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# RESONATING GROUP CALCULATION OF SCATTERING $^3$He($d$, $d$)$^3$He AT $E$ = 1 - 9 MeV

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Distance dependent form of cluster mean field parameters is used for interacting channel fragments in resonating group calculation of elastic scattering $^3$He($d$, $d$)$^3$He. Simple two level approximation of this dependence enables to obtain an essential improving of calculated differential cross sections. In the interaction region the values of cluster radii are near 55 % from far asymptotic phenomenological value, the transition point at studied energy values is placed within interval 11.2 - 12.6 fm of intercluster distance.

*Keywords*: elastic scattering, resonating group method, cluster potential, distance dependent basis.

## 1. Introduction

Microscopic calculations of scattering in system $^2$H + $^3$He are executed at present for energy over 7 MeV by Tang Y.C. with collaborators [1, 2]. Since the first work [1] authors show in a number of publications the more or less close to experiment results of their microscopic calculations corrected with help of fitted optical potentials or, in last versions [2], due to massive including into basis of so-called "deuteron pseudo-states" with arbitrary chosen characteristics. For $^3$He authors [2] do not use the pseudo-states, relying upon its incompressibility. The calculation is additionally complicated through a low threshold of some three-body reaction channels quickly opening at energy over 2.22 MeV. Moreover, for system $^2$H + $^3$He the channel $p$ + $^4$He ($Q$ = 18.35 MeV) is permanently open. Limited success of calculation results in combination with uncertainty in the source physical positions does not stimulate the further development, that means also complication, the ideology [1, 2] since its concepts for the scattering $^3$He($d$, $d$)$^3$He cause more questions than give explanations.

This situation induces to search for other approaches to description of the process within the RGM framework. It seems reasonable to build the adequate representation for wave functions of channel fragments in the assumption that interaction of nuclei at the initial stage results in such changes of nucleon movement within each cluster which can be effectively reproduced through change of parameters of mean cluster potential. The unique parameter of this oscillator potential is radius $\sqrt{\hbar/m\omega}$ which becomes therefore dependent on intercluster distance. It is convenient for an initial estimation to choose this dependency in the simplest step-like form and then define its parameters from fitting of calculated differential sections to experimental data [3, 4]. Present work applies this approach to calculation of scattering $^3$He($d$, $d$)$^3$He. Single-channel calculation with the traditional form of basis in this case so overestimates the values of differential cross sections that there is improbable to explain the discrepancies by influence of competing reaction channels, especially at energy lower than 2.22 MeV where only competing channel $p$ + $^4$He is open and cross section of corresponding reaction $^3$He($d$, $p$)$^4$He is rather small [5]. It means that at least at $E$ < 2.22 MeV the main part of divergences should be eliminated through improvement of single-channel calculation. That is why the single channel calculation is chosen to obtain the parameter values of above-formulated representation for cluster wave functions, and possible influence of ignored reaction channels is the object of following analysis. Necessary resonating group equations for scattering $^3$H($d$, $d$)$^3$H are considered in Section 2 together with used nucleon - nucleon potentials (NNP) and accepted construction of basis as well as determination of its parameters. Section 3 explains the main positions of numerical solution of the obtained equations and describes the comparing of calculated differential cross sections to a set of available experimental data at six energy values from interval 1.2 MeV ≤ $E$ ≤ 8.8 MeV.

