Computersimulation von Demonstrationsexperimenten zur Beugung von Licht, Röntgenstrahlen und Elektronen für Studierende und Doktoranden der Physik

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Zusammenfassung: Ein Mathematica-basiertes Computer-Demonstrationsexperiment soll die Beugung von Licht-, Röntgen- und Elektronenwellen an verschiedenen Medien demonstrieren – einem gewöhnlichen zweidimensionalen optischen Beugungsgitter und einem dreidimensionalen Kristall. Es wird gezeigt, dass trotz der kardinalen Unterschiede dieser Medien in ihrer Natur und Wechselwirkung mit Strahlung das Phänomen der Beugung elektromagnetischer und elektronischer Wellen aus einem einheitlichen Blickwinkel betrachtet wird.
Schlüsselwörter: Demonstrationsexperiment, Computerexperiment, Fraunhofer-Beugung, Schlitzbeugung, Computeralgebrasystem.

Computer simulation of demonstration experiments on the diffraction of light, X-rays, and electrons for undergraduate and graduate students in physics

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Abstract: A Mathematica-based computer demonstration experiment is designed to demonstrate the diffraction of light, X-ray, and electron waves on a different media-an ordinary two-dimensional optical diffraction grating and a three-dimensional crystal. It is shown that despite the cardinal differences of these media in their nature and interaction with radiation, the phenomenon of diffraction of electromagnetic and electron waves is considered from a unified point of view.
Keywords: demonstration experiment, computer experiment, Fraunhofer diffraction, slot diffraction, computer algebra system**.**

In the optics section of the general physics course, students study the phenomena of interference and diffraction of light. In this case, the main attention is paid to Fraunhofer diffraction by slits and diffraction gratings. In such cases, as a rule, the presentation of the question is based on the basic position in which the image given by the lens is always a diffraction pattern arising due to the limitation of the cross section of the light beam. Mathematical analysis of many interesting examples of Fraunhofer diffraction is not difficult and allows us to consider the problem at hand.

The study of the phenomenon of light diffraction by slits and two-dimensional diffraction gratings is a relatively simple task, in which the equality of phases and the equality of amplitudes incident on the diffraction grating and other obstacles greatly simplifies both the graphical and analytical solution of the problem for certain geometries of the chosen experimental scheme [1-3] .

The study of X-ray diffraction, for which the role of an ordinary diffraction grating is played by crystalline bodies, is a relatively difficult task due to their interaction with a specific object. Here, processes such as the interaction of X-rays with individual atoms of matter and the symmetry of the arrangement of atoms in a crystal come to the fore. In the first case, we are dealing with the atomic factor, and in the second case with the structural scattering factor, which have a significant effect on the intensity of the diffracted rays. Along with this, during the diffraction of X-rays, it is necessary to pay attention to the condition characteristic of them, according to which the distance between the atomic planes d, the wavelength λ and the diffraction angle $\theta$are related by the Bragg condition $2d\sin\theta = n\lambda$(n- diffraction order). Here, for the occurrence of the X-ray diffraction maximum, the difference in the path of the rays $d\sin\theta$is $\lambda/2$, and for light, the difference in the path of the rays is λ. However, when determining the total amplitude of the diffracted light and X-ray radiation, the usual procedure for adding the amplitudes of the radiation scattered in each section of the diffraction grating is performed. The intensity is defined as the product of the calculated amplitude and the conjugate value. Both in conventional optics and in X-ray diffraction, the nature of the intensity of scattered radiation near the maximum in the one-dimensional case is given by an expression like:

$$I_{\varphi} = k\frac{\sin^2[(b\pi/\lambda)\sin\varphi]}{[(b\pi/\lambda)\sin\varphi]^2}. \quad (1)$$

In the case of light, the coefficient $k$is the intensity of light coming from a slit wide $b$in the direction of the primary beam. At the same time, for X-rays $k$it also depends mainly on the atomic and structural scattering factors. The φangle between the scattered and primary beams is denoted by.

