Magnetic fingerprints on the spectra of one-electron and two-electrons interacting in parabolic quantum dots

Omar Mustafa and Maen Odeh
Department of Physics, Eastern Mediterranean University
G. Magusa, North Cyprus, Mersin 10 - Turkey
email: omar.mustafa@emu.edu.tr

Abstract

Magnetic fingerprints on the spectra of an electron interacting with a negatively charged ion in a parabolic quantum dot (QD), and of two interacting electrons in such a dot, are investigated via a new pseudoperturbative methodical proposal. The effects of ion - electron and electron - electron interactions on the spectra are studied. The effect of the symmetry of such problem is emphasized. Compared with those obtained by Zhu et al.[6], via a series solution, the results are found in excellent accord. Higher excited - states are also reported.
1 Introduction

Quantum dots (QDs) are essentially quasi-zero-dimensional little islands, populated by two-dimensional (flatland) electrons laterally confined by an artificial potential [1,2]. The variation of their spectra with magnetic field is often called magnetic fingerprints of QDs. Recent intensive experimental and theoretical investigations have been carried out to explore various spectral properties of QDs. Yet such studies are in their infancy and still expanding rapidly [1-15].

The ion-electron and electron-electron interactions in such QDs are of great importance [6,8-11]. The Hamiltonians (section 2-1) of which are known to belong to non-exactly soluble Hamiltonians. One has therefore to resort to approximation methods to study such systems. There has been, in the last few years, an increasing interest in the study of two-electron QDs in a magnetic field [6,12-15]. Among the several eligible and reliable methods for solving the multi-electron problem in QDs exist: exact numerical diagonalization [2,16], numerical simulations based on quantum Monte Carlo techniques [17], Hartree-Fock calculations [16, 18-20], a series solution based on asymptotically physical grounds of the wave functions in the regions $0 < r$ and $r < \infty$ [6,21], etc. It is therefore interesting to carry out systematic studies of the electronic structures in QDs populated by one and two electrons with and without magnetic fields.

Recently, we have introduced a pseudoperturbative (artificial in nature) shifted - $l$ ($l$ is the angular momentum quantum number) expansion technique (PSLET) to solve Schrödinger equation for states with arbitrary number of nodal zeros. It simply consists of using $1/\bar{l}$ as a pseudoperturbation parameter, where $\bar{l} = l - \beta$ and $\beta$ is a suitable shift to be determined [22-27]. Encouraged by its very satisfactory performance (documented in [22-27] through comparisons with direct numerical integration, quasi perturbative,
variational, Hill determinant, etc, methods), we use PSLET recipe, in section 2-2, and study the spectral properties of an electron in a parabolic QD with a negatively charged ion (impurity), and two electrons in such a QD with and without the magnetic field.

In section 3 we compare our results with the ones obtained by Zhu et al.[6], via a series solution, and report on other states that have not been considered before, to the best of our knowledge. The effect of ion-electron (section 3-1) and electron-electron (section 3-2) interactions are also discussed. In the absence of these interactions we show that whilst the magnetic field completely lifts the confinement degeneracy, as it increases from zero, for the one electron case, it partially lifts it for the two-electron case. Moreover, at infinite magnetic fields the energy levels cluster around Landau ones, inducing in effect Landau degeneracy. The inclusion of these interactions, on the other hand, completely lifts the confinement and Landau degeneracies and change levels ordering. Consequently, energy levels crossing occur and spin-singlet spin-triplet oscillations are manifested for two-electron QDs in a magnetic field. Section 4 is devoted for concluding remarks.

2 Hamiltonian models and PSLET recipe

2.1 Hamiltonian models

To a very good approximation, the harmonic oscillator describes the lateral confinement of electrons in some experimentally created QDs. The motion in the z-direction (the growth direction) is always frozen out into the lowest subband [6,28]. The confinement in this direction is assumed to be stronger than that in the xy-plane, and the dots, in effect, can be treated as two-dimensional thin discs [6,21]. Then the Hamiltonian of an electron in such
a parabolic QD with a negatively charged ion center is very well simulated by

\[ H_{i0} = -\nabla^2 + \frac{1}{4} \gamma_{\tilde{a}}^2 \rho^2 + \frac{2}{\rho}, \quad (1) \]

and that of two electrons in the same QD by

\[ H_0 = -\nabla_1^2 - \nabla_2^2 + \frac{1}{4} \gamma_{\tilde{a}}^2 (\rho_1^2 + \rho_2^2) + \frac{2}{|\rho_1 - \rho_2|}, \quad (2) \]

(in effective atomic units) with \( \gamma_{\tilde{a}}^{-1/2} \) related to the confinement region (hence to the quantum size) of the electrons in the QDs. The energy and length are given in effective Rydberg \( R^* \) and effective Bohr radius \( a^* \), respectively.

