CALCULATIONS OF nd-SCATTERING CROSS-SECTIONS BY FADDEEV'S METHOD WITH A HYPERSPHERICAL BASIS

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An approximate method for calculating nd-scattering cross-sections at energies below the deuteron breakup threshold has been developed. The most complicated term Ψ_C of the complete wave function, which describes a three-nucleon system in the interaction region, has been extracted and expanded into a K-harmonic series. The coefficients of such an expansion are the solutions of integral Faddeev equations. Keeping only a term with $K = 0$ in this expansion and taking the quartet phases with $\ell = 0$ and 1 into account, we have calculated nd-scattering cross-sections for the energy of bombarding neutron ranging from 1.0 to 2.5 MeV. The Malfliet–Tjon, Yukawa, and Hulthen local nucleon-nucleon potentials were used in computations. Two fitting parameters, the phase shift for the state with $\ell = 1$ and the normalization coefficient for Ψ_C, were used, which allowed us to obtain a satisfactory agreement between the calculated cross-sections and the corresponding experimental data. The developed approach enables the problem of finding a three-nucleon wave function for the continuous spectrum with nonseparable interaction to be reduced to the problem of solving a one-dimensional integral equation. This circumstance makes it drastically different from the methods based on the direct numerical solution of two-dimensional integral equations in the momentum representation.

1. Introduction

Finding the wave functions of a continuous spectrum for a system of three strongly interacting particles by solving the corresponding Faddeev equations [1–3] numerically is known to be rather a complicated problem. Such wave functions are needed, e.g., for the calculation of the cross-sections of scattering of nucleons and other hadrons by deuterons at low energies, when the available approximate methods turn out inapplicable for this purpose. A substantial contribution to the solution of this problem is given by the works of the so-called Pisa and Bochum-Krakow research groups which use essentially different methods. The Pisa group uses the R-matrix formalism. In the framework of this method, some part of the complete wave function is expanded into a series of hyperspherical polynomials in the interaction region [4]. The corresponding coefficients of this expansion (the radial functions) and the elements of the R-matrix are determined making use of the Kohn–Hulthen variational principle [5] At the same time, the Bochum-Krakow group tries to solve the Faddeev equations in the momentum space [6, 7]. In works [8, 9], both approaches were compared with each other, and the corresponding calculated values for phases, mixing parameters, cross-sections, and polarization characteristics of low-energy nd-scattering turned out close very much.

In work [10], a method was proposed for the calculation of the wave function of the neutron–deuteron system which is based on the expansion of the difference $\Psi - \Phi$ in a series of K-harmonics. Here, Φ is the Faddeev asymptotic wave function which is a product of the internal wave function of the deuteron $\phi_d(|\vec{r}_2 - \vec{r}_3|)$ and a plane wave $\exp(i\vec{k}\vec{x}_1)$, the latter describing the infinite motion of the neutron (the 1-st nucleon) and the deuteron; $\vec{k}$ is the relative momentum of the neutron in the center-of-mass system; $\vec{x}_1 = \vec{r}_1 - (\vec{r}_2 + \vec{r}_3)/2$; and $\vec{r}_j$ is the radius-vector of the j-th nucleon ($j = 1, 2, 3$). The issues how quickly the series of K-harmonics converges and how many of its first terms should be taken into consideration for the solution of specific problems were not discussed in work [10], but the convergence of the series was proved, because the difference $\Psi - \Phi$ diminishes with increase of the hyperspherical radius $\rho = \left(\vec{r}_{23}^{\,2}/2 + 2\vec{x}_1^{\,2}/3\right)^{1/2}$, where $\vec{r}_{ij} = \vec{r}_i - \vec{r}_j$. Also in work [10], a procedure for finding the expansion coefficients in the case $K = 0$ was given as an example. (In work [11] devoted to studying the low-energy proton-deuteron scattering, we also confined the consideration to the case of zero relative momenta).

