

Renormalized perturbation series for quantum dots

This article has been downloaded from IOPscience. Please scroll down to see the full text article.

1994 J. Phys.: Condens. Matter 6 7751

(<http://iopscience.iop.org/0953-8984/6/38/013>)

View [the table of contents for this issue](#), or go to the [journal homepage](#) for more

Download details:

IP Address: 171.66.16.151

The article was downloaded on 12/05/2010 at 20:35

Please note that [terms and conditions apply](#).

Renormalized perturbation series for quantum dots

A Matulis† and F M Peeters‡

† Semiconductor Physics Institute, Gostauto 11, 2600 Vilnius, Lithuania§

‡ Departement Natuurkunde, Universiteit Antwerpen (UIA), B-2610 Antwerpen, Belgium||

Received 10 May 1994, in final form 1 July 1994

Abstract. Convergent renormalized perturbation series in powers of the electron–electron interaction are proposed for calculating the energy of a quantum dot. The method is illustrated by calculating the ground and several excited states of a quantum dot consisting of two electrons. Comparison between the present results and those of an exact numerical integration shows the great accuracy of the proposed method over the whole range of the electron–electron coupling constant values.

1. Introduction

Recently quantum dots containing one, two and more electrons, say quantum dot ‘helium’ and higher ‘elements’ respectively were created and investigated [1, 2, 3]. Exchange and correlation effects were shown to be of great importance [4] in such systems.

Most of the previous approaches can be divided into four categories: (1) there are the ‘exact’ numerical diagonalization approaches which due to computer power are limited to few electron systems [4, 5], (2) numerical simulations based on quantum Monte Carlo techniques [6], (3) approximate schemes which neglect or treat correlation in an approximate way [7], and (4) classical theories in which correlation is fully accounted for but where the quantum mechanical nature of the problem is discarded [8, 9]. The latter approach can handle a large number of electrons.

In the present paper we will concentrate on the correlation effect and propose to treat it in a more simple way making use of the expansion in a power series in the electron–electron (e–e) interaction. It is well known that if one calculates the electron system energy the correlation effects manifest themselves already in second order of that expansion. Actually, the expansion is in powers of the dimensionless e–e interaction coupling constant $\lambda_0 = a_0/a_B$ where a_0 is the characteristic quantum dot dimension, $a_B = \epsilon\hbar^2/m^*e^2$ the Bohr radius in which ϵ is the static dielectric constant of the medium in which the electrons are located and m^* is the electron effective mass. Thus, the effective coupling constant can be easily varied by changing the confining potential. Typically, values $\lambda_0 \geq 2$ are of interest in present day experiments.

The primitive λ -expansion is only useful in the case of small coupling constant, i.e. for very narrow quantum dots. In order to cover the whole range of λ_0 -values we constructed the renormalized λ -expansion as was previously used in the case of the non-parabolic oscillator problem (see, for example, [10]). The renormalized λ -expansion is constructed by means

§ Electronic mail: Algirdas.Matulis@kktl.PFI.lt.

|| Electronic mail: peeters@nats.uia.ac.be.

of two orders of simple λ -expansion: the asymptotic expansion for large λ -values which can be obtained from quasi-classical considerations, and taking into account the symmetric properties of the Schrödinger equation.

For illustrative purposes we consider here the ground state and several excited states of the two-electron system in a parabolic quantum dot. We compare the obtained results with the exact numerical solution. An agreement within 1% was found for all λ -values. One of the advantages of the present approach is that explicit analytic expressions are obtained for the energy which are valid for arbitrary magnetic field.

The present paper is organized as follows. In section 2 the problem is formulated. The λ -expansion technique is outlined in section 3. In section 4 renormalization series are developed which are based on a scaling relation which extends the validity range of the λ -expansion to large λ -values. Through a rescaling of the problem we show in section 5 that our results are easily extended to the case where a magnetic field is present. In section 6 the present approach is applied and tested for the two-electron quantum dot problem, and our conclusions are given in section 7.

2. Formulation of the problem

We shall consider the system of N electrons in a quasi-two-dimensional quantum dot when the electron motion in the z direction is frozen out into the lowest subband. The motion of electrons with the effective mass m^* in the $z = 0$ plane is described by the following Schrödinger equation:

$$\left\{ \sum_{i=1}^N \left[-\frac{\hbar^2}{2m^*} \nabla_i^2 + \frac{1}{2} m^* \omega_0^2 r_i^2 \right] + \frac{e^2}{\epsilon} \sum_{i < j} \frac{1}{|r_i - r_j|} - E \right\} \Psi = 0 \quad (2.1)$$

