Nonlinear Dynamics and Applications. Vol. 14 (2007) 152 - 159

Exact analytical solutions for the dynamics of quantum multilevel molecular systems in laser fields and orthogonal q-polynomials

V. A. Savva*

B. I. Stepanov Institute of Physics, National Academy of Sciences of Belarus, 68 Nezalezhnasts Ave., Minsk 220072 Belarus

In the method with the use of integral transform with orthogonal polynomials to construct exact analytical solutions for dynamics of quantum multilevel systems in laser field algorithm is presented to solve dynamical equations describing excitation by laser pulse with an arbitrary prescribed form. Examples of solutions are given.

It is justified that orthogonal polynomials are adequate and natural instruments for analytical investigation of the dynamics of multilevel quantum systems since orthogonal polynomials and probabilities amplitudes of dynamical equations are connected to one another with Fourier transform.

A brief survey of the theory of q-calculus, the theory of special q-functions and orthogonal q-polynomials as special cases of basic hypergeometric functions is given. Certain orthogonal q-polynomials being q-deformed analogues of classical orthogonal polynomials are presented. Orthogonal q-polynomials are promising mathematical structures for constructing new multilevel quantum systems and for obtaining exact analytical solutions describing their coherent dynamics in laser fields and for other physical problems as well.

PACS numbers: 03.65.Ge; 31.70.Hq; 33.80.Rv; 42.65.Re; 02.30.Gp

Keywords: ultrashort laser pulses, coherent laser excitation, multilevel quantum systems, exact analytical solutions, orthogonal q-polynomials .

1. Objects, Processes, Equations, and Aims of the Investigation

Objects of our investigations are multilevel quantum systems. For more then 40 years two and three level quantum systems were models for many processes in physics of lasers and in resonance nonlinear optics. These models explained on the quantitative level various phenomena of matter-radiation interaction. However there exist many processes which demand multilevel systems as models for adequate description of their dynamics.

Multilevel quantum systems are models of molecules, atoms, resonance media in: (1) vibrational relaxation of molecular gases after laser excitation, (2) selective population of a target molecular vibrational or atomic level by ultrashort high-power laser pulse, (3) laser control of chemical reactions, (4) dynamics of free-electron lasers and others.

In the simplest case a multilevel quantum system has equidistant energy levels:

$$E_n = \hbar\omega_0 n, \quad n = 0, 1, 2, \ldots \quad . \tag{1}$$

*E-mail: v.savva@ifanbel.bas-net.by

Its radiative transitions between neighboring levels are stimulated by laser pulse

$$\mathcal{E}_l\, u(t) \cos \omega_l t \quad . \tag{2}$$

and the transitions are characterized by dipole moments

$$\mu_{n-1,n} = \mu_{0,1} f_n \quad , \tag{3}$$

Where f_n is a dipole moment function. For example the dipole moment function of the quantum harmonic oscillator has the form

$$f_n = \sqrt{n} \quad , n = 1,\, 2,\, \ldots \quad . \tag{4}$$

In (2) $\mathcal{E}_l$ is an amplitude of laser pulse envelope, $u(t)$ is a pulse form, ω_l is a carrier frequency of the laser pulse.

Dynamical equations describing excitation of the multilevel system (1), (3) have the form

$$\begin{gathered} -i\frac{da_n(t)}{dt} = \Lambda(t)\left\{f_{n+1}e^{-i\varepsilon t}a_{n+1}(t) + f_n e^{i\varepsilon t}a_{n-1}(t)\right\}, \\ a_n(t=0) = \delta_{n,0}, \quad n = 0,\ 1, 2,\ \ldots; \end{gathered} \tag{5}$$

$$\Lambda(t) = \mu_{0,1}\mathcal{E}_l u(t)/2\hbar, \quad \varepsilon = \omega_0 - \omega_l.$$

Here $a_n(t)$ are probability amplitudes, ε is a frequency detuning. Probability amplitudes $a_n(t)$ along with level populations

$$\rho_n(t) = a_n^*(t)a_n(t) \tag{6}$$

define the dynamics of a quantum system.

