ELECTRODYNAMICS 2D BOUNDARY PROBLEMS SOLUTION FOR APPLICATION OF NANO-BIO-PARTICLES CHARACTERIZATION

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Abstract - Solutions of electrodynamics two dimensional (2D) boundary problems are applied to study the electromagnetic (EM) field and single nanoscale particles interaction in purpose of characterization near and far EM field distribution. Physical models are elaborated for investigation of optical properties of bio-particles of different morphology. Particles of cylindrical shape are used for modeling rod-like, prolatevirions (e.g. bacteriophage M13, Tobacco Mosaic VirusTMV), extracellular infective forms of viruses. Method of estimation of spectral response on EM field & particles interaction, as well as of resonance wave-length ranges are considered. Theoretical decision of problem is based on rigorous solutions of Maxwell's, Helmholtz's and Bessel's equations. Analytical expressions of EM fields are defined through the relative parameters, diameters over excitation wavelength. It makes possible to apply the classical well-known approach to sub-micro particles characterization. Computer simulation (based on MatLabR2013b software) shows that resonant spectral response is observable on far-field characteristics: scattering cross sections and radiation patterns(RP). Near-field distributions are presented in a form of isolines of EM field amplitudes, indicating the locations of energy maximums inside and outside of particles. Analysis revealed the strong dependence of field characteristics on electrical and geometrical parameters in resonance wave range, possibility for consideration the simulated spectra as the specific signatures of bio-particles of a given parameters. Proposed methodology of estimation EM field characteristics is essential for aerosol and nano-bio-particles spectroscopic studies, bio-particles detection and identification systems.

Keywords - Nanoscale Bio-particles, Simulation, Spectra, Electromagnetic Field.

I. INTRODUCTION

Study of complex biomolecules, bio-structures and bio-particles takes important place in modern trends of applied physics, nanophysics, nanobio science, nanotechnology. There are numerous types of bio-particles: natural-made (bacteria, viruses, mineral composites), artificial (synthesized chemically or shredded) and randomly generated (anthropogenic, industrial), many of that are threatfullbio-agents, transmitted as aerosol and bio-aerosol (containing bacteria and viruses) particles causing the health problems, increasing epidemiological risks.

Elaboration of effective methods for research and estimation of properties and characteristics of sum-micro sized bio-particles is actual and important insensing, detectingand identification systems [1]-[3] aswell as in bio-aerosol studies [4]. Viruses, bacteria, polymers, proteins, DNA and RNA moleculesare composed of different functional groups, structures of great numberof atoms, having the set of characteristicfrequenciesrelated to translation, rotation, vibration, electronic motions.
Determination of frequencies, unique spectral signatures and fingerprints of complex bio-molecular systemsis essential in spectral analysis and biomaterials characterization. Study of optical properties of nano and micro (10^{-9}-10^{-6} m) sized particles is problematic because of limited spectral ranges or operation parameters of experimental, spectroscopic, fluorescent, bio-chemical and immunological techniques, long-term processes of sample preparation and measurements [5], low values of detected signals, variety of particles and overlapping of the sizes in theair and environment, expensive experimental technology. Advanced measuring technics and the methods developed in recent years make opportunity to determine the dielectric permittivity of biomolecules, bio-sells, including viruses [6]-[9].

Characterization of complex biomolecules as one complete physical object instead of characterization of certain segments orstructures, study whole bio-particles behavior in different medium (air, aqua, and otherliquids) is the challenge and main goal of real systems research activities. One of the possible ways for determination of electromagnetic (EM) spectra, unique spectral signatures of nano and micro bio-particles, estimation of vibration and oscillation frequencies, resonan cewave length ranges and spectrometric parameters of bio-particles is the method we propose for consideration. The methodology is based on concept considering a particle of biological origin as a physical object characterized by the set of electromagnetic and geometric parameters [10], [11].Solution of classical electrodynamics two dimensional (2D) boundary problems we applied for obtaining new knowledge and data concerning nanobio-particles physical properties.
Proposed approach and methodologyweuse for investigation of optical properties and estimation of scattering characteristics of viral nanoparticles. In this work, we present for demonstration of elaborated methodology researchoutcomes obtained for virus, bacteriophage M13.

II. METHODOLOGY

Research methodology developed for studying physical properties of bio-particles involves two main directions: elaboration of appropriate models corresponding to morphology of bio-particles and formulation of relevant physical tasks, considering theoretical, numerical or experimental solution.

