كلية العلوم قسم الفيزياء والفلك
مشاريع التخرج --- باكلوريوس
مقرر 499 فيز

Doubly Excited States of Two-Electron Atom in Hyperspherical Adiabatic Approximation

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Introduction

The problem of studying a two-electron atom from the first principlesbased on the separation of variables in the Schrödinger equation for atwo-electron atom. The aim of the work was to study weakly bound Wannier states and to semiclassical calculation of the energy levels of such states. The existence of exact integrals of motion - the total orbital angular momentum of the atom L and parity π it was possible to use theEuler angles describing the rotation of the system as a whole in theseparation of variables. This makes it possible to reduce the problemof analyzing the Schrödinger equation for a two-electron atom foreach definite value of the total orbital angular momentum of the atomL to the solution of a finite system of differential equations in thecollective variables of the problem: the hyperspherical radius hyperspherical angle and the interelectronangle The introduction of these variables makes it possible to use in future their approximate separation, based (and confirmed by numerical and analytical calculations Ojha P. C. [7]) on the hierarchy in the rate of change of the introduced collective variables. The fastest is ,slower α and, finally, the slowest -R. This circumstance, taking into account the localization of the states being explored in the region α≈π⁄4 , ≈π enables us to carry out an approximate adiabaticseparation of the variables , α , R and analytically quantize the two-electron motion with respect to the variables and α. The final solution of the problem consists in quantizing the energy levels of the weakly bound Wannier states of the two-electron atom quasi classical in the hyperradius R.
in this research project we follow the work of Mohamed, A. S. ; Nikitin, S. I. [8] and verify the derivations and calculate some energy values.

Objectives

- Study model of doubly excited states of two electron atom in hyperspherical coordinate system.
- Verification some derivations contained in the original work
- Calculate some energy values
- Compare the results with published calculations.

Theoretical Model

Hamiltonian of the two-electron atom

$$H = -\frac{1}{2}\Delta_1 - \frac{1}{2}\Delta_2 - \frac{Z}{r_1} - \frac{Z}{r_2} + \frac{1}{r_{12}}$$

transformation from a fixed coordinate system to a rotating coordinate system

$$\hat{z} = \left(\vec{r}_1 \times \vec{r}_2\right) / \left|\vec{r}_1 \times \vec{r}\right| \;,\quad \hat{x} = \frac{\vec{r}_1}{r_1} + \frac{\vec{r}_2}{r_2} \;,\quad \hat{y} = \hat{x} \times \hat{z}$$

according to above choice of Euler angles, the Hamiltonian takes the form.

$$H = -1/2 \left\{ \begin{array}{l} \frac{1}{r_1^2}\frac{\partial}{\partial r_1} r_1^2 \frac{\partial}{\partial r_1} + \frac{1}{r_2^2}\frac{\partial}{\partial r_2} r_2^2 \frac{\partial}{\partial r_2} + \left(\frac{1}{r_1^2} + \frac{1}{r_2^2}\right) \\ \left[\frac{1}{\sin\theta_{12}}\frac{\partial}{\partial\theta_{12}}\sin\theta_{12}\frac{\partial}{\partial\theta_{12}} - \frac{\cos\theta_{12}}{2\sin^2\theta_{12}}\left(H_+^2 + H_-^2\right) + \left(\frac{1}{2\sin^2\theta_{12}} - \frac{1}{4}\right)L_z^2 - \frac{L^2}{2\sin^2\theta 12}\right] \\ +i\left(\frac{1}{r_1^2} - \frac{1}{r_2^2}\right)\left[\frac{1}{2\sin\theta_{12}}\left(H_+^2 - H_-^2\right) - L_z\left(\frac{\partial}{\partial\theta_{12}} + \frac{\cos\theta_{12}}{2\sin\theta_{12}}\right)\right] + \frac{2Z}{r_1} + \frac{2Z}{r_2} - \frac{2}{r_{12}} \end{array} \right\}$$

Now transition from variables r_1 and r_2 to hyperspherical coordinates $R = \sqrt{r_1^2 + r_2^2}$, $\alpha = \tan^{-1}(r_1 / r_2)$

the required system of equations will have the form:

$$\left\{ \begin{array}{l} \frac{\partial^2}{\partial R^2} + \frac{1}{R^2}\frac{\partial^2}{\partial\alpha^2} + \frac{1}{R^2\sin^2\alpha\cos^2\alpha}\left[\frac{1}{\sin\theta_{12}}\frac{\partial}{\partial\theta_{12}}\sin\theta_{12}\frac{\partial}{\partial\theta_{12}} - \frac{K^2}{\sin^2\theta_{12}}\right] \\ -\frac{2\left[L(L+1) - 2K^2\right]}{R_{12}^2} + \frac{2Z}{R\sin\alpha} + \frac{2Z}{R\cos\alpha} - \frac{2}{r_{12}} + \frac{1}{4R^2} + 2E \end{array} \right\} f_{LK}^{\pm}(R,\alpha,\theta_{12})$$
$$-\left\{\frac{\sin\theta_{12}}{R_{12}}\frac{\partial}{\partial\alpha} + \frac{2\cos 2\alpha}{R_{12}^2\sin 2\alpha}\left[\cos\theta_{12}\frac{\partial}{\partial\theta_{12}} - \sin\theta_{12} \pm \frac{K+1}{\sin\theta_{12}}\right]\right\}\left[1 \pm \left(\sqrt{2}-1\right)\delta_{K0}\right]\beta_K f_{LK+1}^{\pm}(R,\alpha,\theta_{12})$$
$$+\left\{\frac{\sin\theta_{12}}{R_{12}}\frac{\partial}{\partial\alpha} + \frac{2\cos 2\alpha}{R_{12}^2\sin 2\alpha}\left[\cos\theta_{12}\frac{\partial}{\partial\theta_{12}} - \sin\theta_{12} \mp \frac{K-1}{\sin\theta_{12}}\right]\right\}\left[1 \pm \delta_{K1}\right]\beta_{-K} f_{LK-1}^{\pm}(R,\alpha,\theta_{12}) = 0$$

where

$$\beta_K = \sqrt{(L-K)(L+K+1)} \;,\quad f_{LK}^{\pm}(R,\alpha,\theta_{12}) = R^{5/2}\sin\alpha\cos\alpha\, f_{LK}^{\pm}(r_1, r_2, \theta_{12})$$

