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Asymptotic behavior of numerical solutions of the Schrodinger equation

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Many problems of numerically solving the Schrodinger equation require that we choose asymptotic distances many times greater than the characteristic size of the region of interaction. The problems of resonance diffraction for composite particles or the problem of nucleon scattering by nonspherical atomic nuclei are examples of the need to use a large spatial domain for calculations. If the solution to one-dimensional equations can be immediately chosen in a form that preserves unitarity, the invariance of probability (in the form of, e.g., fulfilling an optical theorem) is a real problem for two-dimensional equations. An addition that does not exceed the discretization error and ensures a high degree of unitarity is proposed as a result of studying the properties of a discrete two-dimensional equation.

The problem for scattering of rigid molecules by the disks was successfully solved using an improved sampling scheme that provides the correct asymptotic behavior. Corresponding diffraction scattering curves are of a pronounced resonance nature.

Key words: Numerov's method, resonance diffraction, Babine's principle.

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1 Introduction

In numerically solving problems whose mathematical notation is expressed in terms of the two-dimensional Schrodinger equation, there is the problem of a loss of accuracy for finite difference schemes. It is associated with the need to travel long distances relative to the characteristic size of the potential range. Such situations arise in the scattering of slow particles at long scattering distances or with the scattering of fast particles with pronounced diffraction when we need to go beyond the region of the diffraction shadow in the calculations.

The problems of resonance diffraction for composite particles [1, 2] or the problem of nucleon scattering by nonspherical atomic nuclei are examples of the need to use a large spatial domain for calculations. Expansion in spherical functions in this case loses both physical and mathematical meaning because of the non conservation of the

angular momentum in the scattering process. The standard approach, which uses amplitude notation in an explicitly unitary form, thus becomes an inoperative tool. We can, of course, choose a solving scheme based on some averaging of the nonspherical potential (by, e.g., means of folding [3]) and leaving the error of the means of solving without any possibility of analysis. This problem arises not only in the two examples given above, and it is solved in different ways for specific cases in theoretical physics, nanostructure physics, and related fields of chemistry, medicine, and atomic interferometry [4-8].

2 Material and methods

Let us write the Schrodinger equation in a two-dimensional axially symmetric case for a scattering problem (here and below, we use a system of units in which the Planck constant and the Boltzmann constant are 1 in analogy with [4])

$$\Delta\Psi(\vec{r}) - V(\vec{r})\Psi(\vec{r}) = -k^2\Psi(\vec{r}), \quad (1)$$

$$\Delta = \frac{\partial^2}{\partial r^2} + \frac{2}{r} \frac{\partial}{\partial r} + \frac{1}{r^2} \frac{1}{\sin(\vartheta)} \frac{\partial}{\partial \vartheta} \sin(\vartheta) \frac{\partial}{\partial \vartheta}$$

Here, $k^2 = 2mE$ is a wave parameter, E is the energy of the system, and $\Psi(\vec{r}) = \Psi(r, \vartheta)$ is the wave function. Note that the energy in the selected system of units is measured in ones that are inverse to the square of the length. The potential is limited in some area $V = 0$ with $r > r_V$. The asymptotic form of the wave function in a region greater than some asymptotic radius $r_{as} : r > r_{as} \gg r_V$,

$$\Psi(\vec{r}) \rightarrow e^{i\vec{k}\vec{r}} + f(\vartheta) \frac{e^{ikr}}{r} \left(1 + O\left(\frac{1}{r}\right) \right),$$

determines scattering amplitude $f(\vartheta)$, which obeys optical theorem [9]

$$\sigma = 2\pi \int_0^\pi |f(\vartheta)|^2 \sin(\vartheta) d\vartheta = \frac{4\pi}{k} \text{Im} f(0),$$

where σ is the total cross section. This ratio (the condition for invariance of probability) can be used as a criterion of accuracy for the numerical solution to the problem. We must choose a sufficiently high value of parameter r_{as} that determines the region of the asymptotic solution in the numerical solution to the scattering problem. Asymptotic distances several hundred units of the problem's length for characteristic values $r_V = 1 - 3$ and $k \leq 30$ must extend beyond shadow region $r_{as} > r_V(kr_V)$ in the problem of the quantum scattering of particles on a nonspherical potential [1].