## 2. Resonating group formulation

In order to build suitable resonating group formalism the variational method is used to minimize values of the matrix elements

$$\left\langle \Psi \middle| H - E_t \middle| \Psi \right\rangle \qquad (1)$$

where $H$ is microscopic Hamiltonian and $E_t$ total energy of the system. Completely antisymmetrized RGM wave function in this case:

$$\Psi = \mathrm{A}\left\{ \sum_{IM_I} F_{IM_I}(\vec{r}) \left[ \Phi_1(\xi_1)\Phi_2(\xi_2) \right]_{IM_I} \mathrm{X}_{IM_I} \right\} \qquad (2)$$

Here $\mathrm{X}_{IM_I}$ is component of spin function with channel spin $I$ and its projection $M_I$. Product of

cluster wave functions $\Phi_1(\xi_1)$ and $\Phi_2(\xi_2)$ is projected on the spin state $IM_I$ what reflects the lower indexes of the square brackets. These functions are the Slater determinants constructed of single-nucleon wave functions taken as products of spatial, spin and isospin functions of each nucleon. Their variables $\xi_1$, $\xi_2$ unite the spatial, spin and isospin variables of all nucleons of corresponding cluster. Antisymmetrized expression in square brackets forms spatial basis for wave function of relative movement of the channel fragments $F_{IM_I}(\vec{r})$, which depends on the distance between fragments $\vec{r}$. After transform to spherical coordinates and expanding $\Psi$ in series over the states of total angular momentum $JM$ with spin $I$ and system parity $\pi$ ($f_l^{JM\pi I}(r)$ are partial coefficients of such series), for radial functions $g_l^{JM\pi I}(r) = r f_l^{JM\pi I}(r)$ by using of variational methods one can obtain the Euler's equations which determine the minimum of functional (1). For each system state $JM\pi I$ (these indexes for functions $g_l(r)$ and coefficients of the equations further are omitted) the dynamic equations have a form

$$\left\{\frac{\hbar^2}{2\mu}\left[-\frac{d^2}{dr^2}+\frac{l(l+1)}{r^2}\right]+V(r)-E\right\}g_l(r)+\frac{1}{2}r\int dr'r'\left\{\frac{\hbar^2}{2\mu}\left[-\frac{\partial^2}{\partial r'^2}N_l(r,r')-\frac{\partial^2}{\partial r^2}N_l(r',r)+\right.\right.$$

$$\left.\left.+N_l(r,r')\frac{l(l+1)}{r'^2}+N_l(r',r)\frac{l(l+1)}{r^2}\right]-E\left[N_l(r,r')+N_l(r',r)\right]+U_l(r,r')+U_l(r',r)\right\}g_l(r')-$$

$$-\frac{\hbar^2}{2\mu}\int dr'\left[r'\frac{\partial}{\partial r}N_l(r',r)+r\frac{\partial}{\partial r'}N_l(r,r')\right]g_l(r')=0\,. \qquad (3)$$

Here $E$ is energy of relative movement of channel fragments. Direct potential for their interaction $V(r)$ is formed of local terms of matrix elements of intercluster interaction taken on basis functions. The non local terms of these matrix elements form the integral kernels $U_l(r,r')$, the non local part of overlap matrix elements produces the kernels $N_l(r,r')$. In the integral part of equations by mathematical transformations during the variational procedures it is possible to replace the action of differential operators on the unknown functions $g_l(r)$ by differentiation of the kernels $N_l(r,r')$. That form of the equations is more convenient for the further numerical solution. Comparatively simple representation for the dynamic equations (3) results from mathematical simplicity of matrix elements obtained with the spatial basis formed with wave functions of channel fragments, nuclei $^2$H and $^3$He, in their ground states. For the same reason the expressions for potential and integral kernels also are rather simple. For oscillator potential of channel fragments these variables are given by expressions with real parameters $\alpha_k$, $\beta_k$, $o_k$, $u_k$, $v_k$:

$$V(r)=\sum_k v_k\exp\left(-\alpha_k^{(v)}r^2\right),$$

$$N_l(r,r')=\sum_k o_k\,h_l(\gamma_k^{(o)}rr')\exp\left(-\alpha_k^{(o)}r^2-\beta_k^{(o)}r'^2\right),$$

$$U_l(r,r')=\sum_k u_k\,h_l(\gamma_k^{(u)}rr')\exp\left(-\alpha_k^{(u)}r^2-\beta_k^{(u)}r'^2\right);$$