The method proposed in work [10] was applied in work [12] for the description of the results of experiments dealing with elastic nd -scattering at the neutron energy $E_n = 3.28$ MeV in the laboratory reference frame. Retaining only the first K-harmonic with $K = 0$ in the expansion of the difference $\Psi - \Phi$, we managed to describe the experimental data only at a qualitative level; in particular, the calculated curves did not agree with experimental dependences at small and large scattering angles. We believed that a satisfactory description of the experiment in the framework of the formalism of work [10] was possible only provided that the terms with $K \neq 0$ were included into the $(\Psi - \Phi)$-expansion, but it would make the calculation procedure for expansion coefficients too complicated.

However, we paid attention that $\Psi - \Phi \sim x_1^{-1}$ at $x_1 \to \infty$; it is associated with the fact that the difference $\Psi - \Phi$ is proportional to a divergent wave $\exp(ikx_1)/x_1$. Therefore, it is reasonable to expand the difference

$$\Psi_C = \Psi - \phi_d(r_{23})\Psi_S(\vec{x}_1)\,, \tag{1}$$

rather than the $\Psi - \Phi$ one into a series of K-harmonics. Here, the function $\Psi_S(\vec{x}_1)$ describes the scattering of a neutron by a deuteron, and, in the asymptotic region, it is a superposition of the incident plane wave and the divergent spherical one. Then, function (1), which describes the state of a system composed of three nucleons located at small distances from each other so that the nuclear interaction is implemented for each pair of nucleons, can be expanded into a series of K-harmonics.

A similar principle of constructing the wave function in the continuum for the nd-systems was used in work [4] and in the interpolation model [3].

2. Formalism of the Theory

The function $\Psi_S(\vec{x}_1)$ which is included into Eq. (1) satisfies the Schrödinger equation (hereafter, the system of units $\hbar = c = 1$ is used)

$$\frac{\partial^2}{\partial \vec{x}_1^{\,2}}\Psi_S(\vec{x}_1) + k^2\Psi_S(\vec{x}_1) = U\Psi_S(\vec{x}_1)\,,$$

$$U = 4m\big(V_{12} + V_{31}\big)/3\,, \tag{2}$$

where $k^2 = 4mE/3$, m is the nucleon mass, $E = 2E_n/3$ is its kinetic energy in the center-of-mass system, $V_{ij} \equiv V(r_{ij})$ with $ij = (12, 23, 31)$ is the pair nucleon-nucleon (NN) potential, $\vec{r}_{12} = \vec{x}_1 - \vec{r}_{23}/2$, and $\vec{r}_{31} = -\vec{x}_1 - \vec{r}_{23}/2$. The coordinate $\vec{r}_{23}$ in Eq. (2) is supposed to be "frozen" for a while, with its absolute value not exceeding the nuclear force action radius.

At $x_1 \to \infty$, we have

$$\Psi_S(\vec{x}_1) = \exp(i\vec{k}\vec{x}_1) + f(\theta)\,\frac{\exp(ikx_1)}{x_1}\,, \tag{3}$$

where

$$f(\theta) = \frac{1}{2ik}\sum_{\ell=0}^{\infty}(2\ell+1)(\exp(2i\delta_\ell) - 1)P_\ell(\cos\theta) \tag{4}$$

is the neutron-deuteron scattering amplitude in the center-of-mass system, ℓ is the orbital moment of the neutron with respect to the deuteron, and δ_ℓ is the corresponding scattering phase. Taking Eq. (3) into account, let us write down function (1) in the asymptotic region as follows:

$$\Psi_C = (\Psi - \Phi) - \phi_d(r_{23})f(\theta)\,\frac{\exp(ikx_1)}{x_1}\,. \tag{5}$$

Now, it is evident from the last equation that, unlike the difference $\Psi - \Phi$, the function Ψ_C does not contain the components proportional to x_1^{-1} at $x_1 \to \infty$.