The limiting accuracy of calculations for such distances is determined by the ignored asymptotic term (i.e., it can be a fraction of a percent). The form of potential $V(\vec{r})$ requires the use of a small parameter for the sampling step. This ensures the accuracy of the solution, but considerably extends the estimated time. Two sampling steps are used to advance the calculations for continuing quantum scattering studies on nonspherical potentials [1,2]. For $r \leq r_s \approx r_V$, we choose fairly small step $\Delta r = 0.001$, which guarantees sufficient

accuracy $O((\Delta r)^2)$ in the range of potentials, and step $\Delta r_2 = 2^n \Delta r$ with $n \sim 4 - 5$ for $r > r_s$. However, this choice results in as much as 10% deviation in fulfilling the optical theorem. These deviations are much larger than the sampling error $O((\Delta r_2)^2)$ for finding the wave function. Such an error in the phase of asymptotic wave function nevertheless results in considerable deviation from the optical theorem.

The importance of loss of accuracy can be expressed in a one-dimensional example. Let us consider a one-dimensional free equation for $\varphi = r\Psi$ and its finite difference approximation

$$\frac{d^2}{dr^2} \varphi + k^2 \varphi(r) = 0 \rightarrow \frac{\varphi(r + \Delta r) - 2\varphi(r) + \varphi(r - \Delta r)}{(\Delta r)^2} + k^2 \varphi(r) + O((\Delta r)^2) = 0$$

Replacing the value of the function at points $\varphi(r \pm \Delta r)$ with a Taylor expansion, we obtain

$$\frac{\partial^2}{\partial r^2} \varphi(r) + \frac{(\Delta r)^2}{12} \frac{\partial^4}{\partial r^4} \varphi(r) + k^2 \varphi(r) + O((\Delta r)^4) = 0$$

The solutions to this equation have the form

$$\exp\left(\frac{\sqrt{2} \sqrt{-3 + \sqrt{9 - 3(\Delta r k)^2}} r}{\Delta r} \right).$$

Expanding the exponent in a series with respect to Δr , we obtain

$$ikr + \frac{1}{24} ikr(\Delta r k)^2 + O(\Delta r^4). \quad (2)$$

Since this expression is in the exponent, the second term can be ignored only if it is small in comparison to unity $\left(\frac{1}{24} k r (\Delta r k)^2 \ll 1 \right)$. This inequality is certainly not satisfied for very large r . For example, phase term $\frac{1}{24} k r (\Delta r k)^2 = 0.05543 r$ at $\Delta r = 0.016$, $k = \sqrt{300}$, and becomes equal to 5.5 when $r = 100$. The problem of the loss of

accuracy is thus due to the incongruity of the exact asymptotic form and the asymptotic behavior when solving the equation in finite differences. The same result can be obtained in general form. Let us find the solution to finite difference equation

$$\frac{\phi(r+\Delta r)-2\phi(r)+\phi(r-\Delta r)}{(\Delta r)^2} + \dots \quad (3)$$

$$+k^2\phi(r)=0$$

by substituting function $\phi = \exp(ik_{eff}r)$ in it.

This leads to the equation for k_{eff} :

$$4\sin^2\left(\frac{k_{eff}\Delta r}{2}\right) = k^2(\Delta r)^2.$$

The finite difference equation thus has an exponential solution with wave parameter k_{eff} :

$$\frac{\left(1 + \frac{(k\Delta r)^2}{12}\right)\exp(ik_{eff}\Delta r) - 2\left(1 + \frac{(k\Delta r)^2}{12}\right) + \left(1 + \frac{(k\Delta r)^2}{12}\right)\exp(-ik_{eff}\Delta r)}{(\Delta r)^2} + k^2 = 0, \dots \quad (4)$$

It yields

$$k_{eff} = \frac{2\arcsin\left(\frac{3k\Delta r}{\sqrt{36+3(k\Delta r)^2}}\right)}{\Delta r},$$

without quadratic terms with respect to Δr as a series expansion

$$k_{eff} = k + \frac{1}{480}k^5(\Delta r)^4 + O((\Delta r)^6) \quad (5)$$

The deviation of the correct asymptotic behavior from the solution to Eq. (4) thus occurs at much greater distances when using Numerov's scheme.