$$\left(\alpha>0,\quad \beta>0\right). \qquad (4)$$

The number of terms in the sum for $N_l(r,r')$ is determined by number of the Gaussians used for representation of nucleon *1s*-sell wave functions in the cluster. In the sums for $V(r)$ and $U_l(r,r')$ this number also depend on the quantity of Gaussians used in expression for nucleon-nucleon potential. The number of terms in the integral kernels additionally increases due to intercluster nucleon permutations at the antisymmetrization of wave function $\Psi$. Functions $h_l(crr')$ in integral kernels appear because of expanding on spherical harmonics according to standard formulae of the exponential factors $\exp\left[\gamma(\vec{r}\vec{r}')\right]$ in exchange matrix elements.

In most of calculations for NNP is applied the expression used in the previous works on scattering in the systems of nuclei $A\le 4$ [1, 2] at small energy, with the same parameter values:

$$v(r_{ij})=\left[\frac{1}{2}\left(1+P_{ij}^{\sigma}\right)V^t(r_{ij})+\frac{1}{2}\left(1-P_{ij}^{\sigma}\right)V^s(r_{ij})\right]\left[\left(1-m\right)+mP_{ij}^{r}\right]+\frac{e^2}{r_{ij}}\frac{1+\tau_{iz}}{2}\frac{1+\tau_{jz}}{2}\,. \qquad (5)$$

Here before the potentials of interaction in nucleon pair *i, j* for spin-triplet ($V^t$) and spin-singlet ($V^s$) states are the corresponding projection operators expressed through the exchange operator of nucleon

spin coordinates $P_{ij}^{\sigma}$. The multiplier responsible for a ratio of direct and spatial-exchange part NNP in the second square brackets is written down in the notation accepted for Volkov NNP, operator $P_{ij}^{r}$ exchanges the spatial coordinates of nucleons, $m$ is the relative contribution of Majorana interaction. Coulomb part is expressed through z-components of isospin operator for nucleons $i, j$ $\tau_{iz}, \tau_{jz}$.

$$V^t(r_{ij}) = V^t e^{-\kappa_t r_{ij}^2}, \qquad V^t = -66.92 \text{ MeV},$$

$$\kappa_t = 0.415 \text{ fm}^{-2},$$

$$V_{ij}^s(r_{ij}) = V^s e^{-\kappa_s r_{ij}^2}, \qquad V^s = -29.05 \text{ MeV},$$

$$\kappa_s = 0.292 \text{ fm}^{-2}.$$

To estimate the sensitiveness of the result to used NNP expression the calculations were carried out also with variant V1 of Volkov potential improved in [3]. Both used NNP expressions are determined only for even states of relative movement in the nucleon pair.

The initial version of spatial basis is built of the wave functions for ground states of nuclei $^2$H and $^3$He. According to [1] for $^2$H this function is a linear combination of three Gaussians:

$$\Phi_k = \sum_{i=1}^{3} C_{ik} \exp\left\{ -\frac{1}{2b_{ik}^2} \sum_{j=1}^{A_k} \left( \vec{r}_j - \vec{R}_k \right)^2 \right\}. \qquad (6)$$

Here $\vec{r}_j$ is coordinate of nucleon $j$, $\vec{R}_k$ is coordinate of the center of mass for cluster with serial number $k$ ($k$ = 1, 2). $A_k$ is mass number of cluster $k$. With NNP (5) and set of values $b_{ik}$ given in [2] the function (6) provides correct values of binding energy and root-mean-square radius for deuteron. For $^3$He authors [1, 2] use here one Gaussian to obtain according to the standard practice the correct radius value only. For elastic scattering, however, calculation with both forms of cluster functions $\Phi_k$ gives, as a rule, the results far from experiment, and with both form for $^2$H wave function the calculation results are rather similar.

