Novel method for solution of coupled radial Schrödinger equations

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Abstract. One of the major problems in numerical solution of coupled differential equations is the maintenance of linear independence for different sets of solution vectors. A novel method for solution of radial Schrödinger equations is suggested. It consists of rearrangement of coupled equations in a way that is appropriate to avoid usual numerical instabilities associated with components of the wave function in their classically forbidden regions. Applications of the new method for nuclear structure calculations within the hyperspherical harmonics approach, are given.

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INTRODUCTION

Systems of coupled Schrödinger equations often appear in problems of quantum mechanics and applications to nuclear physics, quantum chemistry etc. A variety of methods has been developed to solve systems of coupled radial Schrödinger equations. A widespread approach consists of two steps. First, sets of linear independent solutions are calculated and then, exploiting the linearity of the coupled equations, a suitable combination of different sets with the required boundary conditions is found. A major problem in numerical solution of the coupled equations is the difficulty of maintaining the linear independence of the solution vectors. There always exists a region of radii where some components of the wave function are classically forbidden and others not. The components with negative radial kinetic energy will in general consist of an exponentially growing and an exponentially decreasing part. If the integration is continued through a classically forbidden region, the exponentially growing components of the wave function in the most strongly closed channels increase faster and soon start to dominate the entire wave function matrix. The small components become insignificant on the scale of the relative accuracy of the calculation. Eventually different solutions become linearly dependent and, thus, useless for finding linear combinations with required boundary conditions. In the classically allowed region, the uneven growth of the components does not occur, since the components are mainly oscillating. But all problems involve integration through at least one classically forbidden region, and instability from developing nearly dependent solutions causes serious numerical inaccuracy. This difficulty arises from the natural properties of solutions rather then from any particular method for their construction.

To maintain linear independence, different stabilizing transformations during propagation were suggested [1, 2, 3, 4, 5]. After several propagation steps these regularization procedures can be applied to re-establish the linear independence of the columns in the wave function matrix. Usually these transformations are rather awkward and tedious. Another approach to overcome the difficulty is to use a so-called invariant imbedding method, in which the propagated quantity is not the wave function matrix $\mathbf{\Psi} = \{\psi_{in}(r)\}$ but rather its logarithmic derivative $\mathbf{\Psi}'\mathbf{\Psi}^{-1}$ [6, 7] or its inverse matrix $\boldsymbol{R} = \mathbf{\Psi}\mathbf{\Psi}'^{-1}$ [8]. These methods found broad applications, especially for large coupled-channels calculations. In other approaches radial wave functions are expanded in terms of orthonormal basis functions, chosen to account for some dynamical features in the most effective way. Then a solution of the differential equations is reduced to a set of linear equations for expansion coefficients. Such an approach, for example, is realized in program [9].

In the past three decades, a lot of research (see, for example, [10, 11] and references therein) has been performed in the area of numerical integration of the Schrödinger equation. The main goal is to construct numerical methods that are both accurate and computational efficient. The development of these methods is still an active subject. Here, we suggest a novel method for solution of radial Schrödinger equations. It consists in rearrangement of coupled equations in a way that is appropriate to avoid the usual numerical instabilities associated with components of the wave function in their classically forbidden regions. Applications of the new method to nuclear structure calculations within the hyperspherical harmonics approach, are given.

THEORY

Consider the system of the N coupled radial Schrödinger equations

$$\left(\frac{d^2}{dr^2} + \frac{2mE}{\hbar^2} - \frac{\mathscr{L}_i(\mathscr{L}_i+1)}{r^2}\right)\psi_{in}(r) = \sum_{j=1}^{N} V_{ij}(r)\,\psi_{jn}(r) \tag{1}$$

where E is a total energy, $\mathscr{L}_i$ is an angular orbital momentum in the channel i. The first index of $\psi_{in}(r)$ denotes the i-th component of wave functions ($i = 1, \ldots, N$) while the second index n marks different linear independent solutions. The $N \times N$ matrix of coupling potentials $V_{ij}(r)$ is assumed symmetric, i. e. $V_{ij}(r) = V_{ji}(r)$. Note that potentials include the factor $2m/\hbar^2$ and have dimension fm^{-2}. In general, the system (1) of the N linear differential equations of second order has $2N$ linearly independent solutions called the fundamental ones; N solutions have a regular behaviour at the origin while the N others have irregular behaviour. Any solution of the system (1) can be written as a linear combination of these fundamental solutions. Only solutions that satisfy definite boundary conditions imposed at the origin and infinity, have physical meaning. At the origin the boundary condition demands that wave functions have a regular behaviour

$$\psi_{in}(r \to 0) \to 0 \tag{2}$$

while at infinity the boundary condition depends on the sign of energy E. For bound states ($E < 0$) the problem is of the eigenvalue type and for any given eigenvalue (E_n)

the solution of (1) decays exponentially for large values of r

$$\psi_{in}(r \to \infty) \to \exp(-k_n r) \tag{3}$$

where $k_n = \sqrt{2m \mid E_n \mid /\hbar^2}$. For continuum states ($E > 0$) the solutions oscillate at infinity

$$\psi_{in}(r \to \infty) \to H^{(-)}_{\mathscr{L}_i}(k r)\, \delta_{in} - H^{(+)}_{\mathscr{L}_i}(k r)\, S_{in} \tag{4}$$

where $k = \sqrt{2m \mid E \mid /\hbar^2}$. Here $H^{(\pm)}_{\mathscr{L}_i}(x) = G_{\mathscr{L}_i}(x) \pm \imath F_{\mathscr{L}_i}(x)$ are the Coulomb functions of index $\mathscr{L}_i$ [12] describing the in- and out-going spherical waves. $F_{\mathscr{L}_i}(x)$ and $G_{\mathscr{L}_i}(x)$ are regular and irregular Coulomb functions, respectively, $\imath = \sqrt{-1}$. The S_{in} is the S-matrix element for the outgoing amplitude in channel i from an incoming plane wave in channel n.

Our aim is to find solutions of system (1) satisfying boundary conditions (2,3,4) for radius changing from zero to some maximal value $r = r_{max}$. The general method to solve the boundary value problem for coupled equations (1) is to construct a set of linear independent solutions and after that find a linear combination of these solutions which satisfies the required asymptotic behaviour. Numerical integration within a long radial interval tends to accumulate errors and induces a loss of linear independence of solutions. Thus it is convenient to divide the radial space into nonoverlapping domains by points b_I, $0 = b_0 < b_1 < \ldots < b_{max} = r_{max}$ and solve differential equations separately in each of the intervals. Then the partial solutions are assembled into a global solution that is continuous and smooth across the whole region and satisfies the given boundary conditions. The transparent and straightforward way to perform this task is to reformulate the coupled differential equations (1) as a system of coupled integral equations. It has also the advantage that integral equations contain the explicit structure of required solutions.