where ω_0 is the confinement frequency parameter. For future purposes we will introduce dimensionless units by making the following transformation: (1) $r \rightarrow a_0 r$, where $a_0 = \sqrt{\hbar/m^* \omega_0}$, (2) the energy will be measured in units of $\hbar \omega_0$. Using this dimensionless notation we obtain the eigenvalue problem

$$(H - E)\Psi = 0 \quad (2.2)$$

with the following Hamiltonian:

$$H = H_0 + \lambda V \quad (2.3)$$

where

$$H_0 = -\frac{1}{2} \sum_{i=1}^N [\nabla_i^2 - r_i^2] \quad (2.4)$$

$$V = \sum_{i < j} \frac{1}{|r_i - r_j|}. \quad (2.5)$$

Making use of the solutions of the zero-order Hamiltonian H_0 we introduce the second-quantization representation

$$H = \sum_i \varepsilon(i) a_i^\dagger a_i + \frac{\lambda}{2} \sum_{i, i', j, j'} V_{i, j, j', i'} a_i^\dagger a_j^\dagger a_{j'} a_{i'}. \quad (2.6)$$

Here the symbols i, i', j, j' ($i = \{m_i, n_i, s_i\}$) stand for the quantum numbers of one-electron states of a two-dimensional oscillator.

The one-electron energy is

$$\varepsilon(i) = 1 + |m_i| + 2n_i \quad (2.7)$$

and

$$V_{i,j,j',i'} = \delta_{s_i,s_i'} \delta_{s_j,s_j'} \int d^2r_1 \int d^2r_2 \frac{1}{|r_1 - r_2|} \phi^*(i|r_1) \phi^*(j|r_2) \phi(j'|r_2) \phi(i'|r_1) \quad (2.8)$$

is the e-e interaction matrix element calculated with the oscillator functions

$$\phi(i|r) = \frac{1}{\sqrt{2\pi}} e^{im_i\varphi} R(m_i, n_i|r). \quad (2.9)$$

The radial wavefunction can be expressed via the associated Laguerre polynomial

$$R(m, n|r) = \sqrt{\frac{2n!}{(m+n)!}} r^{|m|} e^{-r^2/2} L_n^m(r^2). \quad (2.10)$$

3. The λ -expansion

Due to the fact that according to (2.7) the one-electron eigenstate energies are discrete and equidistant the electron eigenstates are usually degenerate. The simplest way to obtain the λ -expansion for the degenerate eigenstate energy is to use the so-called resolvent operator technique (see, for example, [11]) as was done for the case of 3D atoms in [12]. The energy of the electron system is then defined as a pole of the Green function

$$G_{u,u'}(E) = \langle \Phi_u | (H - E)^{-1} | \Phi_{u'} \rangle \quad (3.1)$$

in the complex E -plane, where

$$|\Phi_u\rangle = a_N^\dagger \dots a_1^\dagger |\Phi_0\rangle \quad (3.2)$$

are the wavefunctions of the non-interacting electron system, where u represents the collections of all electron quantum numbers. The wavefunction $|\Phi_0\rangle$ is the vacuum state without electrons and it can also represent the completely filled inner electron shells.

In a standard way the λ -expansion of function (3.1) is represented as a sum of diagrams the general form of which is represented in figure 1(a). The diagrams are made up of the vertices of figure 1(b), corresponding to matrix element (2.8), connected by electron lines. In general, in the case where $|\Phi_0\rangle$ includes the inner-closed-shell electrons the diagram part without external lines should be added; but one should not take them into account if the quantum dot energy relative to the above closed-shell electron energy is calculated. The diagram contribution includes the energy denominator corresponding to each diagram cutting across electronic lines.

If we wish to calculate the electron system energy as the Green function pole we should deal with the 'dangerous' diagram cuttings corresponding to the degenerate states under consideration. This can be done making use of the Dyson equation and properly diagonalizing the mass operator in the space of the degenerate state functions. Then the electron system energy is given by the following equation:

$$E = E_0 + M^A(E), \quad (3.3)$$

where symbol A stands for the collection of interacting electron system eigenstate quantum numbers,

$$E_0 = \sum_i \varepsilon(i) \eta_i \quad (3.4)$$

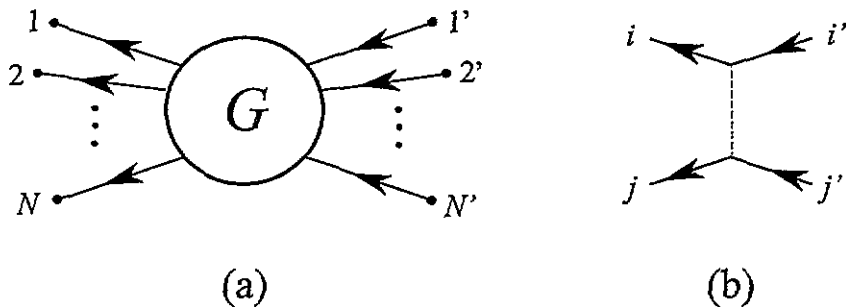


Figure 1. Green function diagram (a) and vertex (b).

