Three-electrons quantum dot with inverse square potential between particles in 2D space

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Abstract

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

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

Keywords:
Quantum computer, quantum dot, hyperspherical functions method, few body system.

The last decade has seen an enormous interest in quantum dots (QD) i.e., a small number of two dimensional (2D) space electrons confined in semiconductor heterostructure [1]; A particular motivation for studying the properties of few electron quantum dots is their relevance to the rapidly developing field of quantum computing [2-5].

One- and Two- electron dots in the (2D) and three-dimensional (3D) spaces [6,7] respectively have been studied in detail. The results on three- and more electron quantum dots (experimental as well as theoretical) are described in [8, 9]; though by the end of the 20th century considerable results have been obtained on few-body systems taking advantage of using nonmodel approach [10 and the references indicated here], 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 quantum dot has been studied theoretically using the above mentioned approach in [11] (where three-electrons QD in the 2D-space is considered with logarithmic potential between the electrons) and in [12] (where four-electrons QD in the 2D-space is considered with Coulomb potential between the electrons).

This work investigates theoretically three-electrons QD in 2D spaces using the method of hyperspherical functions, taking account of inverse square potential between particles. Parabolical type potential has been used as confinement potential.

We consider three identical particles. The appropriate Jacobian coordinates may be represented by the expression:

$$\vec{X}_i = \left(\frac{3}{4}\right)^{1/4}\left(\vec{r}_j - \vec{r}_k\right) \;; \qquad \vec{Y}_i = \left(\frac{4}{3}\right)^{1/4}\left(-\vec{r}_j + \frac{\vec{r}_j + \vec{r}_k}{2}\right) \;; \qquad \vec{R} = \left(\frac{1}{3}\right)^{1/4}\sum_{i=1}^{3} m_i r_i \qquad (1)$$

We introduce hyperspherical coordinates by the following relations:

$$|\vec{X}_i| = \rho\cos\alpha;\ |\vec{Y}_i| = \rho\sin\alpha. \text{ Where } -\infty \le \rho \le +\infty;\ 0 \le \alpha \le \pi/2,$$

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

$$\psi(\rho,\alpha) = \sum_{Kl_1l_2M} \chi_{KL}^{l_1l_2}(\rho)\Phi_{KLM}^{l_1l_2}(\Omega_i) \qquad (2)$$

Where l_1,l_2 are the appropriate orbital moments, K – three body hypermoment. $\Phi^{l_1l_2}_{KLM}(\Omega_i)$ - in the 2D-space, it is eigenfunctions of square four-dimentional angular moment with eigenvalue $K(K+2)$ and may be represented by the expression:

$$\Phi^{l_1l_2}_{KLM}(\Omega_i)=C_o\cos^{l_1}\alpha\sin^{l_2}\alpha P_n^{l_1+l_2+1,l_1+1}(\cos^2\alpha) \quad (3)$$

where $n=(K-l_1-l_2)/2$, $C_o=\left[\frac{2(l_1+1)(l_1+2)...(l_1+n)\Gamma(l_1+l_2+1+n)(l_1+l_2+1+2n)}{\Gamma(l_1+1)\Gamma(l_2+1+n)\Gamma(1+n)}\right]^{1/2}$.

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:

$$\left(\frac{\partial^2}{\partial\rho^2}-\left[\frac{2m}{\sqrt{3}\hbar^2}E+\frac{2mb}{3\hbar^2}\rho^2+\frac{(K+2)^2-0{,}25}{\rho^2}\right]\right)\chi^{l_1l_2}_{RL}(\rho)=\sum_{K'l_1'l_2'M'}W^{l_1l_2l_1'l_2'}_{KK'LL'MM'}(\rho)\chi^{l_1'l_2'}_{K'L'}(\rho) \quad (4)$$

$$\left[-\frac{\hbar^2}{2\mu}\left(\frac{\partial^2}{\partial R^2}\right)+b\frac{R^2}{\sqrt{3}}\right]\psi(\vec{R})=E_R\psi(\vec{R}) \quad (5)$$

where

$$W^{l_1l_2l_1'l_2'}_{KK'LL'MM'}(\rho)=\frac{2m}{\sqrt{3}\hbar^2}\left[J^{l_1l_2l_1'l_2'}_{KK'LL'MM'}+\sum_{\tilde{\tilde{l}}_1\tilde{\tilde{l}}_2}{}^{i}\langle\tilde{\tilde{l}}_1\tilde{\tilde{l}}_2\,|\,l_1l_2\rangle^{j}_{kL}\,{}^{i}\langle\tilde{\tilde{l}}_1'\tilde{\tilde{l}}_2'\,|\,l_1'l_2'\rangle^{j}_{KL}J^{\tilde{\tilde{l}}_1\tilde{\tilde{l}}_2\tilde{\tilde{l}}_1'\tilde{\tilde{l}}_2'}_{KK'LL'MM'}+\right.$$

$$\left.+\sum_{\tilde{\tilde{l}}_1\tilde{\tilde{l}}_2}{}^{i}\langle\tilde{\tilde{\tilde{l}}}_1\tilde{\tilde{\tilde{l}}}_2\,|\,l_1l_2\rangle^{j}_{kL}\,{}^{i}\langle\tilde{\tilde{\tilde{l}}}_1'\tilde{\tilde{\tilde{l}}}_2'\,|\,l_1'l_2'\rangle^{j}_{KL}J^{\tilde{\tilde{\tilde{l}}}_1\tilde{\tilde{\tilde{l}}}_2\tilde{\tilde{\tilde{l}}}_1'\tilde{\tilde{\tilde{l}}}_2'}_{KK'LL'MM'}\right] \text{ and } J^{l_1l_2l_1'l_2'}_{KK'LL'MM'}=\int\Phi^{*l_1l_2}_{KLM}(\alpha)U(\alpha)\Phi^{l_1'l_2'}_{K'L'M'}(\alpha)d\alpha$$

where U – is inverse square potential between particles; b-is related to the confinment region of electrons in quantum dot, Γ- is Gamma function, B- is Beta function, ${}^{i}\langle(\tilde{l})\tilde{K}_3\,|\,(l)K_3\rangle^{j}_{KL}$ -is unitary coefficients of Reynal-Revai [10].