The general solution of Eq. (2) in the whole space of the variable $\vec{x}_1$ can be presented in the form [13]

$$\Psi_S(\vec{x}_1) = \frac{1}{kx_1}\sum_{\ell=0}^{\infty}(2\ell+1)i^\ell\psi_{\ell\,k}(x_1)P_\ell(\cos\theta)\,, \tag{6}$$

where

$$\psi_{\ell\,k}(x_1) = \exp(i\delta_\ell)\big[\cos\delta_\ell\,F_\ell(kx_1) + \sin\delta_\ell\,G_\ell(kx_1)\big]\,, \tag{7}$$

and $F_\ell(kx_1)$ and $G_\ell(kx_1)$ are the regular and irregular, respectively, (at $x_1 \to 0$) solutions of Eq. (2). In the asymptotic region, function (6) with Eq. (7) transforms into function (3) with Eq. (4).

Beyond the range of nuclear force action, the functions $F_\ell(kx_1)$ and $G_\ell(kx_1)$, which are included into Eq. (7), can be expressed in terms of the Bessel and Neumann functions with half-integer indices [14]:

$$F_\ell(kx_1) = \sqrt{\pi kx_1/2}\;J_{\ell+1/2}(kx_1),$$

$$G_\ell(kx_1) = \sqrt{\pi kx_1/2}\;N_{\ell+1/2}(kx_1). \tag{8}$$

In order to determine the function $\Psi_S(\vec{x}_1)$ in the range of nuclear force action in the general case, the inhomogeneous Schrödinger equation (2) has to be solved numerically. However, as was shown in work [15], in the low-energy range where the value of E is much less than the effective potential value, it is a good approximation to consider that the expressions for the functions F_ℓ and G_ℓ in the interaction region look like Eqs. (8).

The three-nucleon function (1) – the solution of the Faddeev equations – can be found by expanding it in a series of hyperspherical polynomials and by retaining only the first term (with $K = 0$) in this expansion:

$$\Psi_C = B(\rho)/\sqrt{\pi^3}\,. \tag{9}$$

Here, the function $B(\rho)$ satisfies the one-dimensional integral equation [10]

$$B(\rho) = \pi^{-1/2}\rho^{-2}m\int d\rho'\,\rho'^3 P(\kappa,\rho,\rho')\times$$

$$\times\int d\Omega\,(V_{12}+V_{31})\,\Phi + \pi^{-2}\rho^{-2}m\times$$

$$\times\int d\rho'\,\rho'^3\,B(\rho')P(\kappa,\rho,\rho')\int d\Omega\;(V_{12}+V_{31}+V_{23})\,, \tag{10}$$

and Ω is the set of five angular variables in the spherical coordinate system which determine the vector $\vec{\rho}$ in the six-dimensional space. The function $P(\kappa,\rho,\rho')$, which is included into Eq. (10), is defined as

$$P(\kappa,\rho,\rho') = -i[J_2(\kappa\rho)\,H_2^{(1)}(\kappa\rho')\,\Theta(\rho'-\rho)+$$

$$+J_2(\kappa\rho')\,H_2^{(1)}(\kappa\rho)\,\Theta(\rho-\rho')],$$

where $\kappa = \sqrt{2m(E-\varepsilon)}$, $\varepsilon = 2.226$ MeV is the deuteron binding energy, $J_2(x)$ and $H_2^{(1)}(x)$ are the Bessel and Hankel, respectively, functions of the second order, and $\Theta(x)$ is the Heaviside function.

By its implication, the function $B(\rho)$ has to be substantially different from zero only in the region of nuclear force action between all the three nucleons.

3. Calculation of Three-nucleon Wave Functions

The wave functions Ψ_C were calculated for the following models of the local NN potential:
1) the Malfliet–Tjon triplet potential (Malfliet–Tjon III) with a repulsive soft core [16]

$$V(r) = -\lambda_A\exp(-\mu_A r)/r + \lambda_R\exp(-\mu_R r)/r \tag{11}$$

with $\lambda_A = 3.22$ fm^{-1}, $\mu_A = 1.55$ fm^{-1}, $\lambda_R = 7.39$ fm^{-1}, and $\mu_R = 3.11$ fm^{-1};
2) the Yukawa triplet potential (Yukawa III) [16, 17]

