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Approximation of the deuteron wave functions and parameters for potential Argonne v18

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The coefficients of analytical forms for the deuteron wave function in coordinate space for Argonne v18 potential have been numerically calculated. The obtained wave functions do not contain any superfluous knots. The designed parameters of the deuteron are in good agreement with the experimental and theoretical data.

Keywords: wave functions, analytical form, deuteron, knot.

Чисельно розраховані коефіцієнти аналітичних форм для хвильової функції дейтрона в координатному представленні для потенціалу Argonne v18. Отримані хвильові функції не містять надлишкових вузлів. Розраховані параметри дейтрона добре узгоджуються з експериментальними і теоретичними даними.

Ключові слова: хвильова функція, аналітична форма, дейтрон, вузол.

Численно рассчитаны коэффициенты аналитических форм для волновой функции дейтрона в координатном представлении для потенциала Argonne v18. Полученные волновые функции не содержат лишних узлов. Рассчитанные параметры дейтрона хорошо согласовываются с экспериментальными и теоретическими данными.

Ключевые слова: волновая функция, аналитическая форма, дейтрон, узел.

Introduction

Deuteron is the most elementary nucleus, which consists of the two strongly interacting particles (a proton and a neutron). The simplicity of the deuteron's structure makes it a convenient laboratory for studying nucleon-nucleon forces. Currently, deuteron has been well investigated both experimentally and theoretically.

The calculations of static characteristics of the deuteron (binding energy, magnetic moment, electric quadrupole moment, etc.) are in good agreement with the experimental data [1]. Despite that, there still are some theoretical inconsistencies. For example, in some theoretical papers [2] one (Bonn potential) or both (Moscow potential) [3] components of the wave function have knots near the origin of the coordinates. Such behavior of a wave function contradicts the common mathematical theorem about the number of knots for the eigenfunctions in boundary value problems [4]. The ground state of the system corresponds to a function without knots in the middle of the interval of boundary value problem. The presence of knots in the wave functions of the basic and the unique state of the deuteron may indicate the existence of certain inconsistencies in the implementation of the numerical algorithms used in these tasks. In Ref. [5] it is shown that the asymptotic behavior of the solution components of the system of equations is not defined by a single orbital angular momentum L , as with individual solutions of the Schrödinger equation, but by the

total orbital moment J and the asymptotic behavior of the tensor potential at short distances, which ensures the binding of Schrödinger equations in the system. The way the choice of numerical algorithms influences the solution is shown in Ref. [5-7]. In Ref. [5] it is shown that input of incorrect asymptotic of wave function could generate superfluous knots of the solution. The calculation of the deuteron wave function in the momentum space are given in Ref. [6]. In Ref. [7] studied the effect of different methods to smooth the experimental curve of yield on the energy dependence of the cross section for the reaction (γ, γ') .

Such potentials of the nucleon-nucleon interaction as Bonn [2], Moscow [3], Nijmegen group potentials (NijmI, NijmII, Nijm93 [8]), Argonne v18 [9] or Paris [10] potential have quite a complicated structure and cumbersome representation. The original potential Reid68 was parameterized on the basis of the phase analysis by Nijmegen group and was called Reid93. The parametrization was done for 50 parameters of the potential, where $\chi^2/N_{data}=1.03$ [8].

Besides, the deuteron wave function can be presented as a table: through respective arrays of values of radial wave functions. It is sometimes quite difficult to operate with such arrays of numbers during numerical calculations. And the program code for numerical calculations is overloaded. Therefore, it is feasible to obtain simpler analytical forms of deuteron wave functions representation.

Analytical form of the deuteron wave functions

The known numerical values of a radial deuteron wave functions in coordinate space can be approximated with the help of convenient expansions [11] in the analytical form:

$$\begin{cases} u_a(r) = \sum_{i=1}^{N_a} A_i \exp(-a_i r^2), \\ w_a(r) = r^2 \sum_{i=1}^{N_a} B_i \exp(-b_i r^2), \end{cases} \quad (1)$$

asymmetric double sigmoidal [7] or approximations of Yukawa type [2, 10, 12]:

$$\begin{cases} u_b(r) = \sum_{j=1}^{N_b} C_j \exp(-m_j r), \\ w_b(r) = \sum_{j=1}^{N_b} D_j \exp(-m_j r) \left[1 + \frac{3}{m_j r} + \frac{3}{(m_j r)^2} \right], \end{cases} \quad (2)$$

where $m_j = \beta + (j - 1)m_0$, $\beta = \sqrt{ME_d}$, $m_0 = 0.9 \text{ fm}^{-1}$. M

- nucleon mass, E_d - binding energy of deuteron.

Despite cumbersome and time-consuming calculations and minimizations of χ^2 (to the value smaller than 10^{-4}), it was necessary to approximate numerical values of deuteron wave functions for potential Argonne v18 [9], the arrays of numbers of which made up 1500x2 values in an interval $r=0-15 \text{ fm}$. The values of coefficients A_i, a_i, B_i, b_i for formulas (1) are shown in Tables 1 and 2 ($N_a=17$).

The asymptotics of deuteron wave functions (1) for $r \rightarrow \infty$ as have been $A_L \exp(-ar^2)$, where A_L are the asymptotic S- or D- state normalizations.

