Phase Shift Analysis in Nuclear Astrophysics

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corresponding member of the Russian Academy of Natural Sciences,
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Translated into English
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By

Sergey Dubovichenko

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INTRODUCTION

In many problems of nuclear physics at low energies and nuclear astrophysics, knowledge of the scattering elastic phase shifts, which can be determined from the differential cross sections of the scattering of various nuclear particles, is necessary [1]. Such phase shifts are used, in particular, for the construction of intercluster interaction potentials, for example, in the potential cluster model (PCM) of light nuclei [2]. The procedure of phase shift analysis consists of the decomposition of the total scattering amplitude in a row by partial waves or amplitudes and the analysis of the parameters that appear at the same time, which are termed scattering phase shifts. Such phase shifts allow us to obtain data about the nature of strong interactions, the structure of resonance states, and the general structure of an atomic nucleus [1].

Two-body processes with the formation of resonances in nuclear physics at low energies can also be investigated by means of phase shift analysis. To solve this problem, it is necessary to consider in detail the energetic behavior of the resonance partial scattering amplitude [1,3]. As a result, phase shift analysis plays a large role in the investigation of nuclear resonances in scattering processes and the determination of their quantum numbers. Research into scattering processes by means of phase shift analysis can help clarify many important aspects of the interactions of nuclear particles, because such analysis is based only on the most general laws of conservation and displays close connections to the experimental data [1,3].

The problem of determining or extracting the nuclear phase shifts from cross sections of elastic scattering in the mathematical plane is reduced to a multiple parameter variation problem. In other words, using the experimental scattering cross sections of nuclear particles and the mathematical expressions obtained in the quantum mechanics, which describe these cross sections according to some δ_L parameters, the nuclear scattering phase shifts can be known. Consequently, a multiple parameter variation problem arises in finding these parameters for the set interval of values while taking into account the generalized Levinson theorem [4]. In different nuclear systems, depending on the energy of the colliding particles, the number of elastic scattering phase shifts can change from 1–3 to 10–20 [5].

This book is directly based on the results of about twenty scientific articles published over the last five to seven years in Russia, Europe, the USA, and the CIS countries. It consists of three chapters. The first chapter is devoted to a description of the general mathematical methods for calculating some nuclear characteristics. The general criteria and methods of creation of the intercluster potentials in a continuous and discrete spectrum, which are used further for the consideration of some nuclei in the three-body model (described in the third chapter), are defined.

The second chapter presents methods and results of the phase shift analysis of elastic scattering of the following nuclear particles at low and astrophysical energies: ^{4}He^{4}He, n^{3}He, p^{6}Li, p^{12}C, n^{12}C, p^{13}C, p^{14}C, n^{16}O, p^{16}O, and ^{4}He^{12}C. These results have been used to construct the potential cluster model (PCM) of pair intercluster interaction potentials in a continuous spectrum. Here, the various experimental measurements, methods of calculating differential cross sections, computer programs, and results of the phase shift analysis of elastic scattering of the stated particles, are all considered. For the first system, ^{4}He^{4}He, only the main expressions for the phase shift analysis, the computer program, and versions of the control account are given at 25–29 MeV. For other systems, the approximate energy range 1–2.5 MeV is considered. In an elastic ^{4}He^{12}C scattering, a phase shift analysis was undertaken in the range 1.5–6.5 MeV. The areas of phase shift analysis given here are defined by the existence of experimental data on differential cross sections for angular distributions or excitation functions.

The results obtained for the three-body single-channel models of some light nuclear nuclei, namely, ^{7}Li, ^{9}Be, and ^{11}B, are given in Chapter Three. They allow one to check the adequacy of the construction of pair intercluster potentials on the basis of the elastic scattering phase shifts and characteristics of the bound states of light atomic nuclei. These results allow us to determine the applicability of the obtained potentials to three-body problems. The checked potentials are thus used for the calculation of some primary characteristics of thermonuclear processes in the preliminary nucleosynthesis of the universe and some solar cycles [2].

We note that the second and, particularly, the third chapters of this book almost completely coincide with the results given in the corresponding chapters of other books by the author, including *Preliminary Nucleosynthesis of the Universe* (2014, Lambert Academy Publ. GmbH & Co. KG: Saarbrucken, Germany, 668 pages) [2]. This material is found in this book (*Phase Shift Analysis in Nuclear Astrophysics*) primarily in order to reduce the size of book [2] and allow the future possibility of its enlargement and the addition of new material on thermonuclear reactions in the next edition. At the same time, the present book can also be extended by the inclusion of new results on phase shift analysis and the three-body model.

I

METHODS OF SOLVING THE SCHRÖDINGER EQUATION

Introduction

The set of problems of theoretical nuclear physics, especially in the field of light atomic nuclei and low energies, requires the ability to solve the Schrödinger equation or the coupled system of equations of this type. A wave function, which describes a quantum state of some system of nuclear particles and, in principle, contains all the information about such state is a result of the solution.

There are many varied mathematical methods for the solution of differential equations or their second-order systems, of which one is the Schrödinger equation. Quite abstract methods of solving such equations, which are rather difficult to apply in the solution of a concrete equation, like the Schrödinger equation type, are usually given in the mathematical literature. The problem usually arises in the choice of the optimum mathematical and numerical method applicable to the consideration of certain problems based on the solutions of the Schrödinger equation.

This chapter is devoted to the solution of these problems and describes some mathematical methods that are directly applicable to locating the wave functions from the Schrödinger equation of scattering problems of nuclear particles and their bound states. The numerical methods applicable to the problems of a continuous and discrete spectrum of states, which allow us to obtain end results with almost complete accuracy, are considered. On the basis of these methods, the possibility of writing computer programs in the BASIC computer language using the Borland Turbo Basic Compiler and the Fortran-90 language is considered, which can assist in solving all problems of nuclear physics considered here.