Integral formulation

Boundary value problems for a system of ordinary differential equations (1) can be reformulated as a system of Fredholm integral equations. For technical reasons it is simpler to solve Volterra integral equations with variable upper or lower limits. System of Volterra equations corresponds to the solution of the initial value problem. If only open channels exist then solutions of Fredholm and Volterra systems are different by a constant matrix. Since the total normalization is not important all solutions are acceptable. If closed and opened channels coexist, then solutions of Volterra equations can not substitute the solutions of Fredholm systems within the entire range of a radial variable. Numerical solutions of Volterra equations with variable upper limit are regular at the origin but at large radii they will have exponentially increasing components in closed channels. Numerical solutions of Volterra equations with variable lower limit can contain exponentially decreasing components in closed channels but can not guarantee the regular behaviour of wave functions at the origin. A solution of this dilemma is well known and commonly used. It consists of a combination of solutions for both type

of Volterra equations: wave functions and their first derivatives are matched at some intermediate radius. Thus the obtained wave functions are solutions of the original system of Schrödinger equations (1) for all radii and satisfy the required boundary conditions. If at least one open channel exists then a matching procedure is always possible. Let $N = N_{op} + N_{cl}$, where N_{op} (N_{cl}) is the number of open (closed) channels. Then, there are N regular solutions for outward integrations of Volterra equations with variable upper limit, while the number of linear independent solutions for Volterra equations with variable lower limit is larger and equal to $N + N_{op} = N_{cl} + 2N_{op}$. This number is composed of the N_{cl} sets with exponentially decreasing components in closed channels, N_{op} sets with components oscillating asymptotically like regular functions F_i or N_{op} sets with components oscillating like irregular G_i. The extra freedom in number of linear independent solutions always allows to match them and define simultaneously necessary S-matrix elements. When only closed channels exist, i. e. for bound state problems, the number of linear independent solutions for inward and outward integration is the same and equal to N. Then matching procedure is only possible at discrete values of the energy which are energies of bound states, respectively.

Consider the following systems of Volterra integral equations with variable upper or lower limit r

$$\psi_{in}(r) - \frac{1}{k}\int_0^r dr' \left(f_i(kr)\,g_i(kr') - g_i(kr)\,f_i(kr')\right) \sum_{j=1}^{N} V_{ij}(r')\,\psi_{jn}(r') = \delta_{in}\,f_i(kr) \qquad (5)$$

$$\psi_{in}(r) + \frac{1}{k}\int_r^\infty dr' \left(f_i(kr)\,g_i(kr') - g_i(kr)\,f_i(kr')\right) \sum_{j=1}^{N} V_{ij}(r')\,\psi_{jn}(r') = \delta_{in}\,g_i(kr) \qquad (6)$$

where δ_{in} is the Kronecker symbol, and where the Green's function $(f_i(kr)\,g_i(kr') - g_i(kr)\,f_i(kr'))/k$ is composed of two linear independent solutions $f_i(kr)$ and $g_i(kr)$ of the free Schrödinger equation

$$\left(\frac{d^2}{dr^2} + \frac{2mE}{\hbar^2} - \frac{\mathscr{L}_i(\mathscr{L}_i+1)}{r^2}\right) f_i(kr) = 0 \qquad (7)$$

Free solutions are normalized by demanding that the Wronskian relation $W(f_i, g_i) = f_i(x)\,g_i'(x) - f_i'(x)\,g_i(x) = -1$. They have explicit representation via Bessel functions [12] of the first J_ν and second Y_ν kinds for $E > 0$

$$f_i(x) = \sqrt{\frac{\pi x}{2}}\,J_{\mathscr{L}_i+1/2}(x) \quad ; \quad g_i(x) = -\sqrt{\frac{\pi x}{2}}\,Y_{\mathscr{L}_i+1/2}(x) \qquad (8)$$

and modified Bessel functions I_ν and K_ν for $E < 0$

$$f_i(x) = \sqrt{x}\,I_{\mathscr{L}_i+1/2}(x) \quad ; \quad g_i(x) = \sqrt{x}\,K_{\mathscr{L}_i+1/2}(x) \qquad (9)$$

The functions $f_i(kr)$ and $g_i(kr)$ have regular and irregular behaviour at the origin, respectively. Hence solutions of Volterra systems (5) and (6) also define sets of N linear independent solutions of the Schrödinger equations (1) with regular or irregular

behaviour at the origin, respectively. Below we consider only system (5), for system (6) a derivation can be made in a similar way.

Labelling the wave function $\psi_{in}(r)$ in the interval I as $\psi^I_{in}(r)$ and using the equations (5) we can write

$$\begin{aligned}\psi^I_{in}(r) &- \frac{1}{k}\int_{b_{I-1}}^{r} dr' \left(f_i(kr)\,g_i(kr') - g_i(kr)\,f_i(kr')\right) \sum_{j=1}^{N} V_{ij}(r')\,\psi^I_{jn}(r') \\ &= f_i(kr)\,A^I_{in} - g_i(kr)\,B^I_{in} \end{aligned} \tag{10}$$

where the constants A^I_{in} and B^I_{in} are equal to

$$\begin{aligned} A^I_{in} &= \delta_{in} + \frac{1}{k}\int_0^{b_{I-1}} dr' g_i(kr') \sum_j V_{ij}(r')\,\psi_{jn}(r') \\ B^I_{in} &= \frac{1}{k}\int_0^{b_{I-1}} dr' f_i(kr') \sum_j V_{ij}(r')\,\psi_{jn}(r') \end{aligned} \tag{11}$$

The wave functions $\psi^I_{in}(r)$ in the interval I can be written as linear combinations of unknown functions $y^I_{ip}(r)$ and $z^I_{ip}(r)$ [13]

$$\psi^I_{in}(r) = \sum_{p=1}^{N} \left(y^I_{ip}(r)\,A^I_{pn} - z^I_{ip}(r)\,B^I_{pn}\right) \tag{12}$$

