Dirasat, Pure Sciences, Volume **36**, No. **1**, 2009

The Energy Eigenvalues of The Quantum Dot Helium Using The Shifted 1/N Expansion Method (Scientific Note)

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ABSTRACT

The eigenenergies of the low-lying energy levels of a two-dimensional quantum-dot helium are calculated. We have used the shifted 1/N expansion method to solve the relative part Hamiltonian of the quantum-dot helium for various values of coulomb to confinement energies ratio in a zero magnetic field. Based on comprehensive comparisons, the shifted method gives accurate energies compared with the corresponding ones obtained by perturbation, variational, full configuration interaction (FCI), Hartree-Fock (HF) and diagonalization methods.

PACS numbers: 73.21La,03.65Ge

Keywords: Quantum-Dot Helium, 1/N Expansion Technique, Eigenenergies.

1. INTRODUCTION

Quantum Dots (QDs), or artificial atoms, have been the subject of intense experimental and theoretical research studies over the last few years (Burkard et al.,1999, Ciftja and Kumar, 2004, Ciftja and Faruk, 2005, Dybalski and Hawrylak, 2005, El-Said, 1996, El-Said, 1995, Geller et al., 2006,Helle et al., 2005,Kyriadis et al., 2002, Kyriakidis, 2005,Loss and Vincenzo, 1998, Xu and Zhu, 2005). These growing interests are motivated by the physical effects and the potential device applications. The modern progress of nanotechnology gives the possibility to produce QDs with controllable parameters, such as the number of charge carriers, the confinement strength, the shape and size of the QDs.These artificially designed semiconductors QDs can be regarded as building blocks for various electronic and optoelectronic devises such as single-electron transistors, semiconductor lasers, ultrahigh-frequency applications, single photon sources and detectors (Geller et al., 2006). In addition, the QDs are very interesting for future single-electron memories and may be used for implementing logic gates in quantum computing [Burkard et al., 1999, Loss and Vincenzo, 1998]. In our early work (El-Said, 1996), we have studied the electronic properties of a quantum dot presented in a magnetic field. The ratio of the electron coulomb repulsion to the confinement energies is an important parameter that can be adjusted experimentally which produces a quantum dot system with controllable physical properties. Encouraged by the accuracy and efficiency of the 1/N expansion method, in this work we shall use this powerful expansion technique to study the energy levels of the 2*e* QD system, called Helium atom, for a wide range of the ratio parameter (λ) in zero magnetic field. The rest of the work is organized as follows. In section II, we have presented the Hamiltonian theory and calculation method. Results and conclusions have been given in the final section.

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2. THEORY AND CALCULATION METHOD

The Hamiltonian for an interacting pair of electrons confined in a two-dimensional quantum dot-helium by a parabolic potential of the form $\frac{1}{2}\omega_0^2 r^2$, in a zero magnetic field, is written as follows,

$$H = \sum_{i=1}^{2}\left[\frac{\mathrm{P}_i^2}{2\mathrm{m}^*} + \frac{1}{2}m^*\omega_0^2\rho_i^2\right] + \frac{e^2}{\kappa\left|\vec{\rho}_2 - \vec{\rho}_1\right|} \qquad (1)$$

where ω_0 is the confinement frequency and κ is the dielectric constant of the medium, GaAs. $\vec{\rho}_1$ and $\vec{\rho}_2$ describe the positions of the first and second electron in the xy-plane. The energy E is measured in unit of $\hbar\omega_0$. λ is the dimensionless parameter defined as the ratio of the coulomb strength to the confining energy, $\lambda = e^2\alpha/\hbar\omega_0$, where $\alpha = \sqrt{\frac{m\omega_0}{\hbar}}$ has the dimension of inverse length, (Ciftja and Kumar, 2004, Ciftja and Faruk, 2005).

The Hamiltonian in equation (1) can be decoupled to a center-of-mass H_R and relative H_R parts upon introducing the standard coordinates and momenta transformations. The CM-part is a Harmonic oscillator type, $H_R = \frac{P^2}{2M} + \frac{1}{2}M\,\omega_0^2 R^2$ with well-known eigenenergy spectra, $E_{cm} = \left(2n_{cm} + |m_{cm}| + 1\right)\hbar\omega_0$, where $n_{cm} = 0,1,2,....$ and $m_{cm} = 0,\pm1,\pm2,...$. The main issue in the present work is to solve the relative Hamiltonian,

$$H_r = \frac{p^2}{2\mu} + \frac{1}{2}\mu\omega_0^2\,\rho^2 + \frac{e^2}{k\rho} \qquad (2)$$

by using the shifted 1/N expansion method. The steps to produce the eigenenergies by the shifted method are clearly presented in previous References, (El-Said, 1996; El-Said, 1995, Imbo et al., 1984, Imbo and Sukhatme, 1983) and will not be repeated here. The necessary expressions to compute the eigenenergies will be given only. The energy eigenvalues in powers of $1/k$ (up to third order) read as,

$$E_{n,m} = \frac{\lambda}{\rho_0} + \rho_0^2 + \frac{\bar{k}^2}{4\rho_0^2} + \frac{1}{\rho_0^2}\left[\frac{(1-a)(3-a)}{4} + \alpha_1\right] + \frac{\alpha_2}{\bar{k}\rho_0^2} \qquad (3)$$