Many problems of nuclear physics can be considered using only the central part of the nuclear forces [6,7]. In this case, we are dealing with only one Schrödinger equation or system of unrelated equations (taking into account the spin-orbital interaction) and the mathematical problem is solved rather simply. The account of tensor components of nuclear forces leads us to the system of bound Schrödinger equations [8,9], the solution of which is slightly more difficult, but quite feasible by many methods, including those described in [10].

We provide the mathematical and numerical methods used for the solution of Schrödinger equations for the central potentials at positive and negative eigenvalues in this chapter. We also consider their application to the analysis of the scattering quantum problem and bound-state energies of nuclear particles. In other words, the methods of investigating nuclear scattering phase shifts and the calculation of bound-state energies of light nuclei within the modified potential two-cluster model (MPCM) [2] are given.

1.1 The general methods of solving the Schrödinger equation

Here the general formulation of the problem for the solution of the Schrödinger equation with positive continuous and negative discrete eigenvalues is considered. Entry and boundary conditions for solving this problem are determined in relation to a description of the physical processes and states in nuclear physics and nuclear astrophysics.

1.1.1 The central real potentials

The Schrödinger equation for the central forces of interaction between two nuclear particles without spin-orbital and tensor potentials has the following form [1,6,7,11]

$$u''(r)+\left[k^2-V_{\mathrm{c}}(r)-V_{\mathrm{coul}}(r)-\frac{L(L+1)}{r^2}\right]u(r)=0\ , \qquad (1.1.1)$$

where r is the scalar relative distance between particles in fm (1 fermi = 10^{-15} m); u is the solution of the equation, i.e. wave function (WF); u'' is its second derivative; $V_{\mathrm{coul}}(r)$ = $2\mu/\hbar^2\ Z_1Z_2/r$ is the Coulomb potential reduced to the dimension of fm^{-2}; $\hbar$ is the Plank constant = 1.055 10^{-34} J s (Joule-second); Z_1 and Z_2 are the charges of particles in terms of their elementary charge (1 e.c. – elementary charge = 1.60 10^{-19} C – Coulomb); the constant $\hbar^2/m_0$ = 41.4686 MeV fm^2 (1 MeV – megaelectronvolt = 1.60 10^{-13} Joule); m_0 is the atomic mass unit (1 amu – atomic mass unit = 1.66 10^{-27} kg.); V_{cf} = $L(L+1)/r^2$ is the centrifugal potential, which depends on the value of the orbital moment of the relative movement of the L particles; $k^2 = 2\mu E/\hbar^2$ is the wave number of the relative motion in fm^2; E is the energy of particles in MeV; $\mu = \frac{m_1 m_2}{m_1 + m_2}$ is the reduced mass of two particles in amu; $V_c(r)$ is the central part of the nuclear potential, equal to $2\mu/\hbar^2\, V_n(r)$; $V_n(r)$ is the radial dependence of the potential, which is often accepted in the form $V_0 \exp(-\alpha r^2)$ or $V_0 \exp(-\alpha r)$; V_0 is the potential depth in MeV; $\eta = \frac{\mu Z_1 Z_2}{\hbar^2 k} = 0.0344476\, Z_1 Z_2/k$ is the Coulomb parameter; the Coulomb potential can be presented in the form

$$V_{coul}(r) = 2\eta k/r = A_c/r.$$

If the spin-orbital interaction is taken into account, then the central potential has the form [1,6,7]

$$V_c(r) = 2\mu/\hbar^2\, [V_n(r) + V_{sl}(r)],$$

$$V_{sl}(r) = (\boldsymbol{SL})\, V_{0sl}\, F(r),$$

where $F(r)$ is the functional dependence of the potential on the relative distance between particles, which can also be accepted in the form of the Gaussian function $\exp(-\alpha r^2)$ or exponent $\exp(-\alpha r)$.

The ***(SL)*** value is called the spin-orbital operator and its values can be found from the well-known expression [6,7]

$$(\boldsymbol{SL})\, u(r) = 1/2\, [J(J + 1) - L(L + 1) - S(S + 1)]\, u(r),$$

where J is the total moment of the system; L is the orbital moment; and S is the spin of the system of particles. Taking into account the spin-orbital interaction, the Schrödinger equation is split into a system of uncoupled equations, each of which allows the finding of the WF for the concrete total moment.

Sometimes, the Coulomb R_c radius is entered into the potential of interaction; then the Coulomb part of the potential takes a slightly different form

$$V_{coul}(r) = \frac{2\mu}{\hbar^2} \begin{cases} \dfrac{Z_1 Z_2}{r} & r > R_c \\ Z_1 Z_2 \left(3 - \dfrac{r^2}{R_c^2}\right) \Big/ 2R_c & r < R_c \end{cases} . \qquad (1.1.2)$$

Equation (1.1.1) forms the Cauchy problem with initial conditions that lie outside physical reasoning The first initial condition demands equality to zero of the WF at $u(0) = 0$. As the WF reflects the probability of some processes or states of the quantum particles, this condition means that two particles cannot completely merge and occupy the same volume. The second statement of the Cauchy problem involves the determination of the value of the first derivative of this function. However, for reasons of physical limitation, it is impossible to determine the value of this derivative; therefore it is taken to equal some constant, which determines the amplitude of the wave function. In numerical calculation, $u'(0) = 0.1–1$ is usually accepted. The real amplitude of the function, which is used for numerous physical calculations, is defined from the asymptotic conditions imposed on this function at long distances of $r \to R$, when the nuclear potential is almost equal to zero.

