Modelling of electromagnetic processes and phenomena in quantum-sized systems in the course of physical and mathematical support of master's programs of the specialty "Electric power engineering, electrical engineering and electromechanics"

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***Abstract*—The article deals with the use of mathematical computer modelling for the study of processes and phenomena in quantum-sized heterosystems.**

The use of computer algebra systems MathCad and Scilab allows us to study the characteristics of electromagnetic oscillations, the representation of periodic signals in the form of harmonic series, as well as to consider the state of electrons in different quantum dots (QD) and to determine the discrete spectrum of natural energies and its dependence on the geometric form and QD parameters.

The results of the research are implemented in the laboratory workshop of the discipline of physical and mathematical support of master's programs for students of the specialty "Power engineering, electrical engineering and electromechanics".

***Index Terms*—Mathematical computer modelling, electromagnetic oscillations, harmonic analysis, quantum dots, discrete model, discipline practice physical and mathematical support of master's programs, specialty "Electric power engineering, electrical engineering and electromechanics".**

I. Problem Statement

Methods of mathematical computer modelling are increasingly used for the study of various systems and phenomena [1]. The development of models for consideration of electromagnetic oscillatory systems, harmonic analysis and the state of the electron in quantum dots is promising. The use of computer simulation in the development of laboratory work on the course of physical and mathematical maintenance of master's programs of the specialty "Electric power engineering, electrical engineering and electromechanics" (EEE) is also relevant. The laboratory workshop provides an opportunity to acquire the necessary skills and abilities, helps to create the foundation for research and creative activity of masters. The introduction of information technology is due to the high level of security, visibility, ease of implementation and organization of laboratory workshops, and the fact that computer technology has become an indispensable tool for researchers in many specialties. In recent years, an intensive introduction of computer-aided mathematics and simulation modeling has been observed at engineering and technical educational institutions all over the world. The Scilab system is adapted to any branch of science and technology, contains tools that are particularly convenient for electrical and radio engineering calculations.

II. Presentation of the Main Material

The course "Physical and mathematical support of master's programs" is aimed at the formation of the masters of the specialty "EEE", a modern scientific worldview, mastering the fundamental knowledge of such sections of higher mathematics and mathematical physics: field theory, Maxwell's equations for the electromagnetic field in the integral and differential form, harmonic analysis and the use of the Fourier's series, equations of mathematical physics and the application of the Schrodinger's equation for stationary states of quantum heterostructures. According to the results of the course, masters

should know:

- characteristics and properties of scalar and vector fields: gradient, divergence and rotor;
- integral theorems: the Ostrogradsky-Gauss theorem, Stokes' and Green's theorems;
- Maxwell's equation in the integral and differential form for an electromagnetic field;
- wave differential equation for electromagnetic waves, characteristics, properties and application of electromagnetic waves;
- basis of harmonic analysis, representation of periodic functions by Fourier's series;
- application of Fourier's series, spectra of periodic functions;
- basic types of equations of mathematical physics and methods of their solution;
- properties and physical content of the wave function, the Schrodinger's equation for stationary states of quantum-sized systems and methods of their solution

be able to:
- determine gradient, divergence and rotor for scalar and vector fields in cartesian coordinates;
- apply the Ostrogradsky-Gauss theorem and Stokes' theorem for the study of various physical fields;
- determine the electric field strength and magnetic field induction by solving Maxwell's equations for the electromagnetic field;
- determine the characteristics of electromagnetic waves: wavelength, velocity of propagation, wave number, the Umov–Poynting vector and others;
- determine the coefficients of the Fourier's series for periodic functions;
- find function spectra;
- apply the Fourier's method to solve partial differential equations;
- find the solution of the Schrodinger's equation for stationary states;
- determine the eigenvalues of the energy of the particle and its own wave functions;
- use the boundary conditions for the wave function;
- simulate the state of the electron in quantum-sized heterostructures heterostructures.

For the modelling of complex physical processes and phenomena in the preparation of future masters in the specialty "EEE" we used MathCad and Scilab systems. Simulation computer modelling of relevant processes is the basis for the development of virtual laboratory work, which allows to intensify the educational process and increase the role of independent work of undergraduates. The laboratory workshop is based on the methods of mathematical computer modeling, which are increasingly used in modern scientific and technical research and in solving various practical problems. Therefore, the acquisition of relevant knowledge and skills in the use of programming (MathCad and Scilab systems) masters specialty "EEE" is an important task.