The aim of our investigation is to construct a method of solving dynamical equations (5) and to obtain exact analytical solution for the dynamics of a quantum system in the field of laser pulse with a prescribed form. It goes without saying an exact analytical solution of equations for dynamics of a multilevel system is an exceptional case along with a difficult problem for any investigator in mathematical physics.

2. Method of solving

After using phase transformation $a_n(t) = b_n(t)\exp(in\varepsilon\, t)$ the dynamical equations (5) with initial conditions take the form

$$\begin{gathered} -i\frac{db_n(t)}{dt} = -n\varepsilon b_n(t) + \Lambda(t)\left\{f_{n+1}b_{n+1}(t) + f_n b_{n-1}(t)\right\}; \\ b_n(0) = \delta_{n,0}\ ; \end{gathered} \tag{7}$$

and energy level populations are $\rho_n(t) = b_n^*(t)b_n(t)$.

We seek a solution in the form of the integral transform with some orthogonal polynomials:

$$b_n(t) = \frac{1}{d_0}A(t)\int_a^b \sigma(x)\,\frac{p_n(x)}{d_n}\,e^{i\,\beta(t)\,x}dx\ , \tag{8}$$

where $\{p_n(x)\}$ is some orthogonal polynomial system, $a \leqslant x \leqslant b$, $\sigma(x)$ is a weight, d_n is a norm. We have to seek $A(t)$, $\beta(t)$. In the course of obtaining these functions we used recurrence relation and differential equation for orthogonal polynomials. And then $b_n(t)$ and $\rho_n(t)$ can be calculated.

3. Example: Laguerre quantum systems

Let $p_n(x)$ be $L_n(x,\alpha)$ — Laguerre polynomials. Then we can construct [1, 2] proper quantum multilevel systems with dipole moment function

$$f_n = \left[\frac{n(n+\alpha)}{\alpha+1}\right]^{1/2}, \quad \alpha > -1\,. \tag{9}$$

More exactly we have not one system with equidistant levels but one parameter (α) family of quantum systems or Laguerre quantum oscillators.

Equations for $A(t)$ and $\beta(t)$ have the forms:

$$\begin{aligned} A^{-1}(t)\frac{dA(t)}{dt} &= (\alpha+1)^{1/2}\Lambda(t)\,[2\beta(t)+i] - (\alpha+1)\varepsilon\beta(t), & A(0) &= 1, \\ \frac{d\beta(t)}{dt} &= q(t)\beta^2(t) + iq(t)\beta(t) - \tfrac{1}{2}\,[q(t)+\varepsilon]\,, & \beta(0) &= 0, \end{aligned} \tag{10}$$

$$q(t) = 2(\alpha+1)^{-1/2}\Lambda(t) - \varepsilon\,. \tag{11}$$

The equation in $\beta(t)$ is Riccati one. One can solve it in some special cases.

3.1. Special case: resonance excitation

If the carrier frequency ω_l of laser pulse is coincident with intrinsic frequency ω_0 of the oscillator i.e. excitation is resonance ($\varepsilon = 0$) the solution sought is given by

$$A(t) = (ch\,z - i\;sh\,z)^{-(\alpha+1)}, \qquad \beta(t) = -\frac{sh\,z}{ch\,z - i\;sh\,z}, \tag{12}$$

$$z \equiv z(t) = \int_0^t (\alpha+1)^{-1/2}\Lambda(t')dt', \tag{13}$$

$$b_n(t) = i^n\left[\frac{\Gamma(\alpha+1+n)}{n!\;\Gamma(\alpha+1)}\right]^{1/2}\frac{sh^n z}{ch^{\alpha+1+n} z}\,; \quad \rho_n(t) = \frac{\Gamma(\alpha+1+n)}{n!\;\Gamma(\alpha+1)}\;\frac{sh^{2n} z}{ch^{2(\alpha+1+n)} z}. \tag{14}$$