The asymptotics of the wave function at long distances, when $V_c(r \to R) \to 0$, offer the solution of equation (1.1.1) without nuclear potential, and can be presented as follows

$$u_L(r \to R) \to F_L(kr) + \mathrm{tg}(\delta_L) G_L(kr), \qquad (1.1.3)$$

or

$$u_L(r \to R) \to \cos(\delta_L) F_L(kr) + \sin(\delta_L) G_L(kr),$$

where F_L and G_L are the scattering Coulomb functions [12,13]. These are partial solutions of equation (1.1.1) without the nuclear part of the potential, i.e. when $V_c = 0$.

Interlacing the numerical solution $u(r)$ of equation (1.1.1) at long distances (R at about 10–20 fm) with these asymptotics, it is possible to find the real amplitude of the function and the scattering phase shift δ_L for each L at the given energy of the interacting particles. The scattering phase shifts in the concrete system of the nuclear particles can be determined from phase shift analysis of the experimental data in terms of their elastic scattering (Chapter 2). Furthermore, variation of the parameters of nuclear potential in the previously determined form in equation (1.1.1) is carried out and those parameters that allow us to describe the results of the phase shift analysis are determined. Thus, the problem of the description of scattering processes of nuclear particles consists of the search for the parameters of the nuclear potential that can describe the results of phase shift analysis and the experimental data for the scattering cross sections.

We consider the procedure of interlacing the wave functions with asymptotics in more detail. At $r = R$, it is possible to write down two equalities for the WF along with their derivatives [14]

$$Nu_L(R) = F_L(kR) + \mathrm{tg}(\delta_L)G_L(kR),$$

$$Nu'_L(R) = F'_L(kR) + \mathrm{tg}(\delta_L)G'_L(kR),$$

where N is a normalizing multiplier. It is possible to consider similar expressions, not for the function and derivative, but only for the function in two different points

$$\begin{aligned} Nu_L(R_1) &= F_L(kR_1) + \mathrm{tg}(\delta_L)G_L(kR_1), \\ Nu_L(R_2) &= F_L(kR_2) + \mathrm{tg}(\delta_L)G_L(kR_2). \end{aligned} \tag{1.1.4}$$

We enter the notations

$F_1 = F_L(kR_1)$, $F_2 = F_L(kR_2)$,
$G_1 = G_L(kR_1)$, $G_2 = G_L(kR_2)$,
$u_1 = u_L(R_1)$, $u_2 = u_L(R_2)$,

and find the value N, for example, from the first equation

$$N = [F_1 + \mathrm{tg}(\delta_L)G_1]/u_1.$$

Substituting this expression into the second equation, we obtain

$$\mathrm{tg}(\delta_L) = (u_1F_2 - u_2F_1)/(u_2G_1 - u_1G_2) = A_L. \tag{1.1.5}$$

then

$$\delta_L = \mathrm{arctg}(A_L).$$

Normalization of the function, for the purposes of investigating phase shifts, is of no importance. However, if we need the normalized WF, i.e. the total scattering function is also required, then it is better to consider the second equation from (1.1.3), written down in the form of (1.1.4) and having performed similar operations to those given above. If the scattering phase shift results in the same expression, then we write the normalization in the form

$$N = [\cos(\delta_L)F_1+\sin(\delta_L)G_1]/u_1,$$

or

$$N = [\cos(\delta_L)F_2+\sin(\delta_L)G_2]/u_2.$$

In so doing, we can completely define the behavior of the wave function, its amplitude and phase shift, in all ranges of solutions for equation (1.1.1), from zero to some large value of R, which define the WF asymptotics.

1.1.2 The central complex potentials

If the inelastic channel of scattering or reactions is open in nuclear processes, then it is necessary to use the complex potential of interaction, taking into account the decrease in the stream of particles from the elastic channel [6]. Now, the potential takes a form

$$V_c = V_r(r) + iV_m(r), \tag{1.1.6}$$

where $V_r(r)$ is the real part of the potential and $V_m(r)$ is its imaginary part. The wave function also becomes complex and can be written in the form

$$u(r) = x(r) + iy(r). \tag{1.1.7}$$

Then, the Schrödinger equation (1.1.1) can be rewritten in the form of a coupled equation system as

$$\begin{aligned} &x''(r) + [k^2 - V_r(r) - V_{coul}(r) - L(L+1)/r^2]x(r) = -V_m y(r), \\ &y''(r) + [k^2 - V_r(r) - V_{coul}(r) - L(L+1)/r^2]y(r) = V_m x(r), \end{aligned} \tag{1.1.8}$$

with initial conditions in the form

$$x(r=0) = 0, \qquad x'(r=0) = \text{const},$$
$$y(r=0) = 0, \qquad y'(r=0) = \text{const}.$$

In the numerical calculations, the value of the constant (const.) for the derivatives of the wave functions is set at the level 0.1–1. The asymptotics of wave functions are represented as follows [6]

$$u(r) = H^{+}(r) + SH^{-}(r) = [F(r) + iG(r)] + S[F(r) - iG(r)], \qquad (1.1.9)$$

where H^{+} is the Hankel function; F and G are the Coulomb functions; and S is the scattering matrix, which has the form

$$S = \mathrm{e}^{2i\delta} = S_1 + iS_2 = \cos(2\delta) + i\sin(2\delta).$$

In taking into account the inelastic processes, the phase shifts of the elastic scattering become complex and are represented as follows

$$\delta = \sigma + i\Delta,$$

where σ and Δ are the real and imaginary parts of the phase shift. Then, the scattering matrix can be rewritten in the form

$$S = \mathrm{e}^{2i\delta} = \mathrm{e}^{-2\Delta}\mathrm{e}^{2i\sigma} = \eta\mathrm{e}^{2i\sigma} = \eta(S_1+iS_2) = \eta[\cos(2\sigma)+i\sin(2\sigma)], \qquad (1.1.10)$$

