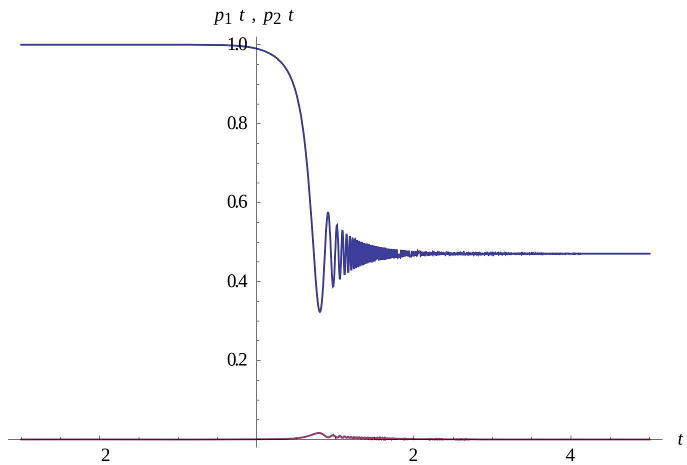

Fig. 4. Occupation probabilities for the ground and excited states (blue and magenta lines, respectively) for the field configuration parameters $U_0 = 0.2$, $\delta_0 = -3$, $\delta_2 = 1$.

From Figs. 3 and 4 we conclude that if the field amplitude is small, then during the interaction the population of the first level decreases, because of the resonance crossing; however, at the end of the process the first level still possesses a remnant population, while the second level always completely empties because of the losses. In other words, if the coupling is weak (that is the Rabi frequency is small), then the interaction is not very intensive (compared to the case presented in Fig. 2), so that by the effective time of the resonance crossing the population of the first level manages not to get fully exhaust.

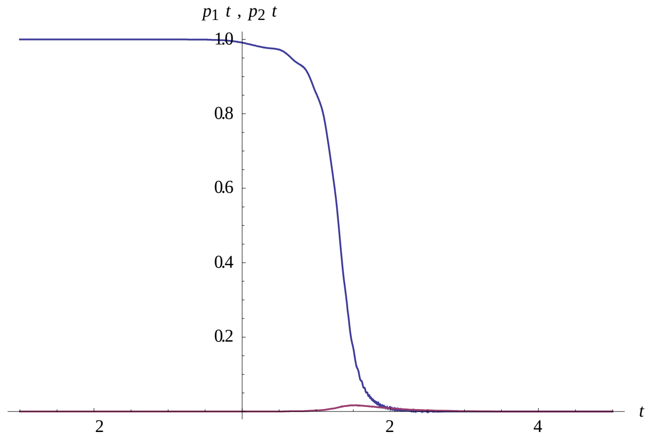

Fig. 5. Occupation probabilities for the first and second levels (blue and magenta lines, respectively) for the weak but long interaction: $U_0 = 0.2$, $\delta_0 = -3$, $\delta_2 = 0.2$.

Finally, even for a weak coupling (small Rabi frequency), complete transition to the second level is possible if δ_2 is sufficiently small (Fig. 5). In this case the system remains near the resonance for a sufficiently long time period, hence, the second level may be well populated thus resulting in complete decay of the population to a third state.

6. Discussion

Thus, we have presented an analytic model of a dissipative semi-classical quantum two-state problem coupled to an external optical field. The physical processes responsible for the dissipation may include photo-induced decomposition of particles, spontaneous emission of photons, collision relaxation, etc. In the model we treat, the excited state is supposed to decay irreversibly out of the system, while the decay transition from the excited to the ground state is neglected.

We have reviewed the specific field configurations for which the time-dependent two-state problem is reduced to the bi-confluent Heun equation which is a second-order ordinary linear differential equation having a regular singularity and an irregular singularity of rank 2. In order to treat the derived solution, we have applied an expansion of the involved bi-confluent Heun function in terms of the non-integer order Hermite functions of a scaled and shifted argument. The expansion is governed by a three-term recurrence relation between the successive coefficients of the expansion. We have discussed the conditions for the derived series to terminate thus resulting in finite-sum solutions.

As an application of such a termination to the two-state problem under consideration, we have identified a conditionally integrable resonance-crossing field configuration for which the termination results in a general solution written through fundamental solutions each of which involves an irreducible linear combination of two Hermite functions. This is a configuration given by an exponentially diverging Rabi frequency and a level-crossing detuning that starts from the exact resonance and exponentially diverges at the infinity. Using the two-term Hermite-function explicit solution, we have studied the population dynamics in different interaction regimes.

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