3.2. Special case: excitation by pulse with rectangular form of envelope

For this pulse $\Lambda(t) \equiv \Lambda_0$ and after going to dimensionless variables

$$t_1 = \Lambda_0(\alpha+1)^{-1/2}t, \qquad \varepsilon_1 = \frac{\varepsilon}{\Lambda_0(\alpha+1)^{-1/2}} \tag{15}$$

the solution for energy level populations is given by the following formulas:

$$\begin{aligned} &\rho_n(t) = \tfrac{\Gamma(\alpha+1+n)}{n!\;\Gamma(\alpha+1)}\;\frac{\sin^{2(\alpha+1)}\varphi\;\; sh^{2n}(t_1\sin\varphi)}{[\sin^2\varphi + sh^2(t_1\sin\varphi)]^{\alpha+1+n}} \\ &for \quad \sin\varphi = \sqrt{1-(\varepsilon_1/2)^2}, \quad 0<\varphi<\pi, \quad |\varepsilon_1/2|<1 \end{aligned} \tag{16}$$

$$\begin{aligned} &\rho_n(t) = \tfrac{\Gamma(\alpha+1+n)}{n!\;\Gamma(\alpha+1)}\;\frac{sh^{2(\alpha+1)}\psi\;\;\sin^{2n}(t_1\,sh\psi)}{[sh^2\psi + \sin^2(t_1\,sh\psi)]^{\alpha+1+n}} \\ &for \quad sh\psi = \sqrt{(\varepsilon_1/2)^2-1}, \quad 0<\psi<\infty, \quad |\varepsilon_1/2|>1 \end{aligned} \tag{17}$$

Here we shell not discuss excitation peculiarities of Laguerre oscillators. Our purpose is to show action of the method and its results.

4. ORTHOGONAL POLYNOMIALS are ADEQUATE and NATURAL INSTRUMENTS for ANALYTICAL INVESTIGATION of the DYNAMICS of MULTILEVEL QUANTUM SYSTEMS

A method to obtain exact analytical solutions for dynamics of multilevel quantum systems is sought, developed and generalized by us for a long time. We constructed the method based on the use of integral transform with orthogonal polynomials. A number of various orthogonal polynomial systems were used among them almost all classical orthogonal polynomials: Hermite, Legendre, Laguerre, Gegenbauer, Jacobi, Charlier, Meixner, Pollaczek, Krawtchouk, Hahn and proper quantum systems were constructed, and exact solutions for their dynamics in laser fields were obtained and at last on the bases on the solutions some interesting properties of these systems and some unexpected phenomena in their dynamics were revealed [1–7] .

The main conclusions from this work are the following:

1. Any system of orthogonal polynomials gives rise to proper multilevel quantum system with proper characteristics: energy levels E_n, dipole moment function f_n, frequency detuning ε_n and so on.

2. Orthogonal polynomial systems are adequate, suitable and natural instruments for constructing multilevel quantum systems and for obtaining exact analytical solutions describing the dynamics of quantum systems in laser fields.

The justification of the last item is orthogonal polynomials are Fourier images of probabilities amplitudes of Schrödinger equation describing dynamics of multilevel quantum systems.

As one knows Fourier transform of a function $a\,(t)$ is

$$Fa\,(t) = \frac{1}{\sqrt{2\pi}} \int_a^b p\,(x) e^{-i\,t\,x} dx \ . \tag{18}$$

Complex valued function $a\,(t)$ of a real variable t is transformed in real function $p(x)$ of a real variable x, which can be continuum or discrete variable. So Fourier transform realizes the transformation from t-space to Fourier x-space. For probability amplitude we have (in simplest case)

$$a_n(t) = \int_a^b \sigma(x)\, \frac{p_0}{d_0}\, \frac{p_n(x)}{d_n}\, e^{-i\,t\,x} dx \ . \tag{19}$$

In so far as $a_n(t) = a_{n,m}(t)$ is amplitude with initial condition $a_n(t=0) = \delta_{n,m}$ it is obvious that the function $a_{n,m}(t)$ and the function $\sigma(x)\, \frac{p_m(x)}{d_m}\, \frac{p_n(x)}{d_n}$ are connected with Fourier transform. Parameters r , $\sigma(x)$ are the coefficients of recurrence formula for polynomials

$$f_{n+1} p_{n+1}(x) + f_n p_{n-1}(x) = (rx + s_n) p_n(x). \tag{20}$$

For every $\{p_n(x)\}$ coefficients f_n, r, s_n are known, They are characteristics of proper quantum system as well.