According to general conception formulated in Introduction the oscillator radii $b_k$ during the rapprochement of channel fragments jump at certain distance $r_x$ from phenomenological far asymptotic values $b_k(e)$ to some values $b_k(i)$ which provide the best possible describing of experimental results for elastic scattering. Achieved proximity of calculated and experimental data is a principal test of accepted procedure.

## 3. Calculations and results

The general method used for solution of the equation system (3) is described in [3, 4] in application to scattering in the system $^4$He + $^4$He. Due to non-zero spin $^2$H and $^3$He there is two possible values $I$ for each $JM\pi$ state and then volume of the calculations approximately doubles. For numerical solution the equation system (3) is written down on the two-dimensional radial grid $r, r'$ with constant step $h$ in the region $\varepsilon \le r \le r_b$, $\varepsilon \le r' \le r_b$ ($\varepsilon$ is a non-zero small constant, $r_b$ denotes a distance where the nuclear interaction of the channel fragments may be neglected compared with the Coulomb one). Coefficients of the equations in each point $r, r'$ are determined from the preliminary computed set of matrix elements (4). Coulomb part for NNP at small $r_{ij}$ values ($\le 6$ fm) have been expressed microscopically according to [3, 4] as linear combination of Gaussians. For bounding values $g_l(r)$ at $r = \varepsilon$ the free movement expressions are used. Matching the general form of internal solution in the far asymptotic region to the usual external Coulomb solution one obtains the collision matrix. With its matrix elements the values of elastic differential cross sections are calculated on standard way for both possible states $I = 1/2$ and $I = 3/2$. Observed $d\sigma/d\Omega$ is obtained as linear combination of these two results with coefficients $1/3$ and $2/3$, correspondingly. Comparing of the cross sections calculated with increasing $r_b$ gives necessary value $r_b$ = 20 fm for considered interval of center mass energy 1.2 MeV $\le E \le$ 8.76 MeV. Admissible $h$ value is found also empirically through comparing of the cross sections calculated with decreasing $h$ value. As in [3] a stable calculation results are obtained at $h \le 0.12$ fm therefore the main calculation set is carried out with $h$ = 0.1 fm, and around the found optimum parameter values the calculations are repeated with $h$ = 0.05 fm. The calculation takes into account required quantity of the $J\pi$ states, $0 \le J \le 10$ of both parities.

The experimental differential cross sections $^3$He($d$, $d$)$^3$He at six characteristic center mass energy values are chosen among available data [6, 7]. First energy point $E$ = 1.2 MeV belongs to "almost single-channel" region where only reaction $^3$He($d$, $p$)$^4$He ($Q$ = 18.354 MeV) with rather small cross section [5] competes with elastic scattering. At next energy point $E$ = 1.8 MeV opens a second competing channel $p + p + t$ ($Q$ = –1.461 MeV). Next two energy values (3 MeV, 4.8 MeV) correspond to open channel $n + p + {}^3$He ($Q$ = –2.224 MeV). At $E$ = = 6.9 MeV an additional competing channel

$p + d + d$ is open ($Q$ = –5.494 MeV). The maximum $E$ = 8.76 MeV lies over the next competing channel $n + p + p + d$ ($Q$ = –7.718 MeV).

At each energy value the differential cross sections first are calculated with NNP (5) on the basis composed of the wave function (6) for the ground state $^2$H and one Gaussian wave function $^3$He, both with parameters [2]. Calculated $d\sigma/d\Omega$ are in general essentially higher than experimental data. Using for $^2$H one Gaussian form (6) with $b_{11}$ = 2.19 fm (with the same root-mean-square radius) gives the result of similar shape. Dashed line in Figs. 1 and 2 shows the latter result. For $^3$He everywhere is used value $b_{12}$ = 1.65 fm [2].

