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ORIGINAL PAPER

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The Spectra of a Two-Electron Quantum Dot: Effects of Dimensionality

Abstract: The shifted 1/D expansion method is used to study the spectral properties of two interacting electrons, confined in a quantum dot of two (2D) and three (3D) dimensions. Based on comparisons, the results calculated by 1/D method are in very close agreement with the exact ones.

Keywords: Quantum Dots, Magnetic Field, 1/D Expansion Method. Packs: 73.21 La; 75.60 Lr; 0.3 Ge.

الطيف لإلكترونين في نقطة كمية: تأثير البعد

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لمستخلص: لقد تم إستعمال طريقة مفكوك 1/D المزاح من أجل دراسة الخصائص الطيفية لزوج من الإلكترونات المتشاده والمحصورة في نقطة كمية ذات بعدين وثلاثة أبعاد. أظهرت المقارنة أن النتائج المحسوبة بواسطة طريقة 1/D هي في إتفاق جيد مع مثيلاتها من النتائج المحسوبة بالطرق الدقيقة الأخرى.

كلمات مدخلية: النقاط الكمية المجال المغناطيسي، طريقة مفكوك 1/D

Introduction

Quantum dots (QDs), or artificial atoms, have been the subject of intense experimental (Drexler, *et al.*1994), (Sikorski and Merkt, 1989), (Demel, *et al.* 1990), (Lorke, *et al.* 1990) and (Ashoori, *et al.* 1993) and theoretical (Makysm and Chakraborty, 1990), (Wagner, *et al.* 1992), (Pfannkuche and Gerhardts, 1993), (De Groote, *et al.* 1992), (Merkt, *et al.* 1991), (Pfannkuche and Gerhardts, 1991), (Zhu and Gu, 1993), (Jhonson and Payne, 1991), (Klama and Mishchenko, 1998), (Zhu, *et al.* 1997), (Rotani, *et al.* 1999), (Dineykhan and Nazmitdinov, 1997), (Bryant, 1987), (Zhu, *et al.* 1999), (Animsimovas and Matulis, 1998), (Matulis and Peeters, 1994), (Blanter, *et al.* 1996), (Peeters and Schweigert, 1996), (Oh, *et al.* 1996), and (El-Said, 1995) research over the last few years motivated by the physical effects and the potential device applications, both as electronic memories as well as optoelectronic devices. Different methods have been used to study the energy spectrum and correlation effects of interacting electrons confined in quantum dots under the effect of an applied magnetic field. One of the most interesting features of the electron correlation is the change of the angular momentum and spin structure in the ground state of this QD-system. In most of these works the authors model the QD as a two-dimensional disk, since the confinement in z-direction is assumed to be stronger than in the xy-plane. Recently, two works (Zhu, *et al.* 1997), (Rotani, *et al.* 1999) have reported the effect of dimensionality on the spectra of two electrons confined with parabolic potentials considered as two-dimensional (2D) and three-dimensional (3D) quantum dots. They have shown, in this study, that the electron-electron coulomb interaction energy strongly depends on the dimensionality of the QD and the spectra changes dramatically.

In this work we shall study the spectral properties of 2D and 3D by using the shifted 1/D expansion method. The results of this work are outlined in the following sections. In section II, we present the Hamiltonian theory for two interacting electrons parabolically confined in QD of D-dimensions. We then proceed to produce an eigenenergy expression for any quantum dot state $|n_r m>$. In section III, we present our computed results and give explanations for the energy level crossings, ordering and the dependence of the electron-electron energy, $V_{e\text{-}e}$, on the confinement strength. We test our results produced by 1/D method against exact ones. The conclusion is given in the final section.

