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Energy spectra of few-electron quantum dots

E Anisimovas^{†§} and A Matulis^{‡||}

[†] Vilnius University, Sauletekio 9, 2054 Vilnius, Lithuania

[‡] Semiconductor Physics Institute, Gostauto 11, 2600 Vilnius, Lithuania

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Abstract. We present the renormalized perturbation series for the energy spectra of parabolic quantum dots with two to five electrons, taking into consideration the ground and the lowest excited states. A complete classification of asymptotic energy levels is performed and the behaviour of energy levels from the quantum to the semiclassical regime is traced. Comparison between the present results and those from exact numerical Hamiltonian diagonalization indicates a fair accuracy of the proposed method over the whole range of the electron–electron coupling constant and magnetic field values. The results obtained indicate that increasing the number of electrons in a dot leads to more classical behaviour of the system.

1. Introduction

Quantum dots have been studied extensively as low-dimension nanostructures, interesting from the intrinsic theoretical point of view and due to their importance to modern electronic devices [1]. Most of the spectroscopy experiments were carried out on quantum dots with soft parabolic confinement potentials [2]. Such parabolic quantum dots attract attention as simple model systems for electron–electron interaction studies. Although the parabolic quantum dots have some disadvantages as indicated by the Kohn theorem [3], which shows that usually only the centre-of-mass motion can be excited (in absorption and even in tunnelling), the confining potential in a dot is very often rather close to the parabolic one. This is why parabolic dots can serve as a good starting point or a reference for investigations of more sophisticated quantum dots. The small non-parabolicity usually helps to reveal peculiarities of the relative-electron-motion spectrum, which is sensitive to the electron–electron interaction.

Only in the case of a quantum dot with two electrons can an exact analytical solution of the eigenvalue problem for the parabolic dot be obtained [4]. Most of the theoretical investigations were mainly based either on mathematical tricks (which are possible in the case of parabolic dots with two and three electrons [5, 6]) or on the straightforward diagonalization of the Coulomb interaction [7]. Although the latter gives an exact solution of the problem, because the calculations are time consuming it can be applied only in cases with small numbers of electrons in the dots. This is why the construction of approximate solutions is of interest. One such was described in [8] where in the case of a high magnetic field rather accurate results were obtained using the moving Eckardt frame. Recently it was shown [9] that an approximate technique based on the renormalized perturbation series can

[§] Present address: Department of Theoretical Physics, University of Lund, Sölvegatan 14A, S-223 62 Lund, Sweden.

^{||} E-mail: matulis@uj.pfi.lt.

be successfully used for energy spectrum estimations over a wide coupling constant range. Another technique based on Padé approximants [10] was shown to be very successful in the case of a parabolic dot with a small number of electrons. Each of these approximations is based on a technique for interpolating between the perturbation series in the coupling constant and the asymptotic expansion valid in the large-coupling-constant range.

In the present paper, in order to obtain a complete picture of the energy spectrum, including the ground and some excited states, we performed a complete classification of the asymptotic energy levels, paying attention to the symmetry properties of the spin-wave-function part, and constructed the renormalized perturbation series for the energies of quantum dots with two to five electrons on the basis of a rather simple two-term expansion for both limiting regions of the coupling constant.

The present paper is organized as follows. In section 2 the problem is formulated and the perturbation series technique is outlined. The asymptotic series are formulated in section 3 and the spin-wave-function part is constructed for the asymptotic region in section 4. The interpolation technique is described in section 5 and in the last section, section 6, the results for quantum dots with two to five electrons are presented and discussed. In appendix A the algebraic expression for the Coulomb matrix element is given and in appendix B all coefficients which are necessary for construction of the renormalized perturbation series are collected together.

2. Perturbation series

Generally the system of N electrons in a quasi-2D quantum dot is described by the following Hamiltonian:

$$H = \sum_{i=1}^N \left[-\frac{\hbar^2}{2m} \nabla_i^2 + \frac{m\omega_0^2}{2} \mathbf{r}_i^2 \right] + \sum_{i<j}^N \frac{e^2}{\epsilon |\mathbf{r}_i - \mathbf{r}_j|}. \quad (1)$$

Here m stands for the effective electron mass, ϵ is the static dielectric constant and ω_0 is the characteristic frequency of the parabolic confinement potential. For convenience we shall scale the coordinates: $\mathbf{r} \rightarrow a_0 \mathbf{r}$ ($a_0 = \sqrt{\hbar/m\omega_0}$), and measure the energies in dimensionless units of $\hbar\omega_0$. After this transformation, we obtain the dimensionless Hamiltonian

$$H = \frac{1}{2} \sum_{i=1}^N (-\nabla_i^2 + \mathbf{r}_i^2) + \lambda \sum_{i<j}^N \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|} = H_0 + \lambda V \quad (2)$$

with the single dimensionless coupling constant $\lambda = a_0/a_B$ ($a_B = \epsilon\hbar^2/me^2$ is the effective Bohr radius) characterizing the energy spectrum of the electrons in the parabolic quantum dot.

The simplest way to solve the eigenvalue problem is just to use the perturbation series in the coupling constant λ :

$$E(\lambda) = E_0 + E_1 \lambda. \quad (3)$$

The first coefficient is the eigenvalue of the unperturbed Hamiltonian H_0 and can be presented as a sum of non-interacting electron energies:

$$E_0 = \sum_{i=1}^N \varepsilon(i) \quad \varepsilon(i) = 1 + |m_i| + 2n_i \quad (4)$$

where $i = (n_i, m_i, s_i)$ labels the one-electron quantum number set.