Target group of ongoing research is viral particles, viruses. Viruses among pathogenic microorganisms are the smallest infectious agents. The sizes of most viruses varies from 20 to 300 nm. Extracellular infective form of a virus is virion, a single stable entire virus particle consisting of an inner core of nucleic-acids (DNA/RNA) and outer protective protein coat called a capsid.To visualize the structure of virions one can use scanning and transmission electron microscopes. Nanoparticles reveal the properties of nano-sized (one dimension < 100 nm) particles quite different from bulk ones. Undoubtedly, nanobio-particles reveal the common and specific properties of both, nanoparticles and bioparticles, which should be reflected in corresponding electromagnetic characteristics. Therefore, we should determine the structure, shape and the set of specific parameters of each nanobio-particle and elaborate the models forestimation of physical properties of nanobio-particles, virions. Mostly bio-particles are characterized by the shapes with irregularities smaller than their size, therefore the approximation of surfaces seems possible by the various geometric surfaces, such are: sphere, ring, tube, ellipsoid, cone, rectangular, and etc. The virion of bacteriophage M13 is un-enveloped having rod-like, prolate shape,length-to-diameter ratio of M13 particle is approximately 126[12].Based on geometry and morphology of M13 particle, we considerthree physical models ofvirus-like particle (VLP) for investigation, namely: long circular cylinder ofA) core-shell structure,B) core-shell structure with core of nonlinear radial dependence of permittivity,and C) homogenous structure without shell. To study bio-particles physical properties and estimateparticles' and fields'characteristics, we considerphysical problem relevant to the processes having place in real spectroscopic experiments and detecting systems. The main actors of scenario: (VLP) particle, waveradiated from EM source, and detected signal, response onEM field &single particle interaction are under consideration.Theoretical solution of single VLP and EM wave interaction can be treated adequately within the framework of infinite cylinder theorythat is linked to classical, electrodynamics (2D) boundary problem's solution. Well-known Maxwell's equations [13], [14] in medium free of surface current and charge take the form

$$\nabla\times\vec{E}=i\omega\mu_q\mu_0\vec{H} \quad (1)$$

$$\nabla\times\vec{H}=-i\omega\varepsilon_q\varepsilon_0\vec{E} \quad (2)$$

where $\vec{E}$ and $\vec{H}$ are electric and magnetic field vectors, correspondingly, ∇ isNabla Operator[14], ω is an angularfrequency of excitation EM wave. For simplicity,we considered plane E-polirized wave of time dependence $\exp(-i\omega t)$ falling at the angle ϑ, through X axis opposite to X>0 direction.Dielectric permittivity $\varepsilon_q(\omega)$ and magnetic permeability $\mu_q(\omega)$ of q mediumgenerally may be defined as complex values:

$$\varepsilon_q(\omega)=\varepsilon_q^0+\frac{i\sigma_q(\omega)}{\omega\varepsilon_0} \quad (3)$$

$$\mu_q(\omega)=\mu_q^0+i\mu_q(\omega) \quad (4)$$

where $\varepsilon_0=8.85\times10^{-12}$ F/m, $\mu_0=1.26\times10^{-6}$ H/m. From (1) and (2), we would get the Helmholtz's (wave) equation:

$$\Delta\vec{E}+k_q^2\vec{E}=0 \quad (5)$$

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Wave vector of q mediumisequal to $k_q=k\sqrt{\varepsilon_q\mu_q}$, where $k=\omega\sqrt{\varepsilon_0\mu_0}$ and $\Delta=\nabla^2$ is Laplace scalar operator [14]. Using the variables separation method [14], [15] (5) can be convertedinto three differential equations. According to the shape and morphology of (VLP),radial equation of radial function $R(\xi)$ is written in cylindrical coordinate system

$$\xi^2R''(\xi)+\xi R'(\xi)+\left(\xi^2-s^2\right)R(\xi)=$$
$$=\frac{k^2}{k_q^2}f\left(\xi/k_q\right)\xi^2R(\xi) \quad (6)$$

$\xi=k_qr_q$, "/" -denotes the derivative with respect to an argument.Function $f(r_q)$ describes inhomogeneity of dielectric permittivity through the radius of cylinder [16].

