HYPERSPHERICAL APPROACH IN FEW-BODY SYSTEMS

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Calculations have been performed for auto-detached one-particle excited $^{1,3}S$-states of negative hydrogenium ion. Adiabatic approach was applied with channel functions, which were obtained using K-harmonics and by solving the two-dimensional boundary problem. It was shown that the rate of convergence for series with K-harmonics is comparatively low. The revealed auto-detached $^{1,3}S$-states for H^- may be observed in the scattering process of electrons on hydrogenium atoms. Comparative investigations of results received by different methods of calculation for ground and lower excited states of H^- and He have been performed. It was shown that energy level shift, conditioned by non-adiabatic potential is about 10^{-3} a.u.

The investigations of the correlation in hyperspherical coordinate method at the small values of the hyperradius were carried out for the first time by T.Gronwall [1], J.Bartlett [2], V. Fock [3] on the basis of studying the ground state of the helium atom. Several works were devoted to the study of correlation in atomic systems at medium and asymptotic values of hyperradius (see, e.g. the reviews [4-6]).

The non-relativistic Schrödinger equation for three particles is equivalent to the system of equations

$$\begin{cases} \left[-\frac{1}{2\mu}\left(\Delta_\rho + \Delta_\tau\right) + V\left(\vec{\rho}_k, \vec{\tau}_k\right)\right]\Phi\left(\vec{\rho}_k, \vec{\tau}_k\right) = E\,\Phi\left(\vec{\rho}_k, \vec{\tau}_k\right), \\ -\frac{1}{2M}\Delta_{\Re}\varphi\left(\vec{\Re}\right) = \left(\tilde{E} - E\right)\varphi\left(\vec{\Re}\right), \end{cases} \quad (1)$$

where $V(R,\alpha,\theta)$ is the operator of potential energies of system, E is the energy of relative motion $\tilde{E}$ is the total energy of the system, ρ ,τ and $\Re$ are relative Jacobi vectors and vectors of center mass system respectively, which are determined by

$$\vec{\rho}_k = d_k^{-1}\left(\vec{r}_j - \vec{r}_i\right),$$

$$\vec{\tau}_k = d_k\left(\vec{r}_k - \frac{m_i\vec{r}_i + m_j\vec{r}_j}{m_i + m_j}\right), \quad (2)$$

$$\vec{\Re} = \frac{m_1\vec{r}_1 + m_2\vec{r}_2 + m_3\vec{r}_3}{m_1 + m_2 + m_3},$$

μ is the reduced mass of the system, d_k and M are constants, which are expressed by the masses of particles

$$\mu = \left(\frac{m_1 m_2 m_3}{M}\right)^{1/2},$$

$$d_k = \left[\frac{m_k}{\mu}\left(1 - \frac{m_k}{M}\right)\right]^{1/2},$$

$$M = m_1 + m_2 + m_3.$$

The first equation in (1) describes relative motion of the particles, the second is the well known equation of Helmholtz which describes the motion of the center-of-mass system. So, full wave function is the product

of the wave function of relative motion and the wave function of center-of-mass motion ($\Psi(\rho,\tau,\Re)=\Phi(\rho,\tau)\varphi(\Re)$). Now the main problem is to find partial solutions of the first equation of the system (1).

For the ^{1,3}S states of helium-like systems the equation of relative motion in these coordinates has the following form [7]:

$$\left\{-\frac{1}{2\mu}\left[\frac{1}{R^5}\frac{\partial}{\partial R}\left(R^5\frac{\partial}{\partial R}\right)+\frac{4}{R^2}\hat{\Lambda}^2\right]+V(R,\alpha,\theta)\right\}\Psi(R,\alpha,\theta)=E\Psi(R,\alpha,\theta), \quad (5)$$

where

$$\hat{\Lambda}^2\equiv\frac{1}{\sin^2\alpha}\left[\frac{\partial}{\partial\alpha}\left(\sin^2\alpha\frac{\partial}{\partial\alpha}\right)+\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)\right]$$

is the operator of ground angular momentum.