where $\eta = \mathrm{e}^{-2\Delta}$ is the inelasticity parameter. For the determination of the scattering phase shifts and the parameter of inelasticity, we can write out the boundary conditions for the functions in two points in the form of a logarithmic derivative

$$\frac{u_1}{u_2} = \frac{H_1^{+} + SH_1^{-}}{H_2^{+} + SH_2^{-}}, \qquad (1.1.11)$$

from which it is easy to find

$$S = \frac{u_2H_1^{+} - u_1H_2^{+}}{u_1H_2^{-} - u_2H_1^{-}}.$$

Substituting the expressions for the Hankel functions given above (1.1.9), and splitting the real and imaginary parts, we obtain

$$S = \frac{C + i\mathrm{D}}{A + iB} = K + iM, \qquad (1.1.12)$$

where

$$K = \frac{AC + BD}{A^2 + B^2}, \qquad M = \frac{AD - BC}{A^2 + B^2}, \tag{1.1.13}$$

and

$A = b - a$, $B = - c - d$,

$C = a + b$, $D = c - d$,

$a = x_2F_1 - x_1F_2$, $b = y_1G_2 - y_2G_1$,

$c = y_2F_1 - y_1F_2$, $d = x_1G_2 - x_2G_1$.

Thus, all elements of the S matrix are expressed through the Coulomb functions and the solutions of the initial Schrödinger equation (1.1.8) with the given nuclear potential.

Comparing the real and imaginary parts of expressions (1.1.10) and (1.1.12), we obtain

$$\begin{aligned} S_1 &= \cos(2\sigma) = K/\eta, \\ S_2 &= \sin(2\sigma) = M/\eta, \end{aligned} \tag{1.1.14}$$

and

$$\begin{aligned} S^2 &= \eta^2(S_1 + S_2)^2 = \eta^2, \\ S^2 &= K^2 + M^2, \end{aligned} \tag{1.1.15}$$

from which we find

$$\eta^2 = K^2 + M^2,$$

giving the inelasticity parameter. Knowing these values, we can obtain

$$A = \mathrm{tg}(\sigma) = \frac{S_2}{1 + S_1}, \tag{1.1.16}$$

then

$$\sigma = \mathrm{arctg}(A). \tag{1.1.17}$$

It is easy enough to check that when $V_m = 0$ and equation (1.1.8) become independent, then $\eta = 1$ and the results for the phase shifts (1.1.5) and (1.1.16) coincide.

For the determination of the normalization of the WF, we use expressions (1.1.9) and (1.1.7)

$$N(x+iy) = H^+(r) + SH^-(r) = [F(r) + iG(r)] + (S_1 + iS_2)\,[F(r) - iG(r)],$$

from which we find

$$N = \frac{Ax + By}{x^2 + y^2} + i\frac{Bx - Ay}{x^2 + y^2},$$

where

$$A = (1 + S_1)F(r) + S_2G(r), \;\; B = (1 - S_1)G(r) + S_2F(r).$$

Generally, normalization of a complex WF can be written down in the form of a complex value as follows

$$Nu(r) = (N_1 + iN_2)(x + iy) = N_1x - N_2y + i[N_1y + N_2x] = v + iw.$$

Here, v and w are already normalized total wave functions of the scattering. Equating the real and imaginary parts, we have

$$N_1 = \frac{Ax + By}{x^2 + y^2}, \qquad N_2 = \frac{Bx - Ay}{x^2 + y^2},$$

which are general expressions for determining the normalization of WF scattering in the case of complex potentials [15].

1.2 The numerical methods of solving the Schrödinger equation

For the numerical solution of the Schrödinger equation, it is possible to use the finite-difference method (FDM) [7], presenting the function and its derivative in the form of the central differences and using the Runge-Kutta method (RKM) [16] or the Numerov method (NM) [17], which allows us to obtain a higher accuracy solution for the initial equation.

1.2.1 The central real potentials

We can write the Schrödinger equation for the central nuclear forces (1.1.1) in the form of [6]

$$u''(r) + [k^2 - V(r)]u(r) = 0. \qquad (1.2.1)$$

To solve it, we can use the finite-difference method, for which the second derivative can be presented as follows [7]

$$u''(r) = [u(r + h) - 2u(r) + u(r - h)]/h^2 = [u(r_{i+1}) - 2u(r_i) + u(r_{i-1})]/h^2, \qquad (1.2.2)$$

where h is a step of the finite-difference grid, for the determination of which the whole interval of h values, from zero to some value of R, are divided into N parts

$$h = R/N.$$

Here, R is the top limit at which the interlacing of the numerical solution of equation (1.2.1) with asymptotics is carried out. Then

$$r_i = hi, \quad u_i = u(r_i),$$

where i changes from 0 to N ($r_0 = 0$ and $r_N = R$). Now, expression (1.2.2) can be rewritten in the form

$$u'' = [u_{i+1} - 2u_i + u_{i-1}]/h^2,$$

and the whole equation is rewritten as

$$[u_{i+1} - 2u_i + u_{i-1}]/h^2 + [k^2 - V(r_i)]u_i = 0,$$

which we find with an order of accuracy $O(h^2)$ equal to h^2, i.e. the method is in proportion to a square of a step [7]

$$u_{i+1} = \left[2 + h^2V(r_i) - h^2k^2\right]u_i - u_{i-1} + O(h^2)\ . \qquad (1.2.3)$$

Here, $i = 1, 2 \ldots. N - 1$. The function at $r = 0$ has to be equal to zero and in the first step it can be accepted as equal to some constant, which defines only a function of normalization without affecting its behavior at various values of r. From here, the WF on the following step of u_2 can be found and this process repeats until i does not become equal to $N - 1$. Such a procedure allows us to find the whole array of WF values at all points from zero to R. Furthermore, we carry out its interlacing in two points, for example, at $r_N = R$ and $r_{N-5} = R - 5h$, as described in paragraph 1.1.1. The second point is defined experimentally in each case and depends on the energy of the particles, but at small energies it usually recedes by 3–5 steps [18].

