New exactly solvable time-dependent quantum two-state models

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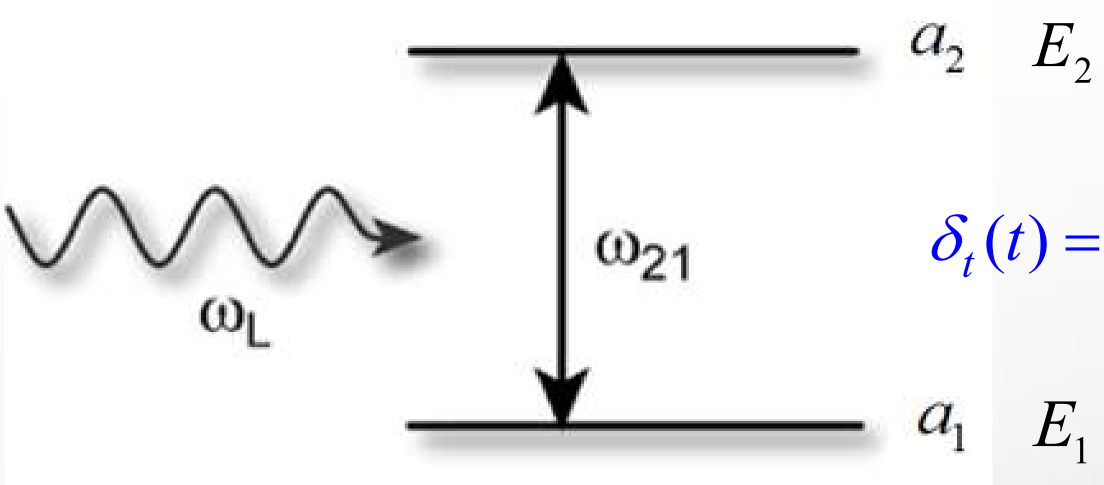
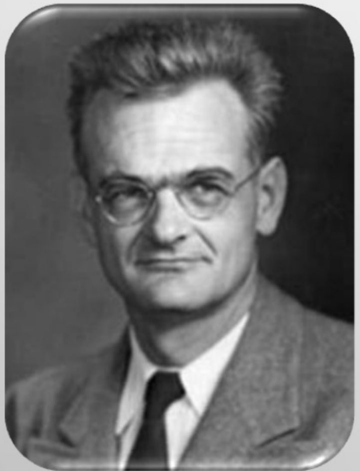
Quantum time-dependent two-state problem

Laser field

$U(t),\ \delta_t(t)$



$\delta_t(t) = \omega_{21} - \omega_L(t)$



Theory of *non-adiabatic* transitions in quantum mechanics

$$\begin{cases} i\dfrac{da_1}{dt} = Ue^{-i\delta}a_2 \\ i\dfrac{da_2}{dt} = Ue^{+i\delta}a_1 \end{cases}$$

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

C. Zener, "Non-adiabatic crossing of energy levels", Proc. Roy. Soc. A 137, 696 (1932).

Non-adiabaticity is due to level-crossing: $\delta_t(t = t_0) = 0 \ \Leftrightarrow\ \omega_L(t_0) = \omega_{21}$

Mathematically, this is because of a singularity of the governing equations

Shortcut to the Schrödinger equation

- Consider the *constant-amplitude* field configuration: $U(z)=U_0=\mathrm{const}$

$$a_{2zz} - i\delta_z a_{2zz} + U_0^2 a_2 = 0$$

- Transform the dependent variable: $a_2 = \varphi(z)\psi(z)$

$$\psi_{zz} + \cancel{\left(2\frac{\varphi_z}{\varphi} - i\delta_z\right)\psi_z} + \left(\frac{\varphi_{zz}}{\varphi} - i\delta_z\frac{\varphi_z}{\varphi} + U_0^2\right)\psi = 0$$

- With $2\varphi_z/\varphi = i\delta_z$ we remove the first-derivative term and obtain the Schrodinger equation

$$\psi_{zz} + \left(E - V(z)\right)\psi = 0$$

- with

$$E = U_0^2$$

$$V(z) = -\frac{\delta_z^2}{4} - i\frac{\delta_{zz}}{2}$$

- The potential $V(z)$ is complex – non-Hermitian Hamiltonian

The two-state problem presents an example of non-Hermitian evolution

Theorem: Class property of solvable models

$$\frac{d^2 a_2}{dt^2} + \left(-i\delta_t - \frac{U_t}{U}\right)\frac{da_2}{dt} + U^2 a_2 = 0 \qquad (1)$$

- Physics equations are usually solved by reducing them to known mathematical equations
- Transformation of dependent and independent variables

$$a_2 = \varphi(z)u(z), \quad z = z(t)$$

- However, in this case the transformation of the independent variable *z(t)* is not needed !
- **Theorem:** Let $a_2^*(z)$ solves the equation $a_{2zz}^* + \left(-i\delta_z^* - \frac{U_z^*}{U^*}\right)a_{2z}^* + U^{*2}a_2^* = 0$ for some functions $\left(U^*(z),\, \delta_z^*(z)\right)$
- Then, $a_2(t) = a_2^*(z(t))$ solves (1) for the field configuration

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

A.M. Ishkhanyan, J. Phys. A **33**, 5539 (2000).

