2nd South Africa – JINR Symposium
Models and Methods in Few - and Many -Body Systems

S. N. Ershov[1], J. S. Vaagen[2], M. V. Zhukov[3]

Novel method for solution of the coupled radial Schrodinger equations

[1] *Joint Institute for Nuclear Research, Dubna, Russia*
[2] *Institute of Physics and Technology, University of Bergen, Norway*
[3] *Fundamental Physics, Chalmers University of Technology, Goteborg, Sweden*

System of the N coupled radial Schrodinger equations

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

$E \Longrightarrow$ total energy

$\mathcal{L}_i \Longrightarrow$ angular orbital momentum in the channel i

$V_{ij} \Longrightarrow$ $N \times N$ symmetric matrix of coupling potentials

the N linear differential equations of the second order

⇓

the $2N$ linearly independent solutions

⇓

the N solutions have a regular behaviour at origin
while the N others have not

Any solution of the system can be written
as a linear combination of fundamental solutions

Physical meanings have only solutions that satisfy definite boundary conditions imposed at origin and infinity

$$\psi_{in}(r \longrightarrow 0) \longrightarrow 0$$

at infinity the boundary condition depends on the sign of energy E :

For bound state ($E < 0$)

the problem is of eigenvalue type and for any given eigenvalue (E_n) the solution decays exponentially for larger values of r

$$\psi_{in}(r \longrightarrow \infty) \longrightarrow \exp\left(-k_n\, r\right)$$

For continuum states ($E > 0$) solutions oscillate at infinity

$$\psi_{in}(r \longrightarrow \infty) \longrightarrow H^{(-)}_{\mathcal{L}_i}(k\, r)\, \delta_{in} - H^{(+)}_{\mathcal{L}_i}(k\, r)\, S_{in}$$

Coulomb functions : $H^{(\pm)}_{\mathcal{L}_i}(x) = G_{\mathcal{L}_i}(x) \pm \imath\, F_{\mathcal{L}_i}(x)$

General method to solve the boundary value problem for coupled equations :

1. construct a set of linear independent solutions
2. find a linear combinations of these solutions which satisfy the required asymptotic behaviour

Numerical integration within a long radial interval :

⇓

tends to accumulate errors

⇓

facilitates a loss of linear independence of solutions

⇓

convenient to divide the radial space into nonoverlapping domains

$$0 = b_0 < b_1 < \ldots < b_{max} = r_{max}$$

⇓

solve the differential equations separately in each of the intervals

Boundary value problems for a system of ordinary differential equations can be reformulated as a system of Fredholm integral equations

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

$$- \frac{1}{k} g_i(kr) \int_r^\infty dr' f_i(kr') \sum_{j=1}^{N} V_{ij}(r') \psi_{jn}(r') = \delta_{in} \left(f_i(kr)\, C_1 + g_i(kr)\, C_2 \right)$$

For technical reasons it is simpler to solve the Volterra integral equations

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

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

the free Green function $G_0(r, r')$

$$G_0(r, r') = \frac{1}{k}\left(f_i(k\,r)\,g_i(k\,r') - g_i(k\,r)\,f_i(k\,r')\right)$$

the two linear independent solutions $f_i(k\,r)$ and $g_i(k\,r)$
of the free Schrödinger equation

$$\left(\frac{\mathrm{d}^2}{\mathrm{d}r^2} + \frac{2\mathrm{mE}}{\hbar^2} - \frac{\mathcal{L}_i(\mathcal{L}_i+1)}{r^2}\right) f_i(k\,r) = 0$$

Wronskian relation: $W(f_i, g_i) = f_i'(x)\,g_i(x) - g_i'(x)\,f_i(x) = 1$

explicit representation via the Bessel functions

$$E > 0: \quad f_i(x) = \sqrt{\frac{\pi x}{2}}\,J_{\mathcal{L}_i+1/2}(x)\ ;\ g_i(x) = -\sqrt{\frac{\pi x}{2}}\,Y_{\mathcal{L}_i+1/2}(x)$$

$$E < 0: \quad f_i(x) = \sqrt{x}\,I_{\mathcal{L}_i+1/2}(x)\ ;\ g_i(x) = \sqrt{x}\,K_{\mathcal{L}_i+1/2}(x)$$