The first-order correction E_1 can be estimated in a standard way (see, for instance, [11]) and presented as a sum of two-electron Coulomb matrix elements:

$$\langle ij|V|j'i'\rangle = \delta_{s_i,s_j} \delta_{s_{j'},s_{i'}} \int d^2r_1 \int d^2r_2 \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|} \phi^*(i|\mathbf{r}_1) \phi^*(j|\mathbf{r}_2) \phi(j'|\mathbf{r}_2) \phi(i'|\mathbf{r}_1) \quad (5)$$

where the one-electron wave functions can be expressed in associated Laguerre polynomials:

$$\phi(n, m|r, \varphi) = \sqrt{\frac{2n!}{2\pi(|m| + n)!}} e^{im\varphi} r^{|m|} e^{-r^2/2} L_n^{|m|}(r^2). \quad (6)$$

For numerical estimation of the Coulomb matrix element (5) we used the analogue of the Girvin and Jach expression [12] which is given in appendix A.

When calculating the first-order correction, the main problem is the degeneracy of the zero-order energy levels, because the good quantum numbers of the total angular momentum M and the total spin S are not sufficient for classification of energy levels. That is why we used numerical diagonalization of the degenerate blocks of the above first-order correction matrix. The results obtained—the coefficients E_0 and E_1 —are collected together in appendix B.

3. Asymptotic expansion

In the $\lambda \rightarrow \infty$ case, the kinetic energy of the electron system is small compared to the potential energy. It is known that such systems are strongly correlated and show a tendency to exhibit Wigner crystallization [13]. Monte Carlo results for classical particles in the parabolic dot [14] show that the particles crystallize in a structure composed of concentric rings. When the number of electrons in a dot is small, $N \leq 5$, they fall into a single ring on which the electrons are located equidistantly, separated by the angle $\alpha = 2\pi/N$. The quantum dynamics of such a Wigner crystal can be described by means of the rotation and vibration modes. The general theory of vibration modes is given in [8]. It is based on introducing the moving Eckardt frame and the diagonalization of the vibrational Hamiltonian in the harmonic approach. In the case of a small number of electrons located on a single ring, the vibrational Hamiltonian and the problem of its diagonalization can be significantly simplified by representing the electron coordinates as complex variables $z = x + iy$ and turning them into local electron coordinates on the ring by means of the following transformation:

$$z_n \rightarrow (R + z_n)e^{i\alpha n}. \quad (7)$$

Here n labels the electrons on the ring. We shall follow the simpler method, restricting our consideration by using the following two-term asymptotic expansion:

$$E(\lambda) = c_0\lambda^{2/3} + c_1. \quad (8)$$

The first term of this expansion can be easily obtained by minimizing the potential in (2). The minimization leads to the equilibrium ring radius $R = (\lambda A)^{1/3}$ (where $A = \sum_{n=1}^{N-1} |4 \sin(\alpha n/2)|^{-1}$) which corresponds to the main term $c_0\lambda^{2/3} = 1.5NR^2$ in the asymptotic energy expansion. The next term in expansion (8) corresponds to the ring oscillations. To obtain it, we insert (7) into Hamiltonian (2) and expand the potential into a z -series. This leads to the following second-order correction to the equilibrium potential:

$$V_2 = \frac{1}{2} \sum_{n=1}^N |z_n|^2 + \frac{N}{32A} \sum_{n=1}^{N-1} (3\gamma_n^2 + 3\gamma_n^{*2} + 2|\gamma_n|^2)$$

where

$$\gamma_{nm} = \frac{z_n e^{i\alpha n} - z_m e^{i\alpha m}}{e^{i\alpha n} - e^{i\alpha m}} = \frac{z_n [1 - e^{i\alpha(n-m)}] + z_m [1 - e^{i\alpha(m-n)}]}{4 \sin^2[\alpha(n-m)/2]} \equiv \gamma_{n-m}.$$

Now let us apply the Fourier transform

$$z_n = \frac{1}{\sqrt{N}} \sum_k e^{ik\alpha n} z_k \quad (9)$$

where $k = 0, 1, \dots, N-1$ denotes the vibration modes. Inserting it into the above potential expression and subsequently into (2), after simple but laborious transformation we obtain the following expression for the asymptotic Hamiltonian with the second-order potential corrections:

$$H = \sum_k H_k = \sum_k \left\{ -2 \frac{\partial^2}{\partial z_k \partial z_k^*} + A_k z_k z_k^* + B_k (z_k z_{-k} + z_k^* z_{-k}^*) \right\} \quad (10)$$

where

$$A_k = \frac{1}{2} + \frac{1}{16A} \sum_{n=1}^{N-1} |\sin(\alpha n/2)|^{-3} \sin^2[(k+1)\alpha n/2]$$

$$B_k = \frac{3}{32A} \sum_{n=1}^{N-1} |\sin(\alpha n/2)|^{-3} [\sin^2(\alpha n/2) - \sin^2(k\alpha n/2)].$$

The Hamiltonian is composed of parts H_k which describe the behaviour of both polarizations of the $\pm k$ -modes as a system of four coupled harmonic oscillators. They can be diagonalized in a standard way, just introducing the appropriate variables. Let us separate the real and imaginary parts of the initial variables, and introduce the new variables in the following way:

$$z_k = x + iy \quad z_{-k} = u + iv. \quad (11)$$

In these variables every part H_k of Hamiltonian (10) splits into two terms. The first term is

$$H_k^{(1)} = -\frac{1}{2} \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial u^2} \right) + A_k x^2 + A_{-k} u^2 + 2(B_k + B_{-k})xu \quad (12)$$

while the other part $H_k^{(2)}$ can be obtained simply by making the replacements $x \rightarrow y$ and $u \rightarrow -v$.

$H_k^{(1,2)}$ both have the same eigenvalues, which can be found by the diagonalization of the symmetric matrix

$$\begin{pmatrix} A_k & B_k + B_{-k} \\ B_k + B_{-k} & A_{-k} \end{pmatrix}$$

which defines the quadratic form of the potential term, and leads to the following expression for the eigenfrequencies:

$$\omega_k^{(\pm)} = \sqrt{A_k + A_{-k} \pm \sqrt{[A_k - A_{-k}]^2 + 4[B_k + B_{-k}]^2}}. \quad (13)$$

Thus, since the transformed Hamiltonian corresponds to the set of independent harmonic oscillators, the corresponding vibration wave function Φ can be constructed in a standard way, introducing the 'phonon' creation ($a_{k,\beta}^\dagger$) and annihilation ($a_{k,\beta}$) operators:

$$\Phi = a_{k_1, \beta_1}^\dagger \cdots a_{k_p, \beta_p}^\dagger |0\rangle. \quad (14)$$

The ‘vacuum’ state $|0\rangle$ corresponds to the system’s ground state and the symbol $\beta = 1, 2$ stands for the polarization.