The transformation of the independent variable is not needed at all !
It can be incorporated afterwards

General reduction procedure

- Rewrite two-state equation for a variable z and functions U^*, δ_z^*

$$a_{2zz}^* + \left(-i\delta_z^* - \frac{U_z^*}{U^*} \right) a_{2z}^* + U^{*2} a_2^* = 0$$

- Transform only the dependent variable: $a_2^* = \varphi(z) u(z)$

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

- Target equation (with rational coefficients):

$$u_{zz} + f(z) u_z + g(z) u = 0$$

- Singularities of this equation: $z_1, z_2, z_3, \ldots, z_m$

- The only possible substitution

$$\varphi = (z - z_1)^{\alpha_1} (z - z_2)^{\alpha_2} \ \ldots \ (z - z_m)^{\alpha_m}$$

$$U^* = U_0^* (z - z_1)^{k_1} (z - z_2)^{k_2} \ \ldots \ (z - z_m)^{k_m}$$

k_m all are integers or half-integers

$$\delta_z^* = \frac{\delta_1}{z - z_1} + \frac{\delta_2}{z - z_2} + \ldots + \frac{\delta_m}{z - z_m}$$

!

A. Ishkhanyan and V. Krainov, Eur. Phys. J. Plus **131**, 342 (2016).

The function z″ /z′ must have the same finite singularities as the target equation

Classical confluent-hypergeometric models

- Kummer equation: $$u_{zz}+\left(\frac{\gamma}{z}-1\right)u_z-\frac{\alpha}{z}u=0$$
- Three classes of solvable models:

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

- For all three: $$\delta_t(t)=\left(\frac{\delta_1}{z}+\delta_2\right)\frac{dz}{dt}$$

A.M. Ishkhanyan, J. Phys. A **33**, 5539-5546 (2000).

- The first Nikitin model: $U=U_0,\quad \delta_t=\delta_1+\delta_2 e^t$ $\longrightarrow$ **Morse potential**

  E.E.Nikitin, Opt. Spectroscopy **6**, 431-433 (1962); Discuss.Faraday Soc. **33**, 14-21 (1962).

- Landau-Zener model: $U=U_0,\quad \delta_t=\delta_1 t+\delta_2/t$ $\longrightarrow$ **Harmonic oscillator**

  L.D. Landau, Phys. Z. Sowjetunion **2**, 46-51 (1932); C. Zener, Proc. R. Soc. London, Ser. A 137, 696-702 (1932).

- The second (standard) Nikitin model: $U=U_0,\quad \delta_t=\delta_1+\delta_2/t$ $\longrightarrow$ **Coulomb**

  E.E. Nikitin and S.Ya. Umanski, *Theory of Slow Atomic Collisions,* Springer, Berlin, 1984.

Three independent confluent-hypergeometric classes

Classical ordinary-hypergeometric models

- Gauss ordinary-hypergeometric equation:

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

- Two classes of solvable models:

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

- For both of them: $$\delta_t(t)=\left(\frac{\delta_1}{z}+\frac{\delta_2}{z-1}\right)\frac{dz}{dt}$$

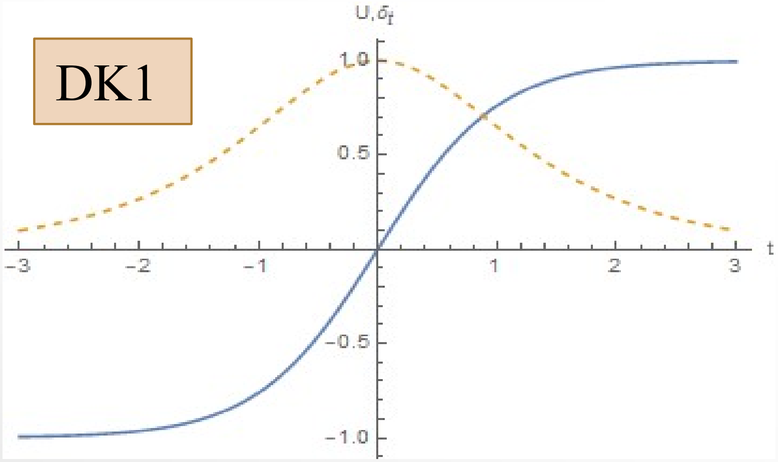
A.M. Ishkhanyan, J. Phys. A **33**, 5539-5546 (2000).

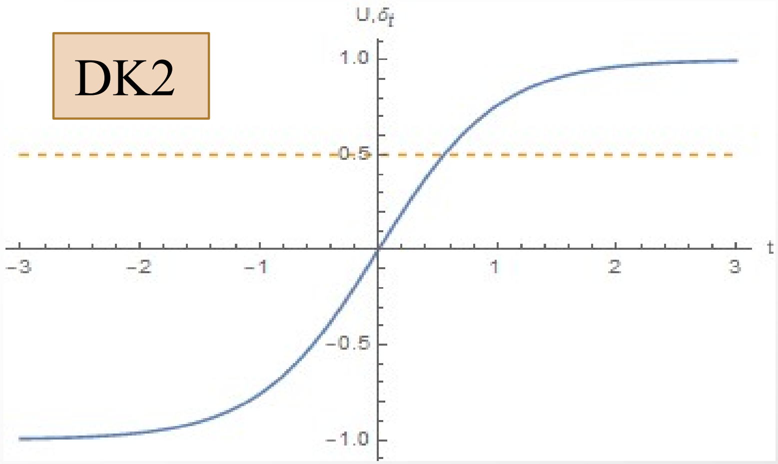
- The first Demkov-Kunike model DK1 $\longrightarrow$ **Pöschl-Teller potential**
- The second Demkov-Kunike model DK2 $\longrightarrow$ **Eckart potential**

1. Yu.N. Demkov and M. Kunike, Vestn. Leningr. Univ. Fis. Khim. **16**, 39 (1969).
2. K.A. Suominen, B.M. Garraway, Phys. Rev. A **45**, 374 (1992).

