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MODELING OF RESONANCE EFFECTS IN ONE-DIMENSIONAL PERIODIC DIFFRACTION GRATINGS CONTAINING GRAPHENE STRIPS Part 1. MATHEMATICAL JUSTIFICATION OF THE SPECTRAL METHOD

Subject and Purpose. This paper presents a theoretical study of the interaction between monochromatic electromagnetic radiation and a one-dimensional periodic strip grating. The grating consists of periodically alternating perfectly conducting and graphene strips located at the boundary of a planar dielectric layer. The aim is to provide a mathematical justification for the spectral method analysis of resonance effects arising during the interaction of electromagnetic radiation with the strip grating.

Methods and Methodology. The mathematical justification of the spectral method is based on the theory of non-self-adjoint compact operators in Hilbert spaces and the theory of compact analytic operator functions. In particular, we apply Keldysh's theorems on the completeness of eigenvectors and associated vectors of non-self-adjoint compact operators, as well as the operator generalization of Rouché's theorem for analytic operator functions.

Results. The spectral approach to solving the diffraction problem of a one-dimensional periodic strip grating, which includes graphene strips, has received a rigorous mathematical treatment. It has been established that the diffraction field can be represented as an expansion in eigenfunctions of the spectral problem, where the spectral parameter (eigenvalue) enters linearly into the boundary condition of conjugation on the graphene strips. The existence of the spectral problem solution has been proved in the case of small widths of the perfectly conducting strips. The completeness of the system of eigenfunctions (eigenvectors) in the corresponding Hilbert space has been demonstrated. As a consequence, in an unbounded region, there is a possibility to expand the diffraction field in resonance terms. An equation for resonance frequencies has been derived, indicating that the imaginary part of the spectral parameter equals the imaginary part of the surface conductivity of the graphene strips in the grating.

Conclusions. The developed spectral method enables effective analysis of resonance effects that occur when electromagnetic radiation interacts with a one-dimensional periodic diffraction grating that includes graphene strips. This method can be used in the mathematical modeling of various devices and systems that utilize such gratings.

Keywords: graphene, one-dimensional periodic diffraction strip grating, compact operator, resonance, Hilbert space, surface conductivity

Introduction

Recent advances in the fabrication of graphene and graphene-based periodic nanostructures have opened up promising opportunities for the develop-

ment of tunable metamaterials and integrated plasmonic devices with potential applications in the terahertz and infrared frequency ranges (see, e.g., [1]). The design of graphene-based devices is fundamentally related to the advancement of modeling tools

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that utilize rigorous solutions of Maxwell's equations and graphene conductivity models. Of particular interest and practical importance is modeling various resonance effects occurring during the interaction between electromagnetic radiation and periodic graphene-based nanostructures. One of the recognized approaches in this field exploits the idea of analytic continuation of a frequency into its complex domain (generally, to a certain Riemannian surface) in terms of the boundary value problem of diffraction governed by Maxwell's equations. The solution of this problem describes the interaction of monochromatic electromagnetic radiation with open resonant-type structures, such as periodic gratings containing graphene. The sense of this analytic continuation procedure is clear, implying that the singularities of the analytically continued solution of the diffraction problem fully determine the behavior of corresponding characteristics of the diffraction field in the domain of real-valued parameters (e.g., real frequency).

The analysis of these singularities is a field of significant research into the nature and physical mechanisms of resonance and anomalous responses of open structures to external excitations. The fundamental concepts and methods of this approach ([2] and the references therein) are believed to be especially effective for studying the diffraction of monochromatic electromagnetic waves by various types of periodic structures [3]. The main drawback is the impossibility of representing the diffraction field as a series expansion in resonance terms, similar to eigenmode expansion in the theory of closed resonators. Although such representations are possible in some special cases (analogous to the Mittag-Leffler expansion in the theory of meromorphic functions of complex variables), they are not generally available. Another weakness is somewhat technical and arises from the fact that the complex frequency domain corresponds to an infinite-sheeted Riemannian surface. (for problems of wave diffraction on periodic structures [3]). In general, a global uniformization of such Riemannian surfaces is not known, which significantly complicates the analysis of diffraction problems. Furthermore, significant challenges arise when the structure physical parameters (dielectric permittivity, graphene surface conductivity in the Kubo formulation, etc.) vary with frequency.

In response to modeling resonance effects in periodic nanostructures, the authors consider an alter-

native approach based on a different idea, which was seemingly first introduced [4] for quantum mechanical scattering problems in terms of the Schrödinger equation. In [4], the Schrödinger equation solution in an unbounded domain is series expanded in eigenfunctions of an auxiliary spectral problem, where the spectral parameter (eigenvalue) is the coupling constant, the factor multiplying the potential energy term. In diffraction theory, this idea allows representing the solution of Maxwell's equations in an unbounded region as a series expansion in eigenfunctions of an auxiliary spectral problem (without sources). This approach has become known as the generalized method of eigenoscillations (see references in [5]). In this formulation, it should be particularly emphasized that (i) the spectral parameter is not a frequency, eigenfunctions of the auxiliary spectral problem satisfy the same radiation condition as the diffraction problem solution does, (ii) the frequency remains real-valued, and there is no need for the analytic continuation of the solution into the complex frequency domain, and (iii) the main concept of the approach is that the spectral parameter is not a frequency (as in the previous approach) but some physical parameter, e.g., the conductivity of graphene. Importantly, the amplitudes of the expansion terms are inversely proportional to the difference between the spectral parameter (eigenvalue) and the corresponding physical parameter in the diffraction problem. Since the spectral parameter depends on frequency, resonances may occur at frequencies where the spectral parameter approaches the physical parameter. This method is akin to the classical technique of eigenmode expansion for diffraction problems in bounded regions (theory of closed resonators).

In this context, a spectral method is developed for modelling resonance effects arising in the interaction of monochromatic electromagnetic radiation with a diffraction grating of periodically alternating perfectly conducting and graphene strips.

Part I presents a rigorous mathematical formulation of the spectral method as applied to a planar strip grating of periodically alternating perfectly conducting and graphene strips. The auxiliary spectral problem (the spectral parameter is the surface conductivity of graphene) is reduced to the eigenvalue-and-eigenvector problem for a non-self-conjugate compact operator in the corresponding Hilbert space. The completeness of the system of eigenvec-

tors is established, which allows the diffraction field in an unbounded region to be expressed as a series expansion in resonant terms.