$\psi^I_{in}(r) \to$ the wave function $\psi_{in}(r)$ on interval I

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

$$= \quad f_i(kr)\,A^I_{in} - g_i(kr)\,B^I_{in}$$

constants A^I_{in} and B^I_{in}

$$A^I_{in} \quad = \quad \delta_{in} + \frac{1}{k}\int_0^{b_{I-1}} dr' g_i(kr') \sum_j V_{ij}(r')\,\psi_{jn}(r')$$

$$B^I_{in} \quad = \quad \frac{1}{k}\int_0^{b_{I-1}} dr' f_i(kr') \sum_j V_{ij}(r')\,\psi_{jn}(r')$$

$\psi^{I}_{in}(r) \rightarrow$ linear combinations of two functions $y^{I}_{ip}(r)$ and $z^{I}_{ip}(r)$

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

the integral equations for functions $y^{I}_{in}(r)$ and $z^{I}_{in}(r)$

$$\begin{aligned} y^{I}_{in}(r) &- \frac{1}{k}\int_{b_{I-1}}^{r} dr' \left(f_i(kr)\, g_i(kr') - g_i(kr)\, f_i(kr') \right) \sum_{j=1}^{N} V_{ij}(r')\, y^{I}_{jn}(r') \\ &= \delta_{in}\, f_i(kr) \\ z^{I}_{in}(r) &- \frac{1}{k}\int_{b_{I-1}}^{r} dr' \left(f_i(kr)\, g_i(kr') - g_i(kr)\, f_i(kr') \right) \sum_{j=1}^{N} V_{ij}(r')\, z^{I}_{jn}(r') \\ &= \delta_{in}\, g_i(kr) \end{aligned}$$

$y^I_{in}(r)$ and $z^I_{in}(r)$ $\rightarrow$ complete system of the $2N$ linear independent solutions of the Schrodinger equations within a radial interval I

the simple recurrence relations for coefficients A^I_{in} and B^I_{in}

$$A^I_{in} = A^{I-1}_{in} + \sum_{p=1}^{N} \left((gVy)^{I-1}_{ip} A^{I-1}_{pn} - (gVz)^{I-1}_{ip} B^{I-1}_{pn} \right)$$

$$B^I_{in} = B^{I-1}_{in} + \sum_{p=1}^{N} \left((fVy)^{I-1}_{ip} A^{I-1}_{pn} - (fVz)^{I-1}_{ip} B^{I-1}_{pn} \right)$$

with initial values $A^1_{in} = \delta_{in}, B^1_{in} = 0$

$$(gVy)^{I-1}_{ip} = \frac{1}{k}\int_{b_{I-2}}^{b_{I-1}} dr' g_i(kr') \sum_{j=1}^{N} V_{ij}(r')\, y^{I-1}_{jp}(r')$$

$$(gVz)^{I-1}_{ip} = \frac{1}{k}\int_{b_{I-2}}^{b_{I-1}} dr' g_i(kr') \sum_{j=1}^{N} V_{ij}(r')\, z^{I-1}_{jp}(r')$$

$$(fVy)^{I-1}_{ip} = \frac{1}{k}\int_{b_{I-2}}^{b_{I-1}} dr' f_i(kr') \sum_{j=1}^{N} V_{ij}(r')\, y^{I-1}_{jp}(r')$$

$$(fVz)^{I-1}_{ip} = \frac{1}{k}\int_{b_{I-2}}^{b_{I-1}} dr' f_i(kr') \sum_{j=1}^{N} V_{ij}(r')\, z^{I-1}_{jp}(r')$$

$f_i(kr)$, $g_i(kr)$ → solutions of the free Schrödinger equation

V_{ii} may be added into the equation to obtain the $f_i(kr)$, $g_i(kr)$

⇓

account a sizeable part of correlations before any attempt to solve the system of coupled equations

⇓

loss a knowledge about analytical properties of $f_i(kr)$, $g_i(kr)$

⇓

a reasonable compromise → constant $V_{ii}(b_{I-1})$ can be added

⇓

$f_i(k_i r)$, $g_i(k_i r)$ → solutions of free Schrödinger equation with the new energy $E_i = E - (\hbar^2/2m)\, V_{ii}(b_{I-1})$ and the linear momentum $k_i = \sqrt{2m|E_i|}/\hbar$

a new integral equations for calculations of local solutions

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

where $V^I_{ij}(r) = V_{ij}(r) - \delta_{ij} V_{ii}(b_{I-1})$

$$a_i, c_i \to y^I_{in}(b_{I-1}) = \delta_{in}\,f_i(kb_{I-1}) \;;\; y^{I\prime}_{in}(b_{I-1}) = \delta_{in}\,k\,f_i'(kb_{I-1})$$

Integral equations define an explicit structure of solutions $y^I_{in}(r)$

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

$\alpha^I_{in}(r), \beta^I_{in}(r) \rightarrow$ **solutions of the system of integral equations**