Below, we give an example of the program written in Fortran-90 to realize the method described. The following designations are set.

U – the array of the WF with a dimension of N,
H – the look-up of the WF,
N – the number of steps,
A0 – the V_0 depth of the central part of the potential in fm^{-2},
R0 – the α width of the central part of the potential in fm^{-2},
L – the orbital moment,
RC – the Coulomb radius R_c in fm,
AK – the Coulomb coefficient A_c in the description of equation (1.1.1),
SK – the wave number of k^2 in fm^{-2}.

```
SUBROUTINE FUN(U,H,N,A0,R0,L,RC,AK,SK)
IMPLICIT REAL(8) (A-Z)
INTEGER N,L,K
DIMENSION U(0:N)
! INITIAL VALUES
U(0)=0.0D0; U(1)=0.1D0; RR=1.0D0/RC
LL=L*(L+1); BB=AK/(2.0D0*RCU); HK=H*H; SHS=SK*HK-2.0D0
! CALCULATION THE VALUES OF THE Vc(R) POTENTIAL
DO K=1,N-1
X=K*H; XX=X*X
V=A0*DEXP(-R0*XX)+LL/XX
IF (X>RC) THEN
V=V+AK/X
ELSE
V=V+(3.0D0-(X*RR)**2)*BB
ENDIF
! CALCULATION THE VALUES OF THE WAVE FUNCTION
Q=V*HK-SHS
```

```
U(K+1)=Q*U(K)-U(K-1)
ENDDO
END
```

The WF $u(r)$ is the calculation result at the given L for the Schrödinger equation (1.2.1) in the range of values from 0 to R.

1.2.2 The central complex potentials

If there is a system of equations (1.1.8) for the complex potential [18]

$$x''(r) + [\, k^2 - V_r(r) - V_{coul}(r) - L(L+1)/r^2\,]x(r) = - V_m y(r),$$
$$y''(r) + [\, k^2 - V_r(r) - V_{coul}(r) - L(L+1)/r^2\,]y(r) = V_m x(r), \qquad (1.2.4)$$

then, using the same representation of a derivative in the finite-difference form

$$u'' = [u_{i+1} - 2u_i + u_{i-1}]/h^2,$$

for functions x and y we obtain

$$x_{i+1} = [\, 2 - A_i h^2\,]x_i - x_{i-1} - h^2 V_m(r_i)y_i,$$
$$y_{i+1} = [2 - A_i h^2\,]y_i - y_{i-1} + h^2 V_m(r_i)x_i, \qquad (1.2.5)$$

where

$$A_i = k^2 - V_r(r_i) - V_{coul}(r_i) - L(L+1)/r_i^2.$$

In addition, setting the values of functions in the two first points

$x_0 = 0$, $x_1 =$ const., $y_0 = 0$, $y_1 =$ const.,

it is possible to find the values of functions in all other points [18], as well as for expression (1.2.3). The interlacing procedure of the numerical function with its own asymptotics in the case of complex potentials is described in paragraph 1.1.2.

1.2.3 The Runge-Kutta method for central real potentials

Here, we consider the other method of solving such equations. This is the fourth-order Runge-Kutta method per step h [16,19,20,21,22]. The standard method of the solution of one differential equation of the first order is

$$y' = f(x,y), \tag{1.2.6}$$

with the initial condition

$$y(x_0) = y_0,$$

which consists of the presentation of the solution on an interval from 0 to some value of R in the form

$$y_{n+1} = y_n + \Delta y_n, \tag{1.2.7}$$

where n can change from 0 to N ($R = x_N = hN$); h is a step in the solution; and Δy_n is obtained from the expression

$$\Delta y_n = 1/6(k_1 + 2k_2 + 2k_3 + k_4), \tag{1.2.8}$$

where

$$k_1 = hf(x_n,y_n), \qquad k_2 = hf(x_n+h/2,\, y_n+k_1/2),$$
$$k_3 = hf(x_n+h/2,\, y_n+k_2/2), \qquad k_4 = hf(x_n+h,\, y_n+k_3).$$

In the case of a system of two differential equations of the first order [16-22], we have

$$\begin{aligned} y' &= f(x,y,z), \\ z' &= g(x,y,z), \end{aligned} \tag{1.2.9}$$

with initial conditions

$$y(x_0) = y_0, \qquad z(x_0) = z_0.$$

The solutions are found from the expressions

$$y_{n+1} = y_n + \Delta y_n, \qquad (1.2.10)$$
$$z_{n+1} = z_n + \Delta z_n,$$

where

$$\Delta y_n = 1/6(k_1 + 2k_2 + 2k_3 + k_4), \qquad (1.2.11)$$
$$\Delta z_n = 1/6(m_1 + 2m_2 + 2m_3 + m_4),$$

and

$$k_1 = hf(x_n,y_n,z_n), \qquad m_1 = hg(x_n,y_n,z_n),$$
$$k_2 = hf(x_n+h/2, y_n+k_1/2, z_n+m_1/2), \qquad m_2 = hg(x_n+h/2, y_n+k_1/2, z_n+m_1/2),$$
$$k_3 = hf(x_n+h/2, y_n+k_2/2, z_n+m_2/2), \qquad m_3 = hg(x_n+h/2, y_n+k_2/2, z_n+m_2/2),$$
$$k_4 = hf(x_n+h, y_n+k_3, z_n+m_3), \qquad m_4 = hg(x_n+h, y_n+k_3, z_n+m_3).$$