For interpolation purposes it is important to know the wave function’s symmetry properties with respect to the rotation of the electronic ring as a whole. Let us denote this operation by the operator \mathcal{P} . It is evident that the ground state is invariant under this operation, i.e. $\mathcal{P}|0\rangle = |0\rangle$. As the above rotation is equivalent to the substitution $n \rightarrow n + 1$, it follows from expression (9) that $\mathcal{P}z_k = \exp(ik)z_k$. Due to the mixing of the two $\pm k$ -modes, the operators $a_{k,\beta}^\dagger$ and wave function (14) obey a more complicated symmetry condition. However, because of the degeneracy of the vibration states obtained, it can be significantly simplified using the appropriate superposition of the eigenstates of the two Hamiltonian parts $H_k^{(1,2)}$. So, we shall assume that a wave-function superposition of this sort is constructed, and consequently that the phonon operators obey the symmetry condition

$$\mathcal{P}a_{k,\alpha}^\dagger = e^{-ik}a_{k,\alpha}^\dagger. \quad (15)$$

We shall use the above symmetry condition for the classification of the asymptotic vibration modes obtained, whose frequencies $\omega_k^{(\beta)}$ are collected together in table 1.

Table 1. The ring vibration frequencies and the asymptotic expansion coefficients.

k	β :	$N: 2$		3		4		5	
		1	2	1	2	1	2	1	2
0		1.7321	0.0	1.7321	0.0	1.7321	0.0	1.7321	0.0
1		1.0	1.0	1.2247	1.0	1.3186	1.0	1.3719	1.0
2				1.2247	1.0	1.4888	0.8852	1.6890	0.7274
3						1.3186	1.0	1.6890	0.7274
4								1.3719	1.0
	c_0	1.1905		3.1201		5.8272		9.2801	
	$c_1^{(0)}$	1.8660		3.0908		4.3716		5.6544	

Two modes with eigenfrequencies $\omega_k^{(\beta)} = 1$ correspond to the centre-of-mass motion. We do not take them into account as we consider the electron-relative-motion energy spectrum only. The mode $k = 0$ corresponds to the ‘breathing’ mode for $\beta = 1$ and to the rotation of the ring as a whole for $\beta = 2$. The latter case should be considered separately. Actually, in the harmonic approximation used, the rotation mode is separated from the vibration modes. Its eigenfunction is $\exp(iM\varphi)$ (φ is an angle determining the rotation of the ring as a whole) and the corresponding energy is $M^2/2NR^2 \sim \lambda^{-2/3}$. It is seen that in the case of large angular momenta M this term becomes crucial and thus it should be included into the main asymptotic energy term, and consequently it leads to the equilibrium ring radius dependence on the total angular momentum M (see [8], for instance). However, the above term is of order $\lambda^{-2/3}$ and lies beyond the approximation (8). Hence considering the states with small M only, we neglect this rotation mode correction (and the dependence of the ring radius on M as well) together with the anharmonicity corrections which are of the same order of magnitude. We should keep in mind, however, that there are many states labelled by different M -values corresponding to every asymptotic vibration term.

Thus, the first-order correction is given by

$$c_1 = c_1^{(0)} + \sum_{k,\beta} n_{k,\beta} \omega_k^{(\beta)}$$

where $c_1^{(0)}$ is the contribution of the ground-vibration-state energy and the symbol $n_{k,\beta}$ stands for the filling factor of the corresponding phonon mode. These coefficients together with the first-term coefficients c_0 are given in the last two lines of table 1.

Separating the rotation mode, we shall represent the total wave function in the asymptotic region as a product of rotation, vibration and spin parts:

$$\Psi = e^{iM\varphi} \Phi \Upsilon. \quad (16)$$

According to Pauli's principle the total wave function should be antisymmetric. In the asymptotic region the classical electron equilibrium positions are separated by high potential barriers. That is why we will restrict ourselves to the physically important permutation—the rotation \mathcal{P} . As the rotation corresponds to an odd permutation in the case of an even number of electrons (and vice versa), the total wave function obeys the following symmetry condition:

$$\mathcal{P}\Psi = (-1)^{N-1}\Psi. \quad (17)$$

According to (14)–(16), the rotation and vibration parts obey the condition

$$\mathcal{P}e^{iM\varphi} \Phi = e^{i\alpha(M-\gamma)} e^{iM\varphi} \Phi \quad \gamma = \sum'_{k,\beta} kn_{k,\beta}. \quad (18)$$

The prime on the summation indicates that the mode corresponding to the ring rotation is excluded. The different factors in the two above conditions should be compensated by the appropriate choice of the spin-function part.

4. The spin-wave-function part

Following [8], we diagonalize the operator \mathcal{P} in the S_z (total spin z -projection operator) eigenfunction space and construct the spin-function part obeying the symmetry condition

$$\mathcal{P}\Upsilon = e^{i\alpha\tau} \Upsilon \quad (19)$$

which, together with (17) and (18), leads to the following selection rule:

$$M + \tau - \gamma = Np. \quad (20)$$

In the case of an odd number N of electrons in a dot, the symbol p stands for an arbitrary integer, while in the case of even N , it should be replaced by $p + 1/2$. The integer parameter τ which characterizes the spin-function-part symmetry properties should be defined for every particular case. In the case in which the above procedure leads to the degeneracy of spin states, the total spin operator S^2 should be diagonalized additionally.

