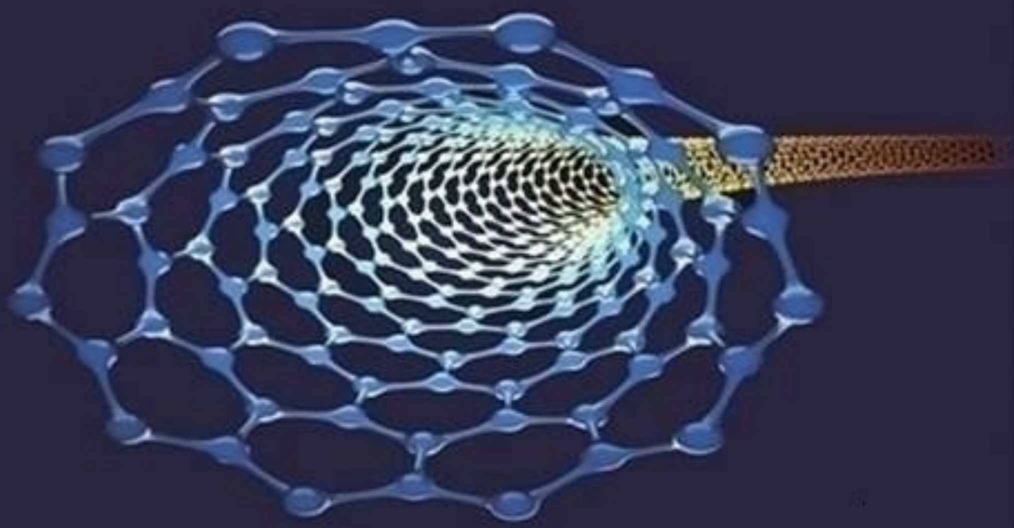
Third International Conference of Mathematics and its Applications

(TICMA 2022)



زانكۆی سەلاحەدین - هەولێر
Salahaddin University-Erbil

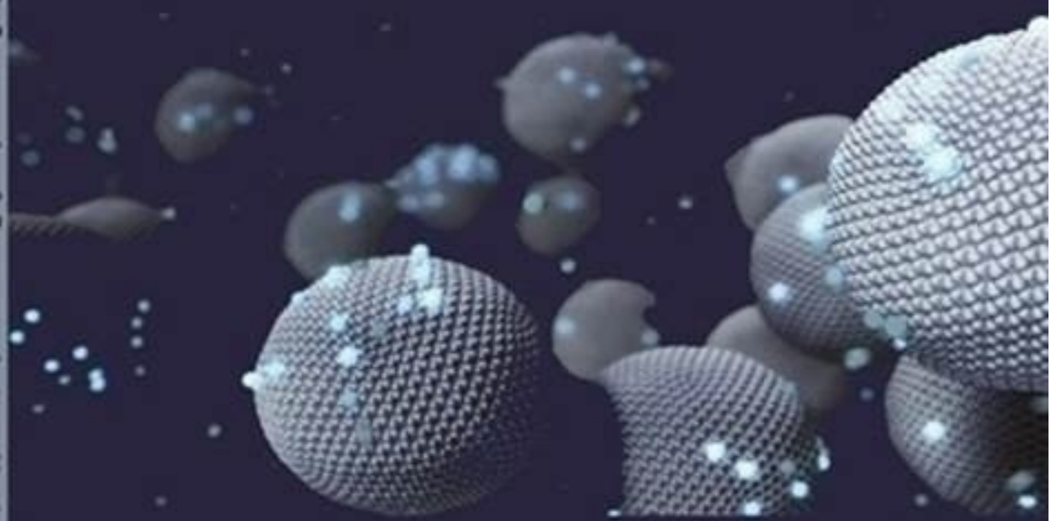
College of science / Mathematics Department