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Model

The effective-mass Hamiltonian, $H^{(D)}$, for two interacting electrons, parabolically confined in a quantum dot with dimension D, is given as,

$$H^{(D)} = \sum_{i=1}^{2}\left[-\frac{\hbar^2}{2m^*}\nabla_i^2 + \frac{1}{2}m^*\omega^2 r_i^2\right] + \frac{e^2}{\varepsilon|\vec{r}_2 - \vec{r}_1|}, \quad (1)$$

where ω is the confinement frequency and ε is the dielectric constant of the medium. Upon introducing the center-of-mass (cm) $\vec{R} = (\vec{r}_1 + \vec{r}_2)/\sqrt{2}$ and the relative coordinates $\vec{r} = (\vec{r}_1 - \vec{r}_2)/\sqrt{2}$,the Hamiltonian in Eq.(1) decoupled to the cm motion Hamiltonian,

$$H_R^{(D)} = -\frac{\hbar^2}{2m^*}\nabla_R^2 + \frac{1}{2}m^*\omega^2 R^2, \quad (2)$$

and the relative Hamiltonian,

$$H_r^{(D)} = -\frac{\hbar^2}{2m^*}\nabla_r^2 + \frac{1}{2}m^*\omega^2 r^2 + \frac{e^2}{\sqrt{2}\,r}. \quad (3)$$

Eq.(2) describes the Hamiltonian of the harmonic oscillator with well known eigenenergies,

$$\mathbf{E}_{n_{cm},m_{cm}} = \left(2n_{cm} + |m_{cm}| + \frac{D}{2}\right)\hbar\omega, \quad (4)$$

labelled by the radial (n_{cm}=0,1,2,...) and the azimuthal (m_{cm}=0±1,±2,...) quantum numbers. The total energy states of the Hamiltonian E = $E_R(n_{cm},m_{cm})+E_r(n_r,m)$ are labelled by the cm and relative quantum numbers $|n_r,m;n_{cm},m_{cm}\rangle$. The problem is reduced to solving the relative Hamiltonian $H_r^{(D)}$. The eigenenergies of Eq. (3) are obtained with the help of the shifted 1/D expansion method [25-28]. In D-spatial dimensions the radial Schrödinger equation for the effective potential $V(r) = \frac{1}{4}\omega^2 r^2 + \frac{\sqrt{2}}{r}$ becomes,

$$\left[-\frac{d^2}{dr^2} + \frac{(\bar{k}+a-1)(\bar{k}+a-3)}{4r^2} + V(r)\right]\psi(r) = \mathbf{E}_{n_r,m}\psi(r), \quad (5)$$

where $\bar{k} = D + 2|m| - a$ and is the shift parameter to be determined later. Following the previous work of the shifted 1/D expansion method (El-Said, 1995), we give here only the energy series expansion which is needed to calculate and understand the spectra of $H_r^{(D)}$. More details on 1/D method can be found in (El-Said, 1995), (Imbo, *et al.* 1984), (Imbo and Sukhatme, 1985) and (Dutt, *et al.* 1986). The eigenenergy expression, for D-dimensional QD, then reads as,

$$\mathbf{E}_{n_r,m} = \mathbf{E}^{(0)}_{n_r,m} + \frac{\bar{k}^2}{4r_0} + \frac{1}{r_0^2}\left[\frac{(1-a)(3-a)}{4} + \alpha_1\right] + \frac{\alpha_2}{\bar{k}_0^2}, \quad (6)$$

$$\mathbf{E}^{(0)}_{n_r,m} = \frac{1}{4}\omega^2 r_0^2 + \frac{\sqrt{2}}{r_0}, \quad (7)$$

$$a = 2 - 2(2n_r + 1)\bar{\omega}, \quad (8)$$

$$\bar{\omega} = \left[3 + r_0\frac{V''(r_0)}{V'(r_0)}\right]^{1/2}, \quad (9)$$

and the roots are determined through the relation,

$$D + 2|m| - 2 + 2(2n_r + 1)\bar{\omega} = \left[2r_0^3 V'(r_0)\right]^{1/2}, \quad (10)$$

α_1 and α_2 are parameters calculated in terms of and a with explicit expressions given in the Appendix.

