The four-electron artificial atom with inverse square potential between electrons in 2D space

Archil Lomidze[1] and Shalva Tsiklauri[2]

[1,2] *I. Javakhishvili Tbilisi State University, Department of Physics, av.3 Chavchavadze, 0128, Tbilisi, Georgia.*

Abstract

This work investigates theoretically four-electron QD in 2D spaces using the method of hyperspherical functions, taking account of inverse square potential between particls. Harmonic oscillator has been used as confinement potential.

We have calculated that the binding energy of four-electron system is monotonically depends on the global quantum number. The account of the inverse square potential considerably changes the disposition of energetic levels.

In recent years there has been a great deal of (as well as a growing) interest throughout the physics community in quantum computation and quantum computers (QC) [1], that also direct conected with artificial atoms i.e. quantum dots (QD)'s. (QD)'s are a small number of two dimensional (2D) space electrons confined in semiconductor heterostructure [2]; A particular motivation for studying the properties of few electron quantum dots is their relevance to the rapidly developing field of quantum computing [3].

One- and Two- electron dots in the two-(2D) and three-(3D) dimensional spaces [4] respectively have been studied in detail.

The results on three- and more electron quantum dots were (experimental as well as theoretical) are described in [5]; though by the end of the 20th century considerable results have been obtained on few-body systems taking advantage of using nonmodel approach [6], which enables us to avoid the model approach to simplify the task and instead of postulating to receive a wave function by the solution the equations in a certain approach. As we know few-electron QD are studied theoretically with the above mentioned approach in [7] (where three-electrons QD in the 2D-space is considered with logarithmic potential between the electrons), in [8] (where four-electrons QD in the 2D-space is considered with Coulomb potential between the electrons) and in [9] (where three-electron quantum dot with inverse square potential between particls in 2D space.

Below we shall generalize the hyperspherical function method suggested in [8] to study four-electron QD problem in the 2D-space. At the same time we use inverse square potential between electrons and parabolic type potential - as confinement potential.

Consider four identical particles. The appropriate Jacobian coordinates may be represented by the expression:

$$\vec{X}_{ijk} = \frac{1}{2^{1/6}}\left(\vec{r}_i - \vec{r}_j\right) \qquad \vec{Y}_{ijk} = \frac{1}{2^{2/3}}\left(\vec{r}_k + \vec{r}_l - (\vec{r}_i + \vec{r}_j)\right)$$

$$\vec{Z}_{ijk} = \frac{1}{2^{1/6}}\left(\vec{r}_k - \vec{r}_l\right) \qquad \vec{R} = \frac{1}{2^{2/3}}(\vec{r}_1 + \vec{r}_2 + \vec{r}_3 + \vec{r}_4) , \qquad (1)$$

We introduce the hyperspherical coordinates by the following relations:

$$|\vec{X}| = \rho \cos\alpha \sin\beta; \ |\vec{Y}| = \rho \sin\alpha \sin\beta; \ |\vec{Z}| = \rho\cos\beta$$

where $\alpha, \beta \in [0, \pi/2]$

Let us expand the four-body wave function in the system of the center mass in a four-body hyperspherical functions:

$$\psi(\rho,\alpha,\beta) = \sum_{KK_3(l)M} \chi_{KL}^{(l)K_3}(\rho)\Phi_{KLM}^{(l)K_3}(\Omega_i) \qquad (2)$$

(l)$\equiv$(l$_1$,l$_2$,l$_3$,l$_{12}$) are the appropriate orbital moments, K_3, K – three and four body hypermoments respectively. $\Phi_{KLM}^{(l)K_3}(\Omega_i)$ - in the 2D-space, it is eigenfunctions of square six-dimensional angular moment with eigenvalue $K(K+4)$ and may be represented by the expression:

$$\Phi_{KLM}^{(l)K_3}(\Omega_i) = N_{K_3}^{l_1,l_2}\,\cos^{l_1}\alpha\,\sin^{l_2}\alpha\,P_n^{l_1+l_2+1,l_1+1}(\cos^2\alpha)\,N_K^{l_3,t}\,\cos^{l_3}\beta\,\sin^t\beta\,P_m^{l_3+t+2,l_3+1}(\cos^2\beta)$$