$$V(r) = -\lambda_{\rm Y}\exp(-\mu_{\rm Y} r)/r \tag{12}$$

with $\lambda_{\rm Y} = 0.36$ fm^{-1} and $\mu_{\rm Y} = 0.71$ fm^{-1}; and
3) the Hulthen potential [18]

$$V(r) = -\lambda_{\rm H}\exp(-\mu_{\rm H} r)/r \tag{13}$$

with $\lambda_{\rm H} = 0.18$ fm^{-1} and $\mu_{\rm H} = 1.15$ fm^{-1}.
Potentials (11) and (12) reproduce well the S-phases of NN-scattering, the deuteron binding energy, the scattering lengths, and other low-energy parameters [16]. As the test ones, they are intensively used by the Pisa, Bochum–Krakow, and Los Alamos research groups in many problems dealing with low-energy nd-scattering [9, 17, 19–21].

The deuteron wave function $\phi_d(r_{23})$ was selected in the form [3]

$$\varphi(r_{23}) = \sqrt{\frac{\alpha\beta(\alpha+\beta)}{2\pi(\beta-\alpha)^2}}\,\frac{\exp(-\alpha r_{23})-\exp(-\beta r_{23})}{r_{23}} \tag{14}$$

with the parameters $\alpha = \sqrt{m\varepsilon}$ and $\beta \simeq 7\alpha$.

When applying expansion (6) in calculations, the phases δ_ℓ were taken into account only for two orbital moments, $\ell = 0$ and 1. The energy dependence of the quartet nd-phase ${}^4\delta_0$ had been studied earlier with a high accuracy in the energy range from zero to a few megaelectronvolts; therefore, its value was considered known (given) [4, 19, 22–24]. Hence, only the values of the P-phases were varied while fitting the calculation results to experimental data. In addition, the calculated functions (9) were normalized in such a way that the scattering amplitude would tend to the known [25] quartet length of nd-scattering $a_4 \approx 6.35$ fm in the limiting case $k \to 0$:

$$\Psi_C = \eta\,B(\rho)/\sqrt{\pi^3}\,, \tag{15}$$

where η is the normalization factor.

In Fig. 1, the functions $B(\rho)$ calculated for potentials (11)–(13) and various energies of a bombarding neutron E are depicted. The corresponding normalization factors η are plotted in Fig. 2 as functions of the energy E. The functions $B(\rho)$ expectedly turned out different from zero only for ρ-values smaller than about 4 fm; beyond this region, $B(\rho) \to 0$.

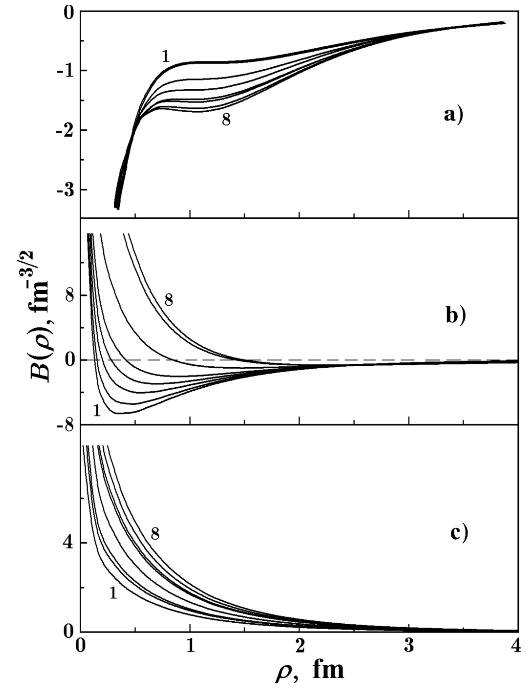

Fig. 1. Families of the calculated functions $B(\rho)$ for the potentials described by (*a*) Eq. (11), (*b*) Eq. (12), and (*c*) Eq. (13). Curves correspond to the neutron energy $E = 10^{-3}$ (*1*), 0.147 (*2*), 0.333 (*3*), 0.5 (*4*), 0.667 (*5*), 1.0 (*6*), 1.333 (*7*), and 1.667 MeV (*8*)