The study of the course "Physical and mathematical support of master's programs" is designed for 3 credits, including 16 hours of lectures, 14 hours of laboratory classes, 30 hours of independent work.

The following examples of laboratory work relate to the sections of fundamental physics and the theoretical foundations of electrical engineering and are their logical development, which is a condition for in-depth study of the course "Physical and mathematical support of master's programs" of the specialty "EEE".

1. Laboratory work "Modelling of fading electromagnetic oscillations". Consider the electromagnetic CRL-oscillatory circuit. The differential equation in the general case has the view [2]:

$$\frac{d^2Q}{dt^2}+2\delta\frac{dQ}{dt}+\omega_0^2Q(t)=\frac{U_0}{L}cos\omega t$$

If U_0=0 та R=0, the extinction coefficient is δ=0 and there are free, non-intermittent oscillations whose own frequency is equal to

$$\omega_0=\frac{1}{\sqrt{LC}}.$$

In the case of $R \neq 0$ there are fading oscillations:

$$Q(t)=Q_0\cdot e^{-\delta t}\cdot\cos(\omega_1 t+\varphi_0)$$

where δ is the attenuation coefficient:

$$\delta=\frac{R}{2L},$$

ω1 - the frequency of fading oscillations:

$$\omega_1=\sqrt{\omega_0^2-\delta^2}.$$

When $\delta>\omega_0$, we obtain the imaginary value ω_1 and the so-called aperiodic electromagnetic oscillations (Fig. 1).

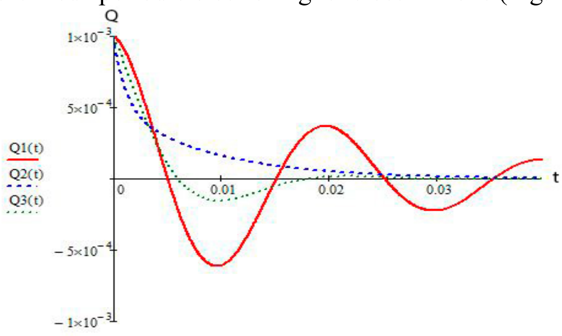


Fig.1. Fusing electromagnetic oscillations: 1 – if R=12 Om, δ=60; 2 – if R=80 Om, δ=400; 3 – if R=40 Om, δ=200.

Forced oscillations are observed when $U_0 \neq 0$, while, if the frequency ω of the external voltage is close to ω_1, there is a resonance phenomenon. The application of the MathCad package provides a study of the dependence of the characteristics of electromagnetic oscillations on the parameters of the oscillatory circuit, the construction of the graphs of the dependence of the current, voltage and energy on the time and the dependence of the amplitude of the oscillations from the cyclic frequency of the external voltage. Using the "Animation" command and the "Frame" variable allows you to demonstrate the dependency of the graphs on the CRL-stake parameters.

Thus, the modelling of electromagnetic oscillatory systems allows us to visualize the process of studying electromagnetic oscillations (non-fading, fading, forced) and the dependence of the characteristics of these oscillations (amplitude, phase, frequency) on the parameters of the electrical circuit (C, L, R), which extends and deepens knowledge of the course of the theoretical foundations of electrical engineering.

2. Laboratory work "Modelling decomposition of periodic function into Fourier's series". In this case, mathematical computer modelling is used to study harmonic analysis [3]. Consider, for example, the representation of an odd periodic function with a period of 2π:

$$f(x) = x, -\pi < x \leq \pi.$$

Determine the Fourier's coefficients:

$$a_0 = \frac{1}{\pi} \cdot \int_{-\pi}^{\pi} x dx = 0\,;$$

$$a_n = \frac{1}{\pi} \cdot \int_{-\pi}^{\pi} x \cdot cosnxdx = 0\,;$$

$$b_n = \frac{1}{\pi} \cdot \int_{-\pi}^{\pi} x \cdot sinnxdx = (-1)^{n+1} \cdot \frac{2}{n} \xrightarrow{n\to\infty} 0.$$

Get the Fourier's series:

$$f(x) = 2\left(sinx - \frac{sin2x}{2} + \frac{sin3x}{3} - \cdots (-1)^{n+1} \cdot \frac{sinnx}{n} + \cdots\right).$$

Determine the partial amount when m=1, 2, …:

$$S_m(x) = 2 \cdot \sum_{n=1}^{m} (-1)^{n+1} \cdot \frac{sinnx}{n} \xrightarrow{m\to\infty} f(x)$$