The case of two electrons is a trivial one. There is the triplet function $|\uparrow\uparrow\rangle$ with $S_z = 1$ corresponding to $\tau = 0$ and the singlet function $\{|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\}/\sqrt{2}$ with $S_z = 0$ corresponding to $\tau = 1$. We shall not consider the functions with $S_z < 0$ as they give no extra information.

The case of three electrons is considered in detail in [8]. There is a quartet state corresponding to $\tau = 0$ and two doublet states with $\tau = \pm 1$.

Applying the same treatment to the systems with four and five electrons we obtain the spin-function parts with the symmetry properties of (19) type. All of the necessary τ -values are collected together in table 2.

Table 2. τ -values for the various multiplets and the ground-state terms.

N	$S = 0$	$S = 1/2$	$S = 1$	$S = 3/2$	$S = 2$	$S = 5/2$	Terms
2	1	—	0	—	—	—	$^1S, ^3P, ^1D, ^3F, \dots$
3	—	1, 2	—	0	—	—	$^4S, ^2P, ^2D, ^4F, \dots$
4	0, 2	—	1, 2, 3	—	0	—	$^{1,3}S, ^3P, ^{1,3}D, ^3F, ^{1,3}G, \dots$
5	—	0, 1, 2, 3, 4	—	1, 2, 3, 4	—	0	$^{2,6}S, ^{2,4}P, ^{2,4}D, ^{2,4}F, ^{2,4}G, \dots$

The above selection rule gives us the possible terms for every vibration state characterized by a γ -value. The terms for the ground vibration state ($\gamma = 0$) are collected together in the last column of table 2. For the sake of brevity we use notation analogous to that adopted in atomic spectroscopy. Thus the capital letters S, P, D, ... indicate the corresponding $M = 0, 1, 2, \dots$ values, and the left-hand superscript symbol stands for the multiplicity ($2S + 1$). The terms corresponding to the excited vibration states with $\gamma \neq 0$ can be easily obtained from those presented in table 2 by applying the shift $M \rightarrow M + \gamma$. Furthermore, we shall label those excited terms with the additional right-hand subscript symbol k , indicating the modes of the phonons present in that state.

5. Interpolation

In constructing the interpolating expression we shall follow [9], where the perturbation series renormalization procedure is given in detail. The main idea is the replacing of (2) by the generalized Hamiltonian

$$H = \frac{1}{2} \sum_{i=1}^N (-\xi^2 \nabla_i^2 + r_i^2) + \lambda \sum_{i < j} \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|} \quad (21)$$

and using the scaling relation for the generalized eigenvalue:

$$E(\xi, \lambda) = \xi E(1, \lambda \xi^{-3/2}). \quad (22)$$

The eigenvalue of the basic problem with Hamiltonian (2) is given as $E(\lambda) = E(1, \lambda)$.

The scaling relation defines the trajectory $\lambda = \lambda_0 \xi^{3/2}$ in the $\xi\lambda$ -plane, as is shown in figure 1. That trajectory enables us to map the vertical dashed line $\xi = 1$ (where we need to obtain the eigenvalue of the basic problem) onto the tilted line KP which we define as

$$\begin{aligned} \lambda &= K\beta & K &= (1 + \tan \phi)/2 \\ \xi &= P(1 - \beta) & P &= (1 + \cot \phi)/2. \end{aligned} \quad (23)$$

For instance, the point λ_0 is mapped to the point (ξ, λ) .

Unlike the line $\xi = 1$, the line KP is located in the finite region of the $\xi\lambda$ -plane ($0 < \beta < 1$), and that is why the energy $E(\xi(\beta), \lambda(\beta))$ can be successfully expanded into a β -series. Adjusting the above series to the λ -series (3) in the region $\lambda \rightarrow 0$ and to the asymptotic expansion (8) in the region $\lambda \rightarrow \infty$, we obtain the final expression for the renormalized series:

$$\begin{aligned} E &= (b_0 + b_1\beta + b_2\beta^2 + b_3\beta^3)/(1 - \beta) \\ \lambda &= \frac{K\beta}{P^{3/2}(1 - \beta)^{3/2}}. \end{aligned} \quad (24)$$

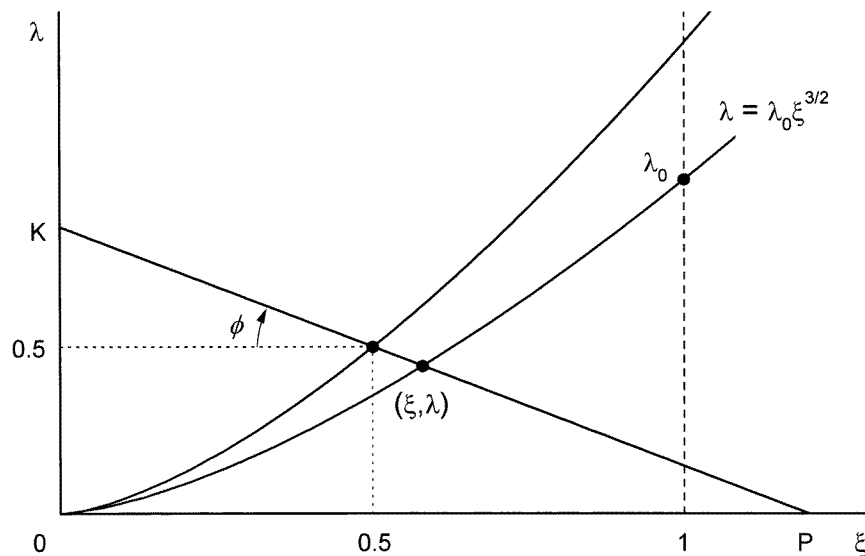


Figure 1. The mapping in the $\xi\lambda$ -parameter plane.