Results and Discussion

Our numerical results are computed for QD made of GaAs and presented in Figs.1 to 4 and Tables I to V. In Figs.1 and 2, we have shown the energies of the states $|n_r,m;n_{cm},m_{cm}\rangle$ for two interacting electrons parabolically confined in the quantum dot as a function of the QD effective length $\ell = \left(\frac{\hbar}{m^*\omega}\right)^{\frac{1}{2}} \sim \omega^{-\frac{1}{2}}$ for 2D and 3D, respectively. These figures coincide with Figs.1 and 2 of Zhu, *et al.* (1997). We observe from the figures that, as $\ell \sim \omega^{-\frac{1}{2}}$ increases the energy level crossings occur and the order of the energy levels significantly changes. For example, the energy levels of 2D QD, calculated at ω 1.0, change their order from: a, b, c, d, e, f, g, h, i, j, k, l, m, n, o, p to: a, b, d, c, h, e, i, f, g, j, k, n, o, p, l, m at ω 0.05. The spectral notations and energies are defined in Table I. The effect of dimensionality on the energy level crossings in the QD spectra is also observed. Calculated results show that the first crossing between the states c= |00;01,0> and d= |0,2;00,0> in the 2D QD occurs at $\omega^{-\frac{1}{2}}$ =2.2 while the same crossing occurs at $\omega^{-\frac{1}{2}} \approx 3.7$ for 3D QD. This finding is in agreement with Rotani, *et al.* (1999). The level crossing can be attributed to the dependence of the electron-electron coulomb interaction energy, $V_{e\text{-}e}$, on the dimensionality of the QD. We have shown, in Fig. 3, $V_{e\text{-}e}$ as a function of ω for different quantum dot states and for D=2 and 3. The coulomb interaction energy, calculated at particular confinement frequency ω, is defined as the difference between the energies of the QD with and without (ω=0) confinement. It is clear from

Figure 3, that the V_{e-e} decreases as the dimensionality of the QD increases. For example, the coulomb interaction energy at ω =0.05 and for |00> relative state is calculated to be 0.1951 R^* and 0.1732 R^* for 2D and 3D QDs, respectively. The coulomb energies for the relative QD-states: |00> , |01> and |02> , calculated at various confinement strength, are also listed in Table II for comparison purposes. Due to the reduction in the electron-electron interaction energy for 3D QD, comparable to 2D QD, the crossing between c and d states in 3D QD occurs at large $\omega^{-\frac{1}{2}} \sim 3.7$ The spectral properties of the QD can be understood from the numerical results listed in Table III and analytical expressions given in Eqs. 6 through 10. In Table III, we have listed the calculated roots r_0 of the 2D and 3D quantum dots for relative states |00> and |03> for various values of confinement frequency ω. The results clearly show that the roots, for fixed ω and particular state, increase as the dimensionality increases from 2 to 3. The dependence of the roots r_0 on the dimensionality D can be also seen from the relation given by Eq.10. The calculations show that, the major contribution (~50%) to the total relative energy $E_{n_r,m}$ is coming from the first energy term Eq.(7), namely,

$$E^{(0)}_{n_r,m} = \frac{1}{4}\omega^2 r_0^2 + \frac{\sqrt{2}}{r_0}, \qquad (7)$$

which is just the sum of parabolic confinement energy $\frac{1}{4}\omega^2 r_0^2$ and repulsive coulomb interaction energy $\sqrt{2}/r_0$. Now, as D increases the roots r_0 also increase and thus the interaction energy decreases. This analytic dependence $v_{e-e} = \sqrt{2}/r_0$ relation of the V_{e-e} on D supports our numerical results and it agrees with the result of Bryant (1987) reported in his significant work. On the other hand the confinement energy, $\frac{1}{4}\omega^2 r_0^2$, enhances as D increases. This energy competition between coulomb and confinement terms leads to the energy level crossings and the transitions in the angular momentum of the ground state of the QD. To see more obviously the influence of dimensionality on the QD spectra, we have ploted in Fig.4 and also listed in Table IV, the ground state eigenenergies |00;00> of the relative Hamiltonian as a function of confinement energy for 2D and 3D QD. It is obvious from the table that the energies enhance as the dimensionality D increases. Our computed results (...) show very good agreement with the exact, perturbation and SH ones reported in Rotani, *et al.* (1999).