Two independent ordinary-hypergeometric classes

The two Demkov-Kunike models





$$U(t) = U_0 \operatorname{sech}(t/\tau)$$
$$\delta_t(t) = \delta_0 + \delta_1 \tanh(t/\tau)$$

$$z = (1 + \tanh t)/2$$

$$U(t) = U_0$$
$$\delta_t(t) = \delta_0 + \delta_1 \tanh(t/\tau)$$

$$z = -e^t$$

1. Yu.N. Demkov and M. Kunike, Vestn. Leningr. Univ. Fis. Khim. **16**, 39 (1969).
2. K.A. Suominen, B.M. Garraway, Phys. Rev. A **45**, 374 (1992).

The solution of the two-state problem for these models is written in terms of ordinary Gauss hypergeometric functions ${}_2F_1(a,b;c;z)$

The second Demkov-Kunike model is unique.
Its symmetric version belongs to both ordinary-hypergeometric classes.

The general Heun equation

Equations of the Heun class

$$(p_0 + p_1 z + p_2 z^2 + p_3 z^3)\frac{d^2u}{dz^2} + (\gamma_1 + \delta_1 z + \varepsilon_1 z^2)\frac{du}{dz} + (\alpha_1 z - q_1)u = 0$$

$$P_3(z) = p_3 \cdot (z - z_1)(z - z_2)(z - z_3)$$

$$z \to s_1 z + s_0 \quad \Rightarrow \quad \boxed{P_3(z) = 1 \cdot z(z-1)(z-a)}$$

1. General Heun equation

$$\boxed{\frac{d^2u}{dz^2} + \left(\frac{\gamma}{z} + \frac{\delta}{z-1} + \frac{\varepsilon}{z-a}\right)\frac{du}{dz} + \frac{\alpha\beta z - q}{z(z-1)(z-a)}u = 0}$$

Riemann P-symbol: $\begin{pmatrix} 0 & 1 & a & \infty & \\ 0 & 0 & 0 & \alpha & z \\ 1-\gamma & 1-\delta & 1-\varepsilon & \beta & \end{pmatrix}$

The four confluent Heun equations

2. Single-confluent Heun equation

$$\frac{d^2u}{dz^2}+\left(\frac{\gamma}{z}+\frac{\delta}{z-1}+\varepsilon\right)\frac{du}{dz}+\frac{\alpha z-q}{z(z-1)}u=0$$

3. Double-Confluent Heun equation

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

4. Bi-Confluent Heun equation

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

5. Tri-Confluent Heun equation

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

The most singular (and hence the most complicated) are the double- and tri-confluent Heun equations

Reduction to the general Heun equation

- Rewrite the two-state equation for a variable z and functions $U^*,\ \delta_z^*$

$$a_{2zz}+\left(-i\delta_z-\frac{U_z}{U}\right)a_{2z}+U^2a_2=0$$

- Transform only the dependent variable: $a_2=\varphi(z)u(z)$

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

- The general Heun equation:

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

There are 35 generator functions $\left\{U^*,\delta_z^*\right\}$

Hence, 35 classes of general Heun models $\left\{U(t),\delta_t(t)\right\}$

A.M. Ishkhanyan, T.A. Shahverdyan, T.A. Ishkhanyan, Eur. Phys. J. D **69**, 10 (2015)

Only 11 classes are independent

Solutions of the general Heun equation in terms of ${}_3F_2$

- If $\gamma = -N$ and accessory parameter q satisfies a certain polynomial equation, the solution of the general Heun equation is written in terms of a single generalized hypergeometric function ${}_rF_s$.

- The simplest non-trivial case is $\gamma = -1$ and

$$q^2 + q\left(a\delta + \varepsilon - 1 - a\right) + a\alpha\beta = 0$$

- Checking the thirty-five general Heun classes of the two-state models, we find that the only class for which these equations are *unconditionally* satisfied is the class defined by the triad

$$(k_1, k_2, k_3) = (1, -1, -1)$$

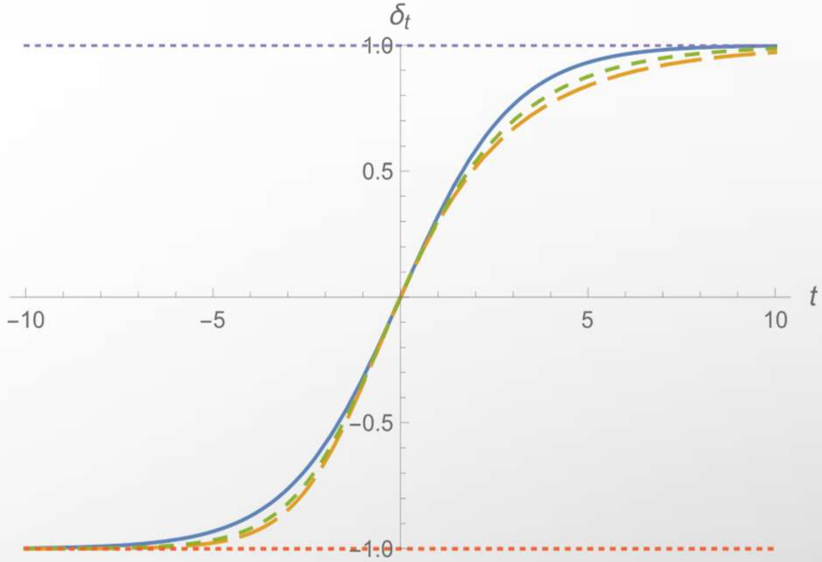
- Corresponding *laser-field* configuration is given as

$$U(t) = \frac{U_0^* z}{(z-1)(z-a)} \frac{dz}{dt} \qquad \delta_t(t) = \left(\frac{\delta_2}{z-1} + \frac{\delta_3}{z-a}\right) \frac{dz}{dt}$$