29-31 August 2022

ZANCO Journal of Pure and Applied Sciences

ZANCO

Journal of Pure and Applied Sciences



زانكۆی سەلاحەدین - هەولێر
Salahaddin University-Erbil

College of science / Mathematics Department

29-31 August 2022

Proceeding of 3rd International Conference of Mathematics and its Applications
TICMA2022
https://conferences.su.edu.krd/su/ticma2022/
DOI: https://doi.org/10.31972/ticma2022

RESEARCH PAPER

Coherent Dynamics of Quantum Systems with Non-Uniform Fourier Space Excited by Laser Radiation

Sary Banjak[1,*] and Vadim Savva[2]
[1,2]Department of Higher Mathematics, Belarusian State Technological University, Minsk, Belarus.

A B S T R A C T:
The algorithm is presented to solve dynamical equations for excitation of molecular models with multiple energy levels. It uses only discrete structures: discrete orthogonal polynomials constructed specially in Fourier space of the probability amplitudes, discrete Fourier transform and leads to exact solution of the differential equations and to discrete distribution of the quantum systems by energy levels.

KEY WORDS: Non-Uniform Fourier Space, Quantum Systems, Coherent Dynamics.
DOI: https://doi.org/10.31972/ticma22.09

1. INTRODUCTION:

The motivation for this work is caused by the fact that Mathematics has significantly changed its appearance in the years after the Second World War. New powerful principles created by discrete mathematics, discrete algorithms, programming, and high–level languages and, of course, computers, computer algebra systems have been added to the former "Mathematical principles of natural science" (as I. Newton called his great book). Newtonian principles (calculus and differential equations, Mathematics of continuous quantities) worked well for 300 years.

Now a rapidly developing branch has been established in mathematics – computer science. The computer algebra system not only performs numerical calculations incredibly quickly, but also performs "analytical calculations", solves algebraic and differential equations. It builds function graphs, works with audio and visual information, competing and collaborating with higher (continuous) Mathematics. Discrete Mathematics can already be considered as Mathematical principles of natural science as well.

Note that the physics of the twentieth century fully recognized the wave-particle duality of the material world. Now this harmony, the unity of the continuous and the discrete, has established itself in mathematics as the language of natural science and technology. Unfortunately, the system of higher education still largely ignores this fact when training most specialists.

The purpose of this work is to apply a discrete algorithm to solve a specific problem - solving a system of differential equations, which, as is known, are usually solved by methods of continuous mathematics, and to show that discrete algorithms give a slightly different perspective, a different view, physically more meaningful.

It was desirable to take a non-"random" problem. As an example, we have chosen one of the fundamental problems of quantum mechanics – the interaction of coherent electromagnetic radiation with quantum systems (models of molecules, atoms, quantum dots and other micro-objects), called the Rabi problem.

It was solved in 1936-37 in a simple, semi-classical version [1, 2], shortly after the creation of quantum mechanics.

*** Corresponding Author: Sary Banjak**
E-mail: bnjk_sary@yahoo.com
Article History:
Received: 01/08/2022
Accepted: 15/09/2022
Published: 07/12/2022

DOI: https://doi.org/10.31972/ticma2022

The solution showed that the influence of radiation on quantum systems should be carried out in a different form than classical physics described it: oscillations of the energy level populations of the molecule should appear while the radiation is active. These oscillations are called Rabi oscillations. The problem is included in textbooks of quantum mechanics and has been the subject of numerous scientific studies for more than 80 years, since it underlies many important, diverse and promising areas of physics, chemistry, and technology. Journal of Physics A: Mathematical and Theoretical devoted a special issue of articles to this anniversary [3, 4].

The Rabi problem has two variants – semi-classical and fully quantum; the first describes radiation (usually given) in terms of classical physics, and the molecule is considered in terms of quantum mechanics. In the second variant, both interacting objects, usually located in the resonator, have a quantum description. This is a more complex option, also because the states of both the field and the microsystem change during interaction.