$$Y_{l_1 m_1}(\vec{x})\,Y_{l_2 m_2}(\vec{y})\,Y_{l_3 m_3}(\vec{z}) \qquad (3)$$

where

$$N_{K_3}^{l_1,l_2} = \left[\frac{2(l_1+1)(l_1+2)...(l_1+n)\Gamma(l_1+l_2+1+n)(l_1+l_2+1+2n)}{\Gamma(l_1+1)\Gamma(l_2+1+n)\Gamma(1+n)}\right]^{1/2}$$

$$N_K^{l_3,t} == \left(\frac{2(l_3+1)(l_3+2)...(l_3+m)\Gamma(l_3+t+2+m)}{\Gamma(l_3+1)\Gamma(t+2+m)}\frac{l_3+t+2+2m}{\Gamma(m+1)}\right)^{1/2}$$

and

$$n = \frac{K_3-l_1-l_2}{2}; \quad m = \frac{K-t-l_3}{2}; \quad t^2 = K_3(K_3+2)$$

After inserting (2) and (3) in Schrodinger equation in the system of center mass in the 2D-space we obtained the following set of equations:

$$\left(\frac{\partial^2}{\partial\rho^2} - \frac{(K+2)^2-0,25}{\rho^2} - \frac{2^{1/3}m}{\hbar^2}\left(\frac{b}{2^{2/3}}\rho^2 - E\right)\right)\chi_{KL}^{l_1l_2l_3}(\rho) = \sum_{K'l'_1l'_2'M'}W_{KK'LL'MM'}^{(l)(l')}(\rho)\chi_{K'L'}^{(l')}(\rho) \qquad (4)$$

$$\left[-\frac{\hbar^2}{2^{4/3}m}\left(\frac{\partial^2}{\partial R^2}\right) + R^2\frac{b}{2^{2/3}}\right]\psi(\vec{R}) == E_R\psi(\vec{R}) \qquad (5)$$

where

$$W_{KK'LL'MM'}^{(l)K_3(l')K'_3}(\rho) = \frac{2^{4/3}m}{\hbar^2}\left[J_{KK'LL'MM'}^{(l)K_3(l')K'_3} + \sum_{(\tilde{l})\tilde{K}_3}{}^i\langle(\tilde{l})\tilde{K}_3|(l)K_3\rangle_{KL}^j\,{}^i\langle(\tilde{l})'\tilde{K}'_3|(l)'K''_3\rangle_{KL}^j\,J_{KK'LL'MM'}^{(\tilde{l})\tilde{K}_3(\tilde{l}')\tilde{K}'_3} + \right.$$

$$\left. + \sum_{(\tilde{\tilde{l}})\tilde{\tilde{K}}_3}{}^i\langle(\tilde{\tilde{l}})\tilde{\tilde{K}}_3|(l)K_3\rangle_{KL}^j\,{}^i\langle(\tilde{\tilde{l}})'\tilde{\tilde{K}}'_3|(l)'K'_3\rangle_{KL}^j\,J_{KK'LL'MM'}^{(\tilde{\tilde{l}})\tilde{\tilde{K}}_3(\tilde{\tilde{l}}')\tilde{\tilde{K}}'_3} + ...\right]; \qquad (6)$$

and

$$J_{KK'LL'MM'}^{(l)K_3(l')K'_3} = 2^{-n}\sum_{k_1=0}^{n}\binom{n+l_3+t+2}{k_1}\binom{n+l_3+1}{n-k_1}\times 2^{-n'}\sum_{k_1=0}^{n'}\binom{n'+l'_3+t'+2}{k'_1}\binom{n'+l'_3+1}{n'-k'_1}\times$$

$$\times(-1)^{n+n'-k_1-k_2}\,B\left(\frac{l_3+l'_3}{2},n+n'-k_1-k_2+\frac{t+t'+4}{2}\right)\times$$

$$\times{}_2F_1\left(\frac{l_3+l'_3}{2},-k_1-k_2,n+n'-k_1-k_2+\frac{t+t'+l_3+l'_3+4}{2};-1\right). \qquad (6')$$

where $b^{-1/2}$- is related to the confinement region of electrons in quantum dot, $_2F_1$- is a generalized hypergeometric function, B - is Beta function, ${}^i\langle(\tilde{l})\tilde{K}_3|(l)K_3\rangle_{KL}^j$ -is unitary coefficients of Reynal-Revai [10].

Equation (5) describes the motion center mass of the system. Equation (4) describes relative motion of four-electron confinement system.

