N-LEVEL QUANTUM SYSTEMS
AND LEGENDRE FUNCTIONS*

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Abstract

An excitation dynamics of new quantum systems of \( N \) equidistant energy levels in a monochromatic field has been investigated. To obtain exact analytical solutions of dynamic equations an analytical method based on orthogonal functions of a real argument has been proposed. Using the orthogonal Legendre functions we have found an exact analytical expression for a population probability amplitude of the level \( n \). Various initial conditions for the excitation of \( N \)-level quantum systems have been considered.

Key words: multilevel quantum systems, analytical solutions, orthogonal functions.

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1 INTRODUCTION

Theoretical investigations of the dynamics of the multiphoton vibrational excitation of polyatomic molecules by an IR laser radiation are based on the analysis of multilevel quantum systems as molecular models. Many other problems of nonlinear optics, spectroscopy and laser physics also lead to the consideration of the dynamics of multilevel systems. Analytical results obtained up to now for multilevel systems dynamics do not cover all the interesting and necessary cases.

In this work an analytical method has been presented that offers new possibility to obtain exact solutions describing the excitation dynamics of a number of new multilevel quantum systems in an infrared laser field. The method uses orthogonal functions to obtain dynamic equations solutions. It generalizes an analytical approach [1] that is based on integral transform and orthogonal polynomials. A particular example with the use of the orthogonal Legendre function is given. Analytical solutions for two different \( N \)-level quantum systems with equidistant levels are found.

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2 ANALYTICAL METHOD

The dynamics of quantum systems in the monochromatic infrared radiation $\mathcal{E}_l \cos(\omega_l t)$ is described by the equations

$$-i \frac{d a_n(t)}{dt} = f_{n+1} e^{-i\epsilon_{n+1} t} a_{n+1}(t) + f_n e^{i\epsilon_n t} a_{n-1}(t),$$

$$a_n(t = 0) = \delta_{n,m}, \quad n = 0, 1, 2, \ldots$$

(1)

for the population probability amplitudes $a_n(t)$ of the level $n$. Here $t = \Lambda \tau$ is the dimensionless time ($\Lambda = \mu_0, 1 \mathcal{E}_l/(2\hbar)$ is the Rabi frequency, $\tau$ is ordinary time). Eqs. (1) are obtained from the Schrödinger equation for a multilevel system with the use of the rotating wave approximation.

In such description the multilevel system has two its characteristics: the dipole moment $\mu_{n-1,n}$ and the dimensionless frequency detuning $\epsilon_n$ for every transition $n-1 \leftrightarrow n$. The dipole moment function $f_n$ describes the dependence of the radiative transitions moments

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

(2)

on the transition number (on energy), $\mu_{0,1}$ is the dipole moment of the lowest transition. The detuning

$$\epsilon_n = (\omega_{n,n-1} - \omega_l)/\Lambda$$

(3)

characterizes the difference of the frequency of the transition $n$ and the laser radiation frequency.

Eqs. (1) for the $N$-level quantum system can be solved by various methods. In work [1] analytical method has been developed on the basis of orthonormal polynomial sequences $p_n(x)/d_n$ ($d_n$ is a norm). The polynomials satisfy the recurrence formula

$$f_{n+1} \frac{p_{n+1}(x)}{d_{n+1}} + f_n \frac{p_{n-1}(x)}{d_{n-1}} = (r x + s_n) \frac{p_n(x)}{d_n}.$$  

(4)

It is supposed that the coefficients $f_n$ in formula (4) and in eq. (1) are identical functions, the coefficients $s_n$ and the frequency detuning are connected in the following way

$$\epsilon_n = s_n - s_{n-1}.$$  

(5)

A number of exact analytical solutions with the help of the expression

$$a_n(t) = \int_A^B \sigma(x) \frac{p_m(x)}{d_m} \frac{p_n(x)}{d_n} \exp[it(r x + s_n)] dx$$

(6)

has been obtained.

Thus, the polynomials $p_n(x)$ are orthogonal on the interval $(A, B)$ with respect to the weight function $\sigma(x)$ and give rise to multilevel quantum systems. The coefficients $f_n$, $s_n$, $r$ of recurrence formula (4) define all characteristics of this quantum systems, i.e. the dipole moment function $f_n$ (2), the frequency detuning $\epsilon_n$ (5) and spacing of the energy levels

$$E_n = E_0 + n\hbar \omega_l + \hbar \Lambda(s_n - s_0).$$

(7)
Let \( \varphi_\alpha(z) \) are some orthogonal functions of one variable \( z \) (in special case, of course, they can be orthogonal polynomials). In contrast to polynomials \( p_n(x) \) which are orthogonal with the Kronecker delta \( \delta_{m,n} \), the functions \( \varphi_\alpha(z) \) can be orthogonal with both the Kronecker delta and the Dirac \( \delta \)-function. The scalar product

\[
D_{\alpha,\beta} \equiv \int_L \varphi_\alpha(z) \varphi_\beta^*(z) \, dM(z) = 0, \quad \alpha \neq \beta
\]  

(8)
can have infinite values. Here \( L \) is an one-dimensional region of the integration, the measure \( dM(z) \) of the integral is non-negative. \( \alpha \) and \( \beta \) are real numbers, not only integer ones. The norm \( d_{\alpha} = \sqrt{D_{\alpha,\alpha}} \) of the orthogonal function can be infinite.