We will very briefly list the scientific and applied research directions for the last decades that have stimulated great interest (analytical, numerical, and experimental) in the Rabi problem. In the early 60s, it was caused by the creation of lasers and the formation of quantum optics. In the 70s - the development of laser isotope separation. In the 80s - the use of ultra-short laser pulses to control chemical reactions, and in spectroscopy - methods for obtaining selectively excited molecules to study the rates of energy redistribution through bonds. A more complex variant - the Rabi quantum problem has become in demand in connection with the development of quantum computers, quantum information transmission networks, modern cryptography and the study of the basics of quantum mechanics.

In our previous works [5-7] devoted to the analytical solution of the semi-classical Rabi problem, in which a discrete spectral algorithm for solving the corresponding equations was proposed, it was shown that it was possible to construct orthogonal discrete polynomials in the corresponding Fourier space of the desired functions and introduce free parameters into their weight function. This opened up an extensive field of use of discrete variable polynomials, which were previously very rarely used in solving physical problems. The presence of free parameters led to a solution for extensive families of quantum systems with various characteristics, including systems with non-equidistant arrangement of energy levels (more real models of molecules and atoms).

In this paper a discrete algorithm for constructing analytical solutions describing the dynamics of excitation is extended to quantum systems with an inhomogeneous Fourier space of the desired functions. It is shown that oscillations of energy level populations can have a more complex form.

They can be non-periodic in time, which is not related to the quantum properties of radiation.

A quantum system with energy levels $E_0, E_1, \dots, E_N$ excited by radiation acting in N transitions between neighbor levels is described with equations:

$$-i\frac{da_n(t)}{dt} = f_{n+1}e^{-i\varepsilon_{n+1}t}a_{n+1}(t) + f_n e^{+i\varepsilon_n t}a_{n-1}(t);$$

$$a_n(t=0) = \delta_{n,0};\ \ n = 0,1,\dots,N. \qquad (1)$$

All variables and coefficients are dimensionless ones. We will consider simple case $N = 2$, two transitions $E_0 \rightleftarrows E_1 \rightleftarrows E_2$, but this is not essential. Coefficients f_1, f_2 describe dipole interaction of radiation with n transition (with normalization $f_1 = 1$); $\varepsilon_1, \varepsilon_2$ are frequency detuning of transition frequency from laser frequency; dimensionless t is time and $a_n(t)$ are functions to be obtained; they are probability amplitudes to find a particle with energy E_n at t moment.

The aim of the paper is to give more general discrete method of solving the equations (1) for quantum systems possessing non-uniform Fourier space of $a_n(t)$ functions in contrast to the method for quantum systems with a homogeneous Fourier space [6].

DOI: https://doi.org/10.31972/ticma2022

3. CONSTRUCTING OBJECTS IN THE DISCRETE FOURIER SPACE OF THE UNKNOWN FUNCTIONS $a_n(t)$

In this example, we define a discrete function $\sigma(x;a,b,c)$ with an argument $x=\{0,1,\sqrt{7}\}$ on an inhomogeneous grid showing another three-level model (irrational, non-periodical dynamics). The function contains free parameters as below:

$$\sigma(x)=\left\{\frac{1}{2}-a, \qquad a, \qquad \frac{1}{2}\right\},$$

$$x=\{0,1,\sqrt{7}\},\quad 0<a<\frac{1}{2} \tag{2}$$

The standard procedure with such a weight function results in a sequence of three discrete orthogonal polynomials $\{\hat{p}(x)\}_{n=0}^{2}$:

- $\hat{P}_0(x)\equiv 1,$
- $\hat{P}_1(x)=\frac{1}{d_1}\left(x-a-\frac{\sqrt{7}}{2}\right),$
- $\hat{P}_2(x)=\frac{1}{d_2}\left(\begin{array}{c}\frac{1}{4}\left(7-4a\left(-1+\sqrt{7}+a\right)\right)x^2\\ +\frac{1}{4}\left(-7\sqrt{7}+2a\left(5+\sqrt{7}+2a\right)\right)x+\left(4\sqrt{7}-7\right)a\end{array}\right).$