On the other hand, when studying the section of atomic physics, as well as the course of quantum mechanics, the focus is primarily on corpuscular-wave dualism , which is its physical basis and according to which any material object - a particle or a wave - has both wave and corpuscular properties. Electron diffraction occurs in the same way as light photon diffraction. Electron waves, when interacting with atoms of crystals, scatter and give a certain diffraction pattern. Therefore, electron diffraction, like the diffraction of light and X-rays, is an important effect, the study of which certainly leads to a deeper understanding of the foundations of all quantum physics. In this case, one should pay attention to the following extremely important moment of the mathematical foundation of quantum mechanics, the essence of which lies in the method of mathematical modeling of quantum mechanical phenomena adopted in quantum mechanics , which makes it possible to calculate the numerical values of quantities and processes observed in quantum mechanics. As a result of the analysis of the results of experiments on electron diffraction, it can be seen that the squared amplitude of de Broglie waves at a given point in space is a measure of the probability of finding a particle at the same point.

Naturally, the processes of interaction between the electron wave and the electrons of the crystal significantly complicate the material under study. As a result, they resort to the study of thin crystalline foil with a thickness not exceeding microns.

Short X-ray waves are used, corresponding to a voltage between the anode and the cathode, in many cases equal to 100,000 volts ($\lambda = 0{,}0370$ Å). Consequently, it is practically necessary to work with wavelengths that are much smaller than the interplanar distances in the crystal and with small diffraction angles. Along with this, a detailed interpretation of electron micrographs and electron diffraction patterns possible only at complete understanding physical factors determining _ intensity Bragg diffracted beams . Therefore, in practice one should consistently calculate amplitude scattering on an atom, elementary cell and on crystal at provided that _ amplitude scattered waves is only small part amplitude falling waves .

We note that when considering the phenomenon of diffraction in crystals, it is very useful to deal with the reciprocal lattice of a crystal, the presentation of the principle of construction of which is not a difficult task. In this case , $\boldsymbol{g}$a c^*strong h, k, ldiffraction a^*maximum $|\boldsymbol{K}| = 2\frac{\sin\theta}{\lambda}$,arises b^*under the condition$\boldsymbol{K} = \boldsymbol{g} = ha^* + kb^* + lc^*$ $|\boldsymbol{g}| = \frac{1}{d_{hkl}}$, d_{hkl}- interplanar distance. In its physical meaning, the vector $\boldsymbol{K}$corresponds to the wave vector. It is natural to assume that in the case $\boldsymbol{K} = \boldsymbol{g} + \boldsymbol{s}$where $\boldsymbol{s}$represents the deviation from the reciprocal lattice node, one can expect a non-zero amplitude of the diffracted radiation. In this case, for the amplitude of the scattered radiation, the expression $A_g = \frac{F_g}{V_c}\int \exp[-2\pi i s \cdot r]d\tau$containing the integral over the crystal is obtained, which is the Fourier transform of the crystal. F_g- structural factor, V_c- unit cell volume. For a rectangular crystal with edges $A, B$and Cthis expression has the form:

$$|A_g| = \frac{F_g}{V_c} \cdot \frac{\sin \pi A u}{\pi u} \cdot \frac{\sin \pi B v}{\pi v} \cdot \frac{\sin \pi C w}{\pi w}. \qquad (2)$$

Here u, v, w, are the components $\boldsymbol{s}$along the directions, respectively x, y, z. The value $|A_g|$characterizes the distribution of amplitudes in the reciprocal space. As noted above, the distribution of the intensity of the diffracted beam is determined by the product Here, we assume $A_g A_g^*$.that the values of the type $\frac{F_g}{V_c}$are constant and equal to unity. Naturally, to solve such problems and to study courses in general and theoretical physics, a relatively solid mathematical background is required.

Now, in accordance with the above reasoning, we can start modeling light on a two-dimensional diffraction grating, X-rays and electron beams in crystalline bodies based on a single computer simulation. We use the Mathematica computer algebra system , with which we constantly used in our previous works [4-5].