Substituting decomposition (12) into equations (10) we obtain the integral equations in the I-th interval for functions $y^I_{in}(r)$ and $z^I_{in}(r)$

$$y^I_{in}(r) - \frac{1}{k}\int_{b_{I-1}}^{r} dr' \left(f_i(kr)\,g_i(kr') - g_i(kr)\,f_i(kr')\right) \sum_{j=1}^{N} V_{ij}(r')\,y^I_{jn}(r') = \delta_{in}\,f_i(kr) \tag{13}$$

$$z^I_{in}(r) - \frac{1}{k}\int_{b_{I-1}}^{r} dr' \left(f_i(kr)\,g_i(kr') - g_i(kr)\,f_i(kr')\right) \sum_{j=1}^{N} V_{ij}(r')\,z^I_{jn}(r') = \delta_{in}\,g_i(kr) \tag{14}$$

According to the driving terms on the right hand side of equations (13) - (14) the functions $y^I_{in}(r)$ and $z^I_{in}(r)$ can be called the regular and irregular solutions in the interval I. They form a complete system of $2N$ linear independent solutions of the Schrödinger equations (1) within the radial interval I. Substituting the decomposition (12) in equations (11), simple recurrence relations for the coefficients A^I_{in} and B^I_{in} can be obtained

$$\begin{aligned} A^I_{in} &= A^{I-1}_{in} + \sum_{p=1}^{N} \left((gVy)^{I-1}_{ip}\,A^{I-1}_{pn} - (gVz)^{I-1}_{ip}\,B^{I-1}_{pn}\right) \\ B^I_{in} &= B^{I-1}_{in} + \sum_{p=1}^{N} \left((fVy)^{I-1}_{ip}\,A^{I-1}_{pn} - (fVz)^{I-1}_{ip}\,B^{I-1}_{pn}\right) \end{aligned} \tag{15}$$

with initial values $A^1_{in} = \delta_{in}$, $B^1_{in} = 0$ and $I \geq 2$. The coefficients of A^{I-1}_{pn} and B^{I-1}_{pn} in (15) are given by

$$\begin{aligned}
(gVy)^{I-1}_{ip} &= \frac{1}{k}\int_{b_{I-2}}^{b_{I-1}} dr' g_i(kr') \sum_{j=1}^{N} V_{ij}(r')\, y^{I-1}_{jp}(r') \\
(gVz)^{I-1}_{ip} &= \frac{1}{k}\int_{b_{I-2}}^{b_{I-1}} dr' g_i(kr') \sum_{j=1}^{N} V_{ij}(r')\, z^{I-1}_{jp}(r') \\
(fVy)^{I-1}_{ip} &= \frac{1}{k}\int_{b_{I-2}}^{b_{I-1}} dr' f_i(kr') \sum_{j=1}^{N} V_{ij}(r')\, y^{I-1}_{jp}(r') \\
(fVz)^{I-1}_{ip} &= \frac{1}{k}\int_{b_{I-2}}^{b_{I-1}} dr' f_i(kr') \sum_{j=1}^{N} V_{ij}(r')\, z^{I-1}_{jp}(r') \qquad (16)
\end{aligned}$$

Thus the original problem (1) is reduced to obtaining a complete set of regular $y^I_{in}(r)$ and irregular $z^I_{in}(r)$ solutions in the interval I. From these solutions, using decomposition (12), global solutions $\psi^I_{in}(r)$ can be obtained. Note that the $y^I_{in}(r)$ and $z^I_{in}(r)$ in the I-th interval are calculated independently of solutions on other intervals. Below we will present the detailed derivation only for regular solutions $y^I_{in}(r)$. For irregular solutions $z^I_{in}(r)$ similar relations can easily be obtained.

The Green's function constructed from the $f_i(kr)$ and $g_i(kr)$ solutions of the free Schrödinger equation (7) was used explicitly in (13) and (14). In reality, any potentials can be added into equation (7) to obtain potential-modified functions $f_i(kr)$ and $g_i(kr)$ in the I-th interval. These potentials must however be subtracted from the diagonal potentials $V_{ii}(r)$ in equations (13) and (14), respectively. For example, the diagonal potentials V_{ii} themselves may be used for $f_i(kr)$ and $g_i(kr)$ calculations. This allows to account for a sizeable part of the correlations induced by the interactions before an attempt is made to solve the system of coupled equations. But now we lose knowledge about analytical properties of $f_i(kr)$ and $g_i(kr)$ functions. As a reasonable compromise, the value of the diagonal potential at any fixed point within the I-th interval (for example, b_{I-1} - the beginning of interval I) can be used to represent the interval. Then functions $f_i(k_i r)$ and $g_i(k_i r)$ will still be solutions of the free Schrödinger equation (7) but with new (scaled) energies $E_i = E$ - $(\hbar^2/2m)\, V_{ii}(b_{I-1})$ and, correspondingly, with new linear momenta $k_i = \sqrt{2m|E_i|}/\hbar$. Then we get new integral equations for calculations of local regular solutions

$$\begin{aligned}
y^I_{in}(r) &- \frac{1}{k_i}\int_{b_{I-1}}^{r} dr' \left(f_i(k_i r)\, g_i(k_i r') - g_i(k_i r)\, f_i(k_i r')\right) \sum_{j=1}^{N} V^I_{ij}(r')\, y^I_{jn}(r') \\
&= \delta_{in}\left(f_i(k_i r)\, a_i - g_i(k_i r)\, c_i\right) \qquad (17)
\end{aligned}$$

where $V^I_{ij}(r) = V_{ij}(r)$ - $\delta_{ij} V_{ii}(b_{I-1})$ and where the constants a_i and c_i in the driving term are fixed by the requirement that $y^I_{in}(r)$ must satisfy the initial values built into equations

(13): $y^I_{in}(b_{I-1}) = \delta_{in}\, f_i(k\, b_{I-1})$ and $y^{I'}_{in}(b_{I-1}) = \delta_{in}\, k f'_i(k\, b_{I-1})$

$$\begin{aligned} a_i &= \frac{k}{k_i} f'_i(k\, b_{I-1})\, g_i(k_i\, b_{I-1}) - f_i(k\, b_{I-1})\, g'_i(k_i\, b_{I-1}) \\ c_i &= \frac{k}{k_i} f'_i(k\, b_{I-1})\, f_i(k_i\, b_{I-1}) - f_i(k\, b_{I-1})\, f'_i(k_i\, b_{I-1}) \end{aligned} \tag{18}$$

When all $k_i = k$, the equations (17) reduce to equations (13). In equations (17) the channel energies E_i depend on values of diagonal potentials $V_{ii}(b_{I-1})$ and thus may have different signs, therefore different channels may be locally open or closed.