The expansion coefficients can be expressed in terms of those in (3) and (8) as

$$\begin{aligned}
 b_0 &= E_0 \\
 b_1 &= KP^{-3/2}E_1 - E_0 \\
 b_2 &= (7/3)K^{2/3}P^{-1}c_0 + c_1 - E_0 - 2KP^{-3/2}E_1 \\
 b_3 &= -(4/3)K^{2/3}P^{-1}c_0 - c_1 + E_0 + KP^{-3/2}E_1.
 \end{aligned}
 \tag{25}$$

As we restricted ourselves to the two-term approximation in both expansions (3) and (8), we introduced the additional adjustable parameter ϕ (as proposed in [15]) for improving the interpolation accuracy. The geometric meaning of that parameter is clear from figure 1—it indicates the rotation angle of the mapping line KP around the point M to which the energy $E(\sqrt{2})$ is always mapped. The rotation changes the relative contributions of the λ -series and the asymptotic expansion to the renormalized series. The value $\phi = 0$ corresponds to the full control of the renormalization procedure by the λ -series and the value $\phi = \pi/2$ to that of the asymptotic expansion.

It was shown in [15] that usually the energy exhibits some plateau as a function of the parameter controlling the mapping line (ϕ in our case). When the number of terms in the λ -series is increased, that plateau shows a tendency to increase, too, thus giving a good basis for the choice of the controlling parameter. In figure 2 the energy at the fixed point $\lambda = \sqrt{2}$ as a function of the parameter ϕ is shown by the solid line in the case of the first excited triplet state of the two-electron system. As our λ -series are rather short, we find no prominent plateau. However, some curve twist is present, and we hope that it is a rather good idea to choose the controlling parameter ϕ somewhere between the points Max and Min. The difference of energy values corresponding to those points can serve as an estimation of the interpolation accuracy. We see that the accuracy is of about 1%.

We used the inflection point of the $E(\sqrt{2})$ versus ϕ curve as the choice for the controlling parameter ϕ . The energy value obtained with that choice is shown by the dashed line in figure 2. Comparing it with the exact result which is known for the two-electron case

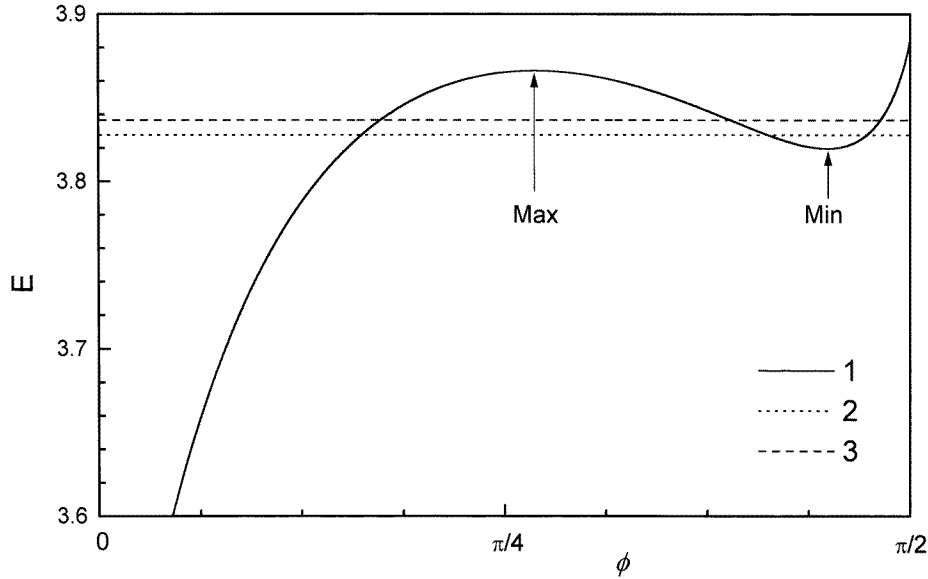


Figure 2. The first excited triplet state for two electrons: (1) the energy versus ϕ plot; (2) the exact result; (3) the energy value at the inflection point.

(dotted line), we see that the accuracy is even better than 1%. The same energy versus ϕ behaviour and the same accuracy were obtained for all other terms considered. The inflection point values of ϕ for all of the terms considered are given in appendix B in tables A1 and A2. They, together with the coefficients E_0 , E_1 and expressions (23)–(25), determine the renormalized perturbation series and enable one to obtain the energies over the whole range of λ -values.

We should note that according to [9] the same parameter values can be used for constructing the renormalized series in the case in which the additional magnetic field B is applied in the direction perpendicular to the quantum dot plane. In that case we have

$$E(\lambda, B) = \sqrt{1 + (\omega_c/2\omega_0)^2} E(\lambda') + M\omega_c/2\omega_0 + g^* \mu_B B S_z / \hbar \omega_0 \quad (26)$$

and

$$\lambda' = \lambda [1 + (\omega_c/2\omega_0)^2]^{-1/4} \quad (27)$$

where the symbol $\omega_c = eB/mc$ stands for cyclotron frequency. Note that there is a misprint in (5.4) of [9]. The last term added in (26) corresponds to the Zeeman energy, where g^* is the effective g -factor and μ_B is the Bohr magneton.

6. Results and discussion

As an illustration of the renormalization technique introduced, we present in figures 3–6 the excitation energy versus λ plot for the relative electron motion for quantum dots with two to five electrons. The inclusion of the centre-of-mass-motion energy is a trivial one. One needs just to shift up the spectra presented by the some integer value, as the centre-of-mass motion is not affected by the electron interaction.