In the case of one differential equation of the second order of the form (1.2.1)

$$y'' = g(x,y,y'), \qquad (1.2.12)$$

with initial conditions

$$y(0) = y_0, \qquad y'(0) = y'_0,$$

we substitute

$$z = y',$$

then we obtain a system of the form

$$y' = z,$$
$$(1.2.13)$$
$$z' = g(x,y,z),$$

with initial conditions

$$y(0) = y_0, \qquad z(0) = z_0.$$

The solution of which $f(x,y,z) = z$ can be presented as follows

$$\Delta y_n = hz_n + 1/6h(m_1 + m_2 + m_3), \qquad (1.2.14)$$

$\Delta z_n = 1/6(m_1 + 2m_2 + 2m_3 + m_4)$,

and

$$\begin{aligned}
k_1 &= hz_n, & m_1 &= hg(x_n,y_n,z_n),\\
k_2 &= h(z_n+m_1/2), & m_2 &= hg(x_n+h/2,\, y_n+k_1/2,\, z_n+m_1/2),\\
k_3 &= h(z_n+m_2/2), & m_3 &= hg(x_n+h/2,\, y_n+k_2/2,\, z_n+m_2/2),\\
k_4 &= h(z_n+m_3), & m_4 &= hg(x_n+h,\, y_n+k_3,\, z_n+m_3).
\end{aligned}$$

The error of the Runge-Kutta method is in the order of O(h^4), which is higher than for the previous case of the FDM.

Below we present an example of the program in Fortran-90 to realize the method described. The following designations are set.

U – the array of the WF with a dimension of N,
H – the look-up of the WF,
N – the number of steps,
A0 – the V_0 depth of the central part of the potential in fm^{-2},
R0 – the α width of the central part of potential in fm^{-2},
L – the orbital moment,
RC – the Coulomb radius R_c in fm,
AK – the Coulomb coefficient A_c in the description of equation (1.1.1),
SK – the wave number k^2 in fm^{-2}.

```
SUBROUTINE FUNRK(U,H,N,A0,R0,L,RC,AK,SK)
IMPLICIT REAL(8) (A-Z)
INTEGER I,N,L
DIMENSION U(0:N)
! THE SOLUTION OF THE SCHRÖDINGER EQUATION BY RUNGE-
KUTT METHOD IN ALL AREA OF VARIABLES
VA1=0.0D0;! VA1 - the value of function in zero
PA1=1.0D-1;! PA1 - Value of a derivative in zero
DO I=0,N-1
X=H*I+1.0D-15
CALL RRUN(VB1,PB1,VA1,PA1,H,X,L,SK,A0,R0)
VA1=VB1; PA1=PB1; U(I+1)=VA1
ENDDO
END
SUBROUTINE RRUN(VB1,PB1,VA1,PA1,H,X,L,SK,A0,R0)
IMPLICIT REAL(8) (A-Z)
INTEGER L
```

```
! THE SOLUTION OF THE SCHRÖDINGER EQUATION BY THE
RUNGE-KUTT METHOD BY ONE STEP
X0=X; Y1=VA1
CALL FA(X0,Y1,FK1,L,SK,A0,R0)
FK1=FK1*H; FM1=H*PA1
X0=X+H/2.0D0; Y2=VA1+FM1/2.0D0
CALL FA(X0,Y2,FK2,L,SK,A0,R0,A1,R1)
FK2=FK2*H; FM2=H*(PA1+FK1/2.0D0); Y3=VA1+FM2/2.0D0
CALL FA(X0,Y3,FK3,L,SK,A0,R0,A1,R1)
FK3=FK3*H; FM3=H*(PA1+FK2/2.0D0); X0=X+H; Y4=VA1+FM3
CALL FA(X0,Y4,FK4,L,SK,A0,R0,A1,R1)
FK4=FK4*H; FM4=H*(PA1+FK3)
PB1=PA1+(FK1+2.0D0*FK2+2.0D0*FK3+FK4)/6.0D0
VB1=VA1+(FM1+2.0D0*FM2+2.0D0*FM3+FM4)/6.0D0
END

SUBROUTINE FA(X,Y,FF,L,SK,A0,R0)
IMPLICIT REAL(8) (A-Z)
INTEGER L,L1
! CALCULATION F (X,Y) FUNCTION IN THE RUNGE–KUTT METHOD
VC=A0*DEXP(-R0*X*X)+A1*DEXP(-R1*X*X)
IF (X>RC) GOTO 1
VK=(3.0D0-(X/RC)**2)*AK/(2.0D0*RCU)
GOTO 2
1 VK=AK/X
2 FF=-(SK-VK-VC-L*(L+1)/(X*X))*Y
END
```

The result of the calculation is the wave function $u(r)$ at a given L, which is the solution of the Schrödinger equation (1.2.1) in the range of values from 0 to R.

1.2.4 The calculation of wave functions by Numerov's method

We still have the Schrödinger equation in the general form

$$u''(r)+a(r)u(r)=0,$$

where

$$a(r) = \left[k^2 - V_{\mathrm{c}}(r)\right],$$

$$V_{\mathrm{c}}(r) = 2\mu/\hbar^2 V_{\mathrm{n}}(r) + 2\mu/\hbar^2 \frac{Z_1 Z_2}{r} + \frac{L(L+1)}{r^2},$$

$$V_{\mathrm{n}}(r) = -V_0 \exp(-\alpha r^2)$$

where V_0 is the potential depth parameter in MeV and α is the parameter of its width in fm^{-2}.