The polynomial norms are:

- $d_1=\sqrt{\frac{7}{4}-a\left(-1+\sqrt{7}+a\right)}$
- $d_2=\frac{1}{2}\sqrt{\left(\frac{7}{2}\left[-a(-1+2a)\left(-7\left(-4+\sqrt{7}\right)+4a\left(11-5\sqrt{7}+\left(-4+\sqrt{7}\right)a\right)\right)\right]\right.}$
  (3)

It is known that orthogonal polynomials satisfy the three-term recurrence relation:

$$\begin{array}{l}\bar{f}_{n+1}\hat{p}_{n+1}(x)+\bar{f}_n\hat{p}_{n-1}(x)=[rx+s_n]\,\hat{p}_n(x);\\ n=0,1,2;\quad \bar{f}_0=0,\ \bar{f}_1=1,\ \bar{f}_3=0.\end{array} \tag{4}$$

Using the well-known formulas of the theory of orthogonal polynomials [3], one can obtain the coefficients of this relation (4):

$$r=\frac{1}{d_1}=\frac{1}{\sqrt{\frac{7}{4}-a\left(-1+\sqrt{7}+a\right)}},$$

$$\bar{f}_1=1,$$

$$f_2=\frac{4\sqrt{14}\sqrt{-(-a+2a^2)(28-7\sqrt{7}+44a-20\sqrt{7}a-16a^2+4\sqrt{7}a^2)}}{(-7-4a+4\sqrt{7}a+4a^2)^2} \tag{5}$$

DOI: https://doi.org/10.31972/ticma2022

Similarly, one can obtain the other coefficients S_0,S_1, S_2.

Numerical values $f_1 = 1$; $f_2 \simeq 0.68$; show the corresponding quantum three-level system has two dipole transitions $f_n = \{1.0; 0.68\}$ and non-equidistant energy levels for all values of $0 < a < \frac{1}{2}$.

The Figures below shows frequency detuning and "Force" $f2$ for different quantum systems of a-family.

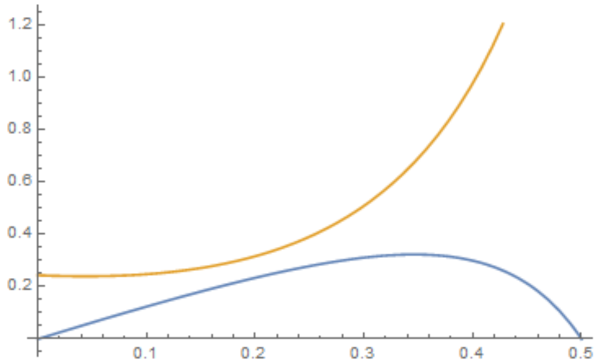


FIGURE 1. The dependence of the frequency tuning of both transitions $(\varepsilon_1, \varepsilon_2)$ for different quantum systems. (ε_2– at the top, ε_1– at the bottom)

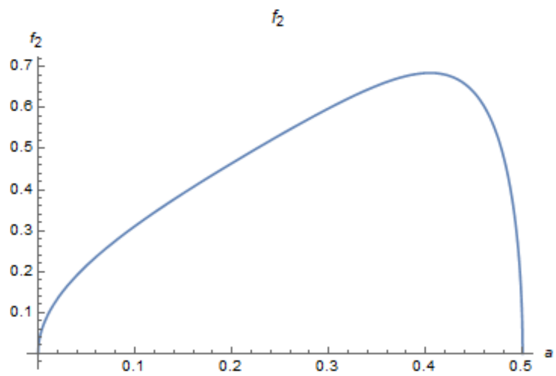


FIGURE 2. The dependence of $f_2(a)$ for different quantum systems of a-family.