The integral equations (17) define an explicit structure for regular solutions $y^I_{in}(r)$

$$y^I_{in}(r) = f_i(k_i\, r)\, \alpha^I_{in}(r) - g_i(k_i\, r)\, \beta^I_{in}(r) \tag{19}$$

where the unknown functions $\alpha^I_{in}(r)$ and $\beta^I_{in}(r)$ are solutions of the following system of coupled integral equations

$$\begin{aligned} \alpha^I_{in}(r) &= \delta_{in} a_i + \frac{1}{k_i} \int_{b_{I-1}}^{r} dr'\, g_i(k_i\, r') \sum_{j=1}^{N} V^I_{ij}(r') \left(f_j(k_j\, r')\, \alpha^I_{jn}(r') - g_j(k_j\, r')\, \beta^I_{jn}(r') \right) \\ \beta^I_{in}(r) &= \delta_{in} c_i + \frac{1}{k_i} \int_{b_{I-1}}^{r} dr'\, f_i(k_i\, r') \sum_{j=1}^{N} V^I_{ij}(r') \left(f_j(k_j\, r')\, \alpha^I_{jn}(r') - g_j(k_j\, r')\, \beta^I_{jn}(r') \right) \end{aligned} \tag{20}$$

Now we return to the differential formulation of the respective equations.

Differential formulation

The system of integral equations (20) for the functions $\alpha^I_{in}(r)$ and $\beta^I_{in}(r)$ is equivalent to a system of the $2N$ coupled ordinary differential equations of the first order

$$\begin{aligned} \frac{d\alpha^I_{in}(r)}{dr} &= \frac{1}{k_i} g_i(k_i\, r) \sum_{j=1}^{N} V^I_{ij}(r) \left(f_j(k_j\, r)\, \alpha^I_{jn}(r) - g_j(k_j\, r)\, \beta^I_{jn}(r) \right) \\ \frac{d\beta^I_{in}(r)}{dr} &= \frac{1}{k_i} f_i(k_i\, r) \sum_{j=1}^{N} V^I_{ij}(r) \left(f_j(k_j\, r)\, \alpha^I_{jn}(r) - g_j(k_j\, r)\, \beta^I_{jn}(r) \right) \end{aligned} \tag{21}$$

with initial values $\alpha^I_{in}(b_{I-1}) = \delta_{in} a_i$ and $\beta^I_{in}(b_{I-1}) = \delta_{in} c_i$. Multiplying the first equation by $f_i(k_i\, r)$ and the second by $g_i(k_i\, r)$, we see that these equations have the special properties, $f_i(k_i\, r)\, d\alpha^I_{in}(r)/dr = g_i(k_i\, r)\, d\beta^I_{in}(r)/dr$. Equations (21) also allow to investigate explicitly the reasons that catalyze loss of linear independence for different solution sets.

We have to estimate the qualitative behaviour of the regular $f_i(x)$ and irregular $g_i(x)$ functions. For closed channels, the regular (irregular) functions (9) are monotonously increasing (decreasing) with increasing arguments. Both functions never equal zero at finite arguments. For open channels there are two regions where functions $f_i(x)$ and $g_i(x)$ (8) have qualitatively different behaviour. At small arguments they have monotonic

behaviour similar to that for closed channels. At large arguments they oscillate like cosine or sine functions. Instead of $f_i(x)$ and $g_i(x)$ functions in the region of oscillations it is convenient to introduce the modulus $M_i(x)$ and phase $\theta_i(x)$ functions [12]

$$M_i(x) = \sqrt{f_i^2(x) + g_i^2(x)}\,; \quad f_i(x) = M_i(x)\cos\theta_i(x)\,; \quad g_i(x) = M_i(x)\sin\theta_i(x) \qquad (22)$$

Modulus $M_i(x)$ is never equal to zero. From the Wronskian relation it also follows that $\theta_i'(x) = -1/M_i^2(x)$.

The presence of centrifugal barriers is natural for dynamics described by Schrödinger equations. It is possible to account for them analytically by introducing regular $f_i(k_i r)$ and irregular $g_i(k_i r)$ solutions of the free Schrödinger equations (7). Explicit centrifugal barriers drop out and their influence on the full solution is described by the $f_i(k_i r)$ and $g_i(k_i r)$ functions in the equations (21). The regular and irregular functions of different orders are mixed in the equations. These functions have quantitatively different behaviour, some may be rather small while others are very large. The difference in absolute values can easily reach many orders of magnitude. Under such circumstances it is difficult to keep an acceptable level of the accuracy in numerical solution of coupled equations. The lack of accuracy leads to loss of the linear independence of different solutions. A possible way out is to make a rearrangement of coupled equations such that the different behaviour of free solutions will be minimized. There exist only three suitable combinations: the product of free functions $f_i(x)\,g_i(x)$ and their logarithmic derivatives $f_i'(x)/f_i(x)$ and $g_i'(x)/g_i(x)$. After rearrangement the necessary requirements to the numerical accuracy for solutions of the new system of coupled equations become significantly weaker. *Such rearrangement of equations is just the main idea of this article*.

To illustrate our point, Figure (1) shows the regular $f_i(x)$ and irregular $g_i(x)$ functions for closed (a) and open (b) channels with $\mathscr{L}_i$ = 3/2, 19/2 and 39/2 represented by the solid, dash and dash-dot lines, respectively. (In the hypersherical harmonics method these values of $\mathscr{L}_i$ correspond to calculations with hypermoment K = 0, 8 and 18, respectively.) We see that changes in scales for absolute values of free solutions can easily span twenty orders of magnitude. (Figure (1) shows variations from 10^{-10} to 10^{+10}). Variations of logarithmic derivatives for these functions, on the other hand, shown in Figure (2), span only a few (2 - 3) orders of magnitude.

Now we assume that in the I-th interval the first N_0 channels have free functions $f_i(x)$ and $g_i(x)$ with arguments x lying in the region of monotonic behaviour. All closed and a part of the open channels are included into this number. The rest, channels from N_0 + 1 to N are open, and arguments of free functions are in the region of oscillations. In the first N_0 channels the absolute values of free solutions may vary over a wide scale while they are restricted to about unity in the last (N - N_0) ones. We will transform the system of equations (21) in such a way that free solutions enter into the new system of equations as logarithmic derivatives with rather restricted variations in absolute scale. For functions with arguments in the region of oscillations the logarithmic derivatives become infinite at the points where the functions have zeros. This is a reason for special selection of such channels. Thus instead of the relation (19) for a regular solution $y_{in}^I(r)$