This is the only family that is exactly solvable in terms of a finite sum of the Gauss hypergeometric functions $\boldsymbol{{}_2F_1}$

A new time-dependent two-state 2F1 model

$U(t) = U_0 = \text{const}$ $\delta_t(t) = \Delta_1 + \dfrac{\Delta_0 - \Delta_1}{z}$



$z(t)$ obeys the algebraic equation $\dfrac{(z-a)^a}{z-1} = e^{-t/\tau}$

For this a=-2 we have a cubic algebraic equation in z, which is resolved as

$$z = -1 + \frac{1}{\left(e^{t/2\tau} + \sqrt{1+e^{t/\tau}}\right)^{2/3}} + \left(e^{t/2\tau} + \sqrt{1+e^{t/\tau}}\right)^{2/3}, \quad z \in (1, +\infty)$$

The detuning varies over the time ***non-symmetrically,*** while the DK2 model is anti-symmetric if $\Delta_0 + \Delta_1 = 0$

$z = 1 + e^{t/\tau}$, $a = 0$ - original DK2 model (solution in terms of ${}_2F_1$)

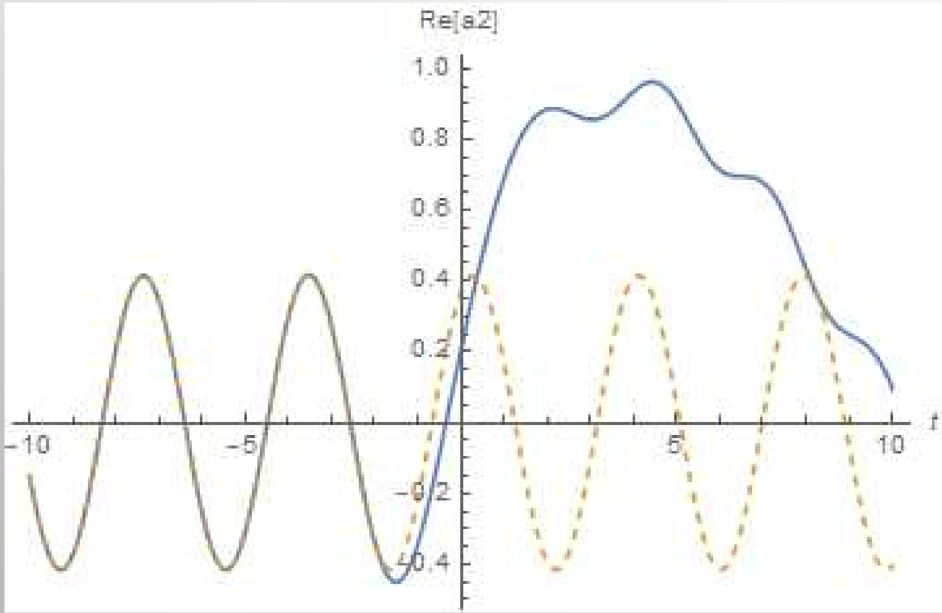
$z = \sqrt{1+e^{t/\tau}}$, $a = -1$ - a first modification of DK2 model (solution in terms of ${}_3F_2$)

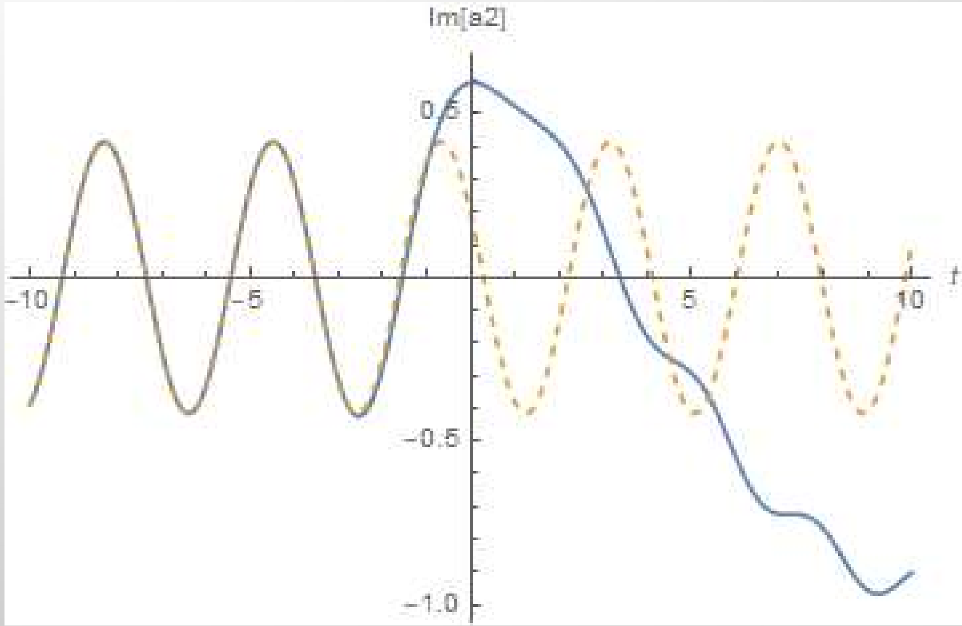
T.A. Shahverdyan, T.A. Ishkhanyan, A.M. Ishkhanyan, J. Contemp. Phys. **56**, 291-296 (2021)