Numerical method for calculation of function $R(\xi)$ when $f(r_q)$ is quadratic type is given in [16].ForVLPmodels (VLP-A) and (VLP-C), function $f\left(\xi/k_q\right)=0$ and we get from (6) the Bessel's equation [14], [17] partial solutions of which are Bessel's $J_s(\xi)$, Neumann's $N_s(\xi)$ and the first kind Hankel's $H_s^{(1)}(\xi)$ cylindrical functions of s-order [17]. EM Fieldsin the areas of VLP are written as the sums of multipole waves, taking into consideration:both the radiation condition outside the area $(kr>>1)$ of (VLP)[14], [15], and thefiniteness of field inside of VLP under the condition $(E_z grad\{\varepsilon_q-f(r_q)\})=0$ .Therefore, EM fields get the following forms:

Outside of (VLP) $b\le r\prec\infty$, $0\le\varphi\le2\pi$

$$E_z^{(out)}=\sum_{s=-\infty}^{\infty}A_sH_s^{(1)}(k_3r)e^{is\varphi-i\omega t} \quad (7)$$

Inside of core $0 \le r \le a$, $0 \le \varphi \le 2\pi$

$$E_z^{(co)} = \sum_{s=-\infty}^{\infty} B_s R_s(k_1 r) e^{is\varphi - i\omega t} \quad (8)$$

Inside of shell $a \le r \le b$, $0 \le \varphi \le 2\pi$

$$E_z^{(sh)} = \sum_{s=-\infty}^{\infty} [C_s J_s(k_2 r) + D_s N_s(k_2 r)] e^{is\varphi - i\omega t} \quad (9)$$

Where $a = d_1/2$, $b = d_2/2$, d_1 and d_2 are inner and outer diameters of shell; k_1, k_2 and k_3 are wave vectors corresponding to core, shell and surrounding medium of VLP.Unknown multipole coefficients $\{A_s\}, \{B_s\}, \{C_s\}, \{D_s\}$ should be defined by solving(2D) boundary problem.Forthis reason, satisfying the continuitycondition of tangent componentsof electric(E_z) and magnetic (H_φ)fieldsat theboundary surfaces of two medium is required. Complicated mathematical transformations leadthe functional equations to the system of algebraic equations. After solving that we get the expressions for multipole coefficients:

$$A_s = -E_o i^{-s} e^{-is\theta} \frac{\{U_s \Im_s - G_s L_s\}}{\{U_s \Gamma_s - G_s \Lambda_s\}} \quad (10)$$

$$B_s = \frac{E_o i^{-s} e^{-is\theta} \dfrac{2i}{\pi k_3 b}}{\dfrac{\pi k_2 a}{2}\{U_s \Gamma_s - G_s \Lambda_s\}} \quad (11)$$

$$C_s = B_s U_s \frac{\pi k_2 a}{2} \quad (12)$$

$$D_s = -\frac{\pi k_2 a}{2} B_s G_s \quad (13)$$

We use in (10)-(13) notations $\Gamma_s, \Lambda_s, \Im_s, L_s, G_s, U_s$ for defining the following functions:

$$\Gamma_s = \mathrm{H}_s^{(1)\prime}(k_3 b) J_s(k_2 b) - W_{23} \mathrm{H}_s^{(1)}(k_3 b) J_s'(k_2 b) \quad (14)$$

$$\Lambda_s = \mathrm{H}_s^{(1)\prime}(k_3 b) N_s(k_2 b) - W_{23} \mathrm{H}_s^{(1)}(k_3 b) N_s'(k_2 b) \quad (15)$$

$$\Im_s = J_s'(k_3 b) J_s(k_2 b) - W_{23} J_s(k_3 b) J_s'(k_2 b) \quad (16)$$

$$L_s = J_s'(k_3 b) N_s(k_2 b) - W_{23} J_s(k_3 b) N_s'(k_2 b) \quad (17)$$

$$G_s = R_s(k_1 a) J_s'(k_2 a) - W_{12} R_s'(k_1 a) J_s(k_2 a) \quad (18)$$

$$U_s = R_s(k_1 a) N_s'(k_2 a) - W_{12} R_s'(k_1 a) N_s(k_2 a) \quad (19)$$

where $W_{pq} = k_p \mu_q / k_q \mu_p$. For model VLP-A,in expressions (7)-(9), (14)-(19) function $R_s(k_1 a)$ should be replaced by function $J_s(k_1 a)$ and $R_s'(k_1 a)$ - by function $J_s'(k_1 a)$.Model (VLP-C) is simplified version of model (VLP-A).For model (VLP-C) we can rewrite EM fields expressions ifuse relations $d_2 = d_1$, $\varepsilon_2 = \varepsilon_1$ and $\mu_2 = \mu_1$ in all formulas.