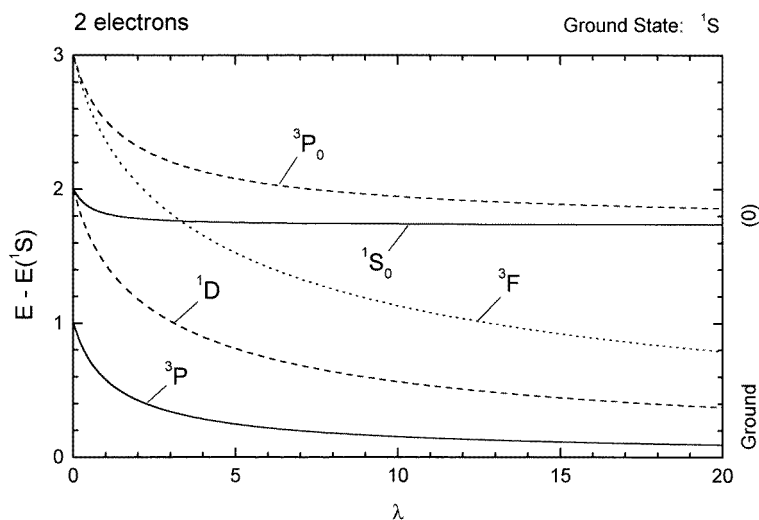


Figure 3. The spectrum for two electrons.

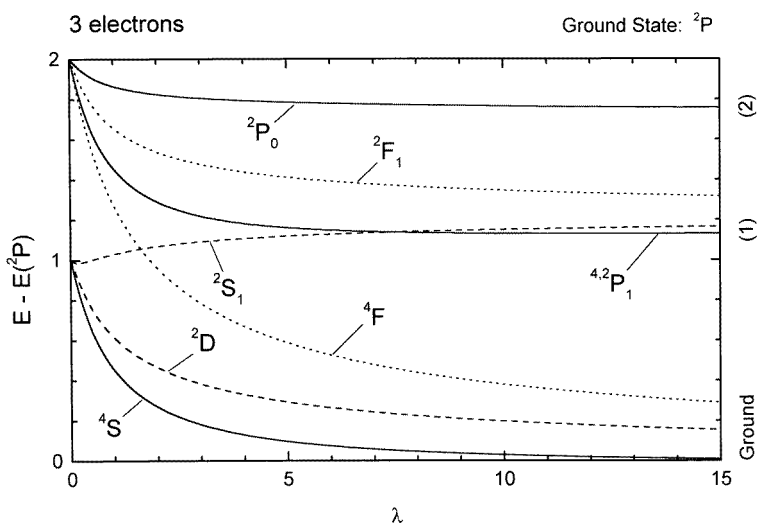


Figure 4. The spectrum for three electrons.

The main problem is that of deciding how the terms in the two regions ($\lambda \rightarrow 0$ and $\lambda \rightarrow \infty$) should be interconnected. Taking into account the fact known from quantum mechanics that two terms with the same good quantum numbers never cross each other, we used the simplest term connection scheme. Starting from the ground state we connected successively each term in the region $\lambda \rightarrow 0$ to the lowest possible unconnected term with the same quantum numbers M and S in the asymptotic region.

In figures 3 and 4 the energy plots for the systems of two and three electrons are presented. The terms with the zero energy exceeding the ground-state energy by 3 and 2, correspondingly, are depicted. In the cases of four and five electrons, the energy plots are given in figures 5 and 6. The degeneracy of the states grows rapidly with the number

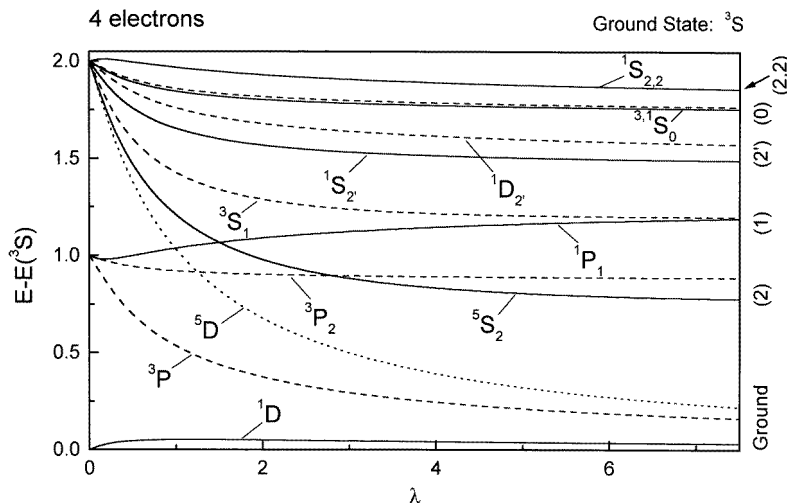


Figure 5. The spectrum for four electrons.

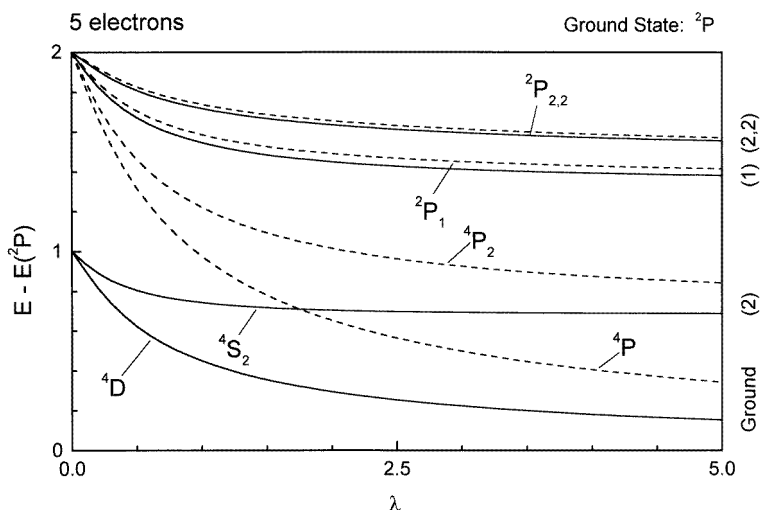


Figure 6. The spectrum for five electrons.

of electrons and thus here we present only the two lowest terms tending to each of the asymptotic vibration states. The asymptotic terms in the above figures are labelled by the numbers in parentheses along the right-hand axis, which indicate the k -values of the phonons present in the state. The phonon state with polarization corresponding to the larger frequency is indicated by a prime.