The MathCad software package provides modelling of the representation of the periodic function in the Fourier's series and allows to construct graphs of partial sums (Fig. 2,3)

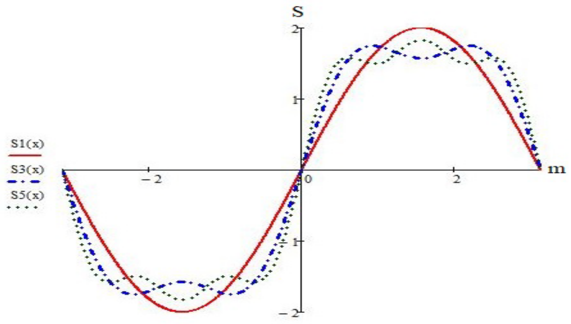


Fig. 2. Graphs of partial sums when m=1, 3, 5

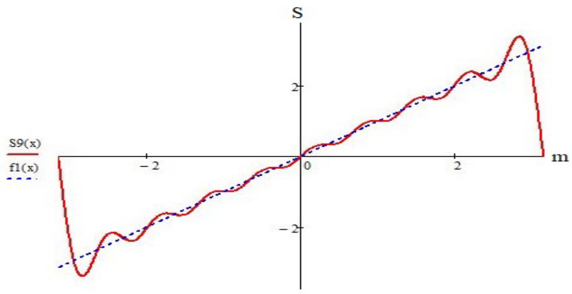


Fig. 3. Graphs of the partial sums when m=9 and $f(x)$.

The use of the MathCad package allows to demonstrate the coincidence of the partial sum of $S_m(x)$ of the Fourier's series of the periodic function $f(x)$ at $m\to\infty$. This is done by animating the $S_m(x)$ graph with the "Animation" command and the corresponding FRAME variable (m: = FRAME) in the MathCad toolbar. Modelling of the Fourier's series obtaining process provides the organization of simulation laboratory work on the course of physical and mathematical support of master's programs. Methods of harmonic analysis are used in electrical engineering and radio engineering to study the filtration, amplification and transformation of various electrical signals.

3. Laboratory work "Modelling of the electron state in a quantum dot". Let us consider the modelling of the state of S-electrons in quantum dots. The wave functions and the discrete spectrum of eigenvolumes depend on the geometric shape and parameters of the quantum dot. For example, for a conical quantum dot (CQD) whose height is H and the radius of the base is R (Pic. 4a) the Schrodinger"s wave equation in a cylindrical coordinate system has the form [4-6]:

$$\frac{\partial^2\psi}{\partial r^2} + \frac{1}{r}\frac{\partial\psi}{\partial r} + \frac{\partial^2\psi}{\partial z^2} + \frac{2mE}{\hbar^2}\psi(r,z) = 0 \qquad (1)$$

To solve the equation (1) in partial derivatives, we use the method of separating the variables (Fourier's method). We are looking for the wave function in the form:

$$\psi(r,z) = A \cdot \varphi_1(r) \cdot \varphi_2(z) = A \cdot J_0(k_1 r) \cdot \sin(k_2 z)$$

where k_1, k_2 – are wave numbers, $J_0(k_1 r)$ – is a zero-order Bessel function.

The electron motion in the approximation of the effective mass is limited in CQD, since the potential energy U is equal (Fig. 4b):

$$U(a,z) = \begin{cases} U_1 = 0, & if \ \ 0 \leq a \leq R, \quad 0 \leq z \leq H \\ U_2 = \infty, & if \ \ a > R, \quad z < 0, \quad z > H \end{cases}$$

where

$$a = r + z \cdot \frac{R}{H}.$$

When

$$\frac{2mE}{\hbar^2} = k_1^2 + k_2^2.$$

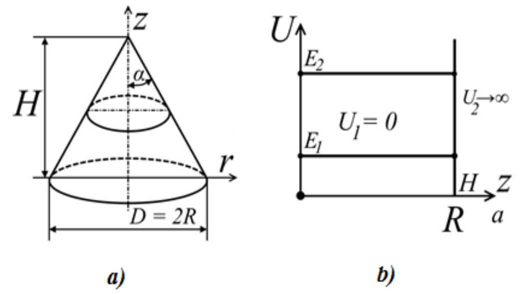


Fig. 4. a) Conical quantum dot; b) the potential energy of an electron: R – radius, H – height.