For studying VLP's physical properties we use near($r < \frac{d_2^2}{\lambda}$ [18]) and far ($kr >> 1$ [15])fields characteristics. EM fields and their characteristics describing response on field &single particle interaction are expressed through dimensionless, relative parameters, diameter of VLP over the value of excitation wavelength (λ). That makes it possible to apply solution,derived above,to nano-sized particles characterization. Near field is estimated by using (7)-(9) formulas. For far field characterization we use an energetic characteristics, describing the scattering ability.Based on Poynting theory [13], using asymptotic expression of Hankel ($H_s^{(1)}(\xi)$)function [17]we derive the formulas for scattering cross section [11], [13], [16]: through the direction of wave propagation that is forward cross section (σ_F) and in opposite directionis backward cross section (σ_B):

$$\sigma_F = 2\pi \left| F(\pi + \vartheta) \right|^2 \text{ and } \sigma_B = 2\pi \left| F(\vartheta) \right|^2 \quad (20)$$

Function $F(\varphi)$, known as radiation pattern (RP), specifies an angular distribution of scattered field

$$F(\varphi) = \sqrt{\frac{2}{\pi k_3}} e^{-i\frac{\pi}{4}} \sum_{s=-\infty}^{\infty} A_s e^{-i\frac{\pi}{2}s} e^{is\varphi} \quad (21)$$

Total (σ_T) cross section defined as

$$\sigma_T = \int_0^{2\pi} F(\varphi) F^*(\varphi) d\varphi$$

gets the form suitable for computing

$$\sigma_T = \frac{4}{k_3} \sum_{s=-\infty}^{\infty} |A_s|^2 \quad (22)$$

Thus, deterministic and rigorous solution of physical task is given in analytical form. Proposed methodology, elaborated computer programs along with modern computing facilities make possible to estimate optical, spectroscopic characteristics of nanobio-particles, obtain data for arbitrary geometric and electromagnetic parameters. In presented work we focus our attention on a method relevant for estimation of resonance wavelength ranges, vibration and oscillation frequencies, so important in determination of bioparticles' specific signatures and fingerprints.

Outcomes of computer simulation studies and experimental data obtained by applying exquisite techniques should complement each other, verify factors (surface roughness, possible anisotropy of core-shell areas of virion) unforeseen in simplified approaches,correct and form accurately VLP models.

III. RESULTS AND ANALYSIS

For studying optical resonant properties of VLP we use computer simulation method based on analytical and numerical solutions of problem. Estimation of scattering and absorption characteristics of nano-micro particles in resonancerangeswas not easily realizable in prior years. Simulation study of VLPspectral properties and EM field characteristics was carried out usingMatLabR2013b software, MatLab library of built in functions. We elaborated and developed script-programsrelevant for computing the spectra and EM field characteristics of nano-micro-sized particles.Determination of number (s) of terms in series (7)-(9), (20)-(22) by empirical formulas in parallel with controlling the convergence of series, accuracy (within 10^{-12})of multipole coefficients were carried out for each set of input parameters through the algorithm. Analysis reveals that the reduction of the relative parameter($\sqrt{\varepsilon_q}d_2/\lambda$) decreases the number of terms in series. In this paper, we present visualized numerical results of modelling VLP-M13 virionby using the possible set of inputparameters: outer diameter of shell - d_2 =6.8 nm, inner diameter of shell - d_1 =3.8 nm [12], dielectric permittivity and magnetic permeability of proteins and DNA[6]-[8] $\varepsilon_1 = 12$, $\varepsilon_2 = 2$, $\varepsilon_3 = 1$, $\mu_q \approx 1$ .Results of simulation study are presented on Fig. 1 and Fig. 2. Angle of incidentwave (ϑ)is equal to 0° . (XOY) plane is perpendicular to the axis of cylinder. Near field distribution in a form of lines of equal field amplitudes (izolines) in the range of ($-\lambda,+\lambda$) along the axes X and Y for (VLP-C) model is shown on Fig. 1 (a,b, c). Scattering cross sections (σ_T , σ_F , σ_B) vs wavelength (λ) in the wavelength range of 3-40 nm are presented on Fig.2(a,b,c), considering two models of M13 virion,(VLP-C) and (VLP-A). Simulation study of EM field characteristics of VLP-M13 reveals the following: expected resonant spectral response is observable on far-field characteristics (Fig.1, 2), values of resonant wavelengths of whole M13 particle may be associated to scattering cross section maximums; the upper limit of expected resonance wavelength range one could define using empirical formula $\lambda < \pi d_2 \sqrt{|\varepsilon_q|}$, where ε_q is dielectric permittivity of VLP;a set of resonant waveleng this is observed in ultraviolet (EUV) range of VLP-M13 particle's spectrum. Graphs describing dependence of scattering cross sections, total (σ_T) , forward (σ_F) and backward (σ_B) vs wavelength are qualitatively similar, with different magnitudes of spectral response on VLP & field interaction (Fig. 2), numbers of peaks and its locationsdepends on values of electromagnetic and geometric parameters of VLP and are quite specific for each VLP modelling virions. Near field distribution in VLP, location and number of maximums and minimums of amplitudes (intensities) highly dependant on values of wavelength (Fig. 1b, Fig. 1c), dielectric permittivity (Fig. 1a and Fig. 1b), also on the relative value of d_2/λ .