and η_i is the electron filling number of electron state i . The mass operator is

$$M^A(E) = \sum_{u,u'} C_u^A M_{u,u'} C_{u'}^{A*} \quad (3.5)$$

where $M_{u,u'}$ denotes the quantity given by the same type of diagram as shown in figure 1(a). In contrast to Green function diagrams these mass operator diagrams have no 'dangerous' cuttings and only the cuttings between vertices should be taken into account. The coefficients C_u^A provide the above-mentioned diagonalization of the mass operator. They should be specified for each eigenstate.

Let us consider the two lowest orders in the λ -expansion. For the sake of simplicity we shall restrict ourselves to the case where Φ_0 corresponds to the vacuum state without electrons. To first order, only diagrams of one type for the mass operator $M^A(E)$ appear, and this consists of the vertex shown in figure 1(b) connected in all various ways with the external electron lines (u, u'). The contribution of these diagrams is given by (2.8).

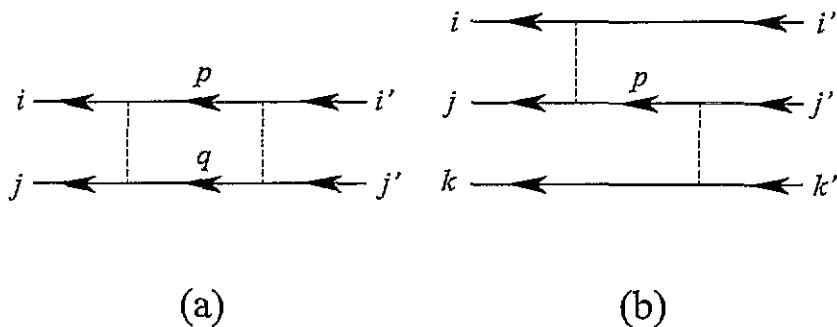


Figure 2. Second-order diagrams.

In second order there are diagrams with two elements which are shown in figure 2. When calculating the contribution of these diagrams the summation over all one-electron states corresponding to the inner electron lines p and q should be carried out. The (a) diagram contribution with one of those electron lines p or q belonging to the electron configuration considered and the contribution of the (b) diagram give the Hartree-Fock approximation, while the remaining (a) diagram contribution should be interpreted as the correlation energy. Thus the electron energy is now made up of each of the electron pair contributions which can be calculated separately:

$$t_{i,j,j',i'} = \sum_{p,q} \frac{v_{i,j,q,p} v_{p,q,j',i'}}{\varepsilon(i') + \varepsilon(j') - \varepsilon(p) - \varepsilon(q)}. \quad (3.6)$$

In order to improve the accuracy of the electron pair energy calculation it is worth replacing the above summation by the solution of a two-electron equation which can be derived in the following way. According to (2.8) the above expression can be transformed into

$$\begin{aligned} t_{i,j,i'} &= \int d^2r_1 \int d^2r_2 \phi^*(i|r_1)\phi^*(j|r_2) \frac{1}{|r_1 - r_2|} \\ &\quad \times [\varepsilon(i') + \varepsilon(j') - H_0]^{-1} \frac{1}{|r_1 - r_2|} \phi(j'|r_2)\phi(i'|r_1) \\ &= \int d^2r_1 \int d^2r_2 \phi^*(i|r_1)\phi^*(j|r_2) \frac{1}{|r_1 - r_2|} \Psi(r_1, r_2) \end{aligned} \quad (3.7)$$

where the electron pair wavefunction satisfies the following equation:

$$[\varepsilon(i') + \varepsilon(j') - H_0] \Psi(r_1, r_2) = \frac{1}{|r_1 - r_2|} \phi(i'|r_1)\phi(j'|r_2). \quad (3.8)$$

In order to take into account the absence of 'dangerous' cuttings in (3.6) the orthogonality condition should be fulfilled:

$$\int d^2r_1 \int d^2r_2 \phi^*(i'|r_1)\phi^*(j'|r_2)\Psi(r_1, r_2) = 0. \quad (3.9)$$

Introducing centre-of-mass coordinates $R = (r_1 + r_2)/2$ and relative coordinates $r = r_1 - r_2$ one can separate the variables and reduce the above equation to a one-dimensional non-homogeneous differential equation. This equation can be easily solved numerically and we found that it gives much better accuracy than to the direct summation of (3.6).