Asymptotes at infinity: $-\infty$

Left asymptote of z(t): $z\big|_{t\to-\infty} \sim 1+(1-a)^a\, e^{t/\tau}$

Left *quasi-energy* *states:* $a_2\big|_{t\to-\infty} \sim e^{i\lambda_L t/\tau}, \quad \lambda_L = \dfrac{\Delta_0}{2} \pm \sqrt{\dfrac{\Delta_0^2}{4} + U_0^2}$

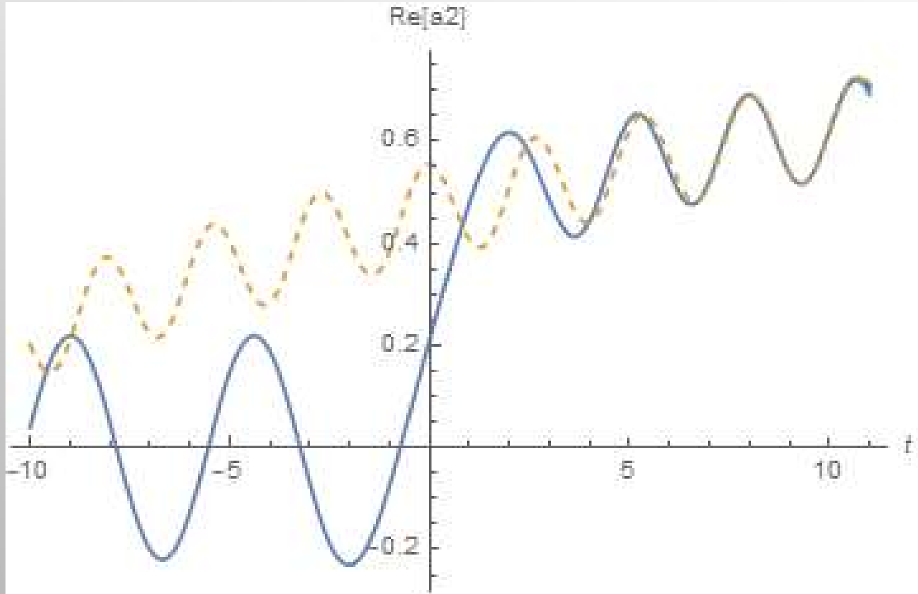


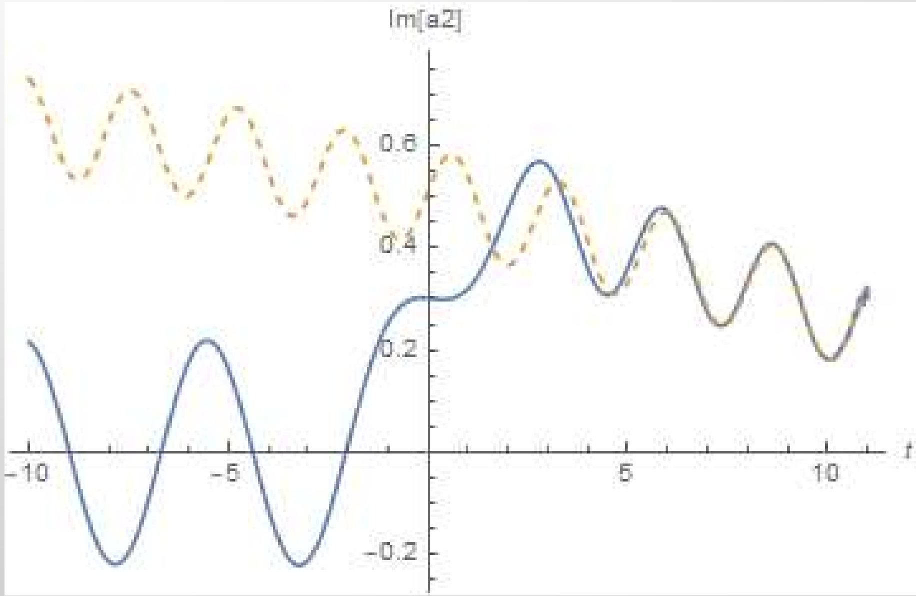


Asymptotes at infinity: $+\infty$

Right asymptote of z(t): $$z\big|_{t\to+\infty} \sim e^{\frac{t/\tau}{1-a}} + (1+a)$$

Right quasi-energy states: $$a_2\big|_{t\to+\infty} \sim e^{i\lambda_R t/\tau}, \quad \lambda_R = \frac{\Delta_1}{2} \pm \sqrt{\frac{\Delta_1^2}{4} + U_0^2}$$





Solution of the two-state problem in terms of the Clausen function

A fundamental solution to equation

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

for field configuration

$$U(t)=U_0,\quad \delta_t(t)=\Delta_1+\frac{\Delta_0-\Delta_1}{z}$$

$$\frac{(z-a)^a}{z-1}=e^{-t/\tau}$$

is explicitly written in terms of a ***Clausen function*** $_3F_2$ *as*

$$a_{2F}=C(z-1)^{\alpha 2}(z-a)^{\alpha 3}\ {}_3F_2\left(\alpha,\beta,1-\frac{\alpha\beta}{q};\delta,-\frac{\alpha\beta}{q};\frac{z-1}{a-1}\right)$$