Comparing VLP models, we have seen that the values of dielectric permittivity of core and shellaffects significantly on formation of spectra and resonance ranges (Fig. 2b and 2c). Protein shell portion of whole M13 particle is 2.2 times greater than the portion of DNA containing core, therefore aninfluence of electromagnetic properties of capsids of M13 virions on EM field distribution should be noticeable. Presence of shell of VLP model makes changes in spectra of VLP (Fig. 2b and Fig. 2c). Thus, in accordance with the proposed concept [10], [11] and based on the solutions of classical electrodynamics boundary-value tasks, numerical experiments and computer simulation, also due to the numerical and graphical analysis of scattering characteristics of VLP, far and near field interpretation, we could state the following outcomes:

a) Sensitivity of system wave-particle towards the changes of electromagnetic and geometrical parameters forcerta in ranges of wave length;

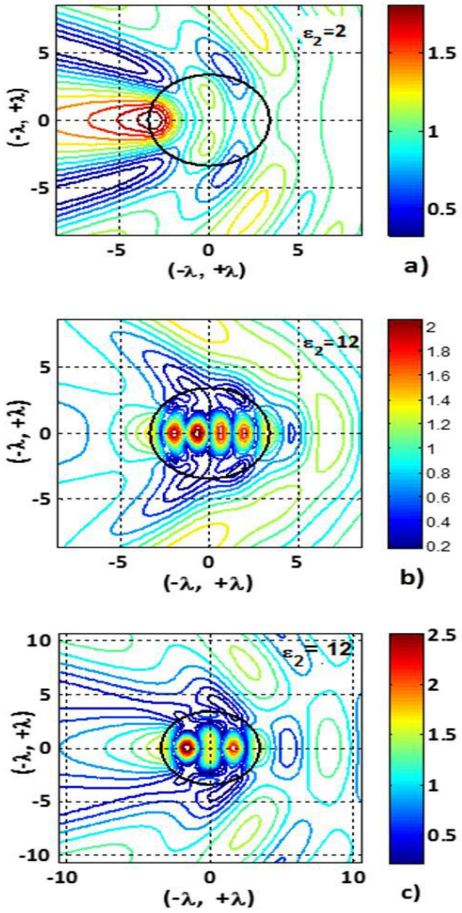


Fig. 1. Isolines of EM field amplitudes of VLP-M13 in wavelength range (- ,+).Angle of incidentwave . Diameter of VLP-C =6.8 nm; dielectric permittivities of surrounding medium andVLP =2 (a), 12 (b, c);excitation wavelength = 8.58 nm (a, b),10.6 nm (c).