In addition to this agreement (Rotani, *et al.* 1999), we compared in Table I the energies of the 2D quantum dot states calculated by 1/D method at various values of against the results calculated by series expansion method (Zhu, *et al.* 1997).The comparison clearly shows that our results are, again, in very good agreement with the results obtained by Zhu, *et al.* (1997) using power series method. Furthermore, the computed eigenenergies of the relative QD states, listed in Table V, recover the exact results of the harmonic oscillator energies as the confinement strength strongly increases: $\omega \to \infty; \omega^{-\frac{1}{2}} \to 0;$ as we mentioned earlier.

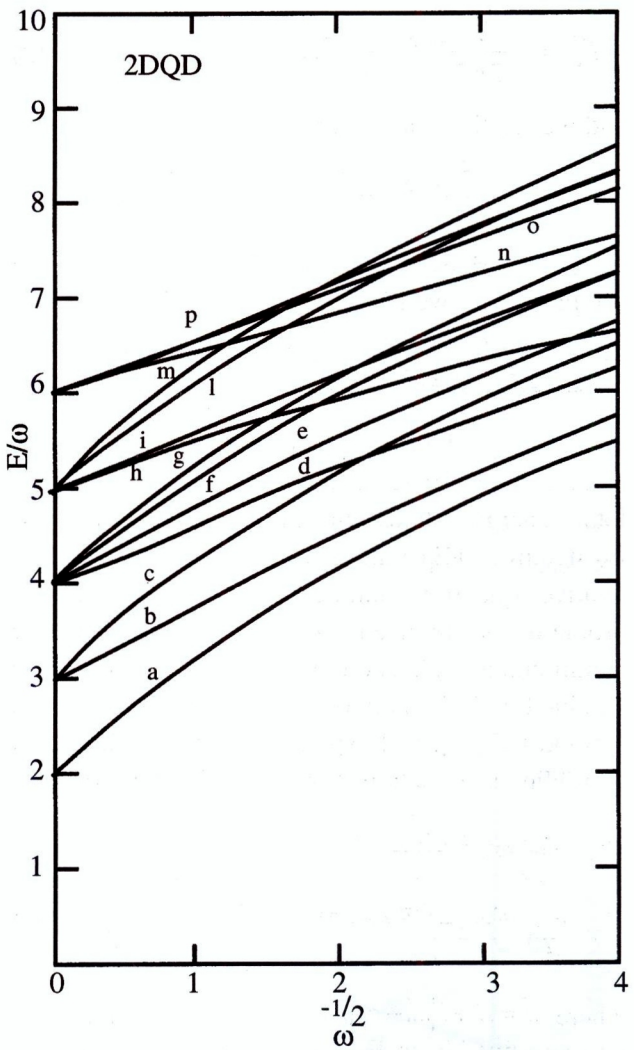

Fig. 1: The energies of the 2D quantum dot scaled bye against, calculated by 1/D expansion method. The spectral notations a,b,c,.... are as defined in Table I.