This is for the case when the system starts from the first quasi-energy state

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The general solution involves two $_3F_2$ functions, each of which can be presented as an irreducible liner combination of two $_2F_1$ functions

Non-transition probability

The first Demkov-Kunike model:

$$P_{DK}=\frac{\sinh\left(\frac{\pi T}{2}\left(E_e-E_a+2b\right)\right)\sinh\left(\frac{\pi T}{2}\left(E_a-E_e+2b\right)\right)}{\sinh\left(\pi t E_a\right)\sinh\left(\pi T E_e\right)}$$

K.A. Suominen, B.M. Garraway, Phys. Rev. A **45**, 374 (1992).

Our result:

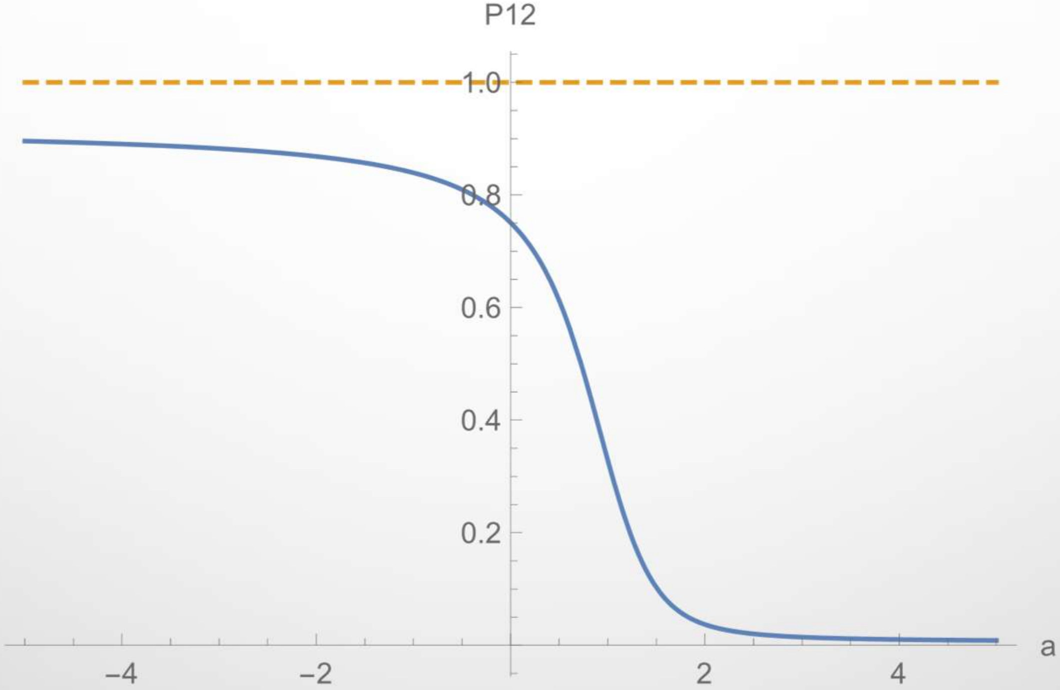
$$P_{I\to I}=\frac{\sinh\left(\frac{\pi\tau}{2}\left(R_L+(a-1)R_R-R\right)\right)\sinh\left(\frac{\pi\tau}{2}\left(R_L+(a-1)R_R+R\right)\right)}{\sinh\left(\pi\tau R_L\right)\sinh\left((a-1)\pi\tau R_R\right)}$$

$$R_L=\sqrt{\Delta_0^2+4U_0^2}\qquad R=\sqrt{(\Delta_0+(a-1)\Delta_1)^2+4a^2U_0^2}\qquad R_R=\sqrt{\Delta_1^2+4U_0^2}$$

This formula is a main new result

A nice plot

Transition probability versus the asymmetry parameter *a*



U_0=0.35, is the original DK2 model, $\Delta_0 = -1,\ \Delta_1 = 1$

- ***a*=0 is the original DK2 model**
- **The new model is more effective at weak fields**

For a<0, this non-symmetric configuration is more effective than the DK2

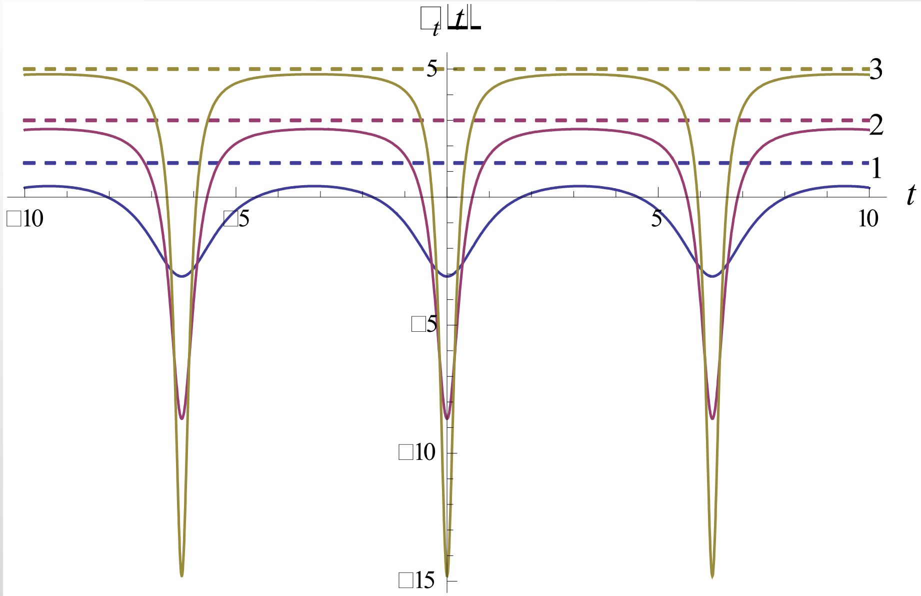
A periodic level-crossing two-state model