Part II is devoted to the extension of the spectral method to the diffraction problem of the aforementioned planar strip grating located at the boundary of a dielectric layer. Mathematical modeling results on resonance effects accompanying the electromagnetic interaction with this grating structure will be reported.

1. The problem formulation, the model problem

1.1. The diffraction problem

The problem of interaction between monochromatic electromagnetic radiation and a planar strip grating composed of periodically alternating perfectly conducting and graphene strips is considered. The grating is supported by a planar dielectric layer (substrate) of thickness h , absolute permittivity $\varepsilon\varepsilon_0$, and permeability μ_0 , with ε_0 and μ_0 being the vacuum permittivity and permeability. In Cartesian coordinate system x, y, z in the Figure, the grating is located in the plane $z = 0$. The strips are parallel and infinite along the x -axis, with period l along the y -axis. The widths of the perfectly conducting and graphene strips are d and $l - d$, respectively. The surface conductivity σ_g of the graphene strips is determined by the Kubo formula [6]

$$\sigma = \sigma_g W_0 = \sigma_1 + \sigma_2, \quad (1)$$

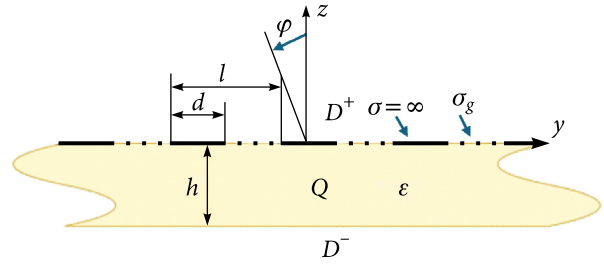
$$\sigma_1 = \frac{i\kappa_p}{\kappa + i\Gamma}, \quad \sigma_2 = \alpha \left(\frac{\pi}{2} + \arctg \xi_- - \frac{i}{2} \ln \frac{\xi_+^2}{1 + \xi_-^2} \right), \quad (2)$$

$$\kappa_p = 2\alpha\kappa_T \ln \left(2ch \left(\frac{\kappa_\mu}{2\kappa_T} \right) \right), \quad \xi_\pm = \frac{\kappa \pm \kappa_\mu}{\kappa_T},$$

$$\kappa = \frac{\omega\sqrt{\varepsilon_0\mu_0}l}{2\pi}, \quad \kappa_\mu = \frac{\mu_c l \sqrt{\varepsilon_0\mu_0}}{\hbar\pi},$$

$$\kappa_T = \frac{k_B T l \sqrt{\varepsilon_0\mu_0}}{\hbar\pi}, \quad \Gamma = \frac{l\sqrt{\varepsilon_0\mu_0}}{2\pi\tau},$$

where ω is the angular frequency, $W_0 = \sqrt{\mu_0/\varepsilon_0}$ is the free space impedance, τ is the relaxation time of charge carriers (electrons) in graphene, μ_c is the chemical potential, \hbar is the Planck constant, k_B is the Boltzmann constant, α is the fine-structure con-



The problem geometry

stant, and T is the temperature ($T \approx 300$ K, the room temperature).

Notably, formula (2) for σ_2 (the contribution of interband transitions to the graphene surface conductivity) is valid for $\kappa_\mu \gg \kappa_T$ ($\mu_c \gg k_B T \approx 0.026$ at the room temperature). Ibidem, $|\sigma_1| \gg |\sigma_2|$ in the frequency range $\omega \ll \omega_0$, where ω_0 is the smallest root of the equation $\text{Im} \sigma = 0$. In the frequency range $\omega < \omega_0$, the real and imaginary parts of the conductivity are positive ($\text{Re} \sigma > 0$, $\text{Im} \sigma > 0$) for all frequencies. The time dependence is $\exp(-i\omega t)$.

The process of the interaction between monochromatic electromagnetic radiation and a strip grating is modeled by the following two-dimensional diffraction problem. Let a TM -polarized monochromatic plane wave propagate in the plane $x = 0$ at an angle φ to the z -axis (the magnetic field strength is parallel to the x -axis),

$$\vec{H}^i = (H_x^i, 0, 0), \quad \vec{E}^i = (0, E_y^i, E_z^i),$$

$$H_x^i = e^{i(\Phi y - \sqrt{\kappa^2 - \Phi^2} z)} \frac{2\pi}{l}, \quad E_y^i = -\frac{W_0 \sqrt{\kappa^2 - \Phi^2}}{\kappa} H_x^i, \quad (3)$$

$$E_z^i = \frac{W_0 \Phi}{\kappa} H_x^i.$$

Here $\Phi = \kappa \sin \varphi$, the frequency parameter κ and factor W_0 are the same as in Eq. (2).

Assuming all quantities x -independent ($\frac{\partial}{\partial x} \equiv 0$, the grating strips are x -infinite), we deal with a two-dimensional problem and seek the diffraction field $\vec{H}^d = (H_x^d, 0, 0)$, $\vec{E}^d = (0, E_y^d, E_z^d)$ resulting from the interaction between the incident wave (3) and the strip grating.

Consider the spatial region $D = D^+ \cup Q \cup D^-$, where

$$D^+ = \{(y, z) : |y| < l/2, 0 < z < +\infty\},$$

$$D^- = \{(y, z) : |y| < l/2, z < -h\},$$

$$Q = \{(y, z) : |y| < l/2, -h < z < 0\}.$$

Let $u_0 = H_x^i$, $u_d = H_x^d$, and $\bar{\varepsilon} = \begin{cases} 1, (y, z) \in D^+ \cup D^-, \\ \varepsilon, (y, z) \in Q. \end{cases}$