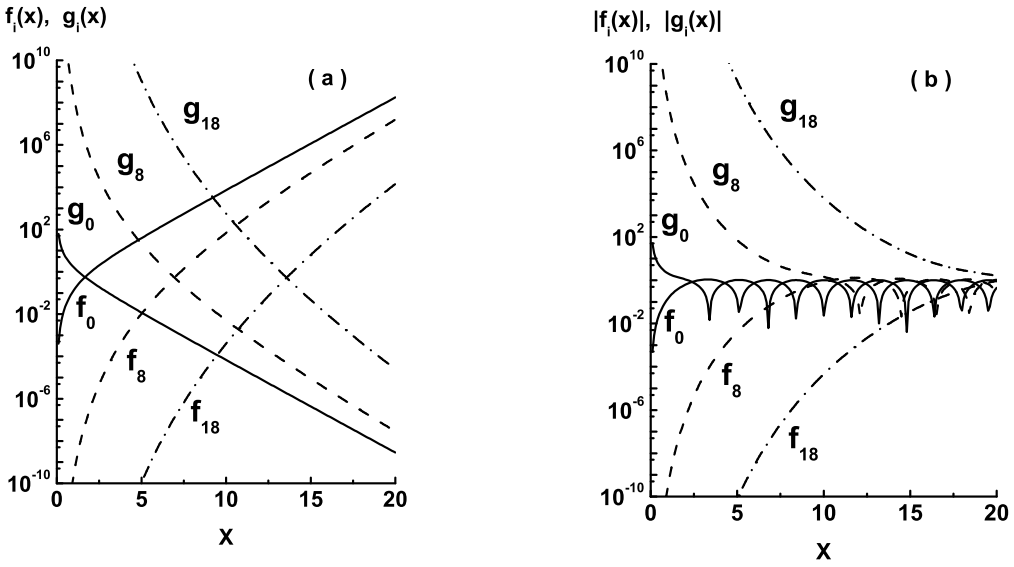

FIGURE 1. The regular $f_i(x)$ and irregular $g_i(x)$ solutions of the free Schrödinger equations for negative (a) and positive (b) energies. The solid, dash and dash-dot lines correspond to calculations with hypermoments $K = 0$, 8 and 18, respectively.

we use a more explicit decomposition for different components i

$$\begin{aligned} y^I_{in}(r) &= f_i(k_i r)\,\alpha^I_{in}(r) - g_i(k_i r)\,\beta^I_{in}(r), \qquad 1 \le i \le N_0 \\ &= M_i(k_i r)\left(\cos(\theta_i(k_i r))\,\alpha^I_{in}(r) - \sin(\theta_i(k_i r))\,\beta^I_{in}(r)\right), \; N_0+1 \le i \le N \end{aligned} \tag{23}$$

Let us first consider the equations for channels $i \le N_0$. Differentiating functions $y^I_{in}(r)$, using equations (21) and the Wronskian relation for free solutions we can get the following set of equations for $i \le N_0$

$$\begin{aligned} \frac{dy^I_{in}(r)}{dr} &= k_i \frac{f_i'(k_i r)}{f_i(k_i r)}\, y^I_{in}(r) + \gamma^I_{in}(r) \\ \frac{d\gamma^I_{in}(r)}{dr} &= -k_i \frac{f_i'(k_i r)}{f_i(k_i r)}\, \gamma^I_{in}(r) + \sum_{j=1}^{N} V^I_{ij}(r)\, y^I_{jn}(r) \end{aligned} \tag{24}$$

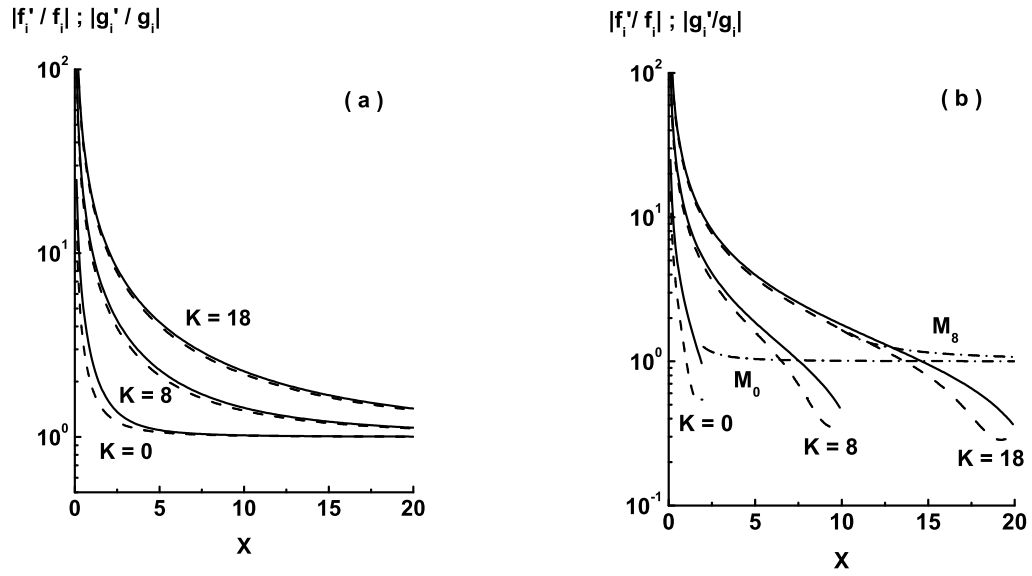

FIGURE 2. Absolute values of the logarithmic derivatives of regular $f_i(x)$ (solid line) and irregular $g_i(x)$ (dash line) solutions of the free Schrödinger equations for negative (a) and positive (b) energies for hypermoments $K = 0$, 8 and 18. The dash-dotted lines show moduli (22) $M_0(x)$ and $M_8(x)$ of free solutions in the region of oscillations.

where the function $\gamma^I_{in}(r) = k_i \beta^I_{in}(r)/f_i(k_i r)$. For $i > N_0$ the following set of equations can be obtained

$$\begin{aligned} \frac{dy^I_{in}(r)}{dr} &= k_i \frac{M_i'(k_i r)}{M_i(k_i r)} y^I_{in}(r) + \gamma^I_{in}(r) \\ \frac{d\gamma^I_{in}(r)}{dr} &= -k_i \frac{M_i'(k_i r)}{M_i(k_i r)} \gamma^I_{in}(r) + \sum_{j=1}^{N} V^I_{ij}(r)\, y^I_{jn}(r) - \frac{k_i^2}{M_i^4(k_i r)} y^I_{in}(r) \end{aligned} \tag{25}$$

where $\gamma^I_{in}(r) = k_i \left(\sin(\theta_i(k_i r))\, \alpha^I_{in}(r) + \cos(\theta_i(k_i r))\, \beta^I_{in}(r)\right)/M_i(k_i r)$. Initial values for functions $y^I_{in}(r)$ and $\gamma^I_{in}(r)$ are equal to

$$\begin{aligned} y^I_{in}(b_{i-1}) &= \delta_{in} f_i(k b_{I-1}) \qquad ; \quad 1 \le i \le N \\ \gamma^I_{in}(b_{i-1}) &= \delta_{in} f_i(k b_{I-1}) \left(k \frac{f_i'(k b_{I-1})}{f_i(k b_{I-1})} - k_i \frac{f_i'(k_i b_{I-1})}{f_i(k_i b_{I-1})} \right) \quad ; \quad 1 \le i \le N_0 \\ \gamma^I_{in}(b_{i-1}) &= \delta_{in} f_i(k b_{I-1}) \left(k \frac{f_i'(k b_{I-1})}{f_i(k b_{I-1})} - k_i \frac{M_i'(k_i b_{I-1})}{M_i(k_i b_{I-1})} \right) \quad ; \quad N_0 < i \le N \end{aligned} \tag{26}$$

