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THE COLLINEAR HELIUM ATOM – HYPERSPHERICAL APPROACH

NENAD SIMONOVIĆ
Institute of Physics, University of Belgrade,
P.O. Box 57, 11001 Belgrade, Serbia
E-mail: simonovic@ipb.ac.rs

Abstract. The collinear helium atom is considered within the quasi-separable hyperspherical approximation. The effective potential curves related to symmetric states are evaluated for the collinear $\theta_{12} = \pi$ configuration. The associated energy levels are found to be in a good agreement with the results obtained using complex rotation calculations.

1. INTRODUCTION

More than forty years ago it was recognized by Macek (1968) that the quasi-separable approximation in hyperspherical coordinates provides a very accurate qualitative description of singly and doubly excited states of two-electron atoms. The two-electron wavefunction is usually described by the six coordinates $r_1, r_2, \hat{r}_1, \hat{r}_2$. In hyperspherical coordinates the individual radial coordinates r_1, r_2 are replaced by the hyperradius $R = (r_1^2+r_2^2)^{1/2}$ and the hyperange $\alpha = \arctan(r_2/r_1)$ ($0 \le \alpha \le \pi/2$) which measure the size of the two-electron state and the radial correlation of the electrons, respectively. The quasi-separable approximation assumes that the R and α-motions are approximately independent what can be justified by inspecting the nodal structure of two-electron wave-function (Starace 1988). The hyperspherical approach is successfully applied in treatments of bound states and resonances of two-electron atomic systems and other Coulomb three-body systems (see Lin 1995 for a review).

Since the radial correlations play a crucial role in the electrons dynamics in atomic systems, for a better understanding sometimes it is more appropriate to consider simplified models where the angular correlations are neglected. In the case of two-electron atoms such models are the collinear models where the mutual angle between the electrons is fixed ($\theta_{12} = 0$ or π). Particularly the most recent semiclassical treatments are based on a collinear model for the classical motion of the electrons (Simonović 2004). However, due to a restricted number of publications regarding an exact quantum-mechanical analysis of collinear models (see e.g. Harabati and Key 2007) the accurate data sets are still incomplete. This work is a contribution in this direction.

2. SCHRÖDINGER EQUATION FOR COLLINEAR TWO-ELECTRON ATOMS IN HYPERSPHERICAL COORDINATES

The Schrödinger equation for the helium-like atom (with the nuclear charge Z) in hyperspherical coordinates reads (in atomic units)

$$\left[-\frac{1}{2}\left(\frac{\partial^2}{\partial R^2}+\frac{5}{R}\frac{\partial}{\partial R}\right)+\frac{\Lambda^2}{2R^2}+\frac{C}{R}-E\right]\Psi=0, \tag{1}$$

where Λ^2 is the so-called grand angular momentum operator (see e.g. Macek 1968 for the full 3D expression) and C/R is the total Coulomb interaction potential among the three charged particles (see e.g. Lin 1995). In the collinear models, however, it is either $\theta_{12} = 0$ or π and, if the total angular momentum is zero, the individual electron's angular momenta are zero, too. In these cases

$$\Lambda^2=-\frac{1}{\sin^2\alpha\cos^2\alpha}\frac{\partial}{\partial\alpha}\left(\sin^2\alpha\cos^2\alpha\frac{\partial}{\partial\alpha}\right), \tag{2}$$

$$C=-\frac{Z}{\cos\alpha}-\frac{Z}{\sin\alpha}+\frac{1}{\sqrt{1\pm\sin 2\alpha}}, \tag{3}$$

where the signs "–" and "+" in Eq. (3) hold for $\theta_{12} = 0$ and π, respectively.

In order to eliminate the first derivative with respect to R in Eq. (1) and simplify the operator Λ^2 we introduce the new function: $\widetilde{\Psi}(R,\alpha)=R^{5/2}\sin\alpha\cos\alpha\,\Psi(R,\alpha)$. Then the Schrödinger equation (1) becomes

$$\left[-\frac{1}{2}\frac{\partial^2}{\partial R^2}-\frac{1}{2R^2}\left(\frac{\partial^2}{\partial\alpha^2}+\frac{1}{4}\right)+\frac{C(\alpha)}{R}-E\right]\widetilde{\Psi}=0\,. \tag{4}$$

For fixed R Eq. (4) reduces to

$$\left[\frac{\partial^2}{\partial\alpha^2}-2RC(\alpha)\right]\Phi_{n_\alpha}(\alpha;R)=U_{n_\alpha}(R)\Phi_{n_\alpha}(\alpha;R), \tag{5}$$

where $\Phi(\alpha;R)$ are the adiabatic eigenfunctions (R appears here as the parameter) and the eigenvalues $U(R)$ ("adiabatic potentials") determine the adiabatic eigenenergies $E(R) = –(U(R)+1/4)/2R^2$. The quantum number $n_\alpha = 0,1,2,\ldots$ labels different solutions of the eigenvalue problem (5). The adiabatic eigenfunctions and eigenvalues are determined by the boundary condition $\Phi_{n_\alpha}=0$ at $\alpha = 0$ (and $\pi/2$).