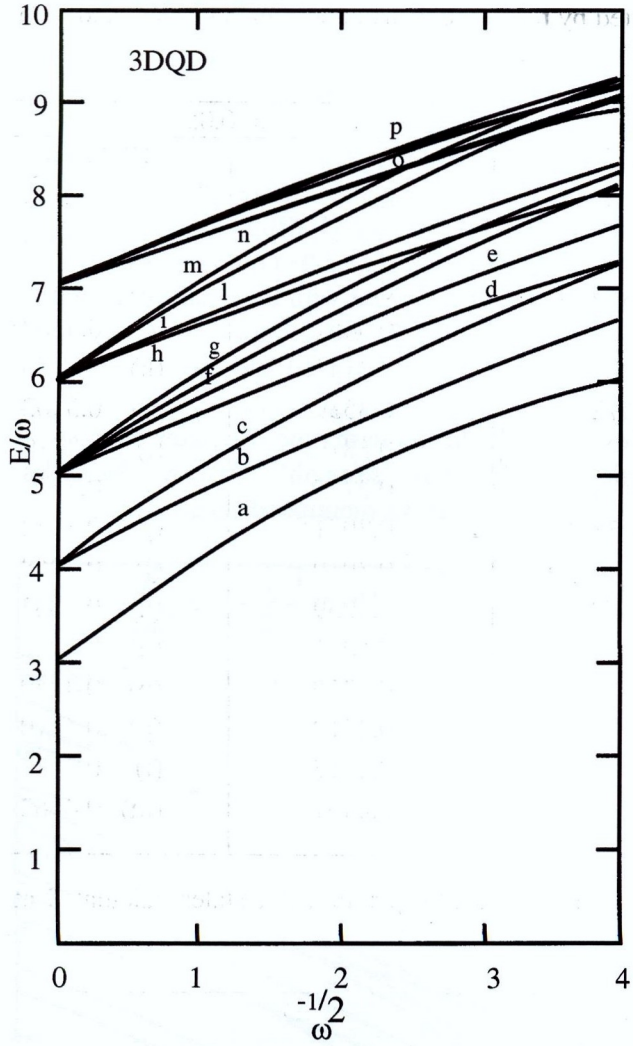

Fig. 2: Same as Fig. 1 except for the energies of the 3D quantum dot.

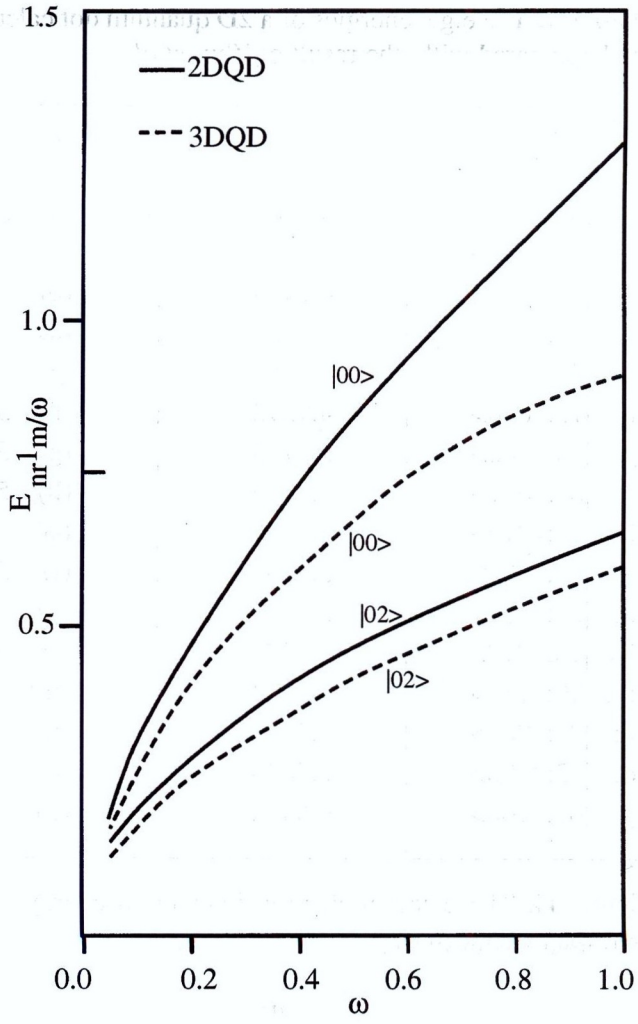

Fig. 3: The electron-electron interaction energies $V_{e\text{-}e}$ in 2D (æ) and 3D (- - -) quantum dots, calculated by the 1/D method at various values of and for |00> and |02> states.