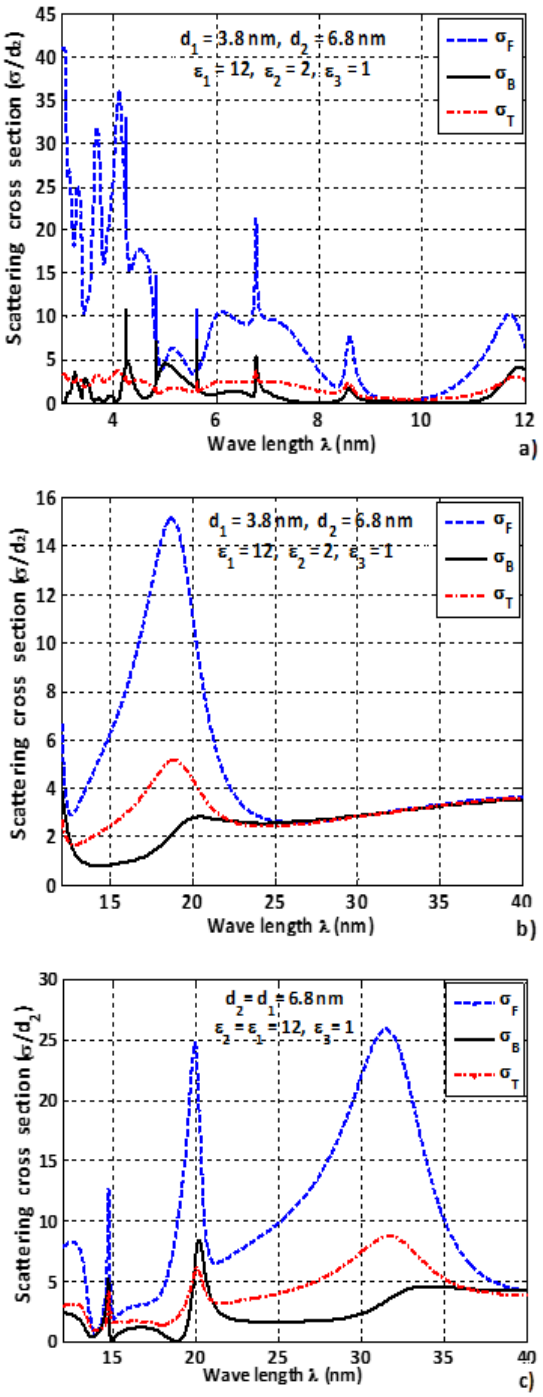


Fig. 2. Simulated spectra of VLP-M13. Scattering cross sections σ : forward (σ_F), backward (σ_B), total (σ_T) vs excitation wave length (λ). Angle of incidentwave $\vartheta = 0^\circ$; Diameters of VLP-M13: inner d_1 =3.8 nm, outer d_2 =6.8 nm (a, b); dielectric permittivities: of core - $\varepsilon_1 = 12$, shell - $\varepsilon_2 = 2$, surrounding medium - $\varepsilon_3 = 1$; models of M13: VLP-A (a, b), VLP-C (c).

b) Possibility of revealing and determining the specific and unique characteristic spectra and signature of each nano-bio-particle;

c) Possibility to estimate the resonance wave length range for given geometry of nano-bio-particle by using the numerical and simulation methods.

Proposed methodology alongsidewith computer simulation analysis make possible to study optical, scattering and absorption properties of bio-particles in different surrounding medium, determine and visualize the spectral response on EM field and particle interaction, have insight visionof particles, perform processes more foreseeable and predictable. Combining analytical and simulation methods, is alternative and efficientway to complex and expensive experimental measurements.

Regarding to models of nano-micro particles we should note, that analytical solution of physical tasks is applicable to particles, preferably of regular geometrical forms, such are: a) Particles of biological origin, virusis, bio-aerosol particles containing viruses, artificially generated bio-agents; b) Micro- and nano-sized solid state particles; c) Hybrid (organic-inorganic) nanoparticles of core-shell structure; d) Particles of non-biological origin, e.g. water drops, ice spheres, asbestos, textile, tar and smoke, atmospheric and aerosol particles, and etc.

Developed methodology and computer programs we may apply for estimation of spectra and resonant frequency ranges of numerous types of virions having the morphology similar to M13, namely rod-like, prolate icosahedral, helical and cylindrical. Proposed concept and methodology of research wesuccessfully use for nanoparticles of spherical shape, virions of spherical icosahedral morphology, on the basis of solutions of relevant physical tasks and elaborated models of nanoparticles [19].

IV. CONCLUSION

Solution of classical electrodymanics (2D) boundary problem we applied for study nanobio-particles' optical properties. Compiuter simulation method based on analitical solutionreveal the possibility to estimate spectroscopic charateristics as well as resonance wave length ranges of viral particles, M13 virons. The set of resonant wave lengths is observable in ultraviolet (EUV)range of VLP-M13 particle's spectrum.

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