In summary, up to second order we found the following λ -expansion for the energy:

$$E = E_0 + \lambda E_1 + \lambda^2 E_2. \quad (3.10)$$

4. Renormalized series

The validity of the above λ -expansion (3.10) is restricted to small λ -values. Here, we will improve the convergence of the λ -expansion obtained using a renormalization procedure. We construct the renormalized λ -expansion following the procedure described in [10]. The main idea of this renormalization is a scaling transformation of the Schrödinger equation which enables us to transform the large- λ -value problem into another problem, which in the present case is the quasi-classical problem, which can be solved.

Let us consider the generalized eigenvalue problem which is described by the Schrödinger equation

$$\left[\sum_{i=1}^N \left(-\frac{\xi^2}{2} \nabla_i^2 + \frac{1}{2} r_i^2 \right) + \sum_{i < j} \frac{\lambda}{|r_i - r_j|} - E(\xi, \lambda) \right] \Psi = 0. \quad (4.1)$$

The difference between this equation and the basic equation with the Hamiltonian (2.3) is the additional parameter ξ which is included in the kinetic part of the Hamiltonian. As a consequence the eigenvalue of this new problem will be a function of two parameters: λ and ξ . The eigenvalue of the basic problem is now given by

$$E(\lambda) = E(1, \lambda). \quad (4.2)$$

The new parameter ξ^2 can be considered as a reciprocal electron mass. Therefore, the limiting case of $\xi \rightarrow 0$ is the quasi-classical approximation to the quantum dot problem which was studied in [8, 9].

After performing the coordinate transformation $r \rightarrow \sqrt{\xi}r$ we find that the eigenvalue satisfies the scaling relation

$$E(\xi, \lambda) = \xi E(1, \lambda \xi^{-3/2}) \quad (4.3)$$

which connects the different eigenvalues on the trajectory $\lambda = \lambda_0 \xi^{3/2}$ in the (λ, ξ) plane (see the thin solid curve in figure 3). Originally, (see (4.2)), we needed the eigenvalue on the line $\xi = 1$ (dashed vertical line in figure 3) but by using the scaling relation (4.3) the problem of large λ_0 can be reduced to the problem of small ξ .

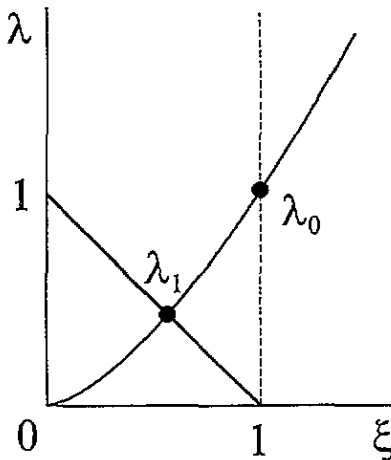


Figure 3. The trajectory in the parameter plane displaying the scaling relation.

This small- ξ problem can be solved in quasi-classical approximation by noticing that in the case with very large electron mass, i.e. when $\xi \rightarrow 0$, the electrons should be located near the minimum of the potential, which is determined from

$$\frac{\partial}{\partial r_k} \left(\sum_{i=1}^N \frac{1}{2} r_i^2 + \sum_{i < j} \frac{\lambda}{|r_i - r_j|} \right) = 0. \quad (4.4)$$

One can show that the minimum is located at $r_k \sim \lambda^{1/3}$ and consequently $E(\lambda) \sim \lambda^{2/3}$, which leads us to propose the following asymptotic eigenvalue expansion:

$$E(\lambda) = c_0 \lambda^{2/3} + c_1. \quad (4.5)$$

Finally, we adjust the eigenvalue $E(\xi, \lambda)$ in order to obtain the λ -series (3.10) and the quasi-classical asymptotic solution (4.5), which are valid in the cases of small λ - and ξ -values, respectively. This can be done following [10] and introducing the mapping of the λ -parameter onto the (ξ, λ) plane

$$\xi = 1 - \beta \quad \lambda = \beta \quad (4.6)$$

with $0 < \beta < 1$, which is shown in figure 3 by the thick solid line. Then every λ_0 -value will be replaced by the λ_1 -value as is indicated in figure 3.