- **A general-Heun periodic level-crossing model (1,0,0)** :

$$U(t) = U_0 = \text{const}, \quad \delta_t(t) = \Delta_1 + \frac{(1-a)\Delta_2}{1+a-2\sqrt{a}\cos\left(\Delta(t-t_0)\right)}$$

- **With** $a = \dfrac{\Delta_1 + 1}{\Delta_1 - 1}$**, an exactly solvable periodic level-crossing 2F1 sub-model**:

$$U(t) = U_0, \quad \delta_t(t) = \Delta_1 - \frac{2}{\Delta_1 - \sqrt{\Delta_1^2 - 1}\cos(t)}$$



- Explicit solution of the two-state problem

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

- where $\qquad z(t) = \sqrt{\dfrac{\Delta_1 + 1}{\Delta_1 - 1}}\, e^{i(t-t_0)}$

G. Saget et al., J. Contemp. Physics (Armenian Ac. Sci.) **52**, 324-334 (2017).

***This is a member of GHE class* (1,0,0)**

Reduction to the confluent Heun equation

- The confluent Heun equation: $$\frac{d^2u}{dz^2}+\left(\frac{\gamma}{z}+\frac{\delta}{z-1}+\varepsilon\right)\frac{du}{dz}+\frac{\alpha z-q}{z(z-1)}u=0$$
- There are 15 classes of confluent Heun models (only 9 are independent)

A.M. Ishkhanyan and A.E. Grigoryan, J. Phys. A 47, 465205 (2014).

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

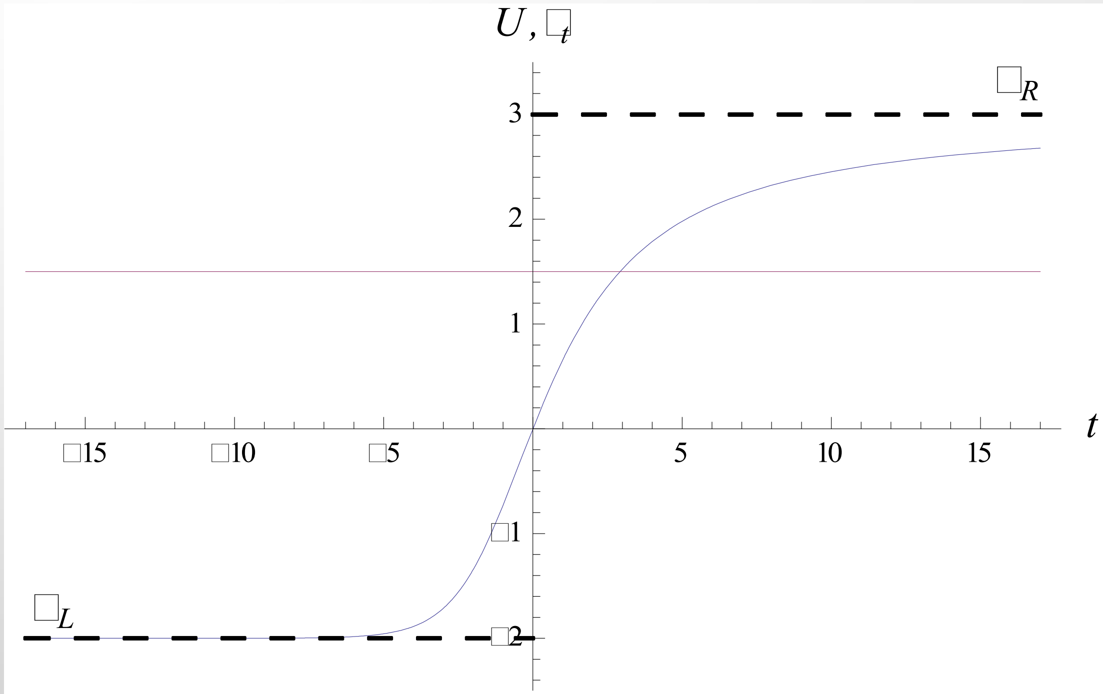
$$\delta_t(t)=\left(\delta_0+\frac{\delta_1}{z}+\frac{\delta_2}{z-1}\right)\frac{dz}{dt}$$

- **Lambert-W model**: $k_{1,2}=-1,1$

$$U(t)=U_0$$

$$\delta_t=\Delta_R+\frac{\Delta_L-\Delta_R}{1+W\left(e^{t/\tau}\right)}$$

$$z=We^W$$



T.A. Ishkhanyan, J. Contemp. Physics (Armenian Ac. Sci.) **54**, 17-26 (2019).