Equation (5) may be solved by using K-harmonics. In this case the wave function $\psi(R,\alpha,\theta)$ is represented in a series

$$\Psi(R,\alpha,\theta)=\sum_{nm}F_{nm}(R)\,\varphi_{nm}(\alpha,\theta), \quad (6)$$

where $F_{nm}(R)$ are unknown radial functions, $\varphi_{nm}(\alpha,\theta)$ are K-harmonics, which are determined by boundary problem

$$\Lambda^2\varphi_{nm}(\alpha,\theta)=-\lambda\varphi_{nm}(\alpha,\theta), \quad (7)$$

with boundary conditions

$$\frac{\partial}{\partial\theta}\varphi_{nm}(\alpha,0)=\frac{\partial}{\partial\theta}\varphi_{nm}(\alpha,\pi)=0,\qquad \varphi_{nm}(0,\theta)=\varphi_{nm}(\pi,\theta)=\delta_{m0}. \quad (8)$$

The problem (7) - (8) may be solved in analytic form and the eigenvalues are given by formula

$$\lambda=(n+m)(n+m+2)=\sigma(\sigma+2), \quad (9)$$

where $\sigma = n + m = 0, 1, 2\ldots$, is quantum number of ground angular momentum, $\rho = m - n$, $(\rho = -\sigma, -\sigma+2,\ldots,\sigma)$ is its project on axis of quantization. Eigenfunctions are given by the formula

$$\varphi_{nm}(\alpha,\theta)=N_{nm}(\sin\alpha)^m\times C_n^{(m+1)}(\cos\alpha)P_m(\cos\theta),$$

where N_{nm} are normalizing factors, $C_n^{(m+1)}(x)$, $P_m(x)$ are Gegenbauer and Legendre polynomials of degree n and m respectively.

We proposed to solve a partial differential equation for the problem of channel functions with corresponding boundary conditions. In the rotation coordinates system for ^{1,3}S-states the equation for adiabatic potentials takes the form [7]

$$\left\{\frac{1}{\sin^2\alpha}\left[\frac{\partial}{\partial\alpha}\left(\sin^2\alpha\frac{\partial}{\partial\alpha}\right)+\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)\right]-\frac{R^2}{2}V(R,\alpha,\theta)+R^2U_\nu(R)\right\}\chi_\nu(R,\alpha,\theta)\equiv L(R,\alpha,\theta)\chi_\nu(R,\alpha,\theta)=0. \quad (10)$$

In adiabatic approach the channel function may be presented as a product of two functions

$$\chi_{nm}(R,\alpha,\theta)=g_n(R,\alpha)f_m(R,\theta), \quad (11)$$

here $g_n(R,\alpha)$ and $f_m(R,\theta)$ are unknown functions, which obey the following conditions

$$\chi_{nm}(0,\alpha,\theta)=g_n(0,\alpha)f_m(0,\theta)=\varphi_{nm}(\alpha,\theta). \quad (12)$$

To solve equation (10) with boundary conditions (12) we take the first step of iteration:

$$\chi_{nm}^{(1)}(R,\alpha,\theta)=g_n^{(1)}(R,\alpha)P_m(\cos\theta),\qquad \left(\chi_{nm}^{(i+j)}(R,\alpha,\theta)=g_n^{(i)}(R,\alpha)f_m^{(j)}(R,\theta)\right) \quad (13)$$

Then to determine $g_n^{(1)}(R,\alpha)$ from (10) we obtain the following equation:

$$\left(f_m^{(0)}, L(R,\alpha,\theta) f_m^{(0)}\right) g_n^{(1)}(R,\alpha) = 0 . \quad (14)$$

Here brackets (,) denote integration over angle θ with the weight function sinθ. By solving equation (14) we obtain $g^{(1)}(\alpha)$ and adiabatic potential $U^{(1)}(R)$. In the second step we put

$$\chi_{nm}^{(2)}(R,\alpha,\theta) = g_n^{(1)}(R,\alpha,\theta) f_m^{(1)}(R,\alpha,\theta) . \quad (15)$$