When a magnetic field \( \vec{B} \) is applied perpendicular to the xy-plane, through the symmetric gauge \( \vec{A} = (-y, x, 0)B/2 \), the Hamiltonians in (1) and (2), respectively, read

\[ H_i = H_{i0} + \frac{1}{4} \gamma^2 \rho^2 + \gamma L_z, \quad (3) \]

and

\[ H = H_0 + \frac{1}{4} \gamma^2 (\rho_1^2 + \rho_2^2) + \gamma L_{z1} + \gamma L_{z2}. \quad (4) \]

Where \( \gamma = \hbar \omega_c/2R^* \) with the cyclotron frequency \( \omega_c \), and \( \gamma L_{z1} \) and \( \gamma L_{z2} \) are the induced Zeeman terms. Obviously, Hamiltonian (4) is separable and can be recast as

\[ H = H_R + H_r, \quad (5) \]
where
\[ H_R = -\nabla^2_R + \frac{1}{2} \Gamma^2 R^2 + \gamma L_{ZR}, \tag{6} \]
and
\[ H_r = -2 \nabla^2_r + \frac{1}{8} \Gamma^2 r^2 + \gamma L_{Zr} + \frac{2}{r}, \tag{7} \]
which represent the center-of-mass (CM) and the relative-motion (RM) Hamiltonians, respectively. Here, \( \Gamma^2 = \gamma^2 + \gamma^2_d \), \( \vec{R} = (\vec{\rho}_1 + \vec{\rho}_2)/2 \), \( \nabla_R = \nabla_1 + \nabla_2 \), \( \vec{r} = \vec{\rho}_1 - \vec{\rho}_2 \), \( \nabla_r = (\nabla_1 - \nabla_2)/2 \), and \( L_{ZR} = -i\partial/\partial\phi \) and \( L_{Zr} = -i\partial/\partial\varphi \) are the \( Z \)- and \( z \)-components of the angular momentum operators in the CM and RM systems, respectively. Effectively, the problem is reduced into two: a quasi-particle of the CM coordinate in a rescaled external field, and a quasi-particle of the RM coordinate in a rescaled external field and a rescaled repulsive Coulomb field (emerging from the electron-electron interaction). The cylindrical symmetry of the attendant problems invites the separability of the wave functions to obtain. Hence, the two-particle wave function in the plane polar coordinate systems is \( \Phi_{K,M}(R)\Phi_{k,m}(r)e^{im\varphi}e^{iM\phi} \). The Pauli principle demands that \( \Phi_{k,m}(r)e^{im\varphi} \) is antisymmetric with respect to inversion \( \vec{r} \rightarrow -\vec{r} \). No restrictions on \( \Phi_{K,M}(R)e^{iM\phi} \) are imposed. One would therefore obtain spin-singlet \( (s = 0) \) and spin-triplet \( (s = 1) \) states for even and odd \( m \), respectively, through the prescription \( s = (1 - (-1)^m)/2 \). Eventually, Schrödinger equation for Hamiltonian (7) reads
\[ \left[ -\frac{d^2}{dr^2} + \frac{m^2 - 1/4}{r^2} + \frac{1}{r} + \frac{1}{16} \Gamma^2 r^2 \right] U_{k,m}(r) = \left[ \frac{E(k, m) - m\gamma}{2} \right] U_{k,m}(r), \tag{8} \]
where $U_{k,m}(r) = \sqrt{r}\Phi_{k,m}(r)$, and $k$ and $m$ are the radial and azimuthal quantum numbers in the RM system, respectively.

It is convenient to define the electron-electron interaction energies as

$$E_{ee}(k, m) = E(k, m) - E_0(k, m),$$

where

$$E_0(k, m) = (2k + |m| + 1)\Gamma + m\gamma$$

are the energies of (8) without the Coulomb interaction. Then the total energies of (4) are

$$E(k, m; K, M) = E(k, m) + E(K, M),$$

where

$$E(K, M) = (2K + |M| + 1)\Gamma + M\gamma$$

are the energies of (6), with $K$ and $M$ the radial and azimuthal quantum numbers in the CM system, respectively.

Similarly, the ion-electron interaction energies are defined as

$$E_{ie}(k, m) = E_i(k, m) - E_{i0}(k, m),$$

where
\[ E_{i0}(k, m) = (2k + |m| + 1) \Gamma + m \gamma \] (14)

are the energies of (3) without the ion-electron interaction and \( E_i(k, m) \) are the eigenenergies of \( H_i \) in (3).

