Vol. 13 (2020) *Acta Physica Polonica B Proceedings Supplement* No 3

EFFECT OF NON-SPHERICAL SCATTERING FOR NUCLEI OF ACTINIDE SERIES*

P.M. Krassovitskiy[a,b], F.M. Pen'kov[b,c]

[a]Joint Institute for Nuclear Research, 141980 Dubna, Russia
[b]Institute of Nuclear Physics, 050032 Almaty, Kazakhstan
[c]al-Farabi Kazakh National University, 050040 Almaty, Kazakhstan

(Received January 28, 2020)

The elastic scattering of neutron on nuclei of actinide group has been investigated. The real part of global optical potential has been used. An algorithm based on direct discretization of a two-dimensional equation is proposed for numerically solving the problem of scattering of axially-symmetrical potential. It has been shown that including of non-spherical form of nuclei gives a significant correction in the description of scattering.

DOI:10.5506/APhysPolBSupp.13.437

1. Introduction

The problem of scattering on an object without spherical symmetry is usually solved numerically. Decomposition in spherical functions then loses both physical and mathematical meaning, due to the nonconservation of angular momentum in the process of scattering; *i.e.*, the standard approach using the amplitude representation in a clearly unitary form cannot be used. The effective scheme of the solution has been used before for different problems [1–3]. In this work, the main parameters were taken for elastic neutron scattering on $^{238-235}$U nuclei. This is known to be one of the well-deformed nuclei and is well-suited for studying a non-spherical object of scattering. The interaction between neutrons and these nuclei is a base of the atomic energy.

Due to the characteristics of the research technique, only one aspect of studying this reaction was examined: the difference between scattering in the model of a non-spherical potential and the model of scattering on a spherically symmetric potential. Note that examples of neutron scattering by a non-spherical atomic nucleus or the problem of diffraction of composite

* Presented at the XXVI Nuclear Physics Workshop *Key problems of nuclear physics*, Kazimierz Dolny, Poland, September 24–29, 2019.

particles [2, 3] do not diminish the relevance of the technique proposed here. In this work, the problem is solved for particular cases using different approaches in theoretical physics, the physics of nanostructures, and in related areas of chemistry, medicine, and atomic interferometry [4–8].

2. General idea of the numerical solution

For the problem of scattering of a spinless particle, we can write the Schrödinger equation in the case of axial symmetry as

$$\varDelta\varPsi(r,\vartheta,\varphi) - V(r,\vartheta)\varPsi(r,\vartheta,\varphi) = -k^2\varPsi(r,\vartheta,\varphi)\,, \tag{1}$$

$$\varDelta = \frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\frac{1}{\sin(\vartheta)}\frac{\partial}{\partial\vartheta}\sin(\vartheta)\frac{\partial}{\partial\vartheta} + \frac{1}{r^2\sin^2(\vartheta)}\frac{\partial^2}{\partial\varphi^2}\,. \tag{2}$$

Here, $k^2 = 2mE$ is the wave number, E is the energy of the system, and $\varPsi(r,\vartheta,\varphi)$ is the wave function. It should be noted that in this system of units, Planck's constant is equal to unity and energy is measured in units of the inverse length squared. The potential is restricted within a certain domain: $V = 0$ at $r > r_V$.

It could be rewritten in the form:

$$\varDelta_m\varPsi_m(r,\vartheta) - V(r,\vartheta)\varPsi_m(r,\vartheta) = -k^2\varPsi_m(r,\vartheta)\,, \quad m = 0, \pm1, \pm2\ldots\,, \tag{3}$$

$$\varDelta_m = \frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\frac{1}{\sin(\vartheta)}\frac{\partial}{\partial\vartheta}\sin(\vartheta)\frac{\partial}{\partial\vartheta} - \frac{m^2}{r^2\sin^2(\vartheta)}\,, \tag{4}$$