For determining $f^{(1)}{}_m(R,\theta)$ the following equation is to be used

$$\left(g_n^{(1)}, L(R,\alpha,\theta) g_n^{(1)}\right) f_m^{(1)}(R,\theta) = 0 . \quad (16)$$

In (16) integration is over angle α with the weight function $\sin^2\alpha$. Solving equation (16) we obtain $f^{(1)}{}_m(R,\alpha)$ and adiabatic potential $U^{(2)}(R)$. Let us continue this process until the condition $\left| U^{(k)}{}_{nm}(R) - U^{(k-1)}{}_{nm}(R) \right| < \varepsilon$ is satisfied, ε being the given precision defining for adiabatic potentials. These functions may be used as basic to obtain partial solutions of equation (5). In this case solutions are represented in a series.

$$\Psi(R,\alpha,\theta) = \sum_{\mu=1}^{\infty} F_\mu(R)\, \chi_\mu(R,\alpha,\theta) . \quad (17)$$

For unknown coefficient F it is easy to obtain the system of differential equations

$$\sum_{\nu=1}^{\infty} \left\{ \left[\frac{1}{R^5} \frac{d}{dR}\left(R^5 \frac{d}{dR} \right) + 4U_\mu(R) - 2E \right] \delta_{\mu\nu} - Q_{\mu\nu}(R) - P_{\mu\nu}(R) \frac{d}{dR} \right\} F_\nu(R) = 0 , \quad (18)$$

here P and Q are nonadiabatic potentials, which are determined by channel functions

$$Q_{\mu\nu}(R) = \left\langle \chi_\mu(R,\alpha,\theta) \left| \frac{\partial^2}{\partial R^2} \chi_\nu(R,\alpha,\theta) \right\rangle, \quad P_{\mu\nu}(R) = \left\langle \chi_\mu(R,\alpha,\theta) \left| \frac{\partial}{\partial R} \chi_\nu(R,\alpha,\theta) \right\rangle \right. .$$

The described process has been realized numerically for lower adiabatic potentials, which describe singlet and triplet states of the helium atom and negative hydrogen ion. The received adiabatic potentials for negative hydrogen ion have potential holes, which ensure formation of bound state in singlet state and autodetachment in singlet and triplet states for basic ^{1,3}S-series.The results of calculation of energies in adiabatic and Born-Oppenheimer approximations are represented in Tables 1–2.

As it is seen from the data presented in Table 1, increasing the dimension of basis allows obtaining better results for energies. Moreover, series expansion in K-harmonics (6) has the same value of convergence rate as using channel functions, which are obtained by reduction of problem (10) to solution of the system of homogenous algebraic equations. If we account correlations using channel functions (11), the results would be better in comparison with those received by solving a system of 36 radial equations [8]. This we may also conclude from the results of calculations for ^{1}S(1s^2) and ^{3}S(1s2s) states of helium atom (see Table 2 and [10]). As it is seen from this table, the energy of ^{3}S(1s2s) state is in a very good agreement with experimental data.

The obtained channel functions and radial wave functions allowed us to calculate average and root-mean-square hyperradius values for singlet and triplet states of negative hydrogen ion:

^{1}S(1s^2): $\langle R \rangle \cong 4.056$ a.u.
$\sqrt{\langle R^2 \rangle} \cong 4.471$ a.u.

^{1}S(1s2s): $\langle R \rangle \cong 11.106$ a.u.
$\sqrt{\langle R^2 \rangle} \cong 12.5$ a.u.

^{3}S(1s2s): $\langle R \rangle \cong 9.9$ a.u.
$\sqrt{\langle R^2 \rangle} \cong 10.42$ a.u.

^{3}S(1s3s): $\langle R \rangle \cong 14.57$ a.u.
$\sqrt{\langle R^2 \rangle} \cong 15.62$ a.u.