That is why orthogonal polynomials are adequate and natural formalism for analytical dynamics of quantum systems.

5. New possibilities to obtain exact analytical solutions with the use of the Basic Hypergeometric Functions

In theoretical studies of many various physical processes hypergeometric functions are every so often used. Well known the Hypergeometric Gauss Function has the next form

$$ {}_2F_1(a,\, b;\; c;\; z) = \sum_{k=0}^{\infty} \frac{(a)_k (b)_k}{(c)_k} \, \frac{z^k}{k!} \, . \tag{21}$$

Symbol $(a)_k$ is defined as

$$ (a)_k = \frac{\Gamma(a+k)}{\Gamma(a)} = \begin{cases} 1, & k=0 \\ a(a+1)\cdots(a+k-1), & k=1,\,2,\,\dots \end{cases} \tag{22}$$

and it is also called the shifted factorial or a Pochhammer symbol. The Hypergeometric functions ${}_rF_s(...)$ give rise to many families of orthogonal hypergeometric polynomials. They are presented in Table 1.

So called the Basic Hypergeometric Series, also called the hypergeometric q-series or hypergeometric q-functions are known much less and they have very small applications in physics though they were constructed about 250 years ago as well.

Basic Hypergeometric Series has more complicated form:

$$ \begin{gathered} {}_r\Phi_s(a_1,\, a_2,\, \dots,\, a_r;\; b_1,\, b_2,\, \dots,\, b_s;\; q,\; z) = \\ = \sum_{k=0}^{\infty} \frac{(a_1;\; q)_k (a_2;\; q)_k ... (a_r;\; q)_k}{(b_1;\; q)_k (b_2;\; q)_k \cdots (b_s;\; q)_k} \, \frac{z^k}{(q;\; q)_k} \left[(-1)^k q^{\frac{k(k-1)}{2}} \right]^{s+1-r} \end{gathered} \tag{23}$$

Here parameter $0 < q < 1$ is known as a base. Symbol

$$ (a;\; q)_k = \begin{cases} 1, & k=0 \\ (1-a)(1-aq)\cdots(1-aq^{k-1}), & k=1,\,2,\,\dots \end{cases} \;, \tag{24}$$

is the q-shifted factorial or a q-Pochhammer symbol. Basic hypergeometric functions are the generalization of proper ordinary hypergeometric functions. For example

$$ \lim_{q\to 1^-} {}_3\Phi_2(q^{a_1},\, q^{a_2},\, q^{a_3};\; q^{b_1},\, q^{b_2};\; q,\; z) = {}_3F_2(a_1,\, a_2,\, a_3;\; b_1,\, b_2;\; z) \tag{25}$$

i.e. basic hypergeometric function goes to hypergeometric function when a base $q \to 1$.

Just as hypergeometric functions give rise to various orthogonal polynomials (see Table 1) so basic hypergeometric functions give rise to various orthogonal q-polynomials presented in Table 2.

Table 1: ASKEY-SCHEME OF HYPERGEOMETRIC ORTHOGONAL POLYNOMIALS

${}_4F_3$	1.Wilson	2.Racah
${}_3F_2$	3.Continuous dual Hahn	4.Continuous Hahn
	5.Hahn	6.Dual Hahn
${}_2F_1$	7.Meixner-Pollaczek	8.Jacobi
	9.Meixner	10.Krawtchouk
${}_1F_1/{}_2F_0$	11.Laguerre	12.Charlier
${}_2F_0$	13.Hermite	

5.1. Elements of q-calculus

For the expired 250 years from the moment of creation of bases of the theory of the hypergeometric functions, the theory of classical orthogonal polynomials based on hypergeometric functions has turned in extensive, in details developed and widely used in theoretical and mathematical physics branch of the theory of special functions. Approximately at the same time the foundation for interesting generalization of the theory hypergeometric functions has been laid. These functions have received the name of basic hypergeometric series (or q-functions). However development of the theory of basic hypergeometric functions went considerably more slowly. Only in the last some decades in this area significant and intensive progress is evident. And at present we have its intensive development [8–10].