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

⇓

differential formulation

$\alpha^I_{in}(r), \beta^I_{in}(r) \rightarrow$ **solutions of the system**

(the $2N$ ordinary differential equations of the first order)

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

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

special properties

$$f_i(k_i r)\, \frac{d\alpha^I_{in}(r)}{dr} = g_i(k_i r)\, \frac{d\beta^I_{in}(r)}{dr}$$

a qualitative behaviour of

the regular $f_i(x)$ and irregular $g_i(x)$ functions

closed channels, $E_i < 0$

$f_i(x) \rightarrow$ monotonously increasing with increasing x

$g_i(x) \rightarrow$ monotonously decreasing with increasing x

open channels, $E_i > 0$

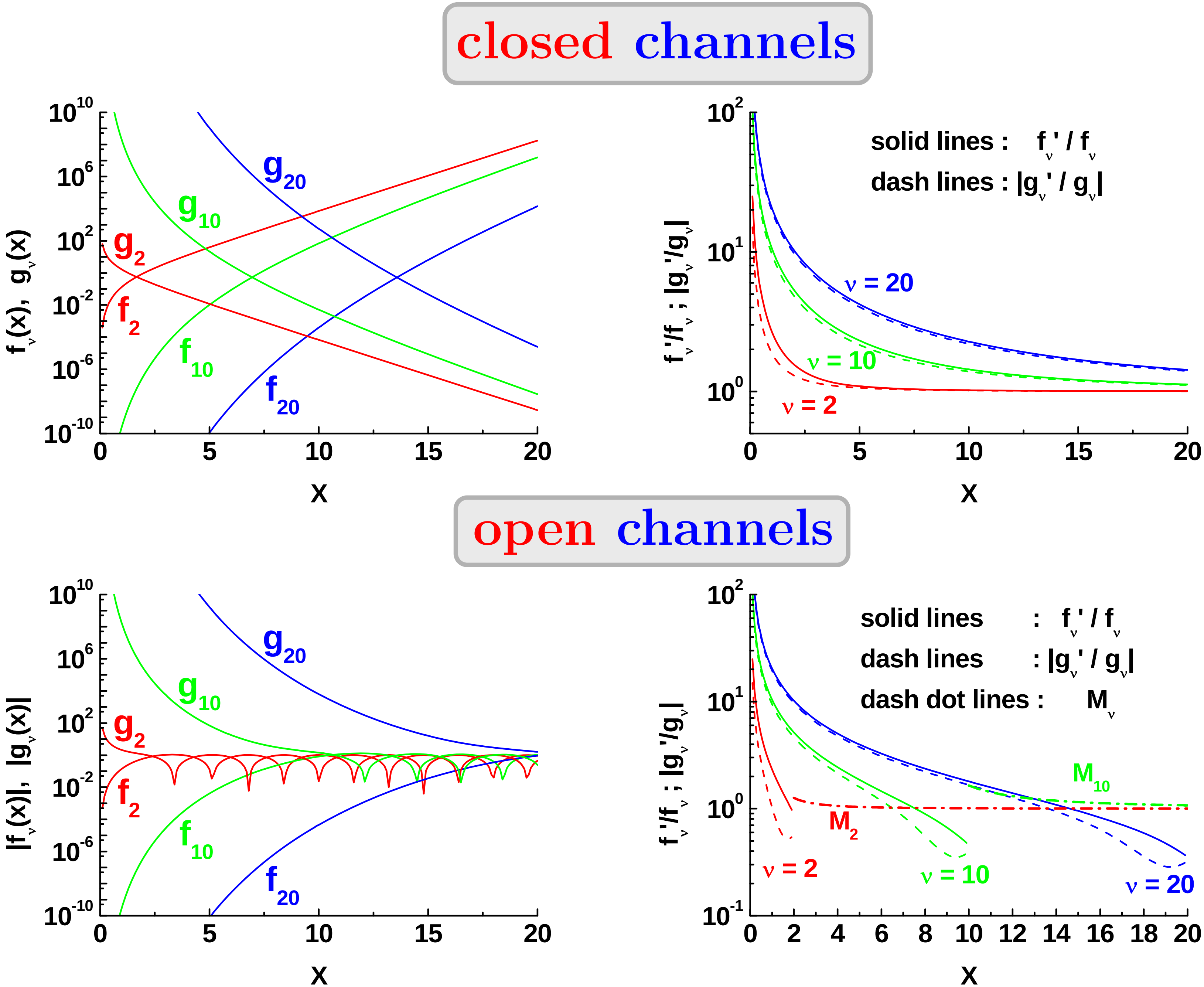
at small arguments

$f_i(x) \rightarrow$ monotonously increasing with increasing x

$g_i(x) \rightarrow$ monotonously decreasing with increasing x

at large arguments $f_i(x)$, $f_i(x) \rightarrow$ oscillate like sin or cos

$$
\begin{aligned}
M_i(x) &= \sqrt{f_i^2(x) + g_i^2(x)} \\
f_i(x) &= M_i(x) \cos\left(\theta_i(x)\right) \\
g_i(x) &= M_i(x) \sin\left(\theta_i(x)\right)
\end{aligned}
$$