Next, we write down the following expansion

$$\begin{aligned} E(1 - \beta, \beta) &= b_0 + b_1 \beta + b_2 \beta^2 + b_3 \beta^3 + b_4 \beta^4 \\ &= (b_0 + b_1 + b_2 + b_3 + b_4) - (b_1 + 2b_2 + 3b_3 + 4b_4)(1 - \beta) + \dots \end{aligned} \quad (4.7)$$

and compare the first part of it with the λ -series (3.10) which is valid for $\beta \rightarrow 0$ ($\lambda \rightarrow 0$). Making use of (4.3) we have

$$\begin{aligned} E(1-\beta, \beta) &= (1-\beta)E\left(1, \frac{\beta}{(1-\beta)^{3/2}}\right) = (1-\beta)\left\{E_0 + E_1\frac{\beta}{(1-\beta)^{3/2}} + E_2\frac{\beta^2}{(1-\beta)^3}\right\} \\ &= E_0 + (E_1 - E_0)\beta + \left(\frac{E_1}{2} + E_2\right)\beta^2 + \dots \end{aligned} \quad (4.8)$$

For $\beta \rightarrow 1$ we may compare the second part of the expansion (4.7) with the asymptotic expansion (4.5) and find

$$\begin{aligned} E(1-\beta, \beta) &= (1-\beta)E\left(1, \frac{\beta}{(1-\beta)^{3/2}}\right) = (1-\beta)\left(c_0\frac{\beta^{2/3}}{1-\beta} + c_1\right) \\ &= c_0 + \left(c_1 - \frac{2}{3}c_0\right)(1-\beta) + \dots \end{aligned} \quad (4.9)$$

Comparing (4.8), (4.9) and (4.7) we obtain the expansion coefficients

$$b_0 = E_0 \quad b_1 = E_1 - E_0 \quad b_2 = \frac{E_1}{2} + E_2$$

$$b_3 = -E_0 - 4E_1 - 2E_2 + \frac{10}{3}c_0 + c_1$$

$$b_4 = E_0 + \frac{5}{2}E_1 + E_2 - \frac{7}{3}c_0 - c_1$$

and finally arrive at the renormalized series for the considered eigenvalue $E^{\text{ren}}(\lambda)$

$$E^{\text{ren}}(\lambda) = (1-\beta)^{-1}(b_0 + b_1\beta + b_2\beta^2 + b_3\beta^3 + b_4\beta^4) \quad (4.10)$$

with

$$\lambda = \beta/(1-\beta)^{3/2}. \quad (4.11)$$

5. Generalization to the case with a magnetic field

The renormalized λ -expansion obtained can be easily generalized to the case of a quantum dot with a parabolic confining potential in the presence of a homogeneous magnetic field perpendicular to the 2D plane. In that case the Schrödinger equation (2.1) becomes

$$\begin{aligned} \left\{ \sum_{i=1}^N \left[-\frac{\hbar^2}{2m^*} \nabla_i^2 + \left(\frac{1}{2}m^*\omega_0^2 + \frac{e^2B^2}{8m^*c^2} \right) r_i^2 + \frac{i\hbar eB}{2m^*c} \left([r_i \times \nabla_i]_z + \frac{igm^*}{m} S_z \right) \right] \right. \\ \left. + \frac{e^2}{\epsilon} \sum_{i < j} \frac{1}{|r_i - r_j|} - E \right\} \Psi = 0 \end{aligned} \quad (5.1)$$

where B is the magnetic field strength and g is the effective gyromagnetic factor.

This eigenvalue problem can be simplified taking into account the fact that our system is invariant under rotation around the z axis. Thus the eigenvalues and wavefunctions can be characterized by the z -components of the total orbital momentum M and spin S . Consequently, rescaling the system via

$$r \rightarrow r \left[1 + \left(\frac{eB}{2m^*c\omega_0} \right)^2 \right]^{-1/4} \quad (5.2)$$

and changing the eigenvalue as follows:

$$E \rightarrow \left[E - B(M + gSm^*/m)/2 \right] \left[1 + \left(\frac{eB}{2m^*c\omega_0} \right)^2 \right]^{-1/2} \quad (5.3)$$

we arrive at the same eigenvalue problem (2.1) with the scaled e-e interaction coupling constant

$$\lambda = \lambda_0 \left[1 + \left(\frac{eB}{2m^*c\omega_0} \right)^2 \right]^{-1/2}. \quad (5.4)$$

Therefore, equations (4.10), (4.11), (5.3) and (5.4) give the renormalized λ -expansion for all values of the coupling constant and the magnetic field strength.

6. Numerical results

In order to illustrate the accuracy of the above λ -expansion we apply this technique to the system of two electrons in a parabolic quantum dot for which there exist exact results to which we can compare our approximate results (see, for example, [13]). Indeed introducing centre-of-mass coordinates $\mathbf{R} = (\mathbf{r}_1 + \mathbf{r}_2)/2$ and relative coordinates $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$ one can separate the variables and reduce the two-electron problem (2.2) into two one-particle equations for the electron wavefunction $\Psi(\mathbf{r}_1, \mathbf{r}_2) = \Psi(\mathbf{R})\Psi(\mathbf{r})$:

$$\left(-\frac{1}{2}\nabla_{\mathbf{R}}^2 + 2R^2 - E_R \right) \Psi(\mathbf{R}) = 0 \quad (6.1)$$

$$\left(-\nabla_{\mathbf{r}}^2 + \frac{1}{4}r^2 + \frac{\lambda}{r} - E_r \right) \Psi(\mathbf{r}) = 0. \quad (6.2)$$

The centre-of-mass equation (6.1) can be solved analytically which gives the eigenvalues

$$E^R = 1 + |M| + 2N \quad (6.3)$$

where the orbital (M) and the radial (N) quantum numbers are integers.