4. nd-scattering Cross-sections. Analysis of the Results Obtained

Since the doublet length of the nd-scattering, $a_2 \approx 0.65$ fm [25], is an order of magnitude smaller than the quartet one a_4, the differential cross-section of the nd-scattering for non-polarized neutrons at $k \to 0$,

$$\sigma(\theta) \equiv \frac{d\sigma}{d\Omega} = \frac{2}{3}\,|a_4|^2 + \frac{1}{3}\,|a_2|^2, \tag{16}$$

is mainly determined by the quartet length. The same can be expected at low enough but finite energies E as well. The fact that the scattering at energies $E \approx 1$ MeV occurs mainly in the quartet state is also confirmed by the data of phase analysis [22, 23], from which it follows that the contribution of the doublet component to cross-section (16) is about 1%. Therefore, we used the formula

$$\sigma(\theta) = \frac{2}{3}\,|A(\theta)|^2, \tag{17}$$

where

$$A(\theta) = \frac{m}{3\pi}\langle\Phi|V_{12} + V_{31}|\Psi\rangle$$

is the scattering amplitude [26], to calculate the cross-sections $\sigma(\theta)$.

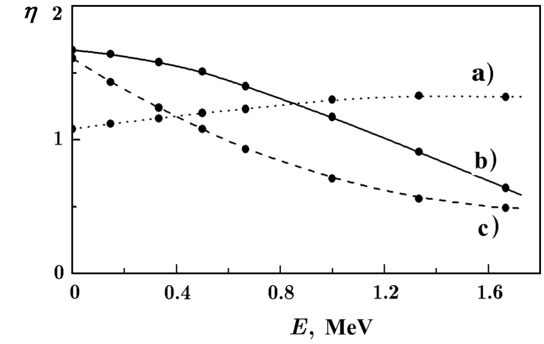

Fig. 2. Normalization factor η as a function of the neutron energy E for the potentials described by (*a*) Eq. (11), (*b*) Eq. (12), and (*c*) Eq. (13)

In Fig. 3, the calculated cross-sections (17) are exhibited for various potentials of NN-interaction and various energies E below the deuteron breakup. Figure 4 demonstrates the corresponding phases ${}^4\delta_1$ which were found while fitting our results to experimental data.

From Fig. 3, one can see that the best agreement in the studied energy range is provided by the Yukawa NN-potential (12). To illustrate the accuracy and the efficiency of the method developed in this work, in Fig. 5, we compare the calculated cross-section (17) with its analog reported in work [27] of the Pisa group, where the data of experiments [22] were also analyzed. Despite that the calculations in work [27] were carried out making use of a realistic $AV18$ NN-potential and the three-particle interaction was taken into consideration as well, the results of our work and work [27] are very close (this also concerns other experimental data of work [22] considered in work [27]). Some difference between the calculated values of P-phases and the corresponding results obtained by other authors (see Fig. 4), as well as the necessity to introduce a normalization factor into Eq. (15), can be explained by the approximate origin of the approach used to solve the problem; namely, only those factors were taken into account, which gave the main contribution to the reaction amplitude.

Figure 5 also demonstrates cross-section (17) calculated for the case $\Psi_C = 0$ (dash-dotted curve). One can see that making allowance for the three-particle interaction is a necessary condition to describe the results of the considered experiments (solid curve) satisfactorily, and that such an agreement cannot be reached at $\Psi_C = 0$ for any values of the phase ${}^4\delta_1$.