For example, the value $\frac{1}{480}r_{as}k(\Delta rk)^4$ at $r_{as} = 100$ is 0.02, determining an error of 2% in the unitarity condition when using the problem parameters $\Delta r = 0.016$, $k = \sqrt{300}$. Such a scheme can be used for a two-dimensional equation with twice differentiable interaction potentials.

$$k_{eff} = 2\arcsin\left(\frac{k\Delta r}{2}\right) / \Delta r.$$

Expanding k_{eff} in a series with respect to Δr , we obtain

$$k_{eff} = k + \frac{1}{24}k(k\Delta r)^2 + \frac{3}{640}k(k\Delta r)^4 + \frac{5}{7168}k(k\Delta r)^6 + O((k\Delta r)^8),$$

As expected, the first terms of the series coincide with Eq. (2). In a similar manner, we can obtain the value of k_{eff} for more complicated problems, e.g., for two-dimensional Schrodinger equation (1), sampled using Numerov's method to an accuracy of $O((\Delta r)^4)$. We must in this case solve the following finite difference equation

Unfortunately, it does not work when using potentials with sharp boundaries. We propose introducing small term $-k^2 \frac{(k\Delta r)^2}{12}$ into Eq. (3). On the one hand, this term has a low degree of discretization error in the range of potentials; on the other, it is the compensating term for the free equation and brings its discretization error down to $O(\Delta r)^4$:

$$\frac{d^2}{dr^2}\phi + k^2\phi(r) = 0 \rightarrow \frac{\phi(r+\Delta r)-2\phi(r)+\phi(r-\Delta r)}{(\Delta r)^2} + k^2\left(1 - \frac{(k\Delta r)^2}{12}\right)\phi(r) = 0.$$

In this case, we obtain for k_{eff} the equation

$$k_{eff} = \frac{2\arcsin\left(\frac{k\Delta r}{12}\sqrt{36+3(k\Delta r)^2}\right)}{\Delta r},$$

whose series expansion

$$k_{eff} = k - \frac{1}{720} k^5 (\Delta r)^4 + O((\Delta r)^6),$$

has a numerical factor in front of $(\Delta r)^4$ that is even less than in expansion (5), ensuring 99–97% unitarity with the most stringent parameters of the problem.

The computational error does not exceed 0.5% in test reductions of the sampling step (down to $\Delta r = 0.008$).

3 Results and discussions

The problem of the scattering of a rigid diatomic molecule on a thin disk was solved by using the correct asymptotic behavior. The barrier potential of a disk in cylindrical coordinates $\rho = r \cos \vartheta$ and $z = r \sin \vartheta$ is written in the form

$$V_b = \begin{cases} V_{b0}: & \rho \leq R \text{ и } |z| \leq a/2, \\ 0: & \rho > R \text{ или } |z| > a/2. \end{cases}$$

Parameters V, a determine the disk size. In analogy with the problem of a rigid molecule passing through a barrier [4], the potential in Eq. (1) for the model of a rigid molecule has the form

$$V_b(\rho, z + d/2) + V_b(\rho, z - d/2),$$

where parameter d corresponds to the size of a scattered rigid molecule. The difference between the scattering of a molecule and a point particle equal to its mass is best seen in backscattering, so not only the scattering cross sections of the molecule but also the backscattering cross section for a particle with a mass equal to that of two atoms are shown in the figures below. This cross section must have the form of monotonic energy and rapidly shrink at energies above that of potential barrier (the disk potential). Barrier height V_{b0} in the above calculations was assumed to be 333.2 \AA^{-2} (4000 K for a hydrogen molecule). The figures show the total cross sections along with those into the front and rear hemispheres. The cross section into the front (rear) hemisphere is determined in the same way as the total cross section, but the limits of integration over the angle are from 0 to $\pi/2$ (from $\pi/2$ to π).