where $\varPsi(r,\vartheta,\varphi) = \sum_m \varPsi_m(r,\vartheta)\mathrm{e}^{im\varphi}$. For scattering problem, if incoming wave has a random wave number $\vec{k}$, then

$$\varPsi(r,\vartheta,\varphi) = \mathrm{e}^{i\vec{k}\vec{r}} + \chi(r,\vartheta,\varphi) = \mathrm{e}^{ikr\cos\tilde{\vartheta}} + \chi(r,\vartheta,\varphi)\,, \tag{5}$$

and equations (3), (4) for $\chi(r,\vartheta,\varphi)$ are

$$\varDelta_m\chi_m(r,\vartheta) - V(r,\vartheta)\chi_m(r,\vartheta) = -k^2\chi_m(r,\vartheta) + V(r,\vartheta)F_m\left(r,\vartheta,\tilde{\vartheta}\right)\,, \tag{6}$$

where $F_m(r,\vartheta,\tilde{\vartheta}) = \int_0^{2\pi}\mathrm{e}^{ikr\cos\tilde{\vartheta}}\mathrm{e}^{im\varphi}\mathrm{d}\varphi$.

The wave-function asymptotics is given by

$$\varPsi\left(r,\vartheta,\varphi\right) \to \mathrm{e}^{ikr\cos\tilde{\vartheta}} + f\left(\vartheta,\varphi\right)\frac{\mathrm{e}^{ikr}}{r}\left(1 + O\left(\frac{1}{r}\right)\right) \tag{7}$$

and determines the scattering amplitude $f(\varOmega) = f\left(\vartheta,\varphi\right)$, which obeys optical theorem [9]

$$\sigma = \frac{4\pi}{k}\mathrm{Im}f\left(\vartheta' = 0\right) \tag{8}$$

in coordinate system ϑ', φ', where direction of free incoming wave is equivalent of the axe $\vartheta' = 0$. There, σ is the total cross section

$$\sigma = \int |f(\Omega)|^2 \, \mathrm{d}\Omega \, .$$

Expression (8) (*i.e.*, the condition of the conservation of probability) can be used as a criterion for the accuracy of the numerical solution of the problem.

The concept behind the technique is that when $r > r_V$, there is a free solution to Eqs. (1), (2) that can be conveniently represented as an expansion in the Legendre polynomials $P_l^m(\cos\vartheta)$

$$\Psi(r,\vartheta) = \exp(ikr\cos\vartheta) + \sum_{lm} a_{lm} i^{l+1}(2l+1) P_l^m(\cos(\vartheta))\, h_l^{(1)}(kr) \qquad (9)$$

with unknown coeffients a_l. Here, $h_l^{(1)}(kr)$ is a spherical Bessel function of the third kind, expressed through a Hankel function of the first kind

$$h_l^{(1)}(kr) = \sqrt{\frac{\pi}{2kr}} H_{l+1/2}^{(1)}(kr) \, .$$

The choice of the radial solution in this functional form is determined by the possibility of satisfying asymptotic condition (7), since

$$h_l^{(1)}(x)|_{x\to\infty} \to (-i)^{l+1} \frac{\exp(ix)}{x} \, ,$$

and function (9) has correct asymptotic form (7) with the amplitude

$$f(\vartheta,\varphi) = \frac{1}{k} \sum_l a_l (2l+1) P_l^m(\cos(\vartheta))\, \mathrm{e}^{im\varphi} \, , \qquad (10)$$

which is expressed through coefficients a_{lm}.