This generalization of the theory goes back to the following generalization of number

$$[n]_q = \frac{1-q^n}{1-q}; \quad 0 < q < 1; \quad [\alpha]_q = \frac{1-q^\alpha}{1-q} \tag{26}$$

with the trivial passage to the limit

$$\lim_{q\to 1} \frac{1-q^\alpha}{1-q} = \alpha. \tag{27}$$

Q-analogues of many classical special functions were constructed as well. For example

$$[n]_q! \ = [1]_q! \ [2]_q! \ ... \ [n-1]_q! \ [n]_q! \tag{28}$$

is generalization of factorial. There exist q-derivative, q-integral, q-analogues of classical functions $\exp_q(z)$, $J_q(z)$, $\sin_q(z)$ and q-hypergeometric function, or basic hypergeometric function etc., including orthogonal q-polynomials. However the theory of special q-functions is little known among physicists and has no adequate applications in physics.

Table 2: SCHEME OF BASIC HYPERGEOMETRIC ORTHOGONAL POLYNOMIALS

1.q-Askey-Wilson	2.q-Racah
3.Continuous dual q-Hahn	4.Continuous q-Hahn
5.Big q-Jacobi	6.Big q-Laguerre
7.q-Hahn	8.Dual q-Hahn
9.Al-Salam—Chihara	10.q-Meixner-Pollaczek
11.Continuous q-Jacobi	12.Continuous q-ultrasoherical
13.Continuous q-Laguerre	14.Big q-Laguerre
15.Little q-Jacobi	16.Little q-Legendre
17.q-Meixner	18.Quantum q-Krawtchouk
19.q-Krawtchouk	20.Affine q-Krawtchouk
21.Dual q-Krawtchouk	
22.Continuous big q-Hermite	23.Continuous q-Laguerre
24.Little q-Laguerre	25.q-Laguerre
26.Alternative q-Charlier	27.q-Charlier
28.Al-Salam—Carlitz I	29.Al-Salam—Carlitz II
30.Continuous q-Hermite	31.Stieltjes-Wigert
32.Discrete q-Hermite I	33.Discreie q-Hermite II

5.2. Some orthogonal q-polynomials

So-called orthogonal q-polynomials represent a special class of orthogonal polynomials. They are expressed through basic hypergeometric functions [8–10] and depend on parameter q. Q-polynomials are generalization of proper well known classical orthogonal polynomials which are given rise to hypergeometric functions. In turn orthogonal q-polynomials are given rise to q-hypergeometric functions and set of families of q-polynomials are quite more numerous as we can see in Table II. Thus it is expected they can have wide field for applications as well.

As an example I show q-analogues of Krawtchouk polynomials of discrete variable. They are 4 families: Quantum q-Krawtchouk polynomials, q-Krawtchouk polynomials, Affine q-Krawtchouk polynomials, Dual q-Krawtchouk polynomials.

For exanple q-Krawtchouk polynomials of discrete variable $x = 0,\ 1,\ \ldots,\ N$ are, in definition,

$$\begin{aligned} \mathrm{K}_n(q^{-x};\ p,\ N;\ q) &:= {}_3\Phi_2(q^{-n},\ q^{-x},\ -pq^n;\ q^{-N},\ 0;\ q,\ q) \\ &= \sum_{m=0}^{n} \frac{(q^{-n};\ q)_m (q^{-x};\ q)_m (-pq^n;\ q)_m}{(q^{-N};\ q)_m} \frac{q^m}{(q;\ q)_m}, \end{aligned} \tag{29}$$

$n = 0,\ 1,\ \ldots,\ N;\quad x = 0,\ 1,\ \ldots,\ N$; parameters are $0 < p < 1,\quad 0 < q < 1$ and natural number N. The q-polynomials obey orthogonality relations

$$\sum_{x=0}^{N} \sigma(x)\ \mathrm{K}_m(q^{-x};\ p,\ N;\ q)\ \mathrm{K}_n(q^{-x};\ p,\ N;\ q) = h_n^2\ \delta_{m,n}\,, \tag{30}$$

and have the following weigh function and square norm

$$\sigma(x) = \frac{(q^{-N};\ q)_x}{(q;\ q)_x}\,(-p)^{-x}, \tag{31}$$

$$h_n^2 = \frac{(q,\ -pq^{N+1};\ q)_n}{(-p,\ q^{-N};\ q)_n}\ \frac{(1+p)}{(1+pq^{2n})}\,(-pq;\ q)_N\ p^{-N} q^{-\frac{(N+1)N}{2}} (-pq^{-N})^n q^{n^2}. \tag{32}$$