α_1 and α_2 are parameters expressed in terms of Q, ϖ and quantum numbers n_r and m, .For more details we refer the interested reader to the work published by El-Said., (El-Said, 1996). $\bar{k} = n + |2m| - a$, where N is the spatial dimension, shift parameter $a = 2 - (2n_r + 1)\varpi$ and $\varpi = \left[3 + \rho_0\frac{V''(\rho_0)}{V'(\rho_0)}\right]^{1/2}$. The roots ρ_0 (where the effective potential has a minimum) are determined for particular quantum state $|n_r m\rangle$ and confining frequency ω_0, through the relation:

$$\left[2\rho_0^3 V'(\rho_0)\right]^{1/2} = Q^{1/2} = \bar{k} = \left(2 + 2|m| - a\right) \qquad (4)$$

After obtaining the roots, ρ_0, the eigenenergies can be computed using Eq.(3). n_r is the radial quantum number related to the principal (n) one by the standard relation: $n_r = n - |m| - 1$.

3. RESULTS AND CONCLUSIONS

Our computed results for quantum dot helium system are presented in Tables (1 and 2) and Figure (1). In Table (1), we have listed the ground state energy $|00;00\rangle$ (in units of $\hbar\omega_0$) produced by the shifted method E(1/N) for a wide range of the ratio parameter λ against the results obtained by first order perturbation theory $E^{(1)}$, three parameter variational method E(var.3),exact numerical diagonalization method E(diag.), full configuration

interaction approach E(FCI) (Rontani et al., 2006), and unrestricted Hartree-Fock method E(HF) (Ciftja and Kumar, 2004, Ciftja and Faruk, 2005). The comparisons clearly show excellent agreements between our results against variational, exact numerical diagonalization and FCI methods. Furthermore, exact energy result $E/\hbar\omega_0 = 2$ is obtained for $\lambda = 0$ (non-interacting case). However, the results calculated by the perturbation theory show a clear discrepancy against other methods. This discrepancy can be understood in this way, as the ratio parameter lambda increases the electron-electron interaction term becomes large compared to the confinement energy term and in this case the applicability of the perturbation theory becomes questionable. This clearly shows the advantage of our method over perturbation theory since the shifted 1/N expansion method is valid for all ranges of the ratio parameter λ. We have also presented in Table II the computed energies for first and second excited states of QD-helium atom. In Fig.1, we have shown the dependence of the excited states, $|00;00\rangle$, $|00;01\rangle$ and $|00;02\rangle$, on the ratio parameter λ. Clear enhancements in the energies are seen as λ values increase. These enhancements in the eigenenergies of the QD system are attributed to the increment in the positive coulomb interaction energy comparable to the parabolic confinement one. The plot for the ground state energy gives very good results compared with Fig.(1) of the reported results, (Ciftja and Kumar, 2004, Ciftja and Faruk, 2005).

In conclusion, we have solved the two-dimensional Hamiltonian which describes 2*e* QD-Helium system, in a zero magnetic filed, using the shifted 1/N expansion method. The low-lying energies for various values of coulomb to confinement ratio parameter are calculated. Based on comparisons with different methods: perturbation, variational, exact, full configuration interaction, and Hartree-Fock theory, the shifted 1/N technique gives accurate results for any degree of coulomb to confinement ratio.

Table 1. The ground state energies $|00;00\rangle$ of the quantum-dot helium system are calculated for various range of ratio parameter, λ. The results are computed by: perturbation theory, variational, exact diagonalization, full configuration interaction (Rontani et al., 2006), Hartree-Fock and 1/N methods, (Ciftja and Kumar, 2004, Ciftja and Faruk, 2005) .

λ	$E^{(1)}(\lambda)$	E(var.3)	E(diag.)	E(FCI)	E(HF)	E(1/N)
0	2.00000	2.00000	2.00000			2.0000
1	3.25331	3.00174	3.00097			2.9556
2	4.50663	3.72565	3.72143	3.7295	4.034	3.6706
3	5.75994	4.32576	4.31872			4.2739
4	7.01326	4.85637	4.84780	4.8502	5.182	4.8114
5	8.26657	5.34141	5.33224			5.3016
6	9.51988	5.79354	5.78429	5.7850	6.107	5.7580
7	10.7732	6.22032	6.21129			6.2069
8	12.0265	6.62674	6.61804	6.6185	6.930	6.6000
9	13.2798	7.01626	7.00795			7.0084
10	14.5331	7.39141	7.38351	7.3840	7.686	7.3700

Table 2. The energies (in unit of $\hbar\omega_0$) of first and second excited states for the QD-helium atom calculated by shifted method for various values of λ .