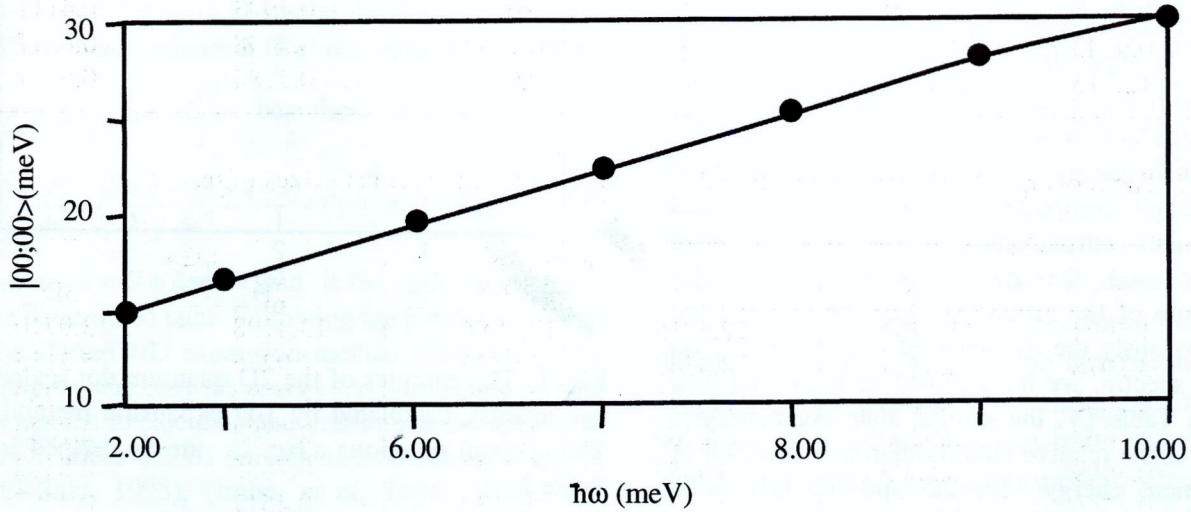

Fig. 4: The ground state energy Ω00;00> calculated by the 1/D method (...) as a function of confinement energy for a) 2D, b) 3D and c) 2D and 3D quantum dots.

Table I: The eigenenergies of a 2D quantum dot calculated by the 1/D expansion method at ω= 1 and 0.05 and compared with the result of Zhu, *et al.*

Quantum Dot State	ω= 1.0		ω= 0.05	
	1/D	Zhu *et.al.*	1/D	Zhu *et.al.*
a: |00; 000	3.2703	(a) 3.3196	0.2952	(a) 0.2962
b: |01; 001>	3.7953	(b) 3.8278	0.3059	(b) 0.3062
c: |00; 010>	4.2408	(c) 4.3196	0.3310	(d) 0.3310
d: |02; 000>	4.6432	(d) 4.6436	0.3451	(c) 0.3462
e: |01; 011>	4.7953	(e) 4.8278	0.3643	(h) 0.3476
f: |10; 000>	4.9292	(f) 5.1472	0.3559	(e) 0.3562
g: |00; 100>	5.2703	(g) 5.3196	0.3810	(ı) 0.3810
h: |03; 001>	5.5136	(h) 5.5174	0.3717	(f) 0.3854
i: |02; 010>	5.6432	(i) 5.6438	0.3951	(g) 0.3962
j: |11; 001>	5.6769	(j) 5.7538	0.3919	(j) 0.3968
k: |01; 101>	5.7953	(k) 5.8278	0.4059	(k) 0.4062
l: |10; 010>	5.9294	(l) 6.1472	0.4061	(n) 0.4066
m: |00; 110>	6.2703	(m) 6.3196	0.4210	(o) 0.4240
n: |04; 000>	6.4782	(n) 6.4693	0.4310	(p) 0.4310
o: |12; 000>	6.5844	(o) 6.5956	0.4217	(l) 0.4354
p: |02; 100>	6.6432	(p) 6.6436	0.4451	(m) 0.4462

Table II. The electron-electron interaction energy $V_{e\text{-}e}$ in 2D and 3D quantum dot states calculated at different values of ω .