4. SOLUTION AND DISCRETE PROBABILITY DISTRIBUTION OF QUANTUM SYSTEMS BY ENERGY LEVELS

Solution of the differential equations (1) is in the form of a discrete Fourier transform:

$$a_n(t) = e^{is_n t} \sum_{x=0}^{2} F_n(x) e^{irxt} \tag{6}$$

where $F_n(x)$ are the Fourier images (spectra) of the amplitudes of the probability of finding a particle at the level E_n at the time t when the radiation is active.

We assume that the Fourier spectra are expressed in terms of the constructed polynomials as follows:

$$F_n(x) = \sigma(x)\hat{p}_0\hat{p}_n(x); \quad n = 0,1,2; \quad x = 0,1,3 \tag{7}$$

The validity of this assumption is proved by substituting (6) and (7) into equations (1), which are satisfied when

$$f_n = \bar{f}_n, \quad \varepsilon_n = s_n - s_{n-1}, \quad n = 1,2 \tag{8}$$

DOI: https://doi.org/10.31972/ticma2022

This one-to-one correspondence establishes a relationship between the coefficients of the equations (1) – on the right and the coefficients of the recurrence relation (4) – on the left for the constructed polynomials. In other words, it is a correspondence between the characteristics of quantum systems and their exciting radiation, on the one hand, and the spectral properties of the probability amplitudes $a_n(t)$.

All values in (6) and 7) are known and one can calculate the Fourier spectra and construct a solution of equations (1).

5. DISCRETE PROBABILITY DISTRIBUTION OF QUANTUM SYSTEMS BY ENERGY LEVELS

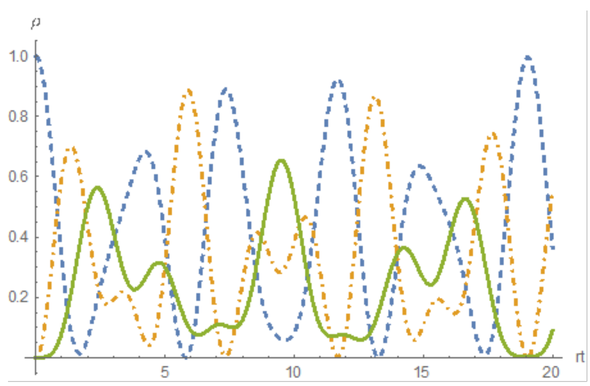
Here we present a discrete statistical distribution of the excited particles over the energy levels. These are time-dependent level populations:

$$\rho_0(t) = \frac{1}{2}\left\{\begin{matrix} 1-2a+4a^2-2a(-1+2a)Cos(rt) \\ +(1-2a)Cos(\sqrt{7}rt)+2aCos(rt-\sqrt{7}rt) \end{matrix}\right\},$$

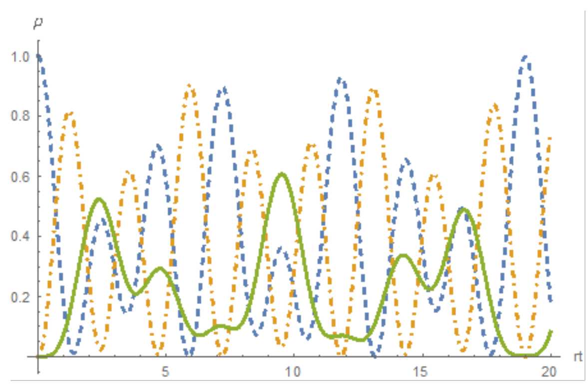
$$\rho_1(t) = \frac{1}{-14+8(-1+\sqrt{7})a+8a^2}\left\{\begin{matrix} -7+14a-40a^2+16\sqrt{7}a^2 \\ +24a^3-16\sqrt{7}a^3-16a^4+2a(-1+2a) \\ (7-2\sqrt{7}+4(-1+\sqrt{7})a+4a^2)Cos(rt) \\ +(7-14a-4a^2+8a^3)\,Cos(\sqrt{7}rt) \\ +(14a-4\sqrt{7}a+8a^2-8a^3)Cos(rt-\sqrt{7}rt) \end{matrix}\right\},$$