In order to obtain the dynamic equation solution we use orthogonal functions \( \varphi_n(z) \) which satisfy the recurrence formula

\[
f_{n+1} \frac{\varphi_{n+1}(z)}{d_{n+1}} + f_n \frac{\varphi_{n-1}(z)}{d_{n-1}} = (r \theta(z) + s_n) \frac{\varphi_n(z)}{d_n}.
\]  

(9)

If \( \theta(z) = x \) and \( \varphi_n(z) \) are the polynomials \( p_n(x) \) then (9) becomes (4).

We shall show that any relation \( (r, A_\alpha, B_\alpha, C_\alpha \) are constants) \n
\[
r \theta(z) \varphi_\alpha(z) = A_\alpha \varphi_{\alpha+1}(z) + B_\alpha \varphi_\alpha(z) + C_\alpha \varphi_{\alpha-1}(z)
\]  

(10)

for orthogonal functions \( \varphi_\alpha(z) \) can be reduced to form (9), when there exists \( \alpha = \alpha_0 \) for which

\[
C_{\alpha_0} = 0.
\]  

(11)

Then (10) can be written as

\[
A_{\alpha_0} \varphi_{\alpha_0+1}(z) = [r \theta(z) - B_{\alpha_0}] \varphi_{\alpha_0}(z),
\]  

(12)

\[
A_{\alpha_0+n} \varphi_{\alpha_0+n+1}(z) = [r \theta(z) - B_{\alpha_0+n}] \varphi_{\alpha_0+n}(z) + C_{\alpha_0+n} \varphi_{\alpha_0+n-1}(z).
\]  

Without any limitation we can take \( \alpha_0 = 0 \). Now it is obviously that the function \( \varphi_n(z) \) has the form

\[
\varphi_n(z) = \varphi_0(z) p_n[\theta(z)]
\]  

(13)

where \( p_n[\theta(z)] \) is a polynomial of the argument \( \theta(z) \).

Any orthonormal polynomial \( p_n(x)/d_n \) satisfies the recurrence formula (4). The functions

\[
\varphi_n(z) = \varphi_0(z) p_n[\theta(z)]/d_n
\]  

(14)

also satisfy formula (4) when \( x = \theta(z) \). And we obtain (9). Systems of functions with infinite norm \( d_n \) have to be considered specially.

Thus, the solution of problem (1) is found in the following way:
(a) with the help of orthogonal functions \( \varphi_{\alpha-\alpha_0}(z) \) (8) we choose such a sequence of functions \( \varphi_n(z) \), \( \alpha - \alpha_0 \equiv n = 0,1,2, \ldots \), which form the complete basis of solutions of the system of the relations (12);

(b) the recurrence formulae (12) reduce to pattern (9);

(c) the coefficients

\[
a_n(t) = \int_L \varphi_m(z) \frac{\varphi_n'(z)}{d_n} e^{it(\theta^*(z)+s_n)} \, dM(z)
\]

of the expansion of the integral transform kernel

\[
U(t, z) = \frac{\varphi_m(z)}{d_m} e^{it(\theta^*(z)+s_n)}
\]

are the solutions of problem (1).

If the expansion of kernel (16) to series of orthogonal functions (polynomials) \( \varphi_n(z) \) is known, the calculation of integral (15) can be avoided.

4 THE ORTHOGONAL LEGENDRE FUNCTIONS

Let’s give a particular example of orthogonal functions which satisfy recurrence formula (9). It’s known that there are systems of functions \( \varphi_m^{(N)}(z) \) among the complete family of the 1st kind Legendre functions \( P_\mu^\nu(z) \)

\[
\varphi_m^{(N)}(z) = (-1)^{N-m-1} \Gamma(N-\mu) P_\mu^{\mu N-1}(z) \bigg|_{\mu=m}
\]

orthonormalized on \([-1,1]\) with the Kronecker \( \delta \)-function

\[
\int_{-1}^{1} \varphi_m^{(N)}(z) \varphi_l^{(N)}(z) \frac{dz}{1-z^2} = \delta_{m,l} d_m^2,
\]

where \( m \) and \( l \) are non-negative integer numbers. \( N \geq 1 \) is an integer parameter (if \( m \geq N \), the right part limit (17) is calculated at \( \mu \to m \)). The norm of these functions

\[
d_m = \left\{ (N+m-1)! \ (N-m-1)! \ /m! \right\}^{1/2}
\]