The functions $\widetilde{\Psi}$ can be expanded in terms of the complete set of adiabatic eigenfunctions Φ_{n_α}

$$\widetilde{\Psi}(R,\alpha)=\sum_{n_\alpha}\Phi_{n_\alpha}(\alpha;R)\,F_{n_\alpha}(R). \tag{6}$$

Substituting this expansion into Eq. (4) one obtains the following set of coupled differential equations for the radial functions F_{n_α}

$$\left[\frac{\partial^2}{\partial R^2}+\frac{U_{n_\alpha}(R)+\frac{1}{4}}{R^2}+2E\right]F_{n_\alpha}+\sum_{n'_\alpha}W_{n_\alpha n'_\alpha}F_{n'_\alpha}=0\,, \tag{7}$$

where

$$W_{n_\alpha n'_\alpha}F_{n'_\alpha}=\left\langle\Phi_{n_\alpha}\left|\frac{\partial^2}{\partial R^2}\right|\Phi_{n'_\alpha}\right\rangle F_{n'_\alpha}+2\left\langle\Phi_{n_\alpha}\left|\frac{\partial}{\partial R}\right|\Phi_{n'_\alpha}\right\rangle\frac{\partial F_{n'_\alpha}}{\partial R}\,. \tag{8}$$

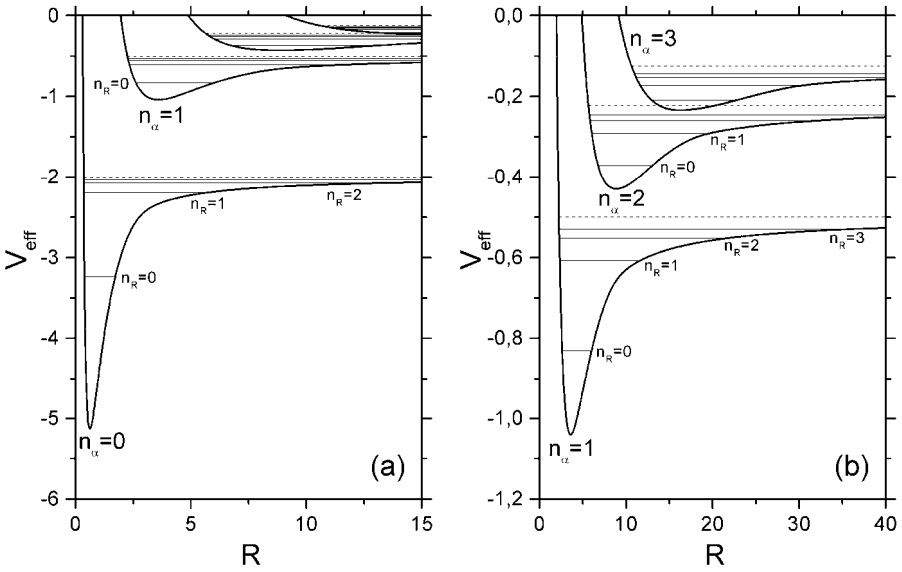

Figure 1: The effective hyperspherical potential curves for the collinear $\theta_{12} = \pi$ helium atom (Z = 2) associated to symmetric states with: (a) n_α = 0,1,2,3 and (b) n_α = 1,2,3, and the corresponding energy levels for n_R = 0,1,2,3 (see also Table 1). The dashed lines denote ionization thresholds.

3. THE QUASI-SEPARABLE APPROXIMATION

Each of the potentials $U_{n_\alpha}(R)$ and the corresponding eigenfunction Φ_{n_α} define a hyperspherical channel n_α. The channels are coupled through the matrix elements $W_{n_\alpha n'_\alpha}$. In a quasi-separable hyperspherical approximation one ignores the coupling terms with $n_\alpha \neq n'_\alpha$ and the radial functions F_{n_α} are solutions of the equation

$$\left[-\frac{1}{2}\frac{\mathrm{d}^2}{\mathrm{d}R^2}+V_{\mathrm{eff}}^{(n_\alpha)}(R)-E_{n_\alpha n_R}\right]F_{n_\alpha n_R}(R)=0\,, \tag{9}$$

where $V_{\text{eff}}^{(n_\alpha)}(R) = -(U_{n_\alpha}(R) + 1/4)/2R^2 - W_{n_\alpha n_\alpha}/2$ are the effective hyperspherical potential curves. For a given hyperspherical channel n_α the quantum number n_R = 0,1,2,… labels different solutions of the radial Eq. (9). Results for symmetric (singlet) states of the collinear helium atom ($\theta_{12} = \pi$ configuration) are shown in Fig. 1 and in Table 1.

Table 1. Energy levels (in atomic units) related to symmetric (singlet) states of the collinear helium atom ($\theta_{12} = \pi$ configuration) calculated using the quasi-separable hyperspherical approximation. The results are compared to results obtained using the more accurate complex rotation treatment.

n_α	n_R	N	n	hyperspherical	complex rotation (Simonović 2004)
0	0	1	1	–3.2388	–3.2459
	1		2	–2.1935	–2.2028
	2		3	–2.0745	–2.0773*
	3		4	–2.0389	–2.0401*
1	0	2	2	–0.8312	–0.8224
	1		3	–0.6091	–0.6098
	2		4	–0.5517	–0.5535*
	3		5	–0.5298	–0.5310*
2	0	3	3	–0.3723	–0.3662
	1		4	–0.2916	–0.2890
	2		5	–0.2595	–0.2603
	3		6	–0.2454	–0.2465*
3	0	4	4	–0.2101	–0.2061
	1		5	–0.1727	–0.1695
	2		6	–0.1529	–0.1532
	3		7	–0.1435	–0.1441

* the complex rotation results obtained by the author

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References

Harabati, C. and Key, K. G.: 2007, *J. Chem. Phys.*, **127**, 084104.

Lin, C. D.: 1995, *Phys. Rep.*, **257**, 1.

Macek, J.: 1968, *J. Phys. B*, **2**, 831.

Simonović, N. S.: 2004, *22th SPIG, Book of Contributed Papers*, ed. Hadžievski Lj. (Vinča Institute of Nuclear Sciences, Belgrade), 97.

Starace, A. F.: 1988, *Fundamental Processes in Atomic Dynamics*, eds. Briggs J.S., Klein-po-ppen H., and Lutz H.O. (Plenum Publishing Corpoation), 235.