The solution involves irreducible linear combinations of two $_1F_1$ functions

Reduction to the biconfluent Heun equation

- The bi-confluent Heun equation: $$\frac{d^2u}{dz^2}+\left(\frac{\gamma}{z}+\delta+\varepsilon z\right)\frac{du}{dz}+\frac{\alpha z-q}{z}u=0$$
- There are 5 classes of biconfluent Heun models $k=-1,-1/2,0,1/2,1$

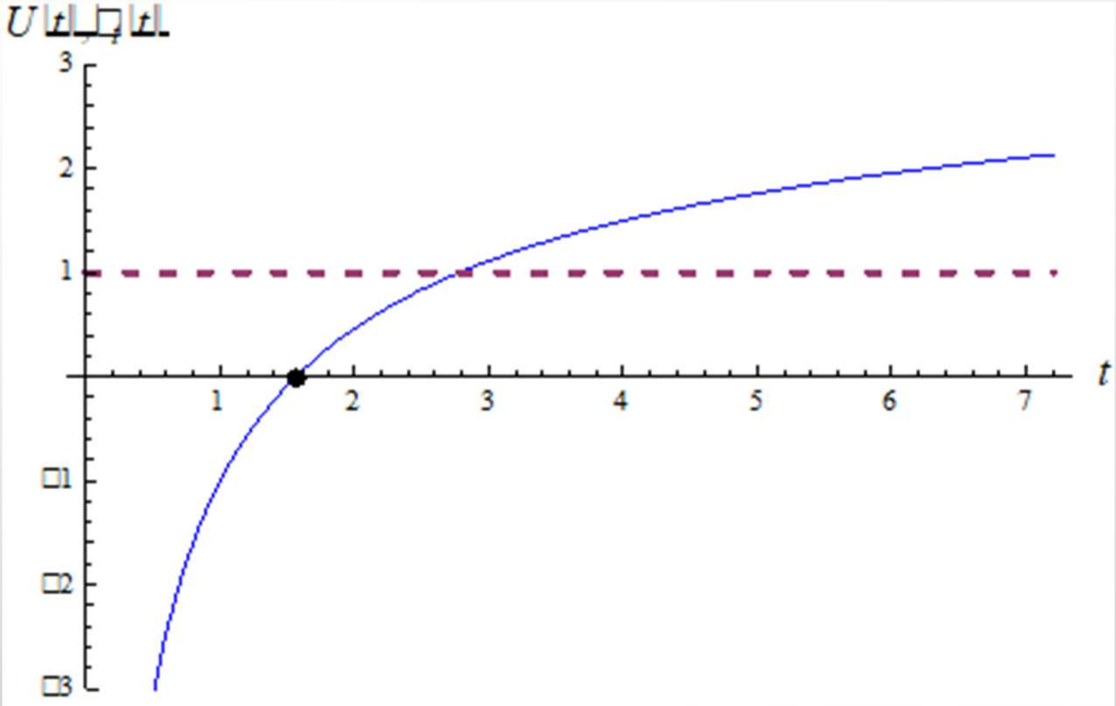
$$U(t)=U_0^* z^k \frac{dz}{dt}$$

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

- **Inverse-square-root model**: $k=1$

$$U(t)=U_0$$

$$\delta_t(t)=\Delta_0+\frac{\Delta_1}{\sqrt{t}}$$



T.A. Ishkhanyan, A.V. Papoyan, A.M. Ishkhanyan, C. Leroy, Las. Phys. Lett. **17**, 106001 (2020)

The solution involves irreducible linear combinations of two Hermite functions

Discussion_1

- Re-examining the analytic solutions of some classical problems. This time, the quantum time-dependent two-state problem.
- The quantum two-state problem is an interesting object, important in the theory of non-adiabatic transitions in quantum mechanics, in atomic, molecular and optical physics, in laser physics, etc.
- This is a slightly more difficult problem than the Schrödinger equation. In a sense, it is between the Schrödinger equation and the Dirac equation (although closer to the Schrödinger equation).
- Analytic solutions to the two-state problem are rare. In the past, they were constructed by reducing the problem to the ordinary- or confluent-hypergeometric equations.
- There are only five classical exactly solvable models: two ordinary- and three confluent-hypergeometric models. These models resemble the famous five classical Schrödinger potentials.
- **Conclusion:** To construct more analytic models, one should appeal to advanced equations that have more singular points. The five Hein equations are just that.

Discussion_2

Reduction of the quantum time-dependent two-state problem to the Heun equations

- Four new exactly solvable models are constructed:

  - Generalized DK2 model (general-Heun, 6-parametric)

  - Periodic level-crossing model (general-Heun, 4-parametric)

  - Lambert-W model (confluent-Heun, 5-parametric)

  - Inverse-square-root model (biconfluent-Heun, 5-parametric)

  Note: all five classical hypergeometric models are 5-parametric.

- The generalized DK2 model is ***unique*** since it has an additional parameter as compared with the classical models. This parameter defines the ***asymmetry*** of the resonance crossing.
- The generalized DK2 model is a constant-amplitude level-crossing field configuration for which the detuning varies asymmetrically in time over a finite interval.
- For all the above models, the general solution of the problem is written in terms of fundamental solutions, each of which is an irreducible linear combination of two functions of the hypergeometric class.
- We have calculated the non-transition probability for generalized DK2 model and have seen that the formula has much in common with that for the original DK2 model.
- It turns out that for relatively weak fields, the transition induced by this non-symmetric configuration is more effective than that by DK2.
- A general conjecture is that the non-symmetric models may suggest more effective tools.

Future directions

- The Dirac equation
- The Klein-Gordon equation
- The mass-dependent Schrodinger equation
- The surface plasmon-polariton equation
- Other non-relativistic and relativistic equations …

Thank you !