The accuracy of parametrization (1) is characterized by:

$$\chi^2 = \frac{\sum_{i=1}^n (y_i - f(x_i; a_1, a_2, \dots, a_p))^2}{n - p}, \quad (3)$$

where n - the number of points of the array y_i of the numerical values of deuteron wave functions in the coordinate space; f - approximating function of u (or w) according to the formulas (1); a_1, a_2, \dots, a_p - parameters; p - the number of parameters (coefficients in the sums of formulas (1)). Hence, χ^2 is determined not only by the shape of the approximating function f , but also by the number of the selected parameters.

The designed the deuteron wave functions $u(r)$ and $w(r)$ on an analytical form (1) in configuration space do not contain superfluous knots (Fig. 1.). The obtained deuteron wave functions well correlate with the data in Ref. [9].

Parameters of the deuteron

Based on the known deuteron wave functions (1) one

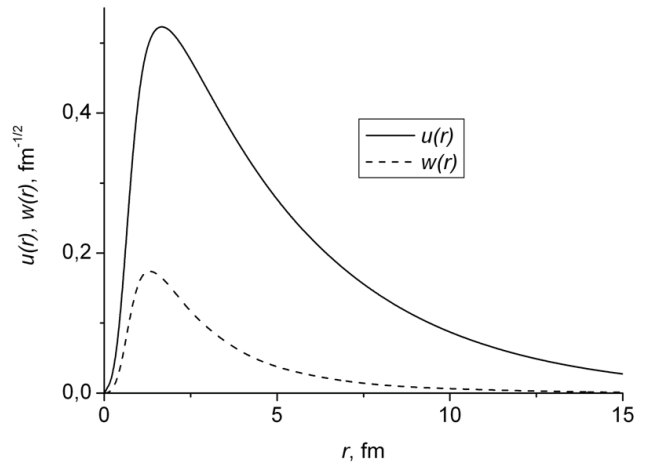


Fig. 1. Deuteron wave functions $u(r)$ and $w(r)$.

can calculate the deuteron parameters [2, 6]:

- the root-mean-square or matter radius r_d :

$$r_d = \frac{1}{2} \left\{ \int_0^\infty r^2 [u^2(r) + w^2(r)] dr \right\}^{1/2}; \quad \text{Table 1}$$

Coefficients A_i, a_i of analytical form (1)

i	A_i	a_i
1	0.3783013556	4.5159833496
2	0.0527547473	0.0047927056
3	0.0588462113	0.0402241853
4	0.0394988588	0.1108640062
5	-0.0983386258	0.9027821990
6	0.0602079746	0.0129223752
7	0.0583622013	0.0395882632
8	0.0395335071	0.1114996980
9	-0.0983386259	0.9027821990
10	0.0562850175	0.0281322415
11	0.0579689851	0.0389768962
12	0.0395253229	0.1113533265
13	-0.0983386258	0.9027821990
14	0.0579715002	0.0132941967
15	0.0586185593	0.0129874337
16	0.0395035425	0.1109524943
17	-0.6972629687	2.5872139842

Table 2

Coefficients B_i, b_i of analytical form (1)

i	B_i	b_i
1	0.0004509483	0.0202568988
2	-0.7761852998	2.8877752389
3	-0.1541927357	1.8739405194
4	0.0315895933	0.8758471679
5	0.6146075529	2.0531580006
6	0.0190358032	0.8868757916
7	-0.1541927357	1.8739405194
8	-0.1541927357	1.8739405194
9	0.1226950521	0.6009934906
10	-0.0216492291	0.9298786972
11	0.0218535866	0.2200515118
12	-0.0028421548	0.9083871303
13	0.6146075529	2.0531580006
14	-0.1541927357	1.8739405194
15	0.0402612414	0.8681178930
16	0.0218416604	0.2230021638
17	0.0066681258	0.0733951961

Table 3

Deuteron parameters					
Potential	P_D (%)	r_d (fm)	Q_d (fm ²)	μ_d	η
Argonne v18 (1)	5.75949	1.96737	0.267685	0.846988	0.0260866
Argonne v18 [9]	5.76	1.967	0.270	0.847	0.0250

- the electric quadrupole moment Q_d :

$$Q_d = \frac{1}{20} \int_0^\infty r^2 w(r) [\sqrt{8}u(r) - w(r)] dr;$$

- the magnetic moment:

$$\mu_d = \mu_s - \frac{3}{2}(\mu_s - \frac{1}{2})P_D;$$

- the D - state probability:

$$P_D = \int_0^\infty w^2(r) dr;$$

- the “ D/S - state ratio”:

$$\eta = A_D / A_S.$$

The designed parameters of a deuteron it is reduced in Table 3. They well agree with the experimental and theoretical datas [1, 9].

Conclusions

The coefficients of the approximating dependencies have been calculated in a new analytic form (1) for the numerical values of deuteron wave functions in the coordinate space for realistic phenomenological Argonne v18 potential. The obtained wave functions do not contain any superfluous knots.

Using the deuteron waves functions in coordinate presentation, were calculated the parameters of the deuteron.

On the designed deuteron wave functions (1) expedient there are calculations of polarization characteristics [13]: a component of a tensor of sensitivity polarization of deuterons T_{20} , polarization transmission K_ρ , tensor analyzing power A_{yy} and tensor-tensor transmission of polarization K_{yy} .

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