λ	$\|00;01\rangle$	$\|00;02\rangle$
0	3.0000	4.0000
1	3.5944	4.4591
2	4.1376	4.8984
3	4.6410	5.3201
4	5.1127	5.7264
5	5.5590	6.1188
6	5.9834	6.4987
7	6.3889	6.8672
8	6.7792	7.2259
9	7.1561	7.5755
10	7.5208	7.9163

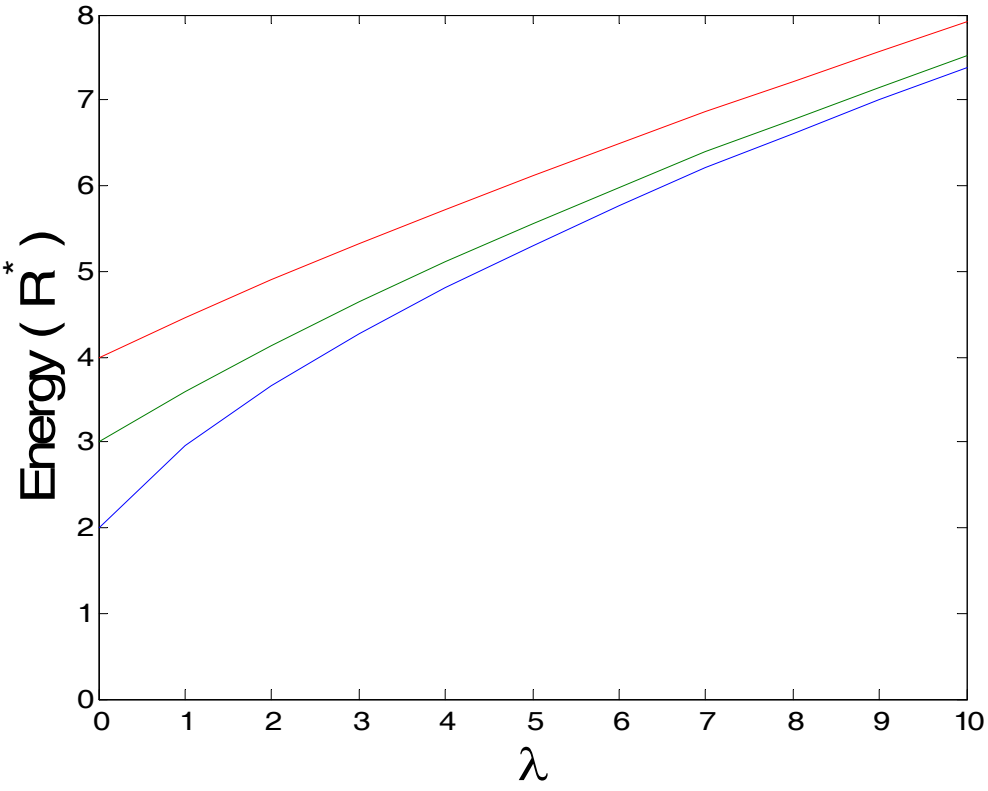

Figure 1. The dependence of the energy levels on the ratio parameter λ for quantum dot Helium. The curves in the plot, starting from the bottom, correspond to: $|00;00\rangle$, $|$ 00:01> and $|00;02\rangle$ states.

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قيم الطاقة المميزة لنقطة هيليوم الكمية باستخدام مفكوك 1/N المزاح
(ملحوظة علمية)

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ملخص

تم حساب قيم الطاقة المميزة لمستويات الطاقة المنخفضة لنقطة هيليوم الكمية ثنائية البعد. قمنا باستخدام مفكوك 1/N المزاح من أجل حل الجزء النسبي من الهاملتونين (دالة الطاقة) لنقطة هيليوم الكمية. حصلنا على الحل وبقيم مختلفة لنسبة طاقة كولوم إلى طاقة الحصر في حالة غياب المجال المغناطيسي. أعطت طريقة المفكوك المزاح قيم طاقة دقيقة مقارنة مع مثيلاتها من النتائج التي تم الحصول عليها بواسطة طرق حسابية متعددة مثل: الاضطراب، التغير، تفاعل الشكل الكامل، هارتري-فوك، الطريقة القطرية.

الكلمات الدالة: نقطة هيليوم الكمية، طريقة مفكوك 1/N وقيم الطاقة المميزة.

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* قسم الفيزياء، كلية العلوم، جامعة حائل، حائل، المملكة العربية السعودية. تاريخ استلام البحث 2007/11/25، وتاريخ قبوله 2008/10/5.