For cases when $k_i = k$ and $i \leq N_0$ the initial values for functions $\gamma^I_{in}(b_{i-1})$ are equal to zero. Finding functions $y^I_{in}(r)$ and $\gamma^I_{in}(r)$ we obtain simultaneously the derivatives $y^{I'}_{in}(r)$ via equations (24) and (25).

The systems of equations (24) - (25) include the bare potentials $V^I_{ij}(r)$ without the multiplications on functions $f_i(k_i r)$ and $g_i(k_i r)$ occurring in equations (21). The free solutions appear in the new equations (24) - (25) only as logarithmic derivatives. Thus huge differences in scales of absolute values that may exist for functions $f_i(x)$ and $g_i(x)$ with different indices i are significantly reduced, to relatively mild variations of absolute values for logarithmic derivatives. Hence requirements on accuracy of numerical methods applied for solving the coupled radial Schrödinger equations become essentially weaker and the loss of linear independence for different solution sets due to insufficient numerical accuracy, is greatly reduced.

Expressions (24) - (25) correspond to calculations of regular solutions $y^I_{in}(r)$. For irregular solutions $z^I_{in}(r)$ we can proceed analogously and get for $i \leq N_0$ the following system of equations

$$\begin{aligned} \frac{dz^I_{in}(r)}{dr} &= k_i \frac{g_i'(k_i r)}{g_i(k_i r)} z^I_{in}(r) + \eta^I_{in}(r) \\ \frac{d\eta^I_{in}(r)}{dr} &= -k_i \frac{g_i'(k_i r)}{g_i(k_i r)} \eta^I_{in}(r) + \sum_{j=1}^{N} V^I_{ij}(r) z^I_{jn}(r) \end{aligned} \tag{27}$$

and for $i > N_0$ equations parallel to those of (25) (by just changing notations: $y^I_{in}(r) \rightarrow z^I_{in}(r)$ and $\gamma^I_{in}(r) \rightarrow \eta^I_{in}(r)$). Initial values for functions $z^I_{in}(r)$ and $\eta^I_{in}(r)$ are equal to

$$\begin{aligned} z^I_{in}(b_{i-1}) &= \delta_{in} g_i(k b_{I-1}) \quad ; \quad 1 \leq i \leq N \\ \eta^I_{in}(b_{i-1}) &= \delta_{in} g_i(k b_{I-1}) \left(k \frac{g_i'(k b_{I-1})}{g_i(k b_{I-1})} - k_i \frac{g_i'(k_i b_{I-1})}{g_i(k_i b_{I-1})} \right) \quad ; \quad 1 \leq i \leq N_0 \\ \eta^I_{in}(b_{i-1}) &= \delta_{in} g_i(k b_{I-1}) \left(k \frac{g_i'(k b_{I-1})}{g_i(k b_{I-1})} - k_i \frac{M_i'(k_i b_{I-1})}{M_i(k_i b_{I-1})} \right) \quad ; \quad N_0 < i \leq N \end{aligned} \tag{28}$$

We see that if in the formulas above for $y^I_{in}(r)$, the regular functions $f_i(x)$ are replaced by the irregular functions $g_i(x)$, we get expressions for calculations of irregular solutions $z^I_{in}(r)$. The new systems (24) and (27) show explicitly why regular and irregular solutions behave in qualitatively different way. The differences of respective equations for $i \leq N_0$ are in the terms that include the logarithmic derivatives of free solutions. Since $f_i'(x)/f_i(x)$ and $g_i'(x)/g_i(x)$ have comparable absolute values and different signs they force solutions to change in opposite directions. For components $i > N_0$ in the regions of oscillations both solutions $y^I_{in}(r)$ and $z^I_{in}(r)$ obey equations where only the modulus function $M_i(k_i r)$ of free solutions appears at the place of $f_i(k_i r)$ and $g_i(k_i r)$.

In practice, it is convenient to scale solutions $y^I_{ip}(r)$ and $z^I_{ip}(r)$ by factors $f_p(k b_{I-1})$ and $g_p(k b_{I-1})$, respectively, for channels p where the functions $f_p(k b_{I-1})$ and $g_p(k b_{I-1})$ have monotonic behaviour (while we do not scale solutions for channels p where their absolute values oscillate around unity)

$$y^I_{ip}(r) = \tilde{y}^I_{ip}(r) f_p(k b_{I-1}) \quad ; \quad \tilde{A}^I_{pn} = f_p(k b_{I-1}) A^I_{pn} \tag{29}$$

$$z^I_{ip}(r) \;=\; \tilde{z}^I_{ip}(r)\, g_p(k\, b_{I-1}) \quad ; \quad \tilde{B}^I_{pn} = g_p(k\, b_{I-1})\, B^I_{pn}$$