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

In the case of noninteracting electron the solution of equation (4) takes form

$$\varphi_{KN}(\rho)=2^{1/2}\{W^{1/2}\rho^2\}^{1/4}\frac{2}{\Gamma(5)}\left(\frac{\Gamma(N+5)}{\Gamma(N+1)}\right)^{1/2}\rho^{-3/2}\{W\rho^2\}^{1{,}75}exp\left\{-\frac{W^{1/2}}{2}\rho^2\right\}\times$$

$$\times F(-N;5;W^{1/2}\rho^2) \quad (6)$$

where $W=\frac{2m}{3\hbar^2}b$; E_o–binding energy.

$$E_o=-\frac{2\sqrt{3}\hbar^2}{m}W^{1/2}(N+2{,}25) \quad (7)$$

where N = 0, 1, 2,... is global quantum number,

We expand exact hyperradial function in terms of basic functions (6):

$$\chi^{l_1l_2}_K(\rho)=\sum_N a^{l_1l_2}_{KN}\varphi^{ol_1l_2}_{KN}(\rho) \quad (8)$$

and the coefficients $a^{l_1l_2}_{KN}$ obey the normalization condition $\sum_{N=0}^{\infty}\left|a^{l_1l_2}_{KN}\right|^2=1$. 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:

$$det\left\|\left(E-E_o^{K'N'}\right)\delta_{KK'}\delta_{l_1l_1'}\delta_{l_2l_2'}\delta_{NN'}-J^{l_1l_1'l_2l_2'}_{KK';LL';MM'}(1-\delta_{KK'}\delta_{l_1l_1'}\delta_{l_2l_2'}\delta_{NN'})\right\|=0, \quad (9)$$

where $J^{l_1l_1'l_2l_2'}_{KK';LL';MM'}$ is matrix elements of total potential energy.

The total energy of the system equals to the sum of center of mass and relative energies. The equations (9) has been solved for the ground state of three-electron system in the singlet state (S=0).

We obtained that the three-electrons QD binding energy is depends monotonically upon the global quantum number, besides taking into account the inverse square potential the disposition of energetic levels is changed.

References:

1. Ch. Sikorski and U. Merkt. Spectroscopy of electronic states in InSb quantum dots. Phys.Rev. Lett. 62, 2164–2167, 1989.

2. Daniel Loss, Eugene V. Sukhorukov, Probing Entanglement and Non-locality of Electrons in a Double-Dot via Transport and Noise. Phys. Rev. Lett. v.84, 1035-1039 (2000). cond-mat/9907129

3. D. Loss and D. P. DiVincenzo, Quantum Computation with Quantum Dots. Phys. Rev. A 57, 120-132 (1998). cond-mat/9701055

4. E. Pazy, E. Biolatti, T. Calarco, I. D'Amico, P. Zanardi, F. Rossi, and P. Zoller Spin-based optical quantum gates via Pauli blocking in semiconductor quantum dots. cond- mat/ 0109337

5. A. Imamoglu, D. D. Awschalom, G. Burkard, D. P. DiVincenzo, B. D. Loss, M. Sherwin, and A. Small, Quantum information processing using quantum dot spins and cavity-QED. Phys. Rev. Lett. 83, 4204 (1999).

6. Jia–Lin Zhu and Jian Wu R. T. Fu, Hao Chen, and Yoshiyuki Kawazoe. Effects of quantum size and potential shape on the spectra of an electron and a donor in quantum dots. Phys. Rev. B 55, 1673–1679 (1997).

7. Jia-Lin Zhu, Zhi-Qiang Li, Jing-Zhi Yu, Kaoru Ohno, Yoshiyuki Kawazoe. Size and Shape effects of quantum dots on two-electron spectra. Phys. Rev. B.55, 15819-15823, (1997).

8. Y. Alhassid. The Statistical Theory of Quantum Dots. Rev. Mod. Phys. 72, 895- 968 (2000), cond- mat/ 0102268

9. K. Varga, P. Navratil, J. Usukura, Y. Suzuki. Properties of few-electron artificial atoms Cond. Matt. 0010 398.

10.R.I. Jibuti, N.B. Krupennikova. metod giperspheric heskix funkcii v kvantovoi mekhanike neckolkikh tel. “mecniereba” Tbilisi, 1984. 180. (in Russion)

11. A Lomidze, Sh. Tsiklauri. The properties of three-electron quantum point. p.758-TU-131. in Proccedings XXI -ICPEAC, Senday, Japan, July, 22-27, II, 1999, 758.

12. A.Lomidze, Sh.Tsiklauri. The properties of four-electron quantum dot. Proceedings of I. Javakhishvili Tbilisi state university. Physics 36, 2001, pp.74-80.