	2D			3D		
w	00>	|01>	|02>	|00>	|01>	|02>
0.05	0.1951	0.1559	1.1310	1.1732	0.1421	0.1219
0.1	0.3048	0.2327	0.1913	0.2634	0.2094	0.1770
0.2	0.4732	0.3440	0.2774	0.3969	0.3059	0.2553
0.3	0.6100	0.4306	0.4348	0.5022	0.3806	0.3155
0.4	0.7290	0.5040	0.3998	0.5921	0.4437	0.3663
0.5	0.8361	0.5690	0.4492	0.672	0.4993	0.4111
0.6	0.9345	0.6278	0.4939	0.7447	0.5498	0.4517
1.0	1.2715	0.8251	0.6433	0.9896	0.7184	0.5871

Table III. The roots r_0 of 2D and 3D quantum dot-states calculated at various values of ω.

	|00>		|01>		|02>	
ω	2D	3D	2D	3D	2D	3D
0.05	11.5694	11.9466	12.3915	12.8884	13.4198	13.9710
0.3	3.7978	4.0514	4.3342	4.6286	4.9236	5.2135
0.5	2.7882	3.0100	3.6841	3.4970	3.7390	3.9739
1.0	1.8463	2.0280	2.2186	2.4069	2.5882	2.7629
10	0.4999	0.5803	0.6553	0.7245	0.7885	0.8482
30	0.2766	0.3271	0.3726	0.4139	0.4517	0.4867
50	0.2112	0.2515	0.2873	0.3195	0.3490	0.3763
70	0.1770	0.2117	0.2422	0.2697	0.2947	0.3178

Conclusion

In conclusion, we have studied the spectral properties of QD for 2D and 3D using the shifted 1/D expansion method. We have shown the dependence of the electron-electron interaction energy on the dimensionality of the QD. An explanation is given for the energy level crossings and transitions in the angular momentum of the ground state of the QD. Based on comparisons, the shifted 1/D expansion method is an accurate and effective tool to produce and explain the spectral properties of the QD.

Table IV. The scaled ground state |00> energy $E_{oo/}$ calculated by 1/D expansion method at various values of for 2D and 3D quantum dots. The exact values of the harmonic oscillator Hamiltonians in 2D and 3D are indicated by stars.

w	2D	3D
0.05	4.9020	4.9640
0.1	4.0480	4.1340
0.2	3.3660	3.4845
0.3	3.0333	3.1733
0.4	2.8225	2.9802
0.5	2.6722	2.8440
0.6	2.5575	2.7412
1.0	2.2715	2.4896
10	1.4744	1.8385
30	1.2859	1.6896
50	1.2246	1.6549
70	1.1914	1.6313
	1.0000*	1.5000*

Table V. The scaled energies of the states |00 ; 00> and |02 ; 10> calculated by 1/D expansion method at various values of for 2D and 3D quantum dots. The exact values of the harmonic oscillator Hamiltonians in 2D and 3D are indicated by stars.

		|00;00>		|02;10>	
w	w	2D	3D	2D	3D
0.05	4.4721	5.9020	6.4640	8.6200	9.4380
0.30	1.8257	4.0333	4.6740	7.1460	8.0516
0.50	1.4142	3.6722	4.3340	6.8984	7.8222
1.00	1.000	3.2715	3.9896	6.6433	7.5871
10.00	0.3162	2.4744	3.3385	6.2079	7.1887
30.00	0.1826	2.2859	3.1989	6.1205	7.1093
70.00	0.1195	2.1914	3.1313	6.0791	7.0717
		2.0000*	3.0000*	6.0000*	7.0000*

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