Hence, the approximate method developed by us for calculating the cross-sections of nd-scattering with simple models of NN-interaction allows a satisfactory agreement with the majority of analyzed experimental

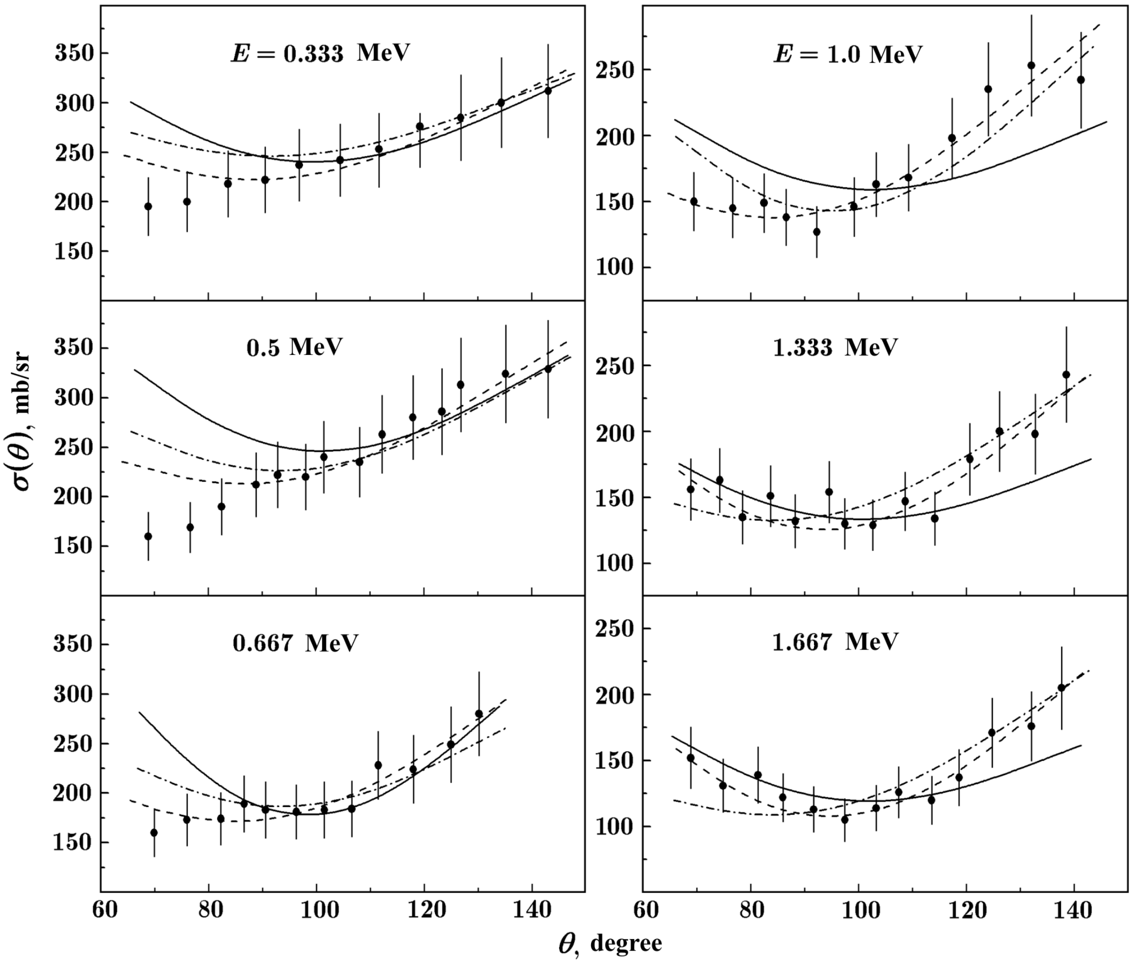

Fig. 3. Differential cross-sections of nd-scattering for various NN-potentials: potential (11) (solid), potential (12) (dashed), and potential (13) (dash-dotted curves). Experimental data were taken from work [22]