The function u_d must satisfy the homogeneous Helmholtz equation

$$\Delta u_d + k^2 \bar{\varepsilon} u_d = 0, (y, z) \in D \quad (4)$$

and the following conditions, including the quasi-periodicity condition

$$\begin{aligned} u_d(-l/2, z) &= e^{i2\pi\Phi} u_d(l/2, z), \\ \frac{\partial u_d(-l/2, z)}{\partial y} &= e^{i2\pi\Phi} \frac{\partial u_d(l/2, z)}{\partial y}, \end{aligned} \quad (5)$$

the boundary conditions on the perfectly conducting grating strips,

$$\frac{\partial u_d^-}{\partial z} = \frac{\partial}{\partial z}(u_0^+ + u_d^+) = 0, z = 0, |y| < \frac{d}{2}, \quad (6)$$

the radiation condition in $D^+ \cup D^-$,

$$u_d = \begin{cases} \sum_{n=-\infty}^{\infty} R_n e^{i\Phi_n \frac{2\pi}{l} y} e^{i\Gamma_n \frac{2\pi}{l} z}, & (y, z) \in D^+, \\ \sum_{n=-\infty}^{\infty} T_n e^{i\Phi_n \frac{2\pi}{l} y} e^{-i\Gamma_n \frac{2\pi}{l} (z+h)}, & (y, z) \in D^-, \end{cases} \quad (7)$$

with $\Phi_n = \Phi + n$, $\Gamma_n = \sqrt{\kappa^2 - \Phi_n^2}$, $\text{Re } \Gamma_n \geq 0$, $\text{Im } \Gamma_n \geq 0$ (this choice of roots Γ_n ensures a physically consistent behavior of the energy characteristics of the diffraction field and guarantees no incoming waves into the region Q), the boundary conditions on the graphene strips

$$u_0^+ + u_d^+ - u_d^- = -\frac{\sigma}{ik} \frac{\partial}{\partial z}(u_0^+ + u_d^+), z = 0, |y| > \frac{d}{2}, \quad (8)$$

$$\frac{\partial}{\partial z}(u_0^+ + u_d^+) = \frac{1}{\varepsilon} \frac{\partial u_d^-}{\partial z}, z = 0, |y| > \frac{d}{2}, \quad (9)$$

and the matching conditions across the dielectric layer (substrate) boundary $z = -h$, $|y| < l/2$,

$$u_d^+ = u_d^-, \frac{1}{\varepsilon} \frac{\partial u_d^+}{\partial z} = \frac{\partial u_d^-}{\partial z}. \quad (10)$$

Hereinafter, u^\pm and $\frac{\partial u^\pm}{\partial z}$ are the limits of the u and $\frac{\partial u}{\partial z}$ functions as $z \rightarrow 0 \pm 0$ ($z \rightarrow -h \pm 0$). Also, $k = \omega \sqrt{\varepsilon_0 \mu_0}$.

The total diffraction field $\vec{H} = (H_x, 0, 0)$, $\vec{E} = (0, E_y, E_z)$ in the region D is defined by the function

$$u = \begin{cases} u_0 + u_d, & (y, z) \in D^+, \\ u_d, & (y, z) \in D^- \cup Q, \end{cases}$$

$$H_x = u, E_y = -\frac{W_0}{ik\bar{\varepsilon}} \frac{\partial u}{\partial z}, E_z = \frac{W_0}{ik\bar{\varepsilon}} \frac{\partial u}{\partial y}.$$

Before constructing a solution to the diffraction problem (3)–(10) by the spectral approach, we take up a model diffraction problem with the view to solve it in closed analytic form using the spectral approach.

1.2. The model diffraction problem and the spectral approach

Let u_0 be a known function in the spatial region $D = D^+ \cup D^-$, where D^+ is as defined above and $D^- = \{(y, z) : |y| < l/2, z < 0\}$. The function u_0 obeys the Helmholtz equation

$$\Delta u_0 + k^2 u_0 = 0, \quad (11)$$

and the quasi-periodicity condition

$$\begin{aligned} u_0(-l/2, z) &= e^{i2\pi\Phi} u_0(l/2, z), \\ \frac{\partial u_0(-l/2, z)}{\partial y} &= e^{i2\pi\Phi} \frac{\partial u_0(l/2, z)}{\partial y}, \end{aligned}$$

where Φ is a known parameter.

The diffraction problem reduces to finding the solution $u = u_0 + u_d$ of Eq. (11), where u_d satisfies the quasi-periodicity condition (5), the boundary condition

$$\frac{\partial u_d^+}{\partial z} = \frac{\partial u_d^-}{\partial z}, z = 0, |y| < l/2, \quad (12)$$

$$u_d^+ - u_d^- = -\frac{\sigma}{ik} \frac{\partial}{\partial z}(u_0^+ + u_d^+), z = 0, |y| < l/2, \quad (13)$$

and the radiation condition

$$u_d = \begin{cases} \sum_{n=-\infty}^{\infty} R_n e^{i\Phi_n \frac{2\pi}{l} y} e^{i\Gamma_n \frac{2\pi}{l} z}, & (y, z) \in D^+, \\ \sum_{n=-\infty}^{\infty} T_n e^{i\Phi_n \frac{2\pi}{l} y} e^{-i\Gamma_n \frac{2\pi}{l} z}, & (y, z) \in D^-. \end{cases} \quad (14)$$

The quantities Φ_n , Γ_n , u^\pm , $\frac{\partial u^\pm}{\partial z}$, k , σ have the same meaning as before. In particular, $\text{Re } \Gamma_n \geq 0$, $\text{Im } \Gamma_n \geq 0$.

Problem (11)–(14) is the problem of diffraction of the u_0 wave (a quasi-periodic source) on a graphene monolayer, $z=0$ in the region D .

Along with the diffraction problem (11)–(14), the following spectral problem (no sources, $u_0 \equiv 0$) in the spatial region D is considered for the values of the spectral parameter γ at which the homogeneous Helmholtz equation

$$\Delta \bar{u} + k^2 \bar{u} = 0,$$

has nontrivial solutions satisfying quasi-periodicity condition (5), radiation condition (14), and the following conditions at $z=0$, $|y| < l/2$,

$$\frac{\partial \bar{u}}{\partial z} = \frac{\partial \bar{u}^+}{\partial z}, \quad (15)$$

$$\bar{u}^+ - \bar{u}^- = -\frac{\gamma}{ik} \frac{\partial \bar{u}^+}{\partial z}. \quad (16)$$

This problem solution can be obtained by separation of variables in the following closed form

$$\gamma_n = -\frac{2\kappa}{\Gamma_n}, \quad n = 0, \pm 1, 2, \dots, \quad (17)$$

$$\bar{u}_n = \frac{1}{\sqrt{l}} \frac{|z|}{z} e^{i\frac{2\pi}{l}(\Phi_n y + \Gamma_n |z|)}, \quad z \neq 0. \quad (18)$$