In Numerov's method [17], the WF at a given energy can be found from the expression

$$u_{\mathrm{n+1}} = \frac{\left(2 - \frac{5}{6}h^2 a_{\mathrm{n}}\right)u_{\mathrm{n}} - \left(1 + \frac{1}{12}h^2 a_{\mathrm{n-1}}\right)u_{\mathrm{n-1}}}{1 + \frac{1}{12}h^2 a_{\mathrm{n+1}}} + O(h^6)\,.$$

Using this method, we can find the WF with a convergence rate of $O(h^4)$ [17] more easily than with the Runge-Kutta method having a convergence of $O(h^4)$. Here,

$u_{\mathrm{n-1}} = u(r_{\mathrm{n-1}})$, $r_{\mathrm{n-1}} = (n-1)h$, $h = R/N$,

where R is the upper limit of integration of the equation; N is the number of steps of integration; and h is the value of a step, n = 1, … N - 1 and

$u(0) = 0, u(1) = \mathrm{const.}$

We present an example of the program written in Fortran-90 to realize the method described. The following designations are set.

U – the array of the WF with a dimension of N,
H – the look-up of the WF,
N – the number of steps,
A0 – the V_0 depth of the central part of the potential in fm^{-2},
R0 – the α width of the central part of potential in fm^{-2},
L – the orbital moment,
RC – the Coulomb radius R_c in fm,
AK – the Coulomb coefficient A_c in the description of equation (1.1.1),

SK – the wave number of k^2 in fm^{-2}.

```
SUBROUTINE FUN(U,H,N,A0,R0,L,RC,AK,SK)
IMPLICIT REAL(8) (A-Z)
INTEGER N,L,I
DIMENSION U(0:N),V(0:N)
! INITIAL VALUES
U(0)=0.0D0; U(1)=0.1D0; Q0=0.0D0; RR=1/RC; HK=H*H; SHS=SK*HK
LL=L*(L+1);             BB=AK/(2.0D0*RC);             AA=1.0D0/12.0D0;
DD=5.0D0/6.0D0
! CALCULATION OF VALUES FOR THE Vc(r) POTENTIAL
DO I=1,N-1,2
X=I*H; XX=X*X; XP=(I+1)*H; XXP=XP*XP
V(I)=A0*DEXP(-R0*XX) +LL/XX
V(I+1)=A0*DEXP(-R0*XXP)+LL/XXP
IF (X>RC) THEN
V(I)=V(I)+AK/X
V(I+1)=V(I+1)+AK/XP
ELSE
V(I)=V(I)+(3.0D0-(X*RR)**2)*BB
V(I+1)=V(I+1)+(3.0D0-(XP*RR)**2)*BB
ENDIF
ENDDO
! CALCULATION OF VALUES FOR THE WAVE FUNCTION
DO I=1,N-1,1
Q1=SHS-V(I)*HK; Q2=SHS-V(I+1)*HK; B=(1.0D0+AA*Q2)
U(I+1)=((2.0D0-DD*Q1)*U(I)-(1.0D0+AA*Q0)*U(I-1))/B; Q0=Q1
ENDDO
END
```

The result is the WF $u(r)$ at a given L, which is the solution of the Schrödinger equation (1.2.1) in the range of values from 0 to R.

1.2.5 Methods of calculating the binding energy of a two-body system

Phase shifts can be used for the construction not only of scattering potentials, but also of bound states (BS): ground (GS) or excited (ES) states. We give two methods for the calculation of the binding energy of a two-body nuclear system. Such a situation arises, for example, in the S wave of the $^4\mathrm{He}^2\mathrm{H}$ system of $^6\mathrm{Li}$, where the BS potential is constructed by the corresponding phase shift and its parameters are then specified according to the values of the binding energy, mean square radius, and asymptotic constant (AC) [23].

1.2.5.1 The finite-difference method

The first approach is based on the finite-difference method, which is described in detail in [7,10]. Here, we briefly present some methods of investigating the binding energy and the WF for the bound states and scattering processes. The Schrödinger equation [7] for the central potential is

$$u'' + [k^2 - V(r)]\, u = 0,$$

with this or that boundary condition at $k^2 < 0$ to form the boundary value problem of the Sturm-Liouville type with the boundary conditions

$$u(r = 0) = u_0 = 0,$$

$$u'(r = R)/u(r = R) = u'_N/\, u_N = f(\eta, L, Z_N),$$

where f is the logarithmic derivative; η is the Coulomb parameter; $Z_N = 2kr_N$; $n = 1,2,\ldots;$ N is the number of steps; and $r_N = R$ is the upper bound of the interval of integration of the equation. At the transition to the second derivative to the final difference [24,25,26]

$$u'' = [u_{n+1} - 2u_n + u_{n-1}]/h^2,$$

which turns into a determined system of linear algebraic equations

$$u_{n+1} + [h^2k^2 - h^2V(r) - 2]u_n + u_{n-1} = 0.$$

The condition of equality to zero of its determinant D_N is

$$D_N = \begin{pmatrix} \theta_1 & 1 & 0 & . & . & . & 0 \\ \alpha_2 & \theta_2 & 1 & 0 & . & . & 0 \\ 0 & \alpha_3 & \theta_3 & 1 & 0 & . & 0 \\ . & . & . & . & . & . & . \\ . & . & . & . & . & . & . \\ 0 & . & 0 & 0 & \alpha_{N-1} & \theta_{N-1} & 1 \\ 0 & . & 0 & 0 & 0 & \alpha_N & \theta_N \end{pmatrix} = 0,$$

allowing one to define the eigen binding energy of the system of two particles of k_0. Here, N is the number of equations; $h = R/N$ is the step of the finite-difference grid; R is an interval of the solution of the equation, for example, from zero to 30 fm, and

$$\alpha_n = 1, \quad \alpha_N = 2, \quad \theta_n = k^2h^2 - V_nh^2 - 2,$$

$$\theta_N = k^2h^2 - V_Nh^2 - 2 + 2hf(\eta,L,Z_N), \quad Z_N = 2kr_N,$$

$$r_n = nh, \quad n = 1,2 \ldots..N, \qquad k = \sqrt{|k^2|},$$

$$f(\eta,L,Z_n) = -k - \frac{2k\eta}{Z_n} - \frac{2k(L-\eta)}{Z_n^2},$$

where $V_n = V(r_n)$ is the potential of the interaction clusters for point r_n. Recording of the boundary conditions in the form of a logarithmic derivative $f(\eta,L,Z_n)$ allows us to consider the Coulomb interaction, i.e. the effects, and an asymptotic of the WF of the Whittaker function for the BS.