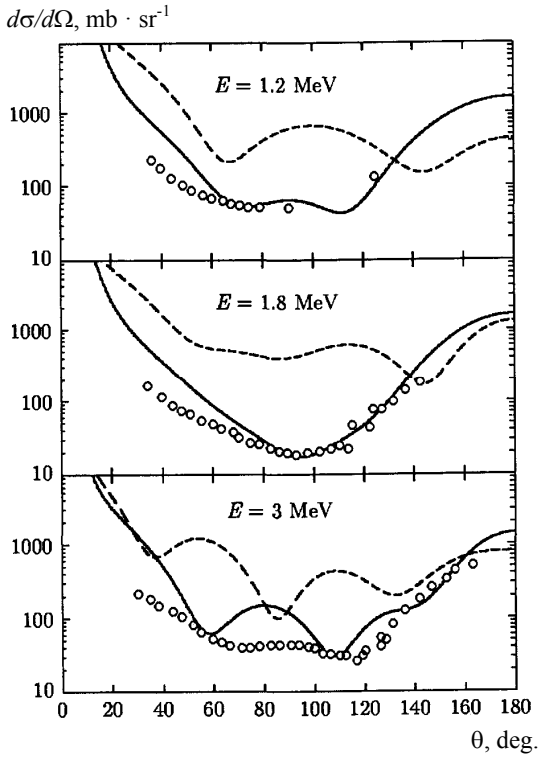


Fig. 1. Differential cross sections for $d + {}^3$He elastic scattering. Solid line represents the values calculated with modified basis. Dashed line corresponds to calculation with usual basis.

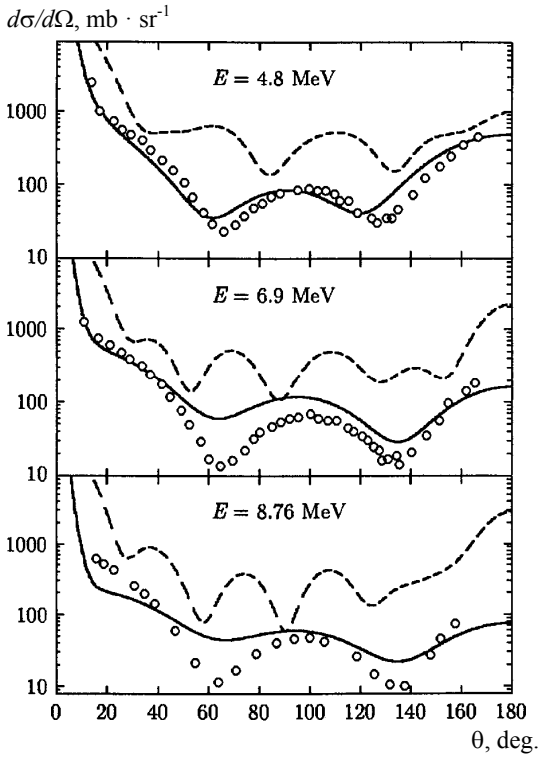


Fig. 2. Differential cross sections for $d + {}^3$He elastic scattering. Solid line represents the result obtained with modified basis and projected wave function Ψ (see text). Dashed line shows the result with usual basis.

Further calculations are carried out according to principles presented in this section. Oscillator radii $b_k(e)$ remain the phenomenological ones: $b_1(e)$ = 2.19 fm, $b_2(e)$ = 1.65 fm. The optimum values $b_k(i)$, $r_x$ at first was found from fitting to the experiment of $d\sigma/d\Omega$ calculated on a rough two dimensional grid 0.7 fm $\le b_k(i) \le$ 6 fm, 1 fm $\le r_x < r_b$ = 20 fm with step values 0.1 fm and 0.2 fm for $b_k(i)$ and $r_x$, correspondingly. Around the found optimum parameter values this procedure was repeated with lesser step of the parametric grid. At the last stage the value of space-exchange parameter was varied within the interval 0.5 $\le m \le$ 0.7.