The relative electron motion equation (6.2) can be integrated numerically. The solution of that equation can be characterized by two quantum numbers: m for orbital motion, and n for radial motion. Keeping in mind that corresponding spin-parts of wavefunctions should be taken into account we see that the even m -values correspond to singlet states and the odd ones correspond to triplet states.

The exact energy for the ground singlet and the excited states—a triplet and two excited singlet states—is depicted in figure 4 by the solid curves.

Now we compare these exact results with the results from our λ -expansion. Due to the degeneracy of the eigenstates of the interacting electron system we are allowed to choose the configurations which are most convenient for the calculation. We take the configurations which are shown in table 1 where the quantum numbers m and the coefficients C_u^A also are given.

The λ -expansion terms obtained are collected in table 2. In this simple two-electron case only the contribution of figure 2(a) diagrams should be taken into account. The corresponding first- and second-order energies are shown in figure 4 by the dotted and dashed curves, respectively. Notice that for the ground state the λ -expansion can be successfully used in the $\lambda < 1$ region, but for $\lambda \geq 1$ it diverges away from the exact result. For the excited states the validity of the λ -expansion technique extends over a larger range of λ -values.

The asymptotic expansion coefficients in (4.5) were calculated by considering the potentials for centre-of-mass and relative electron motion. The coefficient c_0 follows immediately from the minimum in the potential for relative motion, while the second coefficient c_1 is obtained by replacing that potential by an appropriate parabolic one. The

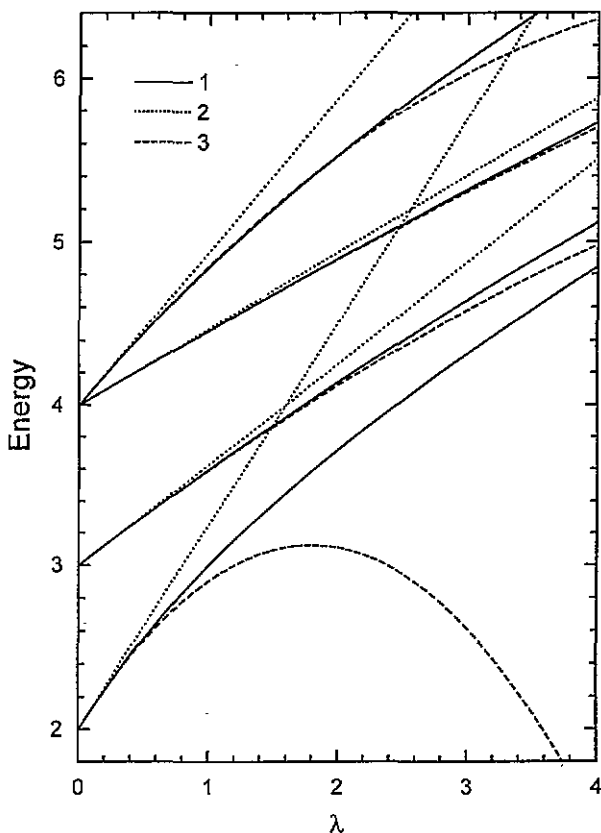


Figure 4. The two electron eigenvalues: 1, exact numerical result; 2, first-order λ -expansion; 3, second-order λ -expansion.

Table 1. Terms and configurations.

Term	m	Configuration $m_1, n_1, s_1; m_2, n_2, s_2$	Coefficients C_u^A
Singlet	0	0 0 1/2; 0 0 -1/2	1
Triplet	1	1 0 1/2; 0 0 1/2	1
Singlet I	2	2 0 1/2; 0 0 -1/2	1/2
		0 0 1/2; 2 0 -1/2	1/2
		1 0 1/2; 1 0 -1/2	$-1/\sqrt{2}$
Singlet II	0	0 1 1/2; 0 0 -1/2	1/2
		0 0 1/2; 0 1 -1/2	1/2
		1 0 1/2; -1 0 -1/2	1/2
		-1 0 1/2; 1 0 -1/2	1/2

asymptotic expansion coefficients obtained are shown in table 2. In table 3 the renormalized λ -expansion coefficients which were calculated according to (4.10) are given.

Table 2. λ -expansion and asymptotic expansion coefficients.