In practice, we search for unknown coefficients. After standard replacement $\Psi(r,\vartheta,\varphi) = r\tilde{\Phi}(r,\vartheta,\varphi)$, separation of the incident and scattered waves $\tilde{\Phi} = \Phi_0 + \Phi$, and reducing the equation obtained from (4) to a discrete form (at this stage, the algorithm is identical to the one in [3]), we use a matrix sweep [10]. It is based on the linear relationship

$$\Phi_{j-1} = Z_j \Phi_j + D_j \qquad (11)$$

between matrix columns $\Phi_j = \overline{(\Phi(r_j,\vartheta_0), \Phi(r_j,\vartheta_1), \ldots, \Phi(r_j,\vartheta_{n_{\max}}))}$, $\vartheta_n = \Delta\vartheta n$ for any point $r_j = \Delta r_j$. The matrix form of the discretized equation with allowance for the boundary condition at $r = 0$ allows matrices Z_j and D_j be determined recursively for any r_j. At boundary $r = r_{\max} > r_V$, relation (11) is transformed into the equation for unknown coefficients a_{lm}.

3. Solution for uranium nuclei

Using a program that executes the specified algorithm, a model problem was solved that demonstrates the possible effects in scattering on a non-spherical potential. The parameters of neutron scattering on the non-spherical $^{235-238}$U nucleus were chosen as the initial data for the problem. Two models were considered for comparison: Model 1, with the boundary of a Woods–Saxon potential in the form of an ellipsoidal surface of revolution, and Model 2, a spherically symmetrical potential. The interaction potential of a neutron with a nucleus in Model 1 in spherical coordinates is written as a function of r_{mod1}, where

$$r_{\text{mod1}} = \frac{b}{\sqrt{1 - e^2 \cos^2 \vartheta}}\,.$$

Parameters of the Woods–Saxon potential and the size of nuclei were found from optical model [12]. The l–s-interaction has not been taken into account. Parameters b, e were determined from the condition of the equality of volume of the sphere and the ellipsoid. This corresponds to the incompressibility of nuclear matter. In addition, the parameter of deformation was used to determine b, e [11]: $1.06\,(a-b)/\,R_0 = \beta, \beta = 0.281$, where a is a major half-axis related to minor half-axis b through eccentricity e. The use of a two-dimensional system of equations to determine $\tilde{\theta}$ can be considered as neutron scattering on spin-oriented targets. Asymptotic (9) has been used for the case of $\tilde{\theta} = 0$ and for Model 1. For $\tilde{\theta} \neq 0$, the asymptotic form of (7) has been used.

Of course, using the parameters of the interaction potential described above the process of neutron scattering on uranium isotopes with a high degree of conditionality because we do not include the Hamiltonian of the nucleus, in which the angular part restores the conservation of angular momentum. However, such a realistic problem can be described in five-dimensional space using a minimal and greatly simplified formulation. The use of two-dimensional scattering on a non-spherical nucleus is thus only part of describing the complete scattering process with the possible transfer of angular momentum to the uranium nucleus. Nevertheless, even such a simplified analysis can show how much the deformation of the nucleus affects the angular dependence of the scattering process.

In figure 1, the calculation for two different models has been shown. The different angles $\tilde{\vartheta}$ have been used. It seems that scattering at spherical potential is very different than the one at potential of ellipsoid. Scattering for all models is lower than for the optical model [12]. It could be explained by the absence of l–s interaction.