Let us compose expressions for visualizing the results of calculations according to formula (1) for the two-dimensional case, we will write the following expression for Mathematica :

$$\text{ContourPlot}\left[\frac{F}{V}\left(\frac{\text{Sin}[\pi\, a\, x]}{\text{Pi}\, x}\right)^2 \left(\frac{\text{Sin}[\text{Pi}\, b\, y]}{\text{Pi}\, x}\right)^2, \{x, 0.5, 5\}, \{y, 0.5, 5\}\right].$$

The $\frac{F}{V} = 1$result of the calculations will be the picture shown in Fig. 1. The resulting picture is a fragment of the reciprocal lattice in the plane (x, y). Profiles of reciprocal lattice sites are seen, the cross sections of which depend on the values of $x$and y, which corresponds to a decrease in the intensity of diffracted radiation depending on the diffraction angle. However, the distances between the nodes of the reciprocal lattice do not change and depend only on $a$and b. Now we can demonstrate the change in the intensity of diffracted radiation in one direction to increase the visibility of the phenomenon under study (Fig. 2).

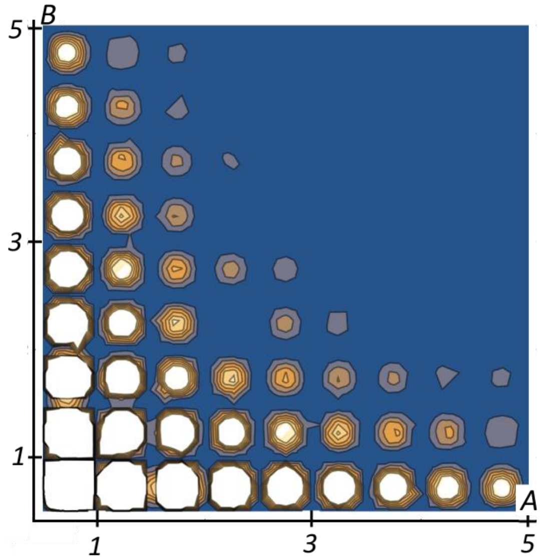

Fig. 1. Fragment of the section of the reciprocal lattice in the plane (xy).

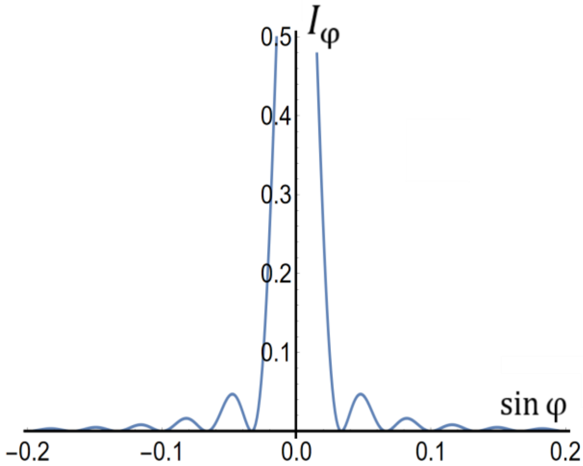

Fig. 2. Intensity distribution of the diffracted wave along A.

Mathematica allows you to manipulate the parameters used directly during the demonstration experiment. So, for example, to use a two-dimensional diffraction pattern, you can get the picture shown in Fig. 3. Here it is possible to change the width of the slit $b$and the number of slits $n$directly during the demonstration of a computer experiment. To get the desired result, enter the command:

$$\text{Manipulate}\left[\text{Plot}\left[\left\{\left(\frac{\text{Sin}\left[\frac{\pi b}{\lambda}\text{Sin}[\varphi]\right]}{\frac{\pi b}{\lambda}\text{Sin}[\varphi]}\right)^2, \left(\frac{\text{Sin}\left[n\frac{\pi b}{\lambda}\text{Sin}[\varphi]\right]}{n\frac{\pi b}{\lambda}\text{Sin}[\varphi]}\right)^2\right\}, \{\varphi, 0, 1\}\right],\right.$$
$$\left.\{b, 0.001, 0.06\}, \{n, 1, 10\}, \text{PlotRange} \to \{0, 0.5\}\right]$$

The conducted studies have shown that the above computer demonstrations can also be used to illustrate other schemes of diffraction experiments, for example, to show the superposition of sound waves, as well as waves propagating on the surface of water. We believe that the proposed development should primarily be used during lectures and independent work of students and undergraduates.