It can be clearly seen how the term structure transforms from that of the weakly interacting quantum system, where the energy levels are governed by the filling of non-interacting single-electron states, to the semiclassical strongly correlated system, where the energy levels correspond to the electronic ring vibration frequencies. Such switching of the dot behaviour can be explained by means of simple dimensional considerations. Namely, the three terms in Hamiltonian (1) can be estimated as $\hbar^2 N/mR^2$, $m\omega_0^2 R^2 N$ and

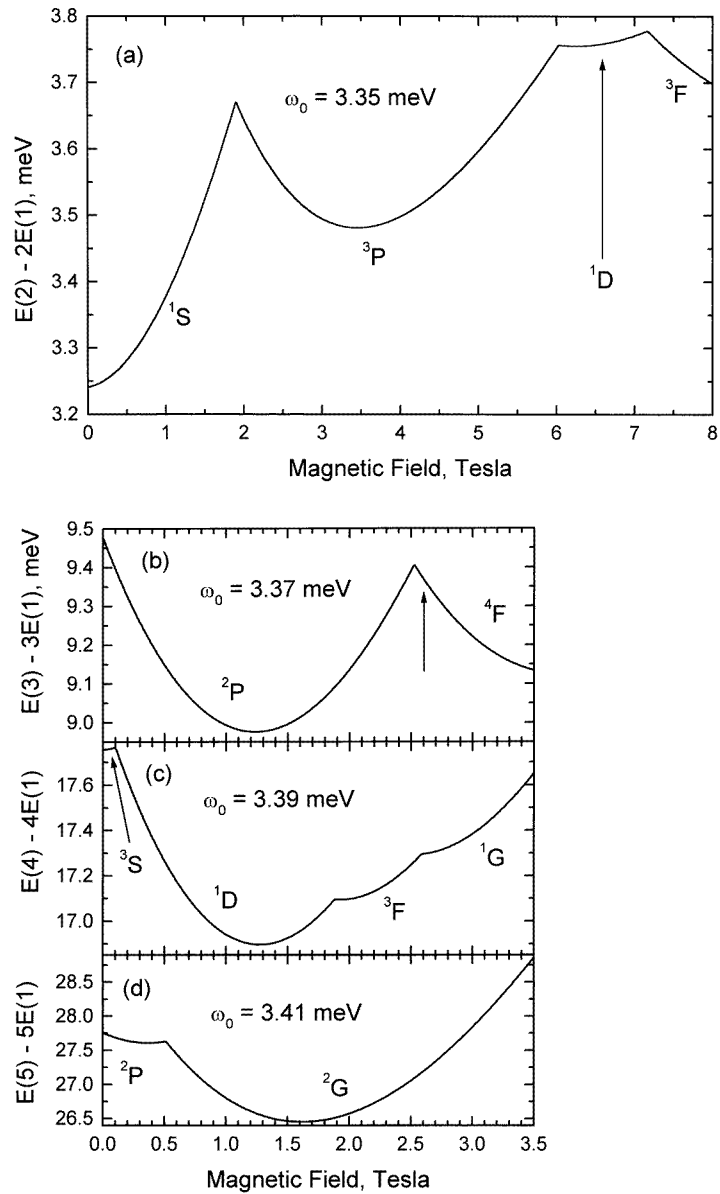


Figure 7. The ground-state energy of a quantum dot in a magnetic field: (a) two electrons; (b) three electrons; (c) four electrons; (d) five electrons. The single-electron ground-state energies $E(1)$ are subtracted.

$e^2N(N-1)/\epsilon R$. Equating them, we define the critical λ -value $\lambda^* \sim 1/(N-1)$ where the above-mentioned switching occurs. This is in agreement with our energy dependencies. As the dimensionless coupling constant λ is proportional to $a_0 \sim 1/\sqrt{\omega_0}$, the above estimation leads to some condition for the confinement potential frequency showing whether the dot behaves like a quantum system or a classical one. When the confinement potential is mainly caused by some positive neutralizing charge located at the rather distant gate, the increase

in the confinement potential frequency ω_0 does not exceed N [7]. In that case, increasing the number of electrons in a dot leads to a more classical system.

As an illustration of the renormalized series technique presented, for the case with a magnetic field (according to (26)) we calculated the ground-state energies versus magnetic field for two to five electrons; these are displayed in figures 7(a)–7(d). The curve in (a) for the two-electron system is in good agreement with that presented in [7] (we choose the parameters as in [7] and also include the fictitious gate charge, but do not subtract the zero-point motion of the centre of mass). It is seen from figures 7(b)–7(d) that on increasing the number of electrons the structure of the dependencies becomes less well resolved and the peaks lose their sharpness. Thus we miss a tiny additional peak in the position marked by an arrow in figure 7(b) which is present in the data from the exact diagonalization. Comparing our results with those obtained in [8], say, for $N = 3$, $B = 20$ T, $S = 3/2$ and $M = 3$, we obtained the ground-state energy value 77.5 meV, and find a good coincidence, which proves that the approximate separation of rotation and vibration modes works fairly well for small angular momenta.

In concluding, we would like to mention that the parabolic quantum dot is, due to the softness of the confinement potential, a rather favourable object as regards constructing the interpolation expressions, in contrast to a hard-wall dot [17], for which the accuracy is much less good.