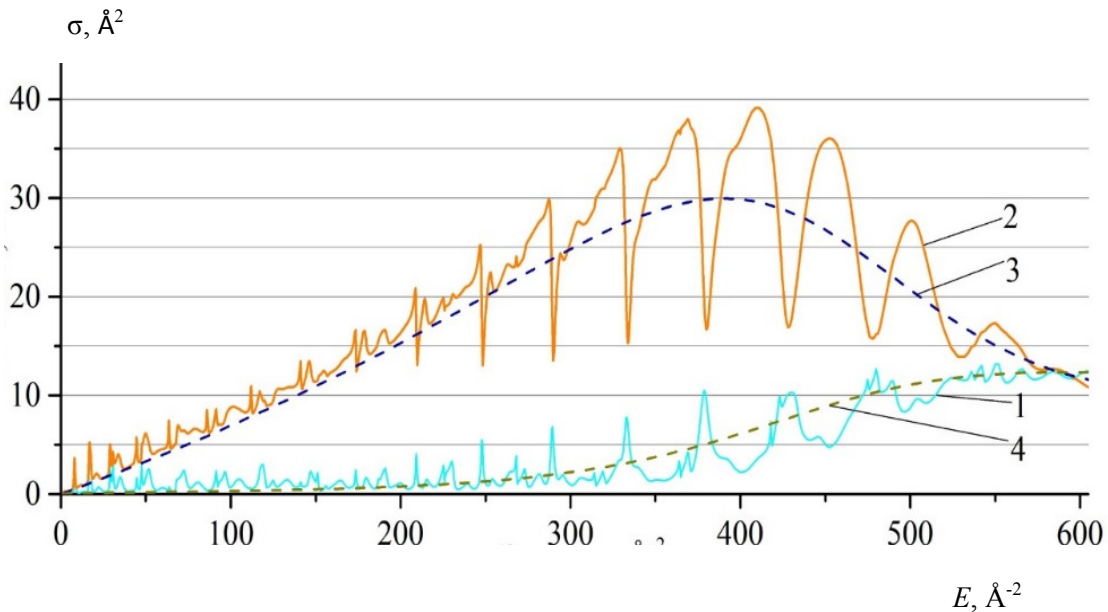


Figure 1 – The scattering cross sections of the hydrogen molecule on the disk at $R = 3 \text{ \AA}$. 1 – σ_t , 2 – σ_f , 3 – σ_b , 4 – backward scattering cross section for a particle with a doubled hydrogen atom mass

Figure 1 shows the results from calculating the dependence of the total scattering cross section of rigid hydrogen molecule H_2 by a thin disk with a radius of 3 \AA and a width of 0.2 \AA on the energy. Parameter d is 0.7416 \AA for hydrogen [10]. It can be seen that the backscattering cross section of the molecule generally repeats the pattern of the scattering cross section for an unstructured particle, but it has characteristic resonance deviations.

The diffraction scattering cross sections of rigid beryllium molecule Be_2 are given for comparison in Figure 2. Parameter d is 2.47 \AA [11, 12]. The

greater number of quasi-bound states are due to the greater distance between atoms that is observed on the cross section by a large number of resonances. The main dips in the cross section (resonances) coincide with the positions of the energy levels in a rectangular one-dimensional well with a width of d , just as in the pattern for the resonant passage of a rigid molecule [4]. This leads to the differences between the scattering of hydrogen and beryllium molecules observed in the figures. The number of minima in the total scattering cross section of a rigid beryllium molecule is much higher.