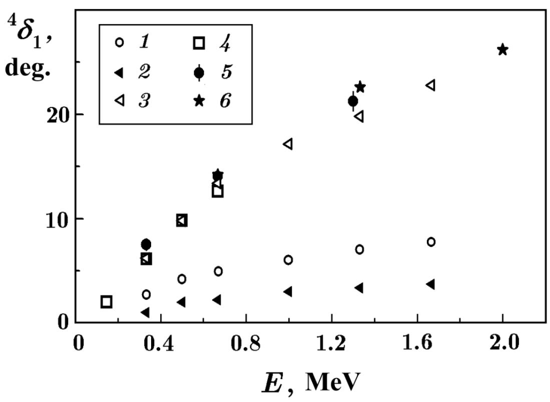

Fig. 4. Quartet P-phase found in the course of fitting our results to the experimental data of work [22] making use of various NN-potentials: potential (11) (*1*), potential (12) (*2*), and potential (13) (*3*). The data of other authors are also presented: work [22] (*4*), work [23] (*5*), and work [4] (*6*)

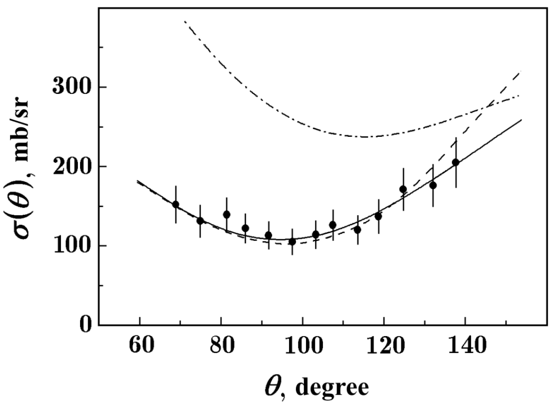

Fig. 5. Differential cross-sections of nd-scattering (17) at E = 1.667 MeV with NN-potential (12). The solid curve was calculated for $\Psi = \Psi_C + \phi_d \Psi_S$, and the dash-dotted one for $\Psi = \phi_d \Psi_S$. The dashed curve corresponds to the results of work [27]. Experimental data were taken from work [22]

data to be obtained. By presenting the complete wave function Ψ of the nd-system as a sum of the asymptotic part and a part that describes the three-nucleon system in the interaction region, we reduced the problem of finding Ψ to the solution of a one-dimensional integral equation, which does not require substantial computer time-resources, in contrast to conventional methods that are based on the direct numerical solution of two-dimensional integral equations in the momentum representation. In general, we may assert that the approach proposed allows the low-energy experiments on nd-scattering to be described well. Hence, in the future, it can serve as a basis for a more rigorous consideration of similar problems, which would take into account terms with $K \neq 0$ in the Ψ_C-expansion, phases with $\ell > 1$, spin-orbit interaction, etc.

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РОЗРАХУНКИ ПЕРЕРІЗІВ nd-РОЗСІЯННЯ В МЕТОДІ ФАДДЄЄВА З ГІПЕРСФЕРИЧНИМ БАЗИСОМ

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Р е з ю м е

Розвинуто наближений метод обчислення перерізів nd-розсіяння при енергіях, нижчих за поріг розвалу дейтрона. В повній хвильовій функції системи виділено найбільш складну її частину Ψ_C, що описує тринуклонну систему в області взаємодії. Цю компоненту розкладено у ряд за K-гармоніками, коефіцієнти розкладу якого є розв'язками інтегральних рівнянь Фаддєєва. Утримуючи в цьому розкладі тільки член з $K = 0$ та враховуючи квартетні фази з $\ell = 0, 1$, ми виконали розрахунки перерізів nd-розсіяння в діапазоні енергій падаючого нейтрона $1,0 \div 2,5$ МеВ з використанням локальних нуклон-нуклонних потенціалів Мальф'є–Тжона, Юкави та Хюльтена. Досягнуто задовільне узгодження з відповідними експериментами, при цьому було використано два підгінних параметри – фазовий зсув у стані з $\ell = 1$ та нормувальний коефіцієнт для Ψ_C. Розвинутий підхід дозволяє звести задачу про знаходження хвильової функції неперервного спектра системи трьох нуклонів з несепарабельною взаємодією до одновимірного інтегрального рівняння, на відміну від методів, які ґрунтуються на безпосередньому чисельному розв'язуванні двовимірних інтегральних рівнянь в імпульсному представленні.