In all energy points the most close to experiment results are obtained with $b_1(i)$ = 1.22 fm ($^2$H), $b_2(i)$ = 0.894 fm ($^3$He), $m$ = 0.55. At starting energy point $E$ = 1.2 MeV $r_x$ = 12.6 fm and fitted in this way $d\sigma/d\Omega$ practically describes the available experimental points for scattering angles $\theta \ge 60^\circ$ (see Fig. 1). At $E$ = 1.8 MeV with $r_x$ = 12.5 fm the calculated cross sections essentially improve, in region $\theta \ge 80^\circ$ one can see a practically complete describing. At $E$ = 3 MeV where the second three body channel ($n + p + {}^3$He) is open the best calculation result ($r_x$ =12.4 fm) is not so close to experiment because of a bump at $\theta \approx 80^\circ$.

At $E > 3$ MeV the calculated $d\sigma/d\Omega$ also changes towards the experimental data but visible discrepancies remain here. For the single channel results that appears quite naturally. In this energy region, however, the calculation results become rather close to experiment after projection of the wave function Ψ on the certain group of the $J\pi$ states. At $E$ = 4.8 MeV this is projection on $\frac{1}{2}^+$, $\frac{3}{2}^+$, $\frac{5}{2}^+$ states with $r_x$ = 12 fm, at $E$ = 6.9 MeV and

$E$ = 8.76 MeV this is projection on the $3/2^+$, $3/2^-$, $5/2^+$ states with $r_x$ = 11.4 fm and $r_x$ = 11.2 fm, correspondingly. Solid lines in Fig. 2 represent these results. Apparently just upper listed states mainly contribute to elastic scattering at studied energies while the rest of the $J\pi$ states are more coupled with others reaction channels. It should be noted that for $\Psi$ with invariables values $b_k(b_1(i) \equiv b_1(e)$ and $b_2(i) \equiv b_2(e))$ projection on the listed $J\pi$_states (or on the another ones) gives the worse results. This means that the modified basis is effective for energies over the single channel region too. The calculation with Volkov NNP at all energy values gives the similar results.

As can be seen the used approach to basis construction is productive with respect to describing of experimental elastic cross sections, and remaining discrepancies may be attributed to influence of the competing reaction channels. Observed proximity of the calculated and experimental $d\sigma/d\Omega$ conforms to the basic assumption about influence of the nucleus-nucleus interaction on the parameters of nuclear mean field. That also attests the efficiency of used simple two-level approximation for dependence of oscillator radius on the distance between interacting nuclei. The weak sensitiveness of the calculated $d\sigma/d\Omega$ to the used NNP form shows that just the transformation of the basis is determinant in this case. In terms of eq. (3) this means that the joint influence of the direct potential $V(r)$ and exchange interaction kernels $U_l(r,r')$ is almost negligible in comparison with contribution of kinetic energy operators. It shows that the interaction between the channel fragments at $r \le r_x$ mainly causes a transformation of the nuclear mean field, and the nucleus-nucleus interaction is of minor importance.

## 4. Conclusion

Single channel calculation of elastic scattering $^3$He($d$, $d$)$^3$He in the energy region 1 - 9 MeV does not give an acceptable describing of the experimental differential cross sections with basis built of the ground states of channel fragments. The modified basis construction considering the possible change of the mean field inside the interacting channel fragments displays a wide capability to improve the calculation results. Important change in the calculated cross sections take place after most simple two-level approximation for dependence of the cluster mean field parameter on the intercluster distance. These results most close to experiment at energy lower 2.22 MeV where the competing reaction channels practically are not expressed. At higher energies a number of open three-body channels effectively compete with elastic scattering and the modified basis improves the results of the single-channel calculation not so much. Within this energy region one can see, however, a selectivity of the elastic scattering with respect to the states of the total angular momentum. Projecting of the wave function on certain group $J\pi$ states leads to a visible improvement of calculated differential cross sections. Observed results show that in framework of accepted approaches inside the interaction region the size of channel fragments essentially decrease but the fragments retain the main features of their initial structure even despite the completely antisymmetrized system wave function.