This type of logarithmic derivative of the wave function of the bound state in the external area can be obtained from the integrated representation of the Whittaker function [27]

$$f(\eta,L,Z) = -k - \frac{2k\eta}{Z} - \frac{2k(L-\eta)}{Z^2}S,$$

where

$$S = \frac{\int\limits_0^\infty t^{L+\eta+1}(1+t/z)^{L-\eta-1}e^{-t}dt}{\int\limits_0^\infty t^{L+\eta}(1+t/z)^{L-\eta}e^{-t}dt}.$$

The calculations show that the S value does not exceed 1.05 and its influence on the binding energy of the two-body system is negligible.

The calculation of a determinant of D_N is carried out on recurrent formulas of the form

$$D_{-1} = 0, D_0 = 1, \qquad (1.2.15)$$

$D_n = \theta_n D_{n-1} - \alpha_n D_{n-2}$,
$n = 1 \ldots N$.

To find the wave functions of bound states, another recurrent process is used

$$u_0 = 0, \quad u_1 = \text{const.}, \tag{1.2.16}$$
$$u_n = -\theta_{n-1} u_{n-1} - u_{n-2},$$
$$n = 2 \ldots N,$$

where const. is any number—this is usually set in the range 0.01–0.1.

As such, at the given energy of the system it is possible to find the determinant and wave function of the bound state. With the energy leading to zero determinants of

$$D_N(k_0) = 0,$$

it considers the eigen energy of system and the wave function at this energy presents the eigenfunctions of the problem.

The last recurrence relation is used also to search for the WF in the case of a continuous spectrum of eigenvalues, i.e. at the previously given energy ($k^2 > 0$) of particle scattering [10]. The text of the computer program written in Fortran-90 is given in [28].

1.2.5.2 The variation method

The second method for discovering the binding energy is based on variation of the decomposition of the wave function on a non-orthogonal Gaussian basis (VM). We briefly give a description of this method and the computer program written in Fortran-90 is provided in [28]. More detailed statements can be found in [10]. Wave functions in the matrix elements for the ground and resonance states are presented through decomposition on a non-orthogonal Gaussian basis of the form

$$\Phi_L(r) = \frac{\chi_L(r)}{r} = r^L \sum_i C_i \exp(-\beta_i r^2),$$

found by the variation method for the bound states or by the approximation of Gaussian functions of the numerical wave functions of resonance levels [29].

For the determination of the spectrum of eigen energies and wave functions in the standard variation method of decomposition of the WF on an orthogonal basis, the matrix problem is solved on the eigenvalues [30]

$$\sum_i (H_{\mathrm{ij}} - EI_{\mathrm{ij}})C_{\mathrm{i}} = 0 ,$$

where H is a symmetric Hamiltonian matrix; I is a unity matrix; E stands for the eigenvalues; and C stands for the eigenvectors of the problem.

In this case, on the non-orthogonal basis of the Gaussian functions, we come to a generalized matrix problem of the form [31]

$$\sum_i (H_{\mathrm{ij}} - EL_{\mathrm{ij}})C_{\mathrm{i}} = 0 ,$$

where L is the matrix of overlapping integrals, which, on an orthogonal basis, is turned into a unity matrix I.

By using the WF in the form given above, we can easily find the expressions for all two-body matrix elements [31]

$$H_{\mathrm{ij}} = T_{\mathrm{ij}} + V_{\mathrm{ij}} + \left\langle j \left| \frac{Z_1 Z_2}{r} \right| i \right\rangle + \left\langle j \left| \frac{\hbar^2 L(L+1)}{2\mu r^2} \right| i \right\rangle ,$$

$$N_0 = \left[\sum C_{\mathrm{i}} C_{\mathrm{j}} L_{\mathrm{ij}} \right]^{-1/2} ,$$

$$T_{\mathrm{ij}} = -\frac{\hbar^2}{2\mu} \frac{\sqrt{\pi}(2L-1)!!}{2^{\mathrm{L+1}} \beta_{\mathrm{ij}}^{\mathrm{L+1/2}}} \left\{ L(2L+1) - L^2 - \frac{\beta_{\mathrm{i}}\beta_{\mathrm{j}}(2L+1)(2L+3)}{\beta_{\mathrm{ij}}^2} \right\} ,$$

$$V_{\mathrm{ij}} = \int V(r) r^{2\mathrm{L}+2} \exp(-\beta_{\mathrm{ij}} r^2) ,$$

$$L_{\mathrm{ij}} = \frac{\sqrt{\pi}(2L+1)!!}{2^{\mathrm{L+2}} \beta_{\mathrm{ij}}^{\mathrm{L+3/2}}} ,$$

$$\left\langle j \left| \frac{Z_1 Z_2}{r} \right| i \right\rangle = \frac{Z_1 Z_2\, L!}{2\beta_{\mathrm{ij}}^{\mathrm{L+1}}} ,$$

$$\left\langle j \left| \frac{\hbar^2 L(L+1)}{2\mu r^2} \right| i \right\rangle = \frac{\sqrt{\pi}(2L-1)!!}{2^{\mathrm{L+1}} \beta_{\mathrm{ij}}^{\mathrm{L+1/2}}} \frac{L(L+1)\hbar^2}{2\mu} , \qquad \beta_{\mathrm{ij}} = \beta_{\mathrm{i}} + \beta_{\mathrm{j}}.$$