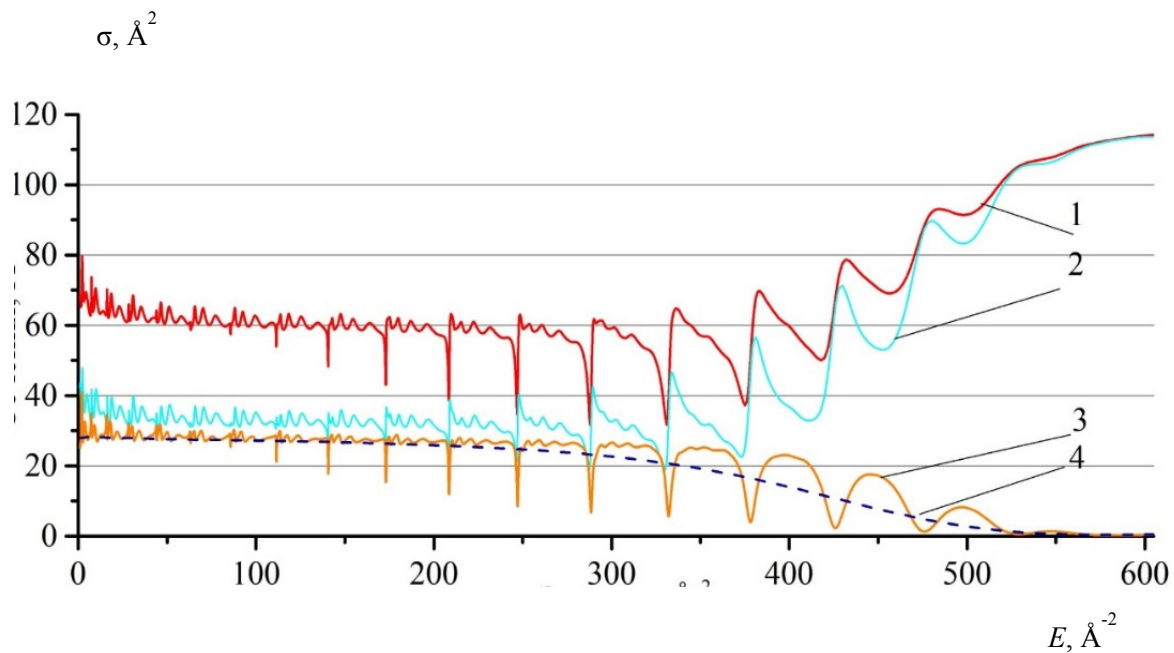


Figure 2 – The scattering cross sections of the Beryllium molecule on the disk at $R = 3 \text{ \AA}$. Numerical lines are like one in Figure 1.

The calculation of two-dimensional scattering at non-symmetrical center can be used for problem of scattering at holes in infinity wall. The

Babinet's principle [13] has been used for it. The numerical example is presented by Figure 3.