$$\rho_2(t) = \frac{2a(-1+2a)}{-7(-4+\sqrt{7})+(44-20\sqrt{7})a+4(-4+\sqrt{7})a^2}\left\{\begin{matrix} -39+12\sqrt{7} \\ +(35-11\sqrt{7})Cos[rt] \\ +(11-5\sqrt{7})Cos(\sqrt{7}rt) \\ +(-7+4\sqrt{7})Cos(rt-\sqrt{7}rt) \end{matrix}\right\} \quad (9)$$

Expression (8) defines all the coefficients of equations (1), i.e. the quantum systems whose dynamics are described by the constructed solution. This is a a family of particle models with different dipole moments of transitions and with a different arrangement of energy levels, including a non-equidistant arrangement, which is typical for molecules. These systems are excited by radiation having different sets of parameters – the carrier frequency and the amplitude.



(a)



(b)

FIGURE 3. The dependence of populations $\rho_n(rt)$ of the three-level quantum systems on time rt; ρ_0, ρ_1, ρ_2 are dashed, dot-dashed, and thick. (Where a =1/√7 in figure (a) and a =1/5 in figure (b))

6. CONCLUSIONS:

In this section we welcome you to include a summary of the end results of your research. Font should be Times New Roman, 10 pt. The discrete algorithm allows one to obtain a solution of equations of the form (1) for a variety of quantum systems with both homogeneous and inhomogeneous Fourier space of the desired functions (probability amplitudes of the excited quantum systems). The method is close to the physical content of the problem under consideration and corresponds to the main goal – to obtain a discrete distribution of particles over energy levels. The method does not require searching for already studied polynomials in order to apply them, but allows one to construct a sequence of polynomials for the quantum models under consideration. It is quite simple to introduce additional parameters leading to a solution describing the coherent dynamics of a family of quantum systems.

Note that the simple function $\sigma(x)$ (2) of the discrete argument x defines all the other structures associated with equations (1). It "generates" the corresponding system of orthogonal polynomials in the Fourier space of functions $a_n(t)$.

The work was carried out with the support of the Belarusian State Technological University, Minsk, Belarus and the SABIS® International School, Erbil, Kurdistan- Iraq.

REFERENCES

[1] Rabi, I.I., 1936. On the process of space quantization. *Physical Review*, 49(4), 324.

[2] Rabi, I.I., 1937. Space quantization in a gyrating magnetic field. *Physical Review*, 51(8), 652.

[3] Braak, D., Chen, Q.H., Batchelor, M.T. and Solano, E., 2016. Semi-classical and quantum Rabi models: in celebration of 80 years. *Journal of Physics A: Mathematical and Theoretical*, 49(30), 300301.

[4] Xie, Q., Zhong, H., Batchelor, M.T. and Lee, C., 2017. The quantum Rabi model: solution and dynamics. *Journal of Physics A: Mathematical and Theoretical*, 50(11), 113001.

[5] Banjak, S., 2019. Solving method without integration of some differential equation systems for coherent dynamics of quantum media excited by laser radiation. *Journal of Interdisciplinary Mathematics*, 22(6), 1051-1059.

[6] Banjak S., Savva V. The role of discrete orthogonal polynomials in constructing solutions of the dynamical equations describing coherent excitation of quantum systems in the field of laser radiation. AIP Conference Proceedings 2213, 020189 (2020). DOI 10.1063/5.0000104.

[7] Savva, V.A. and Banjak, S., 2020. Fourier Spectra of Quantum Systems Excited by Laser Radiation and the Exact Solution of their Dynamics Equations without Integration. *Journal of Applied Spectroscopy*, 87(5), 805-811.