Term	m	E_0	E_1	E_2	c_0	c_1
Singlet	0	2	1.2533	-0.3454	1.1906	1.8660
Triplet	1	3	0.6267	-0.0328	1.1906	1.8660
Singlet I	2	4	0.4700	-0.0112	1.1906	1.8660
Singlet II	0	4	0.9400	-0.0872	1.1906	3.5981

Table 3. Renormalized λ -expansion coefficients.

Term	m	b_0	b_1	b_2	b_3	b_4
Singlet	0	2	-0.7467	0.2772	-0.47954	0.1397
Triplet	1	3	-2.3733	0.2806	0.3947	-0.1101
Singlet I	2	4	-3.5300	0.2238	-0.0229	0.5197
Singlet II	0	4	-3.0600	0.3828	-0.0188	-0.1137

The energy plots of versus λ for all of those terms are presented in figure 5. Notice that the results from the renormalized λ -expansion method (curve '5' in figures 5 (a)–(d)) agree very well with the exact result. The agreement is better than 1% for all λ -values. For the ground state the dotted curve in figure 5(a) shows the second-order Hartree–Fock λ -expansion. The second order Hartree–Fock contribution was calculated according to the diagram shown in figure 2(a) with one internal line p or q belonging to the ground state configuration. We found that the Hartree–Fock contribution gives only half the value of the second-order correction.

7. Conclusions

In conclusion, we have proposed a new approach, which is based on the λ -expansion technique, including electron–electron correlation in the calculation of the energy levels of a quantum dot. This technique was illustrated for the two-electron quantum dot problem for which exact results are available in the literature. Our numerical results indicated that this expansion is good in the case where $\lambda < 1$ for the ground state and is valid over a larger λ -range for the excited states. In the range where $\lambda > 1$ the λ -expansion tends to diverge. The latter artefact is remedied by making use of the asymptotic expansion $\lambda \rightarrow \infty$ which was obtained from the quasi-classical approximation. This led us to construct the renormalized λ -expansion. We found that the renormalized λ -expansion calculated up to second order coincides within 1% with the exact result for all e–e interaction coupling constant values.

We notice that the main reason for the ease with which we could apply the proposed renormalization technique is the simple power dependence of the confining potential and the Coulomb electron interaction potential in the electron coordinate operator. We expect that for systems with a larger number of electrons a level of accuracy in the eigenvalues of a quantum dot to that similar in the present two-electron system can be reached. The incorporation of a non-parabolic confining potential and/or the extent of the electron wavefunction in the z direction is not straightforward. Nevertheless, the proposed technique can be useful in those cases too if the electron–electron interaction dominates the other non-scalable corrections which can then be considered as small perturbations.