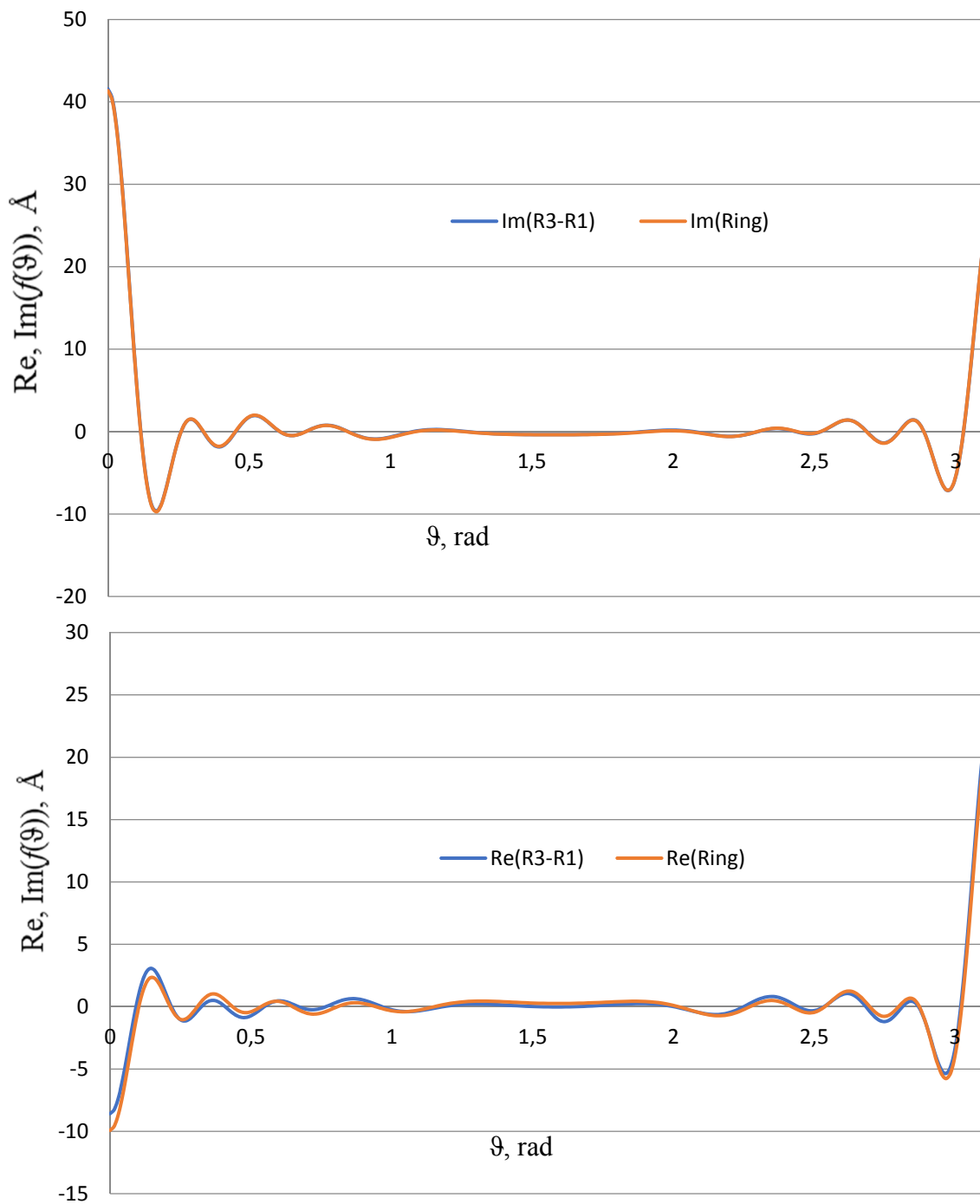


Figure 3 – Comparison of beryllium atom scattering at an energy of 100 \AA^{-2} . R3 is the scattering on a disk of 3 \AA , R1 is scattering on a disk of 1 \AA , Ring is scattering on a ring 3 \AA wide with a hole of 1 \AA .

It can be seen, that calculated scattering on the disk with big radius is equivalent a sum of scattering on ring with external radius which equal big disk's one and little disk with radius which equal hole's one.

The calculation of scattering on hole is presented at Figure 4.

It can be seen that the resonance structure is exist here too.

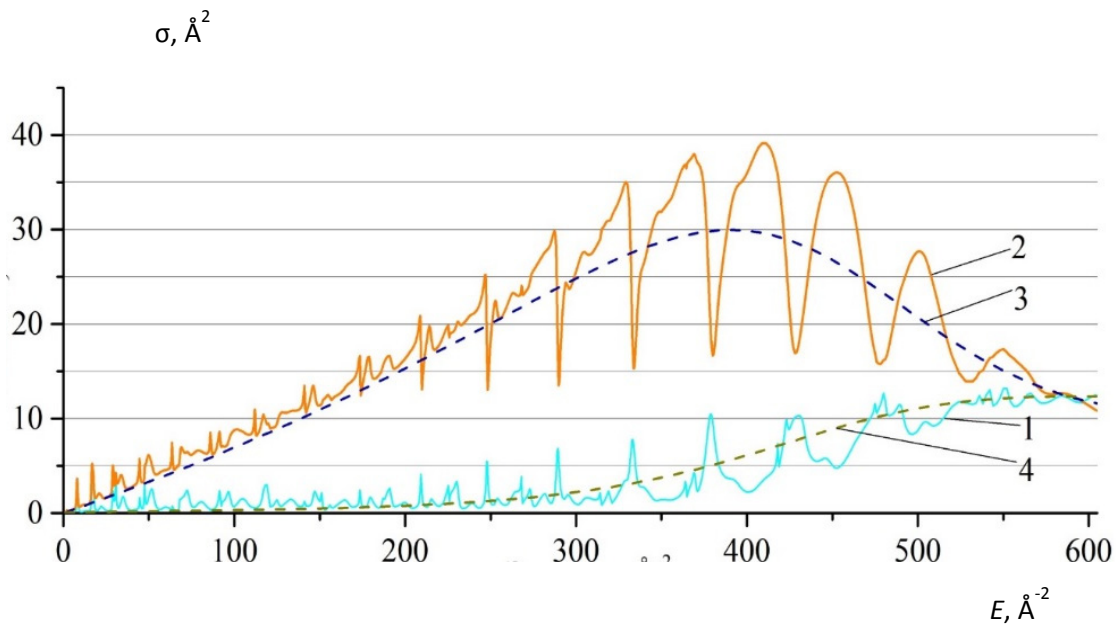


Figure 4 – Diffraction of beryllium on hole $R=2 \text{ \AA}$.
Numerical line are liked one in Figure 1

4 Conclusions

The problem for scattering of rigid molecules by the disks was successfully solved using an improved sampling scheme that provides the correct asymptotic behavior. The result could be useful for analogical topics of investigation [14-22]. Corresponding diffraction scattering curves are of a pronounced resonance nature. The units of the

problem length E were determined by the interaction parameters. A femtometer (fm) is inconveniently chosen as units of length in problems of nuclear physics. The proposed way of correcting for the wave parameter in asymptotic behavior can thus be applied in different areas that study diffraction using two-dimensional differential equations (e.g., in studying particle scattering by nonspherical atomic nuclei).

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