closed channels
$f_\nu(x)$, $g_\nu(x)$
g_{20}
g_{10}
g_2
f_2
f_{10}
f_{20}
x
solid lines : f_ν' / f_ν
dash lines : $|g_\nu' / g_\nu|$
f_ν'/f_ν ; $|g_\nu'/g_\nu|$
$\nu = 20$
$\nu = 10$
$\nu = 2$
x
open channels
$|f_\nu(x)|$, $|g_\nu(x)|$
g_{20}
g_{10}
g_2
f_2
f_{10}
f_{20}
x
solid lines : f_ν' / f_ν
dash lines : $|g_\nu' / g_\nu|$
dash dot lines : M_ν
f_ν'/f_ν ; $|g_\nu'/g_\nu|$
M_{10}
M_2
$\nu = 2$
$\nu = 10$
$\nu = 20$
x

the first N_0 channels $\rightarrow f_i(x), g_i(x)$ with monotonic behaviour
(all closed and a part of open channels)
the channels from N_0+1 to N with oscillating behaviour
(a part of open channels)

regular solution $y^I_{in}(r)$

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

for $i \leq N_0$

$$\frac{dy^I_{in}(r)}{dr} = k_i\,\frac{f_i'(k_i\,r)}{f_i(k_i\,r)}\,y^I_{in}(r) + \gamma^I_{in}(r)$$

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

where the function $\gamma^I_{in}(r) = k_i\,\beta^I_{in}(r)/f_i(k_i\,r)$

regular solution for $i > N_0$

$$\frac{dy^I_{in}(r)}{dr} = k_i \frac{M'_i(k_i\, r)}{M_i(k_i\, r)} y^I_{in}(r) + \gamma^I_{in}(r)$$

$$\frac{d\gamma^I_{in}(r)}{dr} = -k_i \frac{M'_i(k_i\, r)}{M_i(k_i\, r)} \gamma^I_{in}(r) + \sum_{j=1}^{N} V^I_{ij}(r)\, y^I_{jn}(r) - \frac{k_i^2}{M_i^4(k_i r)} y^I_{in}(r)$$

where $\gamma^I_{in}(r) = \frac{k_i}{M_i(k_i r)} \left(\sin\left(\theta_i(k_i r)\right) \alpha^I_{in}(r) + \cos\left(\theta_i(k_i r)\right) \beta^I_{in}(r) \right)$

$$y^I_{in}(b_{I-1}) = \delta_{in} f_i(k b_{I-1}) \quad ; 1 \leq i \leq N$$

$$\gamma^I_{in}(b_{I-1}) = \delta_{in} f_i(k b_{I-1}) \left(k \frac{f'_i(k b_{I-1})}{f_i(k b_{I-1})} - k_i \frac{f'_i(k_i b_{I-1})}{f_i(k_i b_{I-1})} \right) \; ; i \leq N_0$$

$$\gamma^I_{in}(b_{I-1}) = \delta_{in} f_i(k b_{I-1}) \left(k \frac{f'_i(k b_{I-1})}{f_i(k b_{I-1})} - k_i \frac{M'_i(k_i b_{I-1})}{M_i(k_i b_{I-1})} \right) ; i > N_0$$

irregular solution $z^{I}_{in}(r)$

for $i \leq N_0$

$$\frac{dz^{I}_{in}(r)}{dr} = k_i \frac{g'_i(k_i r)}{g_i(k_i r)} z^{I}_{in}(r) + \gamma^{I}_{in}(r)$$

$$\frac{d\gamma^{I}_{in}(r)}{dr} = -k_i \frac{g'_i(k_i r)}{g_i(k_i r)} \gamma^{I}_{in}(r) + \sum_{j=1}^{N} V^{I}_{ij}(r)\, z^{I}_{zn}(r)$$