The direct calculation easily confirms that the function \bar{u}_n meets the normalization condition

$$\int_0^l |u^+(y, 0+0)|^2 dy = 1.$$

The essence of the spectral approach to the diffraction problem (11)–(14) is constructing its solution through a series expansion over the system of functions $(\bar{u}_n)_{n=-\infty}^{\infty}$ (see Eq. (18)),

$$u = u_0 + \sum_{n=-\infty}^{\infty} A_n \bar{u}_n. \quad (19)$$

If the series in Eq. (19) can be differentiated term by term repeatedly, at least twice (with respect to y and z), and the resulting series converge, then the function in Eq. (19) satisfies the Helmholtz Eq. (11). Furthermore, radiation condition (14), quasi-periodicity condition (5), and condition (12) are automatically fulfilled. To determine the unknown coefficients $(A_n)_{n=-\infty}^{\infty}$, simply substitute Eq. (19) into boundary condition (13) and utilize the orthogonality property of the system of functions $(\bar{u}_n^+)_{n=-\infty}^{\infty}$ on the interval

$(-l/2, l/2)$ along with boundary condition (16) for \bar{u}_n . After some transformations,

$$A_n = \frac{i\sigma a_n \sqrt{l}}{2\pi \Gamma_n (\sigma - \gamma_n)}, \quad n = 0, \pm 1, \pm 2, \dots, \quad (20)$$

where

$$a_n = \int_0^l e^{-i\frac{2\pi}{l}\Phi_n y} \frac{\partial u_0^+}{\partial z} dy.$$

$$\text{Here } \frac{\partial u_0^+}{\partial z} = \frac{\partial u_0(y, 0+0)}{\partial z}.$$

As follows from Eqs. (17) in view of (1) and (2), the vanishing of the denominators in Eq. (20) is out of the rule for real-valued $\kappa \geq 0$ and $\Phi \geq 0$. Indeed,

$$\Gamma_n (\sigma - \gamma_n) = \Gamma_n \sigma + 2\kappa.$$

Radiation condition (14) gives $\text{Re } \Gamma_n \geq 0$, $\text{Im } \Gamma_n \geq 0$. Taking

$$\Gamma_n \sigma + 2\kappa = 0 \quad (21)$$

yields

$$\text{Re } \Gamma_n = -\frac{2\kappa \text{Re } \sigma}{(\text{Re } \sigma)^2 + (\text{Im } \sigma)^2},$$

$$\text{Im } \Gamma_n = \frac{2\kappa \text{Im } \sigma}{(\text{Re } \sigma)^2 + (\text{Im } \sigma)^2}.$$

As $\text{Re } \sigma > 0$ (see Eqs. (1) and (2)), equality (21) cannot be fulfilled for κ and Φ real-valued. Nonetheless, we can let the modulus of the denominator in Eq. (20) to a minimum for finding the values of the parameters $\kappa > 0$ and $\Phi > 0$ at which $|\sigma - \gamma_n|$ attains its minimum with the index $n = 0, \pm 1, \pm 2, \dots$ fixed. It follows from Eq. (17) that $\text{Re } \gamma_n \leq 0$ and $\text{Im } \gamma_n \geq 0$. Therefore, these κ and Φ must satisfy the equation

$$\text{Im } \sigma - \text{Im } \gamma_n = 0$$

and will be referred to as resonance values. In the vicinity of the resonance values of these parameters in Eq. (19) for the diffraction field, it would suffice to retain a single series term with index n ,

$$u = u_0 + A_n \bar{u}_n.$$

Thus, the spectral problem not only aids in constructing a diffraction problem solution but also identifies the frequency parameter $\kappa = \frac{\omega l}{2\pi} \sqrt{\varepsilon_0 \mu_0}$ values at which one can expect the diffraction field resonance behavior as a function of the excitation monochromatic wave frequency.

2. The spectral problem. Mathematical justification of the spectral method

Let us consider the spectral problem, beginning with the case of the relative permittivity $\varepsilon = 1$ of the layer (substrate). The periodic structure is a planar strip grating of alternating perfectly conducting and graphene strips in the plane $z=0$ in the Figure.

The problem is to identify the spectral parameter γ values, at which non-trivial solutions \bar{u} of homogeneous Helmholtz equation (4) exist in the region D and satisfy the quasi-periodicity condition (5), the boundary condition on the perfectly conducting strips of the grating,

$$\frac{\partial \bar{u}^+}{\partial z} = \frac{\partial \bar{u}^-}{\partial z} = 0, \quad z = 0, \quad |y| < \frac{d}{2}, \quad (22)$$

the radiation condition (7), and the boundary conditions on the graphene strips,

$$\frac{\partial \bar{u}^+}{\partial z} = \frac{\partial \bar{u}^-}{\partial z}, \quad z = 0, \quad \frac{l}{2} > |y| > \frac{d}{2}, \quad (23)$$

$$\bar{u}^+ - \bar{u}^- = -\frac{\gamma}{ik} \frac{\partial \bar{u}^+}{\partial z}, \quad z = 0, \quad \frac{l}{2} > |y| > \frac{d}{2}. \quad (24)$$

Here \bar{u}^\pm and $\partial \bar{u}^\pm / \partial z$ are the limiting values of \bar{u} and $\partial \bar{u} / \partial z$ as $z \rightarrow 0 \pm 0$.

We meet the radiation condition (7) and seek a solution to this problem in the form

$$\bar{u} = \begin{cases} \sum_{n=-\infty}^{\infty} R_n e^{i\Phi_n \frac{2\pi}{l} y} e^{i\Gamma_n \frac{2\pi}{l} z}, & z > 0, \\ \sum_{n=-\infty}^{\infty} T_n e^{i\Phi_n \frac{2\pi}{l} y} e^{-i\Gamma_n \frac{2\pi}{l} z}, & z < 0. \end{cases} \quad (25)$$

From conditions (22) and (23), it follows the relationship between the unknown coefficients R_n and T_n ,

$$R_n = -T_n, \quad n = 0, \pm 1, \dots \quad (26)$$

From conditions (22) and (24) in view of (26), we obtain

$$\begin{aligned} \gamma \sum_{n=-\infty}^{\infty} \Gamma_n R_n e^{i\Phi_n \frac{2\pi}{l} y} &= \\ &= \begin{cases} 0, & |y| < \frac{d}{2} \\ -2\kappa \sum_{n=-\infty}^{\infty} R_n e^{i\Phi_n \frac{2\pi}{l} y}, & l/2 > |y| > \frac{d}{2}. \end{cases} \end{aligned} \quad (27)$$