At last three terms recurrence relation for them as known as well

$$A_n \mathrm{K}_{n+1}(q^{-x}) + C_n \mathrm{K}_{n-1}(q^{-x}) = \left[(A_n + C_n) - R_n(1 - q^{-x})\right]\ \mathrm{K}_n(q^{-x}), \tag{33}$$

$$\mathrm{K}_n(q^{-x}) := \mathrm{K}_n(q^{-x};\ p,\ N;\ q), \tag{34}$$

with the coefficients

$$A_n = \frac{(1-q^{n-N})(1+pq^n)}{(1+pq^{2n})(1+pq^{2n+1})},\quad C_n = -pq^{2n-(N+1)} \frac{(1+pq^{n+N})(1-q^n)}{(1+pq^{2n-1})(1+pq^{2n})},\quad R_n \equiv 1. \tag{35}$$

In addition

$$\lim_{q \to 1^-} \mathrm{K}_m(q^{-x};\ p,\ N;\ q)\ =\ \mathrm{K}_n(x;\ \frac{1}{1+p},\ N). \tag{36}$$

This is all almost to use these q-polynomials in physical problems. Now one can construct proper multilevel quantum systems, study their properties and obtain exact analytical solutions for their dynamics.

Orthogonal q-polynomials are wonderful and promising mathematical structures for constructing new multilevel quantum systems and for obtaining exact analytical solutions describing their coherent dynamics in laser fields and for other physical problems as well.

References

[1] V. I. Zelenkov, V. A. Savva. *Analytical solutions of the problem on multiphoton excitation of multilevel systems with a fast grower dipole moment of radiative transitions.* Doklady Academy of Science of Belarus **36**, pp. 504–507 (1992) /in Russian/.

[2] V. A. Savva, V. I. Zelenkov, A. S. Mazurenko. *Orthogonal polynomials in analytical method of solving differential equations describing dynamics of multilevel systems.* Integral Transforms and Special Functions **10**, pp. 299–308 (2000). arXiv:math.CA/0101105 v1 .

[3] V. A. Savva, V. I. Zelenkov, A. S. Mazurenko. *Analytical methods in dynamics of multiphoton excitation of molecules by infrared laser radiation (Review).* Journal of Applied Spectroscopy (Minsk) **58**, pp. 256–270 (1993) /in Russian/.

[4] V. A. Savva, V. I. Zelenkov, A. S. Mazurenko. *Dynamics of multilevel systems and orthogonal polynomials.* Optics and Spectroscopy (St. Petersburd) **74**, pp. 949–956 (1993) /in Russian/.

[5] V. A. Savva. *Analytical solutions for dynamics of multlevel molecular systems excited by IR laser radiation.* Infrared Phys. Technol. **36**, pp. 381–386 (1995).

[6] V. A. Savva, V. I. Zelenkov, A. S. Mazurenko. *Analytical methods in dynamics multilevel quantum systems.* Quantum Systems: New Trends and Methods (QS 96). World Scientific. Singapore (1997) pp. 217–221.

[7] V. A. Savva, V. I. Zelenkov, O. V. Khlus. *Orthogonal Krawtchouk oscillators and their dynamics in high-power laser field.* Development of the Mathematical Ideas of Mykhailo Kravchuk (Krawtchouk). Ed. by N. Virchenko et al. Kyiv–New York (2004) pp. 242–258 /in Russian/.

[8] G. Gasper, M. Rahman. *Basic Hypergeometric Series.* Cambridge University Press, Cambridge (1990)

[9] G. Gasper. *Lecture Notes for an Intoductory Minicourse on q-Series.* arXiv:math. CA/9509223 - v1 - 25 Sep. (1995).

[10] R. Koekoek, R. F. Swarthouw. *The Askey-scheme of hypergeometric orthogonal polynomials and its q-analogue.* arXiv:math. CA/9602214 - v1 -20 Feb. (1996).