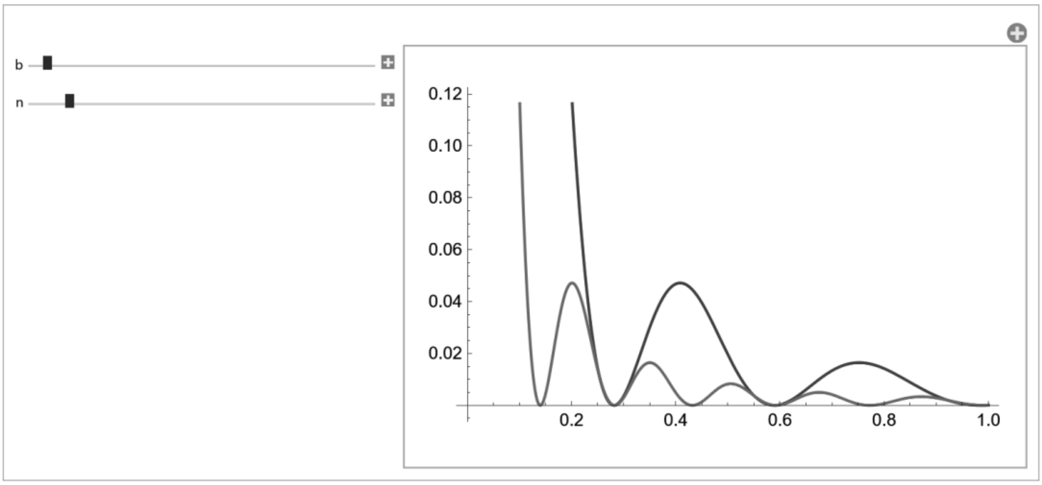

Fig. 3. Picture showing changes in the profile of diffraction lines with a change in the width and number of slits.

Thus, on the basis of the research carried out, the following conclusions can be drawn:

Regardless of the nature of the waves, it is possible to visually demonstrate many diffraction phenomena that are directly related to both classical and quantum physics with the help of one software development. At the same time, students and undergraduates can receive specific knowledge about the features of, for example, sound, light, X-ray and electronic waves, as well as their interactions with a conventional diffraction grating, crystal, and other kinds of obstacles. The data obtained testify to the unity and fundamental nature of many physical phenomena studied in various branches of physics. At the same time, from the point of view of the methodology of teaching physics, the requirements of the principle of continuity in education are clearly manifested, according to which the educational process is built in the form of a certain system and sequence of learning. At the same time, it should be taken into account that the goal of any education is the training of a comprehensively developed specialist, which can be organized only with the active use of both modern computer technologies and the competent use of the most advanced software tools. Here, naturally, there is a need for a worldview orientation of the program of the subject being studied and the educational literature used, as well as the generalization of educational material on the leading and main physical theories.

References

1. P.V. Kazarin, Yu.V. Polushtaitsev, N.F. Uslugin. Lecture experiments on the demonstration of light diffraction in the system of university physical education. Bulletin of the Nizhny Novgorod University. N.I. Lobachevsky. Series: Social Sciences, 2017, No. 3 (47), p. 143–147.

2. Lecture demonstrations in physics / Ed. V.I. Iveronova. M.: Nauka, 1972. 640 p.

3. Maciej Lisicki, Ludmila Buller, Michal Oszmaniec, Krzysztof Wojtowicz. Dynamic transition between Fresnel and Fraunhofer diffraction patterns - a lecture experiment. arXiv:0803.0120v2 [physics.optics] 22 Apr 2009.

4 Stephen Wolfram. An Elementary Introduction to the Wolfram Language. second edition. Champaign, IL, USA: Wolfram Media, Inc. 2017. 339 p.

5. Gerd Baumann. Mathematica for theoretical physics. 2. Electrodynamics, quantum mechanics, general relativity, and fractals. Springer. 2005. 942p .

6. Khozhanazarova R.M. Methodology of the origin and development of the concept quantum of light // Berlin Studies Transnational Journal of Science and Humanities ISSN 2749-0866 Vol.2 Issue 1.5 Pedagogical sciences, Germany. 01. 2022. http://berlinstudies.de/

7. Joraev M., Abdikamalov B., Khozhanazarova R. methodical questions holding computer experiment a for demonstrations optical a on a log a motion a needles in area potential threshold // Path nauka, ISSN 2311-2158 International a native on a scientific Zhurnal, No. 5 (75), 2020, Impact - factor 0.543. Volga a city 2020, pp. 68-70 .