If the spectral parameter is $\gamma = 0$, then Eq.(27) in view of (22) yields

$$\sum_{n=-\infty}^{\infty} |R_n|^2 \Gamma_n = 0.$$

When $\Gamma_n = \sqrt{\kappa^2 - \Phi_n^2} \neq 0$, $n = 0, \pm 1, \dots$, then $R_n = 0$ and, therefore, the spectral parameter $\gamma = 0$ only matches a trivial solution ($\bar{u} = 0$) of the spectral problem. In the opposite case $\Gamma_n = 0$, there exist non-trivial solutions at some n, κ , and Φ . It can be easily checked that these n, κ , and Φ satisfy the equation

$$\kappa = |n + \Phi|. \quad (28)$$

From the perspective of wave diffraction theory for periodic structures [2, 3], these values of the frequency parameter κ (see Eq. (28)) are related to Wood's anomalies [7]. Namely, for $\kappa > |n + \Phi|$, the diffraction harmonic (Floquet wave) $\exp\left(i \frac{2\pi}{l} (\Phi_n y \pm \Gamma_n z)\right)$ is a plane homogeneous wave, while for $\kappa < |n + \Phi|$, it is a plane inhomogeneous wave that exponentially decays as $z \rightarrow \pm\infty$. Near these frequency parameter values $|n + \Phi|$, the diffraction characteristics can change abruptly. Therefore, the nontrivial solutions matching the spectral parameter $\gamma = 0$ are physically associated with Wood's anomalies.

In what follows below, we assume without loss of generality that $\Gamma_n \neq 0$, $n = 0, \pm 1, \dots$, i.e., $\kappa \neq |n + \Phi|$. Furthermore, suppose that for some $\Phi \geq 0$, there exists a nontrivial solution \bar{u} , $\gamma \neq 0$ of the spectral problem (see Eq. (25)). Then at $\Phi \pm m$ (m is an integer), a nontrivial solution \bar{u}_\pm , $\gamma \neq 0$ exists,

$$\bar{u}_\pm = \begin{cases} \sum_{n=-\infty}^{\infty} R_{n \mp m} e^{i\Phi_n \frac{2\pi}{l} y} e^{i\Gamma_n \frac{2\pi}{l} z}, & z > 0, \\ \sum_{n=-\infty}^{\infty} T_{n \mp m} e^{i\Phi_n \frac{2\pi}{l} y} e^{-i\Gamma_n \frac{2\pi}{l} z}, & z < 0, \end{cases}$$

where the coefficients R_n and T_n are the same as those of the nontrivial solution \bar{u} (see Eq. (25)).

This property allows the range of the parameter Φ to be limited to the interval $[0, 1)$.

The next step in constructing the spectral problem solution is to derive the coefficients R_n ($T_n = -R_n$) from Eq. (25). Make use of the orthogonality of the functions $\exp\left(i \frac{2\pi}{l} \Phi_n y\right)$, $n = 0, \pm 1, \dots$ on the interval $(-l/2, l/2)$. Then Eq.(27) yields the following

infinite system of linear algebraic equations for the coefficients R_n , $n = 0, \pm 1, \dots$,

$$\gamma R_m = 2\kappa \sum_{n=-\infty}^{\infty} A_{mn} R_n, \quad m = 0, \pm 1, \dots \quad (29)$$

Here, the $\|A_{mn}\|_{m,n=-\infty}^{\infty}$ matrix elements are

$$A_{mn} = \frac{1}{\Gamma_m} \begin{cases} \frac{d}{l} - 1, & m = n, \\ \operatorname{sinc}\left(\frac{\pi d}{l}(n-m)\right) \frac{d}{l}, & n \neq m, \end{cases} \quad (30)$$

where $\operatorname{sinc} X = \frac{\sin X}{X}$, and, according to the radiation condition (7), the coefficients $\Gamma_m = \sqrt{\kappa^2 - \Phi_m^2}$, $\Phi_m = m + \Phi$ satisfy the inequalities $\operatorname{Re} \Gamma_m \geq 0$ and $\operatorname{Im} \Gamma_m \geq 0$.

Rewrite system (29) in the matrix form

$$\gamma R = 2\kappa A R, \quad (31)$$

where $A = \|A_{mn}\|_{m,n=-\infty}^{\infty}$ and R is a column vector.

Let us define the space of sequences to which solutions of the matrix equation (31) must belong. Given the grating strip edges, the set of conditions listed above should be supplemented with the edge condition that the solution of the spectral problem must satisfy in the grating edge vicinity. We assume that the column vectors $R^T = (R_n)_{n=-\infty}^{\infty}$ (T is a transpose operation) belong to the space of the sequences

$$\bar{l}_2 = \left\{ R^T = (R_n)_{n=-\infty}^{\infty} : \sum_{n=-\infty}^{\infty} |R_n|^2 (1 + |n|) < \infty \right\}. \quad (32)$$

As shown in [2], this condition provides a physically consistent behavior of the function \bar{u} (see Eq. (25)) near the grating strip edges.

As $R^T \in \bar{l}_2$, we can change over to the new unknown vectors $X^T = (X_n)_{n=-\infty}^{\infty}$ by the formula

$$R_n = \frac{X_n}{\sqrt{|n|} + 1}. \quad (33)$$

From Eqs. (32) and (33) it follows that X^T belongs to the space of square-summable sequences, $X^T \in l_2$.

In terms of the new unknown vectors X , Eq. (31) becomes

$$\gamma X = 2\kappa \bar{A} X, \quad (34)$$

where the elements of the matrix $\bar{A} = \|\bar{A}_{mn}\|_{m,n=-\infty}^{\infty}$

are related to the elements of the matrix $A = \|A_{mn}\|_{m,n=-\infty}^{\infty}$ as

$$\bar{A}_{mn} = A_{mn} \frac{\sqrt{|m|} + 1}{\sqrt{|n|} + 1}. \quad (35)$$

Equation (34) should be considered in the space l_2 . It can be proved that the matrix \bar{A} defines a compact operator in this space l_2 (as a product of a compact and a bounded operators).

Thus, the initial spectral problem has been reduced to the eigenvalue γ and eigenvector $X^T \in l_2$ problem for the compact operator $2\kappa \bar{A}$ in the Hilbert space l_2 . As known [8], if \bar{A} is a self-adjoint compact operator, there exists an eigenvector basis of this operator. Therefore, a solution of the equation

$$2\kappa \bar{A} X = \gamma X + b \quad (36)$$

exists (if $\bar{\gamma} \neq 0$ and is distinct from eigenvalues) and can be written in the series form

$$X = \sum_{n=-\infty}^{\infty} \frac{a_n}{\gamma_n - \gamma} X_n.$$

Here $2\kappa A X_n = \gamma_n X_n$, b is a known vector from the space l_2 , $a_n = (b, X_n)$, and $(,)$ is a scalar product in l_2 .