Then, wave functions $\psi^I_{in}(r)$ (see (12)) on interval I can be written as linear combinations of the $\tilde{y}^I_{ip}(r)$ and $\tilde{z}^I_{ip}(r)$ functions

$$\psi^I_{in}(r) = \sum_{p=1}^{N} (\tilde{y}^I_{ip}(r)\, \tilde{A}^I_{pn} - \tilde{z}^I_{ip}(r)\, \tilde{B}^I_{pn}) \tag{30}$$

where the initial values for functions $\tilde{y}^I_{ip}(r)$ and $\tilde{z}^I_{ip}(r)$ at the radius $r = b_{I-1}$ are reduced to the Kronecker symbol. The integrals in (16) can be scaled in similar ways, for example $(gVy)^I_{ip} = g_i(k\, b_{I-1})\, (\widetilde{gVy})^I_{ip}\, f_p(k\, b_{I-1})$ etc. Thus, the recurrence relations (15) for coefficients A^I_{in} and B^I_{in} are transformed, and read

$$\begin{aligned}
\tilde{A}^I_{in} &= \frac{f_i(k\, b_{I-1})}{f_i(k\, b_{I-2})} \left\{ \tilde{A}^{I-1}_{in} + f_i(k\, b_{I-2})\, g_i(k\, b_{I-2}) \sum_{p=1}^{N} \left((\widetilde{gVy})^{I-1}_{ip}\, \tilde{A}^{I-1}_{pn} - (\widetilde{gVz})^{I-1}_{ip}\, \tilde{B}^{I-1}_{pn} \right) \right\} \\
\tilde{B}^I_{in} &= \frac{g_i(k\, b_{I-1})}{g_i(k\, b_{I-2})} \left\{ \tilde{B}^{I-1}_{in} + f_i(k\, b_{I-2})\, g_i(k\, b_{I-2}) \sum_{p=1}^{N} \left((\widetilde{fVy})^{I-1}_{ip}\, \tilde{A}^{I-1}_{pn} - (\widetilde{fVz})^{I-1}_{ip}\, \tilde{B}^{I-1}_{pn} \right) \right\}
\end{aligned}$$

This scaling gives significant reduction of the absolute value variations within radial interval I for all functions and coefficients in the formulas above.

Matching and normalization

For bound state case ($E < 0$) we have two sets of the N linear independent solutions of systems (5) and (6), regular $\psi^{reg}_{in}(r)$ and irregular $\psi^{irr}_{in}(r)$, respectively. Wave functions $\psi^{reg}_{in}(r)$ are regular at the origin while $\psi^{irr}_{in}(r)$ vanish at infinity. We demand that at some (matching) point r_m a linear combinations of wave functions and derivatives for both sets become equal to a each other

$$\begin{aligned}
\sum_{n=1}^{N} \psi^{reg}_{in}(r_m)\, \lambda_n &= \sum_{n=1}^{N} \psi^{irr}_{in}(r_m)\, \mu_n \\
\sum_{n=1}^{N} \psi^{reg'}_{in}(r_m)\, \lambda_n &= \sum_{n=1}^{N} \psi^{irr'}_{in}(r_m)\, \mu_n
\end{aligned} \tag{31}$$

Here $\{\lambda_n\}$ and $\{\mu_n\}$ are unknown mixing coefficients that must be found from solving the homogeneous system of $2N$ linear equations (31). A solution exists only if the determinant of the system constructed from wave functions and derivatives equals to zero. This may only happen at a discrete value of the energy E, which is the energy of a bound state. Hence we have a procedure searching for the energy of bound states. First, the energy intervals, where the determinant changes sign, are defined. Then the search for zero of the determinant within the energy interval gives the bound state

energy. Knowing sets of solutions for this energy we can arbitrarily fix one of the mixing coefficients (say by putting it equal to unity) and the rest of them can be found by solving the inhomogeneous system of $(2N-1)$-equations obtained from (31). Finally a bound state wave function, obtained as linear combination of $\psi_{in}^{reg}(r)$ and $\psi_{in}^{irr}(r)$, is normalized to have unit norm.

For continuum states ($E > 0$) the asymptotic form ($r \to \infty$) for linear combinations of radial wave functions from system (5) may be written as

$$\begin{aligned} \sum_{p=1}^{N} \psi_{ip}(r)\,\lambda_{pn} &= F_i(k\,r)\,\delta_{in} + G_i(k\,r)\,K_{in} \\ \sum_{p=1}^{N} \psi'_{ip}(r)\,\lambda_{pn} &= k\left(F_i'(k\,r)\,\delta_{in} + G_i'(k\,r)\,K_{in}\right) \end{aligned} \tag{32}$$

Solutions of this system allow us to define the $\boldsymbol{K}$-matrix elements K_{in} and matrix of mixing coefficients $\{\lambda_{pn}\}$ for normalization of linear independent sets of radial functions $\psi_{ip}(r)$. The $\boldsymbol{K}$-matrix is related to the scattering $\boldsymbol{S}$-matrix appearing in formula (4) by the equation

$$\boldsymbol{S} = (1 + \imath\boldsymbol{K})(1 - \imath\boldsymbol{K})^{-1} \tag{33}$$

This procedure gives the $\boldsymbol{S}$ (or $\boldsymbol{K}$) matrix and N independent sets of radial wave functions with necessary asymptotic behaviour.

DISCUSSION

The centrifugal potentials are an important part of the dynamics described by the system of coupled radial Schrödinger equations and usually singled out explicitly. Numerical solutions of Schrödinger equations in regions where motions are under barriers lead to mixing of large and small components that coexist at these conditions. When accuracy of numerical integration is not enough for tracing of different solutions, such mixing may lead to loss of linear independence. This is one of the major problems in numerical solutions of coupled system of equations. The method suggested here, tries to remedy this, and consists of two steps. First, the radial domain is split into finite intervals. A complete set of fundamental solutions has to be obtained at every interval independently on solutions in other intervals. The second step consists in a rearrangement of equations to a set which is less prone to developing numerical instabilities. To this end, the second order equations are reduced to a system of the first order equations. In mathematical textbooks on ordinary differential equations, the general method to transform second order equations $y'' = F(x,y)$ into a double systems of first order equations is usually formulated via introduction of new variables $\gamma = y'$ for the first derivative of solutions y. In our scheme this general idea is developed further taking into account the specific structure of Schrödinger equations. If the function f is a solution of the free Schröedinger equation with centrifugal barrier then the special transformation $\gamma = y'$ - $k\,(f'/f)\,y$ accounts for the influence of centrifugal barriers explicitly and in a most effective way. As the result, centrifugal barriers drop out from the final system of first order differential equations,