Calculations

In the case of Se-state: L=0 , K=0 , $\beta_K = \sqrt{(L-K)(L+K+1)}$ =0

$$\left[\begin{array}{l} \frac{\partial}{\partial R^2} + \frac{1}{R^2}\frac{\partial^2}{\partial\alpha^2} + \frac{1}{R^2\sin^2\alpha\cos^2\alpha}\left(\frac{1}{\sin\theta_{12}}\frac{\partial}{\partial\theta_{12}}\sin\theta_{12}\frac{\partial}{\partial\theta_{12}}\right) \\ +\frac{2z(\sin\alpha + \cos\alpha)}{R\sin\alpha\cos\alpha} - \frac{2\lambda}{R\sqrt{1 - \sin 2\alpha\cos\theta_{12}}} + \frac{1}{4R^2} + 2E_{00} \end{array} \right] f_{00}^{+}(R,\alpha,\theta_{12}) = 0$$

separation of variables allows

$$f_{00}^{+}(R,\alpha,\theta_{12}) = f_{00}^{+}(\theta_{12}) . f_{00}^{+}(R,\alpha)$$

$$\left[\left(\frac{1}{\sin\theta_{12}}\frac{\partial}{\partial\theta_{12}}\sin\theta_{12}\frac{\partial}{\partial\theta_{12}}\right) - \frac{\lambda R}{2\sqrt{1 - \cos\theta_{12}}} + \frac{RZ'}{\sqrt{2}} + \frac{\mu' R^2}{2} + \frac{1}{16}\right] f_{00}^{+}(\theta_{12}) = 0$$

quantum number m=1,2,3,…

$$\left[\frac{\partial^2}{\partial R^2} + \frac{1}{R^2}\frac{\partial^2}{\partial\alpha^2} - \left(c_1 + c_2(\alpha - \pi/4)^2\right) + 2E_{00}\right] f_{00}^{+}(R,\alpha) = 0$$

approximate adiabatic separation of variables allows us

$$f_{00}^{+}(R,\alpha,) = f_{00}^{+}(\alpha) . f_{00}^{+}(R)$$

where $(\alpha - \pi/4) = x = 1$

$$\left[\begin{array}{l} \frac{\partial^2}{\partial x^2} + \left(\nu R^2 + \left(8Z\sqrt{2} - 1/\sqrt{2}\right)R - (2m + 1 + \sqrt{R/\sqrt{2}})^2 + 5/4\right) \\ +\left(\left(24Z\sqrt{2} - 10\sqrt{2}\lambda\right)R - 8\left(2m + 1 + \sqrt{R/\sqrt{2}}\right)^2 + 6\right)x^2 \end{array} \right] f_{00}^{+}(x) = 0$$

Where integer n = 1,2,3, …
Differential equation depending only on the hyperradius

$$\left[\frac{\partial^2}{\partial R^2} + \frac{A}{R} + \frac{B}{R^{3/2}} + \frac{C}{R^2} + 2E_{00}\right] f_{00}^{+}(R) = 0$$

Now the Bhor-Sommerfield quantization condition is:

$$\int_{R_1}^{R_2} \sqrt{E_o - U(R)}\, dR = \pi(2k+1)$$

$$F + J(2E)^{1/2} + H(2E) = 0$$

where the coefficients F, J, H depend in a complex way on the quantum numbers n and m and k.

Results

Energy values for the S-state

K	n	m	-E	R1,1,3Se(N,nα)	R2,1Se (n1,n2)	R3, 1Se(N,n,T,*K*)
2	3	3	0.735	0.775 1Se(2,2a)		
3	3	3	0.585			0.5621Se(3,4,0,2)
6	3	3	0.313	0.3151Se (3,3b)	0.3171Se(3, 3)	
7	3	3	0.265	0.2703Se (3,4b)		
1	4	4	0.310			0.3011Se(4,6,0,3)
2	4	4	0.248		0.2571Se(3, 3)	
3	4	4	0.207			0.2001Se(5,7,0,4)
2	2	3	0.640	0.615 1Se(2,2b)	0.6211Se(2, 2)	
3	2	3	0.502			0.5111Se(3,5,0,2)
5	2	3	0.417			0.4011Se(4,4,0,3)
6	2	3	0.278	0.280 1Se(3,4a)		
7	2	3	0.199			0.2001Se(5,6,0,4)

Conclusions

1-The scheme of separation of variables in the Schrodinger equation, based on a special choice of Euler angles, made it possible to obtain a finite system of differential equations with respect to the dynamic variables of the problem
(θ_{12}, α, R) describing the states of a two-electron atom.
2-Verification of derivations showed consistency with the original work
3-The obtained results for the energy values are in good agreement with the published numerical calculations.

Acknowledgements:

I would like to take this opportunity to thank. Prof. Abdelhay Salah for his guidance in the past few months**.**

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