The outlined idea underpins the spectral method for constructing the diffraction problem solution (vector b in Eq. (36) is determined by the excitation wave in the diffraction problem).

As is readily observed, operator \bar{A} in Eq. (34) (see also Eqs. (30) and (35)) is a non-self-adjoint operator in the space l_2 , suggesting that the strip grating structure is open and radiates energy into free space. The question of whether an eigenvector basis exists for such an operator is not trivial. Below, it will be shown that the eigenvector system of the operator $2\kappa \bar{A}$ is complete in the space l_2 . This means that any vector $X \in l_2$ can be approximated by a linear combination of eigenvectors. In particular, a solution of Eq. (36) can be sought as a Fourier series expansion with respect to the system of eigenvectors of operator \bar{A} .

Let us examine some properties of eigenvalues and eigenvectors of the operator $2\kappa \bar{A}$ and begin with the matter of eigenvalue existence in the case of a sufficiently small parameter $d/l \ll 1$, where d is the width of the perfectly conducting strips of the grating. As follows from Eqs. (30) and (35), the

matrix operator \bar{A} can be represented by the sum of two operators

$$\bar{A} = D_0 + \frac{d}{l} \bar{V}. \quad (37)$$

Here $D_0 = \left\| -\frac{\delta_{mn}}{\Gamma_m} \right\|_{m,n=-\infty}^{\infty}$, $\bar{V} = \left\| \bar{V}_{mn} \right\|_{m,n=-\infty}^{\infty}$,

$$\bar{V}_{mn} = \frac{\sin c \left(\frac{\pi d}{l} (n-m) \right) \sqrt{|m|+1}}{\sqrt{|n|+1} \Gamma_m}, \text{ and } \delta_{mn} \text{ is the}$$

Kronecker delta.

It is readily seen that the matrix operator D_0 is compact in l_2 because $1/\Gamma_m \rightarrow 0$ as $|m| \rightarrow \infty$.

Since $\sum_{m,n=-\infty}^{\infty} |\bar{V}_{mn}|^2 < \infty$, the operator \bar{V} is also

compact. From Eq. (37) it follows that as $d/l \rightarrow 0$, the operator \bar{A} converges to D_0 in the operator norm. In particular, $\bar{A} = D_0$ for $d/l = 0$ (no perfectly conducting grating strips). In this case, Eq. (34) becomes

$$\gamma X = 2\kappa D_0 X. \quad (38)$$

From Eq. (38), it follows that the eigenvalues $\gamma_m^0 = -\frac{2\kappa}{\Gamma_m}$, $m = 0, \pm 1, \dots$ exist along with the corresponding eigenvectors $x_m^T = (\delta_{nm})_{n=-\infty}^{\infty}$. It is obvious that the system of the eigenvectors x_m^T , $m = 0, \pm 1, \dots$ forms an orthonormal basis in the space l_2 . The values of the spectral parameter γ_m^0 coincide with the values of the spectral parameter defined in Eq. (17) of the model spectral problem (15)–(18).

If the parameter d/l ($d/l \neq 0$) is sufficiently small, a circle with the center at γ_m^0 locates an eigenvalue of the operator \bar{A} (see Eq. (37)). To prove that, we introduce the operator-functions

$$B(\gamma) = C(\gamma) - 2\kappa \frac{d}{l} \bar{V}, \quad C(\gamma) = \gamma I - 2\kappa D_0,$$

of the complex spectral parameter γ , with I being an identical operator in l_2 .

The operator-functions $B(\gamma)$ and $C(\gamma)$ are analytic functions of the parameter γ in the complex plane. The equations

$$B(\gamma)X = 0, \quad C(\gamma)X = 0$$

are equivalent to Eqs. (34) and (38), respectively.

Now we have nothing to do but make use of the operator generalization of Rouché's theorem [9] (see

[3] and the references therein). Let γ_m^0 be an eigenvalue of the operator $2\kappa D_0$. A circle with the center at γ_m^0 only contains eigenvalue γ_m^0 , and the inverse

operator $C^{-1}(\gamma) = \left\| \left(\gamma + \frac{2\kappa}{\Gamma_m} \right)^{-1} \delta_{mn} \right\|_{m,n=-\infty}^{\infty}$ exists

on its boundary. Since γ is located on the boundary of the circle, then $\gamma = \gamma_m^0 + re^{i\varphi}$, $0 \leq \varphi \leq 2\pi$. Therefore, the operator norm $C^{-1}(\gamma)$ at $\gamma = \gamma_m^0 + re^{i\varphi}$ satisfies the inequality $\|C^{-1}(\gamma)\| \leq \frac{1}{r}$.

According to the operator generalization of Rouché's theorem, if the inequality

$$\left\| C^{-1}(\gamma) \frac{2\kappa d}{l} \bar{V} \right\| \leq 1 \quad (39)$$

holds on the boundary of the circle, then an eigenvalue of the operator-function $B(\gamma)$ exists inside this circle and, hence, so does an eigenvalue of the operator-function $2\kappa \bar{A}$.

If $d/l \rightarrow 0$, then the inequality

$$\frac{2\kappa d}{r} \left\| \bar{V} \right\| < 1$$

is true, and so is inequality (39). Thus, for each eigenvalue γ_m^0 , $m = 0, \pm 1, \dots$ of the operator D_0 , there exists a circle that locates a single eigenvalue of the operator $2\kappa \bar{A}$. This fact allows the eigenvalues of the operator $2\kappa \bar{A}$ to be numbered in the same way as γ_m^0 .