REFERENCES


1. *Chwieroth F.S., Brown R.E., Tang Y.C., Thompson D.R.* Study of $d$ + $^3$H and $d$ + $^3$He systems with resonating-group method // Phys. Rev. - 1973 - Vol. C8. - P. 938 - 950.
2. *Kanada H., Kaneko T., Tang Y.C.* Multi-configuration resonating-group study of the five- nucleon system // Nucl. Phys. - 1989. - Vol. A504. - P. 529 - 548.
3. *Козырь Ю.Е.* Структура сталкивающихся ядер $^4$He // Изв. РАН. Сер. физ. - 2006. - Т. 70. - С. 294 - 301.
4. *Kozyr Yu.E.* A spatial RGM basis for scattering $^4$He($\alpha$, $\alpha$)$^4$He // Ukr. J. Phys. - 2006. - Vol. 51. - P. 750 - 757.
5. *Chulik G.S., Kim Y.E., Rice R.A., Rabinowitz M.* Extended parameterization of nuclear-reaction cross sections for few-nucleon nuclei // Nucl. Phys. - 1993. - Vol. A551. - P. 255 - 268.
6. *Jenny B., Gruebler W., Konig V.* Analyzing power and cross-section measurement for $^3$He($d$, $d$)$^3$He scattering // Nucl. Phys. - 1979. - Vol. A324. - P. 99 - 108.
7. *Roy R., Seiler F., Conzett H.E., Rad F.N.* Cross section and vector analyzing power $iT_{11}$ of the processes $^3$He($\vec{d}$, $d$)$^3$He $^3$He($\vec{d}$, $p$)$^4$He between 15 and 40 MeV // Phys. Rev. - 1981. - Vol. C24. - P. 2421 - 2434.


## РОЗРАХУНОК РОЗСІЯННЯ $^3$He($d$, $d$)$^3$He ПРИ $E$ = 1 - 9 МеВ ЗА МЕТОДОМ РЕЗОНУЮЧИХ ГРУП

**Ю. Ю. Козир**

Розрахунки пружного розсіяння $^3$He($d$, $d$)$^3$He за методом резонуючих груп виконано в припущенні залежності параметрів кластерних потенціалів фрагментів каналу від відстані між ними. Проста дворівнева

апроксимація цієї залежності дає змогу істотно поліпшити розрахункові значення диференціальних перерізів. В області інтенсивної взаємодії кластерів значення їхніх радіусів зменшуються до приблизно 55 % від значень на дальній асимптотиці, дистанція переходу монотонно спадає від 12,6 до 11,2 фм при збільшенні енергії в межах дослідженого інтервалу.

*Ключові слова*: пружне розсіяння, метод резонуючих груп, кластерний потенціал, дистанційно-залежний базис.

## РАСЧЕТ РАССЕЯНИЯ $^3$He($d$, $d$)$^3$He ПРИ $E$ = 1 - 9 МэВ ПО МЕТОДУ РЕЗОНИРУЮЩИХ ГРУПП

**Ю. Е. Козырь**

Расчеты упругого рассеяния $^3$He($d$, $d$)$^3$He по методу резонирующих групп выполнены в предположении зависимости параметров кластерных потенциалов фрагментов канала от расстояния между ними. Простая двухуровневая аппроксимация этой зависимости позволяет существенно улучшить расчетные дифференциальные сечения. В области интенсивного взаимодействия кластеров значения их радиусов уменьшаются до примерно 55 % от значений на дальней асимптотике, дистанция перехода монотонно убывает от 12,6 до 11,2 фм при возрастании энергии в пределах рассмотренного интервала.

*Ключевые слова*: упругое рассеяние, метод резонирующих групп, кластерный потенциал, дистанционно-зависимый базис.

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