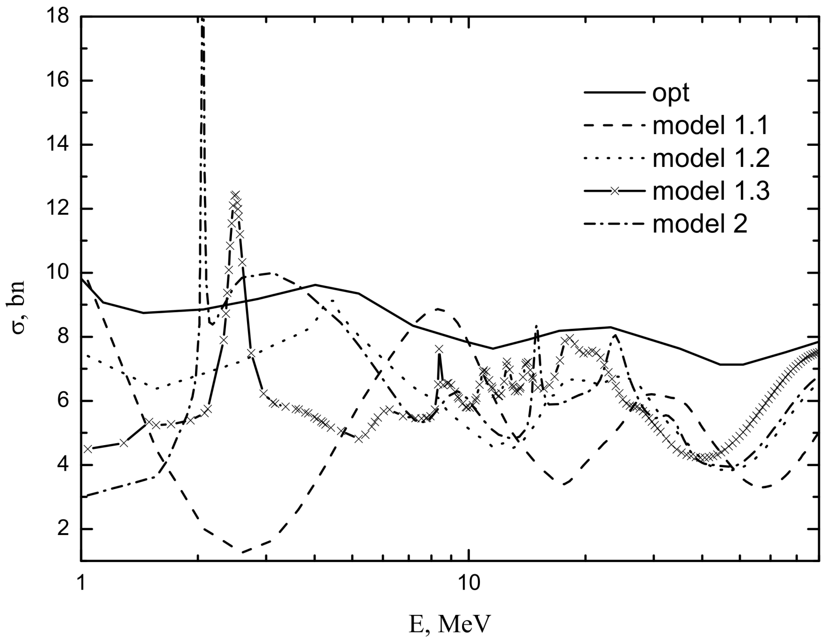

Fig. 1. Comparision of the different calculation model. 'opt' — calculation by optical model from [12], 'model 1.1–1.3' — for angles $\tilde{\vartheta}$ 0, $\pi/4$ and $\pi/2$, respectively.

Another point is a difference between possible averaged result of scattering at non-spherical potential and the one at spherical potential. For 5–10 MeV, full averaged cross section of Model 1 will be more than cross section of Model 2.

4. Conclusion

The program for calculating the cross sections of two-dimensional equations in spherical coordinates was modernized as a result of expanding the solution according to free solutions. The modernization results in a considerable saving of computer resources, a reduction in computation time, and new ways of calculating the wave function in the region of the geometric shadow.

The program was tested on an ellipsoidal Woods–Saxon potential of the uranium nuclei. Calculations of neutron scattering differ considerably from those of scattering in the model of a spherically symmetric potential. Nucleon–nuclear spherically symmetric interaction thus cannot be used to describe elastic neutron scattering on the uranium nucleus (for spin-oriented targets) even as a first approximation.

This work was supported by the representative of the Republic of Kazakhstan at the Joint Institute for Nuclear Research, grant No. 434 of 2018. The major part of the calculations has been done by cluster HYBRILIT JINR (`hybrilit.jinr.ru`).

REFERENCES

[1] P.M. Krassovitskiy, F.M. Penkov, *Bull. Russ. Acad. Sci.: Phys.* **83**, 420 (2019).

[2] P.M. Krassovitskiy, F.M. Penkov, *Bull. Russ. Acad. Sci.: Phys.* **81**, 730 (2017).

[3] P.M. Krassovitskiy, F.M. Penkov, *Bull. Russ. Acad. Sci.: Phys.* **82**, 669 (2018).

[4] P.M. Krassovitskiy, F.M. Penkov, *J. Phys. B* **47**, 225210 (2014).

[5] R. Mathaes, *et al.*, *Expert Opin. Drug Delivery* **12**, 481 (2015).

[6] A.N. Ikot *et al.*, *Commun. Theor. Phys.* **65**, 569 (2016).

[7] A. Statt, P. Virnau, K. Binder, *Mol. Phys.* **113**, 2556 (2015).

[8] O. Chuluunbaatar *et al.*, *Bull. Russ. Acad. Sci.: Phys.* **82**, 654 (2018).

[9] L.D. Landau, E.M. Lifshitz, «Kvantovaya mekhanika (nerelyativistskaya teoriya) (Quantum Mechanics: Non-Relativistic Theory)», *Nauka*, Moscow 1989.

[10] R.P. Fedorenko, A.I. Lobanov (Ed.) «Vvedenie v vychislitel'nuyu fiziku (Introduction to Computational Physics)», *Intellekt*, Dolgoprudny 2008.

[11] O.F. Nemets, Yu.V. Gofman, «Spravochnik po yadernoi fizike (Nuclear Physics Handbook)», *Naukova Dumka*, Kiev 1975.

[12] Yinlu Han *et al.*, *Phys. Rev. C* **81**, 024616 (2010).