Now let us prove that the system of eigenvectors of the operator $2\kappa \bar{A}$ is complete in the space l_2 . Using Eqs. (30) and (35), represent Eq. (34) as follows

$$\frac{i}{2\kappa} \gamma X = (I + D) V X, \quad (40)$$

where operators D and V have the following matrix representations

$$D = \left\| d_m \delta_{mn} \right\|_{m,n=-\infty}^{\infty}, \quad V = \left\| V_{mn} \right\|_{m,n=-\infty}^{\infty},$$

$$d_m = \begin{cases} \frac{i(|m|+1)}{\sqrt{\kappa^2 - \Phi_m^2}} - 1, & \kappa > |\Phi_m|, \\ \frac{|m|+1}{\sqrt{\Phi_m^2 - \kappa^2}} - 1, & \kappa < |\Phi_m|, \end{cases} \quad (41)$$

$$V_{mn} = \begin{cases} \frac{1}{|m|+1} \left(\frac{d}{l} - 1 \right), & m = n, \\ \sin c \left(\frac{\pi d}{l} (n-m) \right) \frac{d}{\sqrt{|n|+1} \sqrt{|m|+1}}, & m \neq n. \end{cases}$$

From Eq. (41) it comes that, first, $d_m \rightarrow 0$ as $m \rightarrow \infty$ and, hence, D is a compact operator in the space l_2 . Second, $V_{mn} = V_{nm}$ and $\sum_{m,n} V_{mn}^2 < \infty$.

Hence, V is a self-adjoint Hilbert-Schmidt operator in the space l_2 .

According to the results obtained in [10] (see [3] and the references therein), the structure of the operator from Eq. (40) guarantees that its system of eigenvectors and associated vectors is complete in the space l_2 . Let the associated vectors be absent. This assumption has some basis because no such vectors exist as $d/l \rightarrow 0$ (narrow perfectly conducting grating strips). The numerical calculations in the general case $0 \leq d/l \leq 1$ confirm this assumption.

Thus, the eigenvector system of the operator from Eq. (40) is complete. Hence, the spectral method can be applied to solving the diffraction problem.

For the efficient application of the spectral method, the eigenvectors must be orthogonal. Ensure that eigenvectors corresponding to distinct eigenvalues are orthogonal in a sense. Let X_p and X_q be eigenvectors with $\gamma_p \neq \gamma_q$. Introduce vectors X_p^* and X_q^* whose components are complex conjugates of the components of the vectors X_p and X_q . From Eq. (40),

$$\frac{i}{2\kappa}(\gamma_p - \gamma_q)(\bar{D}X_p, X_q^*) = (VX_p, X_q^*) - (VX_q, X_p^*). \quad (42)$$

Here (\cdot, \cdot) is a scalar product in the space l_2 ,

$$\bar{D} = (I - D)^{-1} = \|\bar{d}_m \delta_{mn}\|_{m,n=-\infty}^{\infty},$$

$$\bar{d}_m = \begin{cases} -\frac{i\sqrt{\kappa^2 - \Phi_m^2}}{|m|+1}, & \kappa > |\Phi_m|, \\ \frac{\sqrt{\Phi_m^2 - \kappa^2}}{|m|+1}, & \kappa < |\Phi_m|. \end{cases}$$

Since V is a self-adjoint operator, the right-hand side of Eq. (42) is zero. So, if $\gamma_p \neq \gamma_q$,

$$(\bar{D}X_p, X_q^*) = 0. \quad (43)$$

Equality (43) is the condition of the orthogonality of eigenvectors of the operator $(I + D)V$ (or $2\kappa\bar{A}$). Let $X_p^T = (X_n^{(p)})_{n=-\infty}^{\infty}$ and $X_q^T = (X_n^{(q)})_{n=-\infty}^{\infty}$. Then Eq. (43) can be written as

$$\sum_{n=-\infty}^{\infty} \bar{d}_n X_n^{(p)} X_n^{(q)} = 0.$$

From here on, the eigenvectors X_p are $\sqrt{(\bar{D}X_p, X_p^*)}$ normalized. Then, for the normalized eigenvectors, the orthogonality condition takes the appearance

$$(\bar{D}X_p, X_q^*) = \delta_{pq}. \quad (44)$$

Let $X_p^T = (X_n^{(p)})_{n=-\infty}^{\infty}$ be an eigenvector and γ_p be an eigenvalue. The solution of the spectral problem given by Eqs. (4), (5), and (22)–(24) can be represented in the following form

$$\bar{u}_p = \frac{|z|}{z} \sum_{n=-\infty}^{\infty} \frac{X_n^{(p)}}{\sqrt{|n|+1}} e^{i\Phi_n \frac{2\pi}{l} y} e^{i\Gamma_n \frac{2\pi}{l} |z|}, \quad z \neq 0. \quad (45)$$

We will apply the spectral method to construct a solution of the diffraction problem (4)–(10). Here we restrict ourselves to the scenario without a dielectric layer, $\varepsilon = 1$. The case $\varepsilon \neq 1$ is left to Part II of the paper.

According to radiation condition (7), we obtain

$$u = \begin{cases} u_0 + \sum_{n=-\infty}^{\infty} \frac{X_n}{\sqrt{|n|+1}} e^{i\Phi_n \frac{2\pi}{l} y} e^{i\Gamma_n \frac{2\pi}{l} z}, & z > 0, \\ -\sum_{n=-\infty}^{\infty} \frac{(X_n - \delta_{0n})}{\sqrt{|n|+1}} e^{i\Phi_n \frac{2\pi}{l} y} e^{-i\Gamma_n \frac{2\pi}{l} z}, & z < 0. \end{cases} \quad (46)$$

Equation (46) accounts for the boundary condition (9) on the graphene strips. Having substituted (46) into the boundary conditions (8) and (9), one arrives after some transformations at

$$\begin{aligned} \sum_{n=-\infty}^{\infty} \Gamma_n \frac{(X_n - \delta_{0n})}{\sqrt{|n|+1}} e^{i\Phi_n \frac{2\pi}{l} y} = \\ = \begin{cases} 0, & |y| < \frac{d}{2}, \\ -\frac{2\kappa}{\sigma} \sum_{n=-\infty}^{\infty} \frac{X_n}{\sqrt{|n|+1}} e^{i\Phi_n \frac{2\pi}{l} y}, & |y| > \frac{d}{2}. \end{cases} \end{aligned} \quad (47)$$

As in the spectral problem case, Eq. (47) reduces to the system of linear algebraic equations in $X^T = (X_n)_{n=-\infty}^{\infty}$ (X is a column vector, X^T is a row vector, and T is a transpose operation). This system of equations in the operator form is

$$X = b + \frac{2\kappa}{i\sigma}(I + D)X. \quad (48)$$

The matrix operators D and V are the same as in Eqs. (40) and (41), and $b^T = (\delta_{0n})_{n=-\infty}^{\infty}$. The unknown column vector X is sought in the space l_2 .