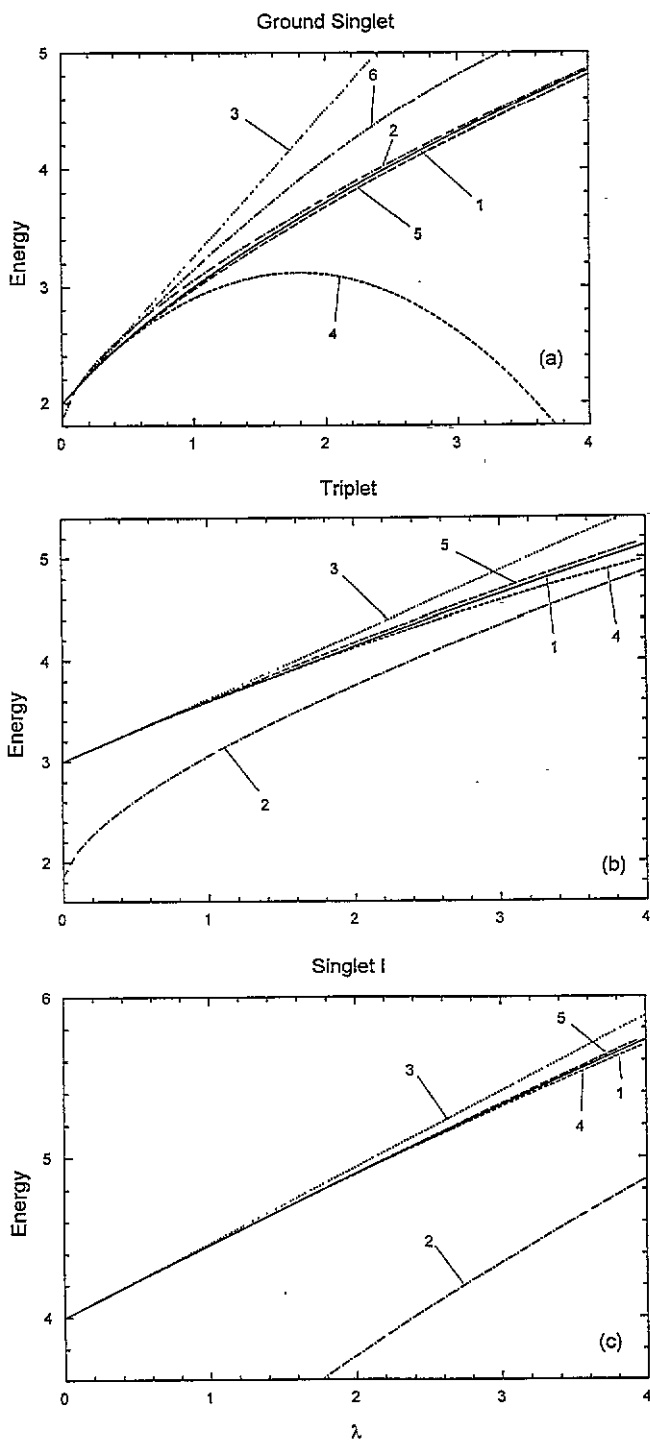


Figure 5. Continued on following page.

Finally we would like to mention that the renormalization technique can be applied to the

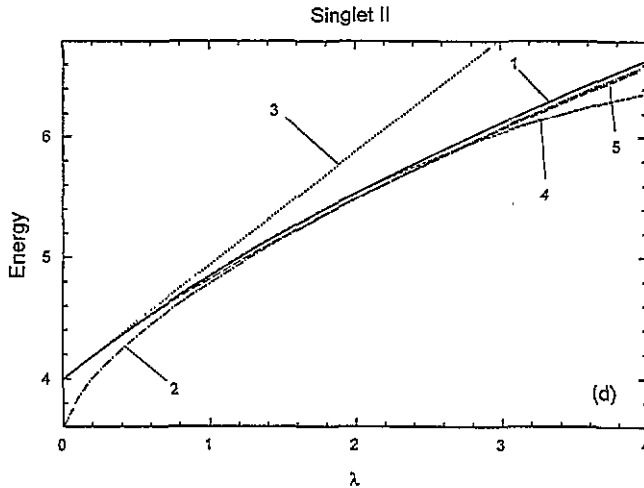


Figure 5. A plot of energy versus λ for: (a) the ground singlet; (b) the first excited triplet; (c) excited singlet I, and (d) excited singlet II. The different curves are: 1, exact numerical result; 2, quasi-classical asymptotic expansion; 3, first-order λ -expansion; 4, second-order λ -expansion; 5, second-order renormalized λ -expansion; 6, second-order Hartree-Fock λ -expansion.

calculation of matrix elements of operators when they have a simple power-type dependence in the electron position coordinates or momentum. This is the case for the dipole matrix element which is used in calculations of the oscillator strength in optical absorption. In that case the corresponding λ -expansion for matrix elements could be constructed in a similar way to what was done in [14] for the case of 3D atoms.

Acknowledgments

This work was supported by the Belgian National Science Foundation (NFWO) and the Interuniversity Microelectronics Centre (IMEC, Leuven).

References

- [1] Sikorski Ch and Merkt U 1989 *Phys. Rev. Lett.* **62** 2164
- [2] Lorke A, Kotthaus J P and Ploog K 1990 *Phys. Rev. Lett.* **64** 2559
- [3] Ashoori R C, Stormer H L, Weiner J S, Pfeiffer L N, Pearton S J, Baldwin K W and West K W 1992 *Phys. Rev. Lett.* **68** 3088
- [4] Pfannkuche D, Gudmundsson V and Maksym P 1993 *Phys. Rev. B* **47** 2244
- [5] Maksym P A and Chakraborty T 1990 *Phys. Rev. Lett.* **65** 108
- [6] See, e.g.,
Bolton F 1994 *Solid-State Electron.* **37** 1159
- [7] Pfannkuche D, Gudmundsson V, Hawrylak P and Gerhardt R R 1994 to be published
- [8] Bolton F and Rössler U 1993 *Superlatt. Microstruct.* **13** 139
- [9] Bedanov V M and Peeters F M 1994 *Phys. Rev. B* **49** 2667
- [10] Fernández F M, Artega G A, Maluendes S A and Castro E 1984 *Phys. Lett.* **103A** 19
- [11] Kumar K 1962 *Perturbation Theory and the Nuclear Many Body Problem* (Amsterdam: North-Holland) ch 2
- [12] Matulis A, Naslenas E and Bandzaitis A 1965 *Litovskii Fiz. Sbornik* **5** 289 (in Russian)
- [13] De Groot J-J S, Hornos J E M and Chaplik A V 1992 *Phys. Rev. B* **49** 12773
- [14] Matulis A and Bandzaitis A 1965 *Litovskii Fiz. Sbornik* **5** 453 (in Russian)