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Appendix A. Coulomb matrix elements

In [12], the algebraic expression for calculation of the two-particle matrix element of the Coulomb interaction of electrons in the lowest Landau level (corresponding to $n_i = 0$ in our case) was used (see the comments in [16]). In a more general ($n_i \neq 0$) case, the analogous Girvin and Jach expression can be derived, employing the same centre-of-mass and relative-motion complex-coordinate technique after expanding the associated Laguerre polynomials in sums and representing the terms in the form

$$(r_1 e^{-i\varphi_1})^{\gamma_1} (r_2 e^{-i\varphi_2})^{\gamma_2} (r_2 e^{i\varphi_2})^{\gamma_3} (r_1 e^{i\varphi_1})^{\gamma_4} \frac{e^{-(r_1^2 + r_2^2)}}{|\mathbf{r}_1 - \mathbf{r}_2|}.$$

Here the symbols γ_i stand for numbers:

$$\begin{aligned} \gamma_1 &= j_1 + j_4 + (|m_1| + m_1)/2 + (|m_4| - m_4)/2 \\ \gamma_4 &= j_1 + j_4 + (|m_1| - m_1)/2 + (|m_4| + m_4)/2. \end{aligned} \quad (\text{A1})$$

The symbols j_i are integer summation indices running from 0 to n_i . γ_2 and γ_3 can be obtained from (A1) by performing the following replacement of indices: $1 \rightarrow 2$ and $4 \rightarrow 3$. The final expression reads

$$\begin{aligned} \langle 12|V|34 \rangle &= \delta_{s_1, s_4} \delta_{s_2, s_3} \delta_{m_1 + m_2, m_3 + m_4} \left[\prod_{i=1}^4 \frac{n_i!}{(|m_i| + n_i)!} \right]^{1/2} \sum_{(4)j=0}^n \frac{(-1)^{j_1 + j_2 + j_3 + j_4}}{j_1! j_2! j_3! j_4!} \\ &\times \left[\prod_{i=1}^4 \binom{n_i + |m_i|}{n_i - j_i} \right] \frac{1}{2^{(G+1)/2}} \sum_{(4)l=0}^{\gamma} (-1)^{\gamma_2 + \gamma_3 - l_2 - l_3} \end{aligned}$$

Table A1. Coefficients for quantum dots with $N = 2$ and $N = 3$ electrons.

Term	$N = 2$			Term	$N = 3$		
	E_0	E_1	ϕ		E_0	E_1	ϕ
1S	2	1.2533	0.3571	2P	4	2.8200	0.5871
3P	3	0.6267	1.2211	4S	5	1.8800	1.0722
1D	4	0.4700	1.3993	2D	5	2.2325	0.9358
1S_0	4	0.9400	0.7204	2S_1	5	2.5850	0.5836
3F	5	0.3917	1.4651	4F	6	1.7037	1.1984
3P_0	5	0.5483	1.3065	4P_1	6	1.8212	1.0783
				2P_1	6	1.8413	1.0698
				2F_1	6	2.2618	0.8991
				2P_0	6	2.5942	0.7067

Table A2. Coefficients for quantum dots with $N = 4$ and $N = 5$ electrons.

Term	$N = 4$			Term	$N = 5$		
	E_0	E_1	ϕ		E_0	E_1	ϕ
3S	6	5.0133	0.6105	2P	8	8.3032	0.4913
1D	6	5.2483	0.5800	4D	9	7.4416	0.6649
1S	6	5.4832	0.5527	2S	9	7.4812	0.6607
3P	7	4.3608	0.8333	4S_2	9	7.6765	0.6409
3F	7	4.6412	0.7828	2S_2	9	7.7647	0.6325
1P_1	7	4.6999	0.6087	2G	9	7.8234	0.6270
3P_2	7	4.8628	0.6482	2D	9	7.8284	0.6265
5D	8	3.5641	1.0635	2D_2	9	8.1710	0.5969
5S_2	8	3.6816	0.9920	2S_2	9	8.3125	0.5263
3S_1	8	3.9491	0.8956	4P	10	6.7149	0.8303
1S_2	8	3.9822	0.9218	4F	10	6.8596	0.8110
3D_2	8	4.0215	0.9130	4P_2	10	6.9609	0.7980
1G	8	4.0919	0.9543	2F	10	6.9615	0.7980
3G	8	4.1320	0.9466	2P_2	10	7.1355	0.7768
1D_2	8	4.3311	0.8487	4F_2	10	7.2010	0.7224
3D_1	8	4.3783	0.8004	2P_2	10	7.2489	0.7168
$^1S_{2'}$	8	4.3866	0.7810	2H	10	7.2543	0.7631
3S_1	8	4.5628	0.7656	2F_2	10	7.3103	0.7568
3D_1	8	4.5642	0.7654	4P_2	10	7.3563	0.7046
1G_2	8	4.6678	0.7885	2P_1	10	7.4043	0.6993
$^1D_{2'}$	8	4.7087	0.7220	2P_1	10	7.5375	0.6783
3S_0	8	4.7653	0.6836	2F_2	10	7.6303	0.6757
1S_0	8	4.8182	0.6751	2F_1	10	7.6670	0.6720
1D_0	8	5.0062	0.6472	$^2P_{2,2}$	10	7.9283	0.6407
$^1S_{2,2}$	8	5.2186	0.6140	$^2P_{2,2}$	10	8.0142	0.6331

$$\times \delta_{l_1+l_2, l_3+l_4} \left[\prod_{i=1}^4 \binom{\gamma_i}{l_i} \right] \Gamma\left(1 + \frac{\Lambda}{2}\right) \Gamma\left(\frac{G - \Lambda + 1}{2}\right) \quad (\text{A2})$$

where

$$\sum_{(4)j=0}^n \equiv \sum_{j_1=0}^{n_1} \sum_{j_2=0}^{n_2} \sum_{j_3=0}^{n_3} \sum_{j_4=0}^{n_4} \quad G = \sum_i \gamma_i \quad \Lambda = \sum_i l_i \quad \binom{n}{m} = \frac{n!}{m!(n-m)!}.$$

Although the above expression involves terms with alternating signs and leads to numerical difficulties in the case of large quantum number values [16], we found it rather convenient and accurate in the cases of quantum dots with small numbers of electrons.

Appendix B. Expansion coefficients

Here, in tables A1 and A2, the coefficients E_0 and E_1 of the perturbation series (3), and the inflection point angle ϕ are presented for all terms under consideration. These values, together with the asymptotic expansion (8) given in table 1 and expressions (23)–(25), are sufficient for constructing the renormalized perturbation series.

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