Let γ_p and y_p be eigenvalues and eigenvectors. Then we have $\frac{i}{2\kappa}\gamma_p y_p = (I + D)Vy_p$. The eigenvectors are normalized and satisfy the orthogonality condition (44)

$$((I + D)^{-1}y_p, y_q^*) = \delta_{pq}. \quad (49)$$

As established above, the system of eigenvectors is complete in the space l_2 . This fact allows us to seek a solution of Eq. (48) in the series expansion form

$$X = \sum_{n=-\infty}^{\infty} A_n y_n, \quad (50)$$

where A_n are the unknown coefficients.

To identify A_n , we substitute Eq. (50) into Eq. (48) and impose the orthogonality condition (49) to have

$$A_n = \frac{(\bar{D}b, y_n^*)\sigma}{\sigma - \gamma_n}.$$

Then,

$$X = \sum_{n=-\infty}^{\infty} \frac{(\bar{D}b, y_n^*)\sigma}{\sigma - \gamma_n} y_n.$$

Here

$$\bar{D} = (I + D)^{-1}, \quad (\bar{D}b, y_n^*) = \bar{d}_0 y_0^{(n)}, \quad y_n^T = (y_m^{(n)})_{m=-\infty}^{\infty},$$

and

$$\bar{d}_0 = \begin{cases} -i\sqrt{\kappa^2 - \Phi^2}, & \kappa > |\Phi|, \\ \sqrt{\Phi^2 - \kappa^2}, & \kappa < |\Phi|. \end{cases}$$

In the diffraction problem, $\Phi = \kappa \sin \varphi$ and hence $\bar{d}_0 = -i\kappa \cos \varphi$. Then the solution of Eq. (48) takes the form

$$X = -i\kappa \cos \varphi \sum_{n=-\infty}^{\infty} \frac{y_0^{(n)}}{\sigma - \gamma_n} y_n. \quad (51)$$

Substituting Eq. (51) into Eq. (46) and using Eq. (45), we have the initial diffraction problem solution as follows

$$u = u_0 - i\kappa \cos \varphi \sum_{n=-\infty}^{\infty} \frac{y_0^{(n)}}{\sigma - \gamma_n} \bar{u}_n. \quad (52)$$

It can be shown that the eigenvalues γ_n satisfy the conditions $\text{Re} \gamma_n \leq 0$, $\text{Im} \gamma_n \geq 0$. Since $\text{Re} \sigma > 0$, $\text{Im} \sigma > 0$ in the frequency range $\kappa < \kappa_0$ ($\text{Im} \sigma(\kappa_0) = 0$), then for some index n_0 , there exist such κ and Φ values (in the diffraction problem, $\Phi = \kappa \sin \varphi$) for which

$$\text{Im} \sigma - \text{Im} \gamma_{n_0} = 0.$$

At these values of the frequency parameter, the term (52) with index n_0 dominates. Therefore, the diffraction field in the vicinity of these frequency parameter values is approximately

$$u = u_0 - i\kappa \sigma \frac{y_0^{(n_0)}}{\sigma - \gamma_{n_0}} \bar{u}_{n_0} + \dots$$

The structure of the diffraction field is determined by the solution of the spectral (source-free) problem.

Thus, the spectral method allows us to model the resonance behavior of the diffraction field as a function of the frequency parameter.

Conclusion

The spectral method for solving problems of electromagnetic wave diffraction by one-dimensional periodic diffraction gratings with graphene strips has been developed. This method allows us to represent the diffraction field as a series of eigenfunctions of a homogeneous spectral problem with a spectral parameter (eigenvalue) included in the boundary condition on graphene strips. The amplitudes of the series terms are inversely proportional to the difference between the imaginary parts of the spectral parameter and the surface conductivity of the graphene strips. Therefore, at an external source frequency when these differences become zero, the amplitude of one of the series terms becomes dominant, making a diffraction field resonance. In essence, Part I has presented a rigorous mathematical interpretation of the spectral method as applied to a planar strip grating formed by alternating perfectly conducting and graphene strips.

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МОДЕЛЮВАННЯ РЕЗОНАНСНИХ ЕФЕКТІВ В ОДНОВИМІРНИХ ПЕРІОДИЧНИХ ДИФРАКЦІЙНИХ ҐРАТКАХ, ЩО МІСТЯТЬ СТРІЧКИ ГРАФЕНУ Частина 1. ОБҐРУНТУВАННЯ СПЕКТРАЛЬНОГО МЕТОДУ

Предмет і мета роботи. Теоретично досліджується проблема взаємодії монохроматичного електромагнітного випромінювання з одновимірною періодичними стрічковими ґратками. Ґратки утворено ідеально провідними та графеновими стрічками, що періодично повторюються, які розташовано на межі плоского діелектричного шару. Метою роботи є обґрунтування спектрального методу для дослідження резонансних ефектів, що виникають при взаємодії електромагнітного випромінювання зі стрічковими ґратками.

Методи та методологія. Для обґрунтування спектрального методу використано результати теорії несамоспряжених компактних операторів у гільбертових просторах і теорії компактних аналітичних операторів-функцій. Зокрема, теореми Келдиша про повноту власних і приєднаних векторів несамоспряжених компактних операторів і операторне узагальнення теореми Руше для аналітичних операторів-функцій.

Результати. Наведено строгі математичні трактування спектрального підходу до розв'язання задач дифракції на одновимірною періодичних стрічкових ґратках, що містять стрічки графену. Встановлено, що дифракційне поле можна задати у вигляді ряду за власними функціями спектральної задачі, в якій спектральний параметр (власне значення) лінійно входить у граничну умову спряження на графенових стрічках. Доведено існування розв'язань спектральної задачі для випадку малих ширин ідеально провідних стрічок. Доведено повноту системи власних функцій (векторів) у відповідному гільбертовому просторі. І, як наслідок, обґрунтовано представлення дифракційного поля в нескінченній області у вигляді ряду резонансних членів. Отримано рівняння для резонансних частот — рівність уявних частин спектрального параметра та поверхневої провідності графенових стрічок ґратки.

Висновки. Розроблений спектральний метод дозволяє ефективно досліджувати резонансні ефекти, що супроводжують взаємодію електромагнітного випромінювання з одновимірною періодичними дифракційними ґратками, які містять стрічки графену. Його можна застосовувати для математичного моделювання різних приладів і пристроїв, що використовують стрічкові ґратки, які містять стрічки графену.

Ключові слова: графен, одновимірною періодичні дифракційні стрічкові ґратки, компактний оператор, резонанс, гільбертів простір, поверхнева провідність.