The proper values of the wave numbers $k_{1,n}$, $k_{2,n}$ and the energy E_n of the electron are found using the boundary conditions. For example, when

$$H = \frac{R}{tg\alpha} = \sqrt{3}R \ (\alpha = 30^0),$$

$$z_1 = \frac{R - r_1}{tg\alpha} = \sqrt{3(R - r_1)}\,:$$

$$\psi_1(r_1, z_1) = A \cdot \varphi_1\left(R - \frac{R}{H} \cdot z_1\right) \cdot \varphi_2(z_1)$$

$$= A \cdot J_0\left(k_1\left(R - \frac{R}{H} \cdot z_1\right)\right) \cdot sin(k_2 z_1) = 0$$

From:

$$k_{1,n} = \frac{b_n H}{R(H - z_1)}$$

where b_n – zero-order Bessel function.

$$k_{2,n} = \frac{\pi n}{z_1}$$

The proper values of the electron energy in the CQD depend on the coordinate z:

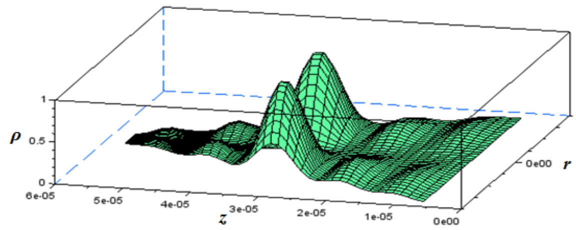
$$E(z) = \frac{\hbar^2}{2m}(k_1^2 + k_2^2) = \frac{\hbar^2}{2m}\left(\frac{3b_n^2}{(H-z)^2} + \frac{n^2\pi^2}{z^2}\right)$$

The 3D graphs of the probability density of finding an electron in a given region of the CQD for various axial and radial modes at A=1 are presented on Fig. 5. $A = 1$:

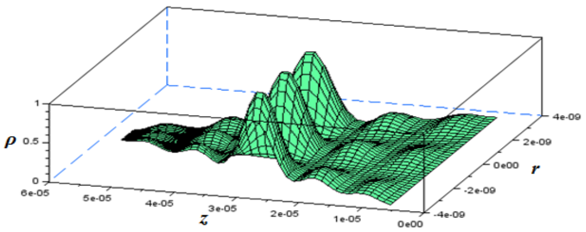
$$\rho(r,z) = |\psi(r,z)|^2 = J_0^2(k_1 r) \cdot sin^2(k_2 z)$$

To construct 3D graphs of probability density, methods of generating discrete models of geometric objects using the Scilab program package are used [7].

Thus, mathematical computer modelling allows to study the state of the electron and the dependence of its own energy on the type and size of the quantum dot. This is the basis for the development and implementation in the educational process of laboratory work: "Modelling the state of the electron in a spherical quantum dot", "Modelling the state of the electron in a cylindrical quantum dot", "Modelling the state of the electron in a conical quantum dot." The use of quantum dots in modern solar cells is a promising way of developing the electric power industry.



a)



b)

Fig. 5. The density of the probability of finding an electron in a conic quantum dot for different axial and radial modes: a) n_1=3, n_2=2; b) n_1=3, n_2=3

III. Conclusion

The modelling of electromagnetic oscillations allows to investigate the characteristics and their dependence on the parameters of the electromagnetic circle, to construct graphs of the dependence of the current and voltage on time for various types of electromagnetic oscillations (non-fading, fading, forced).

Methods of harmonic analysis of periodic signals are widely used in electrical and radio engineering. Mathematical modelling of the process of representation of various periodic functions by Fourier's series provides automation and visualization of this process.

The state of the electron in a conic quantum dot with completely opaque walls, the solution of the Schrodinger's equation for the wave function is considered, the dependence of the electron energy on the parameters of the CQD is investigated, and graphs of the density of the probability of finding an electron in a given region are constructed. A simulation of various radial and axial states of S-electrons is performed when there is no orbital moment (l=0).

Numerical methods can be used to solve the Schrodinger's equation and determine the eigenvalues of the electron energy, as well as to solve the system of Maxwell's equations in differential form (FDTD-method).

Subsequently, the study of quantum dots (cylindrical, spherical, conical) with a shell and a variety of limiting potential is of great interest.

Alternative energy sources, such as solar panels, use quantum dots to increase the limits of the absorption spectrum and the value of the efficiency factor. In addition, the development of a variety of sensors based on quantum dots is promising.

Thus, the laboratory workshop with the use of mathematical computer modelling provides training of highly qualified specialists in the field of knowledge "Electrical engineering".

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