Table 1. Dependence of energies (-E a.u.) of ground $^{1,3}S$ – states of H^- on n-dimensional basis for channel functions

States	$n(\sigma)$	AA CF [8]	SR CF[8]	Present calculations		
			KH [9]	B-O CF	AA CF	B-O TDB
H^- $^1S(1s^2)$	1(0)			0.3851		0.52686
			0.3854			
	4(2)	0.48084	0.4807	0.4832	0.4793	
			0.4808			
	9(5)	0.50118	0.5026	0.5077	0.5021	
			0.5026			
	36(10)	0.5188	0.5207	0.5283	0.5208	
			0.5251			
	72(15)			0.5320		
			0.52668*			
H^- $^3S(1s2s)$	9(5)			0.3885		0.478
	16(7)			0.4158	0.4128	
	36(11)			0.4455	0.4419	
	64(15)			0.4609		
	100(19)			0.4702		

AA CF - adiabatic approximation using channel functions;
SR CF – system of radial equations using channel functions;
KH – K-harmonics method;
B-O CF – Born-Oppenheimer approximation using channel functions;
B-O TDB – Born-Oppenheimer approximation using two-dimension basis.

Table 2. Dependence of energies (-E a.u.) of ground $^{1,3}S$- states of He on n-dimensional basis for channel functions

States	$n(\sigma)$	KH [9]	Present calculation		Experiment
			B-O CF	B-O TDB	
^1S $(1s^2)$	9(5)	2.8502	2.8670	2.9109	2.9037
	36(10)	2.8936	2.9169		
	121(20)	2.9037			
^3S (1s2s)	9(5)		1.8975	2.175	2.1752
	12(6)		1.8976		
	30(10)		1.8978		

KH - K-harmonics method.

It must be pointed out that the obtained average and root-mean-square hyperradius values slightly depend on the dimension of basis, which is used for obtaining adiabatic potentials and channel functions.

So, we may state that the two-dimensional basis is effective for description of angular and some radial correlations. For more complete account of these correlations one has to solve a system of radial equations (18). Such calculations we are going to perform in our further investigations.

References

1. T.H.Gronwall, *Phys. Rev.* **51**, 655 (1937).
2. J.H.Bartlett, *Phys. Rev.* **51**, 661 (1937).
3. V.A.Fock, *Izv. Acad. Nauk. Ser. Fiz.* **18**, 161 (1954).

4. U.Fano, *Rep. Prog. Phys.* **46**, 97 (1983).
5. C.D.Lin, *Adv. Atom. Mol. Phys.* **22,** 77 (1986).
6. C.D.Lin, *Phys.Rep.* **257**, 1 (1995).
7. M.I.Haysak, M.M.Dovhanich, V.I.Lengyel, V.V.Onysko, *J. Phys. Studies* **1**, 521 (1997).
8. R.Chattopadhyay, T.P.Das, *Phys.Rev. A* **56**, 1281 (1997).
9. T.P.Das, R.Chattopadhyay, *Phys.Rev. A* **50**, 3521 (1994).
10. M.I.Haysak, M.M.Dovhanich, V.V.Onysko, *Uzh. Univ. Scient. Herald, Ser. Phys.* **2**, 61 (1998).

ГІПЕРСФЕРИЧНИЙ ПІДХІД У МАЛОЧАСТИНКОВИХ СИСТЕМАХ

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Вперше проведено розрахунки автовідривних одночастинково збуджених $^{1,3}S$-станів негативного іона водню в адіабатичному наближенні з використанням К-гармонік і розв'язанням двовимірної крайової задачі. Показано, що швидкість збіжності ряду з К-гармоніками досить низька. Виявлені автовідривні $^{1,3}S$-стани для H^- можуть спостерігатись у процесі розсіювання електронів на атомах водню. Проведено порівняння результатів розрахунків енергій основних та нижчих збуджених станів для H^- та He, отриманих різними методами. Показано, що зміщення енергетичних рівнів, зумовлених неадіабатичним потенціалом, становить величину порядку 10^{-3} а.о.