is infinite when \( m = 0 \). Therefore the reducing known recurrence formulae for the functions \( P_\mu^\nu(z) \) to relation (9) requires the use of the linear dependence properties of the Legendre functions with the integer parameters \( \mu \equiv m \) and \( \nu \equiv n \). As a result, the functions (17) satisfy the relation

\[
f_{m+1} \frac{\varphi_m^{(N)+1}(z)}{d_{m+1}} + f_m \frac{\varphi_m^{(N)-1}(z)}{d_{m-1}} = r(z) \frac{\varphi_m(z)}{d_m}.
\]
Here \( d_m \) is norm (18), \( \theta(z) = z/\sqrt{z^2 - 1} \), and
\[
f_m = r \left\{ \frac{(N - m) (N + m - 1)}{m (m - 1)} \right\}^{1/2}, \quad m > 0,
\]
\[
r = 2 \{(N - 2)(N + 1)/2\}^{-1/2}.
\]
As in (1), the coefficient \( f_m \) at \( m = 0 \) is equal zero. Since \( f_{m=N} = 0 \), we have the system of \( N \) linearly independent recurrence formulae of form (9) (at \( s_n = 0 \)). In this work the relation (20) for values \( m \geq N \) is not considered.

\[ \textbf{5} \quad \text{N-LEVEL QUANTUM SYSTEMS} \]

Let’s use functions
\[
\varphi_m^{(N)}(z), \quad m \geq 0, \quad N \geq 1,
\]
which form the complete system of solutions of \( N \) equations (20) (when \( m < N \)), in order to obtain new solutions of problem (1).

Let’s integrate expression (15) written for functions \( \varphi_m^{(N)}(z) \) (\( m < N \)) which are orthogonal on \([-1, 1]\) if \( \theta(z) = z/\sqrt{z^2 - 1} \).
\[
a_n(t, N) = \int_{-1}^{1} \frac{\varphi_m^{(N)}(z) \varphi_n^{(N)}(z)}{d_n \ d_n} \frac{e^{irt(z/\sqrt{z^2 - 1})}}{1 - z^2} \ dz = \]
\[
= 2^{m-n+1} \sqrt{\pi} \left\{ m (N + m - 1)! (N - m - 1)! \right\}^{1/2} \times \]
\[
\left\{ \frac{n (N + n - 1)!}{(N - n - 1)!} \right\}^{1/2} e^{irt} \frac{(irt)^{n+m}}{n!} \times \sum_{k=0}^{N-m-1} \frac{\Gamma(N - k - \frac{1}{2}) (-2irt)^{N-m-1-k}}{(N + m - k - 1)! (N - m - k - 1)! k! \Gamma(N + n - k)} \times \]
\[
z F_2 \left( N + n, n + \frac{1}{2} ; N + n - k, 2n + 1, -2irt \right).
\]
This solution describes the resonant excitation of a \( N \)-level quantum system with the equidistant energy spectrum
\[
E_n = E_0 + n \hbar \omega_l
\]
where \( E_0 \) is the zero level energy. The dipole moment of this system depends on \( n \) according to (21). At the initial time moment \( t = 0 \) only \( m \)-level is excited.

Let’s obtain another solution of problem (1) for another dependence on \( n \) of the dipole moment function. We can always consider reverse numeration of levels for finite level quantum systems,
because the choice of "upper" and "lower" level is arbitrary in such a case. Let's renumber the levels of the quantum system: $n \to (N - 1 - n)$.

As a result, we obtain an analytical solution with the help of formulae (21) and (23)

$$a_n(t, N) = 2^{m+n-N+2} \sqrt{\pi} \left\{ m (N + m - 1)! (N - m - 1)! \right\}^{1/2} \times$$

$$\left\{ \frac{(N-n-1) (2N-n-2)!}{n!} \right\}^{1/2} e^{irt} (irt)^{N-n+m-1} (N-n-1)! \times$$

$$\sum_{k=0}^{N-m-1} \frac{\Gamma(N-k-\frac{1}{2}) (-2irt)^{N-m-1-k}}{(N+m-k-1)! (N-m-k-1)! k! \Gamma(2N-n-k-1)} \times$$

$$\sqrt{\frac{2}{\pi}} 2F_2 \left( 2N-n-1, N-n-\frac{1}{2}, 2N-n-k-\frac{1}{2}, 2N-2n+1; -2irt \right) \qquad (25)$$

which describes the resonant excitation of a $N$-level quantum system also with the equidistant energy spectrum, but with different dipole moment function

$$f_n = \frac{n (2N-n+1)}{(N-n+1) (N-n)} \left\{ \frac{1}{(N-1)/2} \right\}^{-1/2}, \quad n < N, \quad (26)$$

Thus, new analytical method for obtaining exact solutions of the problem of the radiative excitation of multilevel quantum systems has been proposed. It allows to model the excitation of systems with more complex dynamics for the description of which both orthogonal polynomials and orthogonal functions have to be used. With the help of the orthogonal Legendre functions exact solutions for two various $N$-level quantum systems have been obtained.

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