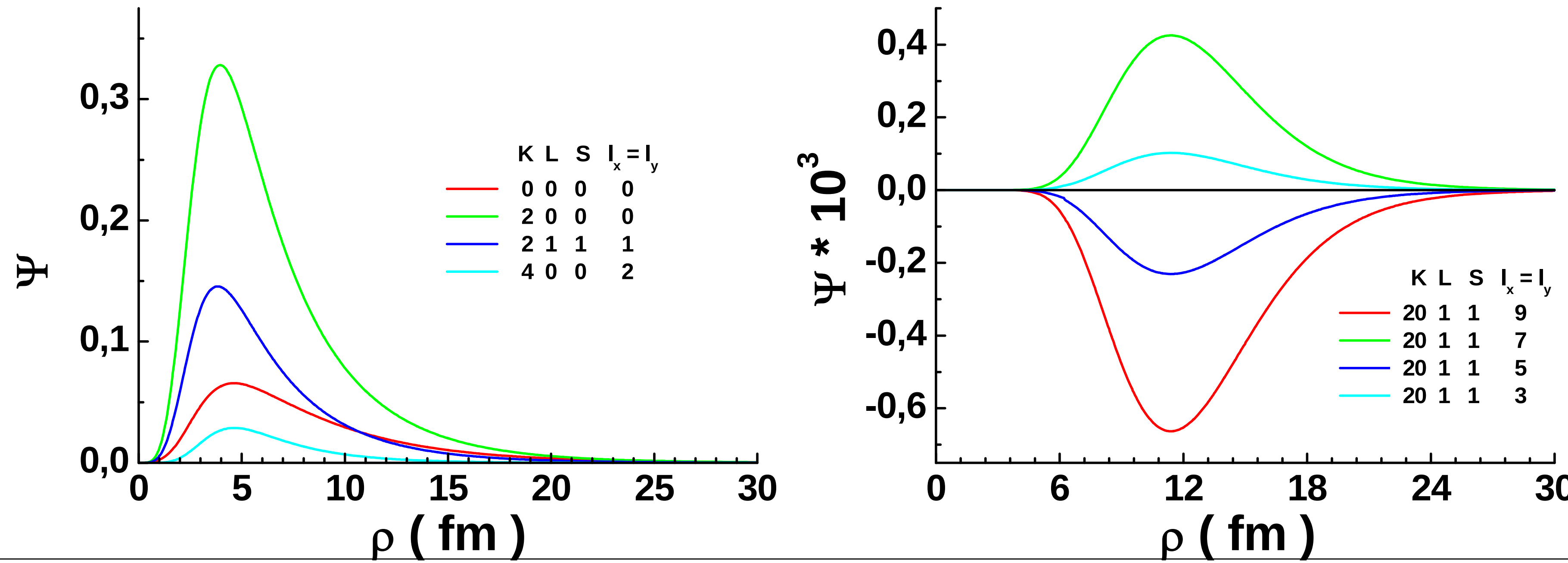
for $i > N_0$ the same system of equations as for regular solution $y^{I}_{in}(r)$

$$z^{I}_{in}(b_{I-1}) = \delta_{in} g_i(kb_{I-1}) \qquad ;1 \leq i \leq N$$

$$\gamma^{I}_{in}(b_{I-1}) = \delta_{in} g_i(kb_{I-1}) \left(k \frac{g'_i(kb_{I-1})}{g_i(kb_{I-1})} - k_i \frac{g'_i(k_i b_{I-1})}{g_i(k_i b_{I-1})} \right) \; ; i \leq N_0$$

$$\gamma^{I}_{in}(b_{I-1}) = \delta_{in} g_i(kb_{I-1}) \left(k \frac{g'_i(kb_{I-1})}{g_i(kb_{I-1})} - k_i \frac{M'_i(k_i b_{I-1})}{M_i(k_i b_{I-1})} \right) ; i > N_0$$

the three-body wave function of the ^{6}He ground state



K L S L	0 0 0 0	2 0 0 0	2 1 1 1	4 0 0 2	20 1 1 9	20 1 1 7	20 1 1 5	20 1 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	$5.\ 10^{-4}$	$2.\ 10^{-4}$	$6.\ 10^{-5}$	$1.\ 10^{-5}$

$\langle r^2 \rangle^{1/2} = 5.55$ fm

CONCLUSIONS

Dynamics of the system of coupled radial Schrodinger equations might be, from one side, very versatile and complicated due to coupling potentials and, from other side, have general features due to universality of the kinetic energy operator. These universal properties are described by 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.

The novel method consists of such a rearrangement of coupled equations that free solutions come in combinations with minimal variations of absolute values. As a result, the new system is less prone for a development of numerical instabilities.