We have solved equation (4) in two ways and in both cases we made calculations for zero approximation.

1. In the case of no interacting electron the solution of equation (4) takes form:

$$\psi(\rho) = \frac{G^{(K+3)/4}\rho^{(2K+5)/2}}{\left(\Gamma(N+1)\right)^{1/2}} \exp(-(G)^{1/2}\rho^2/2)\, \frac{1}{\Gamma(N+K+3)} L_N^{K+2}\left((G)^{1/2}\rho^2\right) \tag{7}$$

where $G = \dfrac{m}{\hbar^2}\dfrac{b}{2^{1/3}}$; $L_N^\alpha(\rho)$ -Lager polynomial. E_o –binding energy.

$$E_o = -\frac{\hbar^2(4N+2K+7)}{2^{1/3}\,m}\sqrt{G} \tag{8}$$

We expand exact hyperradial function in terms of basic functions (7):

$$\chi_{KN}^{(l)K_3}(\rho) = \sum_N a_{KN}^{(l)K_3}\psi_{KN}^{0(l)K_3}(\rho) \tag{9}$$

where $\mu = \dfrac{m}{\sqrt[3]{4}}$, N=0, 1, 2,... is global quantum number, the coefficients $a_{KN}^{l_3K_3}$ obey the

normalization condition $\displaystyle\sum_{N=0}^{\infty}\left|a_{KN}^{l_3K_3}\right|^2 = 1$. Then the energy eigenvalues of the relative motion are obtained from the requirement of making the determinant of the infinite system of linear homogeneous algebraic equations vanish:

$$\det\left\|\left(E - E_o^{K'N'}\right)\delta_{KK'}\delta_{(l)(l')}\delta_{K_3K_3'}\delta_{NN'} - I_{KK';LL';MM'}^{(l)(l');K_3K_3'}(1 - \delta_{KK'}\delta_{(l)(l')}\delta_{K_3K_3'}\delta_{NN'})\right\| = 0, \tag{10}$$

where $I_{KK';LL';MM'}^{(l)(l');K_3K_3'}$ is matrix elements of total potential energy.

We have calculated the total energy of the system which equals to sum of motion energy of the system mass center and relative motion energy.

2. In the case of interacting electron the exact solution of equation (4) takes form:

$$\varphi(\rho) = (-1)^{2+2\sqrt{4+G_1}}\left(\frac{2\left(1+\sqrt{4+G_1}\right)G^{1/4}}{\Gamma\left(N+\sqrt{4+G_1}+2\right)\Gamma\left(N+2\sqrt{4+G_1}+3\right)}\right)^{1/2}$$

$$\times \rho^{-5/2}\left\{G^{1/2}\rho^2\right\}^{0.25+0.5\sqrt{4+G_1}}\exp\left\{-\frac{G^{1/2}}{2}\rho^2\right\} L_{1+\sqrt{4+G_1}+N}^{1+\sqrt{4+G_1}}\left((G)^{1/2}\rho^2\right) \tag{11}$$

Where G_1 equal expression (6) for zero approximation.
Binding energy is:

$$E = -\frac{2^{2/3}\hbar^2}{m}G^{1/2}\left(2N+3,5+\sqrt{4+G_1}\right) \tag{12}$$

The dependence of the binding energy of the four-electron system upon the global quantum number (for the ground state S=0) obtained in the results of the solution of expression (8), equation (10) and equation (12) are given in the table.

Dependence of the binding energy of the four-electron system in 2D space upon the global quantum number

Global quantum number N	Binding energy for confinement potential E_o^N (a.u.). [expression (8)]	Binding energy for taking into account inverse square interactions E (a.u.) [equation (10)]	Binding energy according equation (12) taking into account inverse square interactions, E (a.u.)
0	6,3756	6,3756	9,4746
1	10,0188	11,4697	12,6596
2	13,6520	14,2334	15,8446
3	17,2952	18,1268	19,0296
4	20,9384	21,2632	22,2146
5	24,5716	24,9832	25,3996

As it is seen from the table the four-electron system binding energy calculated by the above mentioned two methods are depended monotonically upon the global quantum number, but they differ from each other and this difference decreases with the increase of the global quantum number.

We conclude that the four-electron system binding energy depends monotonically upon the global quantum number. The account of the inverse square potential considerably changes the disposition of energetic levels.

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