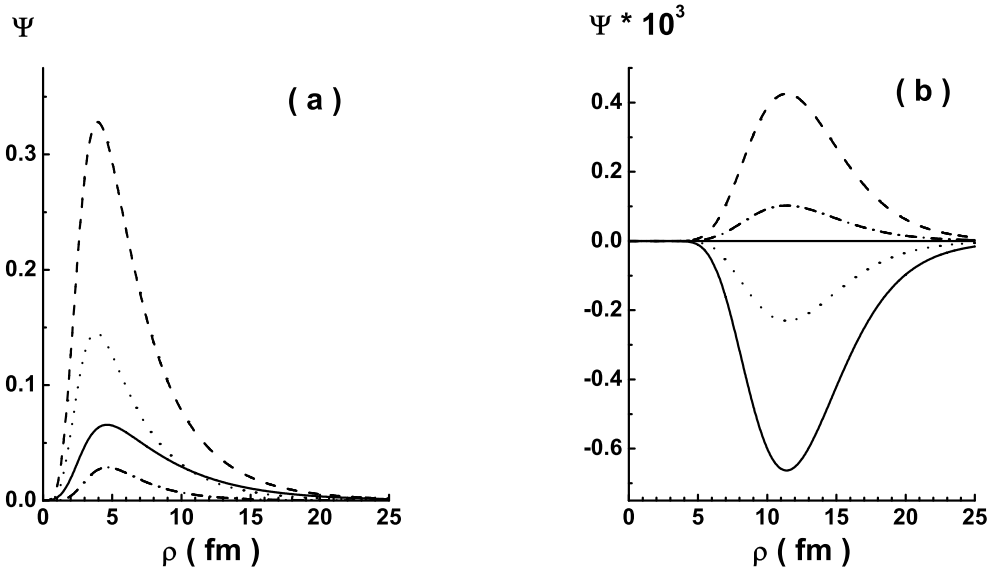

FIGURE 3. Different components of the ^{6}He ground state wave function $\psi^{J\pi}_{KLSl_xl_y}(\rho)$. The solid, dash, dot and dash-dot lines show components with quantum numbers $(K, L = S, l_x = l_y)$ equal to: a) (0, 0, 0), (2, 0, 0), (2, 1, 1) and (4, 0, 2), respectively; and b) (20, 1, 9), (20, 1, 7), (20, 1, 5) and (20, 1, 3), respectively.

and their influence on dynamics appears only via the free solutions appearing as logarithmic derivatives. Since variations of the magnitude of logarithmic derivatives for free solutions are essentially milder, compared to the variations of their absolute values, the conditions for developing numerical instabilities are strongly suppressed.

TABLE 1. Root mean square (r.m.s.) values of hyperradii ($\langle\psi^{J\pi}_{KLSl_xl_y}|\rho^2|\psi^{J\pi}_{KLSl_xl_y}\rangle^{1/2}$) and weights of different components of the ^{6}He ground state wave function. The r.m.s. hyperradius for the whole ground state wave function is equal to 5.55 fm.

K, L = S, $l_x = l_y$	0 0 0	2 0 0	2 1 1	4 0 2	20 1 9	20 1 7	20 1 5	20 1 3
r.m.s. (fm)	6.80	5.40	5.22	5.75	12.36	12.36	12.36	12.36
weight, %	4.1	77.0	14.5	0.6	5.10^{-4}	2.10^{-4}	6.10^{-5}	1.10^{-5}

Below we will demonstrate an application of the new method to solution of a concrete physical problem. A good example is the calculation of the ground state wave functions for light nuclei within cluster few-body models [14]. The method of hyperspherical harmonics is very convenient for description of three-body structure of two-neutron halos

that appears in some nuclei, like the Borromean nuclei ^{6}He, ^{11}Li, etc, at the very edge of nuclear stability (see recent works [15, 16] and references therein for more detailed discussion of successes and challenges of this approach). The relative motion of three clusters is described in the space of hyperspherical coordinates (ρ, Ω_5) and the nuclear wave function $\Psi^{J\pi}$ is decomposed on a basis of hyperspherical harmonics $\Upsilon_{K\nu}(\Omega_5)$ [14], $\Psi^{J\pi}$ = $\sum_{K\nu} \psi^{J\pi}_{K\nu}(\rho)\,\Upsilon_{K\nu}(\Omega_5)$. Here ρ, Ω_5 and K are the hyperradius, hyperangles and the hypermoment, respectively. The index ν denotes all quantum numbers which are necessary, in addition to K, for a complete identification of the basis. If the Schrödinger equation for wave function $\Psi^{J\pi}$ is multiplied by hyperspherical harmonics $\Upsilon_{K\nu}(\Omega_5)$ from the left and integrated over hyperangles Ω_5, a system of coupled hyperradial differential equations similar to (1) is obtained. In this system the effective orbital angular momenta $\mathscr{L}_i$ = K_i + 3/2, where K_i is hypermoment in the i-th channel, and matrix elements $V_{ij}(\rho)$ of the all intercluster interactions in the basis of hyperspherical harmonics, depend only on the hyperradius ρ. More details about development of the model and applied interactions can be found in [17]. As an example, we will consider the calculation of the 0^+ ground state wave function of the ^{6}He nucleus. All possible hyperharmonics up to a value of K = 20 are included in the wave function decomposition, giving a system of Schrödinger equations with $\sim$ 70 coupled channels. A few wave function components with lowest and highest values of hypermoment K are shown in Figures (3(a)) and (3(b)), respectively. Table (1) also gives weights of the respective components and also shows their r.m.s. values of the hyperradius ρ. It is interesting to note the different localization (in hyperradius ρ) of components with different values of the hypermoment K, hence of the generalized orbital angular momentum. Components with larger values of K are more strongly suppressed at small values of the hyperradius, while their maxima are shifted to larger ρ. The r.m.s. values of the hyperradius for each hyperharmonic component are for the largest K values more then two times the value for small K. Note that weights of components that peak far out in the exterior region are rather small. This behaviour is in accordance with intuitive expectations about the role that (centrifugally suppressed) components with high K values should play in the wave function decomposition.

Some questions, important for practical applications, are not discussed in this article. For example, what numerical methods are suited for solving the new system of equations, what partitions of whole radial domain into smaller parts are the most effective (the formulation above was for arbitrary radial intervals) and so on. It is clear that these questions can be answered in different ways and practical prescriptions should take into account the specific features of the problem and should be optimized for any concrete model. To cover these issues, the physical models must be explicitly formulated and thus the scope of this article would have to be essentially expanded. Since our main aim was to present the general idea of the method, these important practical questions will have to be illuminated elsewhere.

CONCLUSION

The dynamics of a system of coupled radial Schrödinger equations may be very versatile and complicated due to coupling potentials, but also carry general features due to universality of the kinetic energy operator. These universal properties are contained in

different centrifugal barriers and lead to appearance of difficulties in numerical solutions of coupled equations in regions where the motion for some channels is classically forbidden. Such classically forbidden regions exist even in cases when coupling potentials are absent, and solutions within such regions are described by Bessel functions with known analytical properties. The absolute scales for free solutions may be very different. Coupling potentials mix and modify free solutions with different absolute values when they are propagated via forbidden regions. If numerical accuracy is not high enough, the propagation leads to development of numerical instabilities in solution vectors. The novel method suggested in this paper rearranges the coupled equations such that free solutions only enter in combinations with minimal variations of absolute values. As a result, the new system is less prone to develop numerical instabilities.

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