### 2.2 PSLET recipe

In the underlying radical radial time-independent Schrödinger equation, in \( \hbar = m = 1 \) units,

\[
\left\{ -\frac{1}{2} \frac{d^2}{dq^2} + \frac{l(l + 1)}{2q^2} + V(q) \right\} \Psi_{k,l}(q) = E_{k,l} \Psi_{k,l}(q),
\] (15)

the isomorphism between orbital angular momentum \( l \) and dimensionality \( D \) invites interdimensional degeneracies to obtain. Which, in effect, adds a delicate nature to this equation and allows us to generate the ladder of excited states for any given \( k \) (number of the nodal zeros in the wave function) and nonzero \( l \) from the \( l = 0 \) result, with that \( k \), by the transcription \( D \rightarrow D + 2l \). For more details the reader may refer to ref.s [26,29-31].

Our recipe starts with shifting the angular momentum quantum number \( l \) in (15) through \( \bar{l} = l - \beta \) and use \( 1/\bar{l} \) as a pseudoperturbation expansion parameter. Hence, equation (15) reads

\[
\left\{ -\frac{1}{2} \frac{d^2}{dq^2} + \frac{\bar{l}^2 + (2\beta + 1)\bar{l} + \beta(\beta + 1)}{2q^2} + \frac{\bar{l}^2}{Q} V(q) \right\} \Psi_{k,l}(q) = E_{k,l} \Psi_{k,l}(q),
\] (16)

where \( Q \) is a constant that scales the potential \( V(q) \) at large - \( l_D \) limit and
is set, for any specific choice of $l_D$ and $k$, equal to $\bar{l}^2$ at the end of the calculations. Here $l_D = l + (D - 3)/2$, to incorporate the interdimensional degeneracies. Hence, $\bar{l} \rightarrow \bar{l} = l_D - \beta$ and $D = 2$ (with $l = |m|$) throughout this paper. Next, we shift the origin of the coordinate system through $x = \bar{l}^{1/2} (q - q_o)/q_o$, where $q_o$ is currently an arbitrary point to be determined below. Expansions about this point, $x = 0$ (i.e. $q = q_o$) would lead to

\[ \left[ -\frac{1}{2} \frac{d^2}{dx^2} + \frac{q_o^2}{\bar{l}} \bar{V}(x(q)) \right] \Psi_{k,l}(x) = \frac{q_o^2}{\bar{l}} E_{k,l} \Psi_{k,l}(x), \quad (17) \]

with

\[ \frac{q_o^2}{\bar{l}} \bar{V}(x(q)) = q_o^2 \bar{l} \left[ \frac{1}{2q_o^2} + \frac{V(q_o)}{Q} \right] + \bar{l}^{1/2} B_1 x + \sum_{n=0}^{\infty} v^{(n)}(x) \bar{l}^{-n/2}, \quad (18) \]

where

\[ v^{(0)}(x) = B_2 x^2 + \frac{2\beta + 1}{2}, \quad (19) \]

\[ v^{(1)}(x) = -(2\beta + 1)x + B_3 x^3, \quad (20) \]

\[ v^{(n)}(x) = B_{n+2} x^{n+2} + (-1)^n \left( 2\beta + 1 \right) \frac{(n+1)}{2} x^n \]

\[ + \left( -1 \right)^n \frac{\beta(\beta+1)}{2} (n-1) x^{(n-2)}; \quad n \geq 2, \quad (21) \]

\[ B_n = (-1)^n \left( \frac{n+1}{2} \right) + \left( \frac{d^n V(q_o)}{dq_o^n} \right) \frac{q_o^{n+2}}{n!Q}, \quad (22) \]
It is then convenient to expand $E_{k,l}$ as

$$E_{k,l} = \sum_{n=-2}^{\infty} E_{k,l}^{(n)} \bar{l}^{-n}. \quad (23)$$

Equation (17), along with (18)-(22), is evidently the one-dimensional Schrödinger equation for a harmonic oscillator $\Omega^2 x^2/2$, with $\Omega^2 = 2B_2$, and the remaining terms in Eq.(17) as infinite power series perturbations to the harmonic oscillator. One would then imply that

$$E_{k,l}^{(-2)} = \frac{1}{2q_o^2} + \frac{V(q_o)}{Q} \quad (24)$$

$$E_{k,l}^{(-1)} = \frac{1}{q_o^2} \left[ \frac{2\beta + 1}{2} + (k + \frac{1}{2})\Omega \right] \quad (25)$$

Where $q_o$ is chosen to minimize $E_{k,l}^{(-2)}$, i.e.

$$\frac{dE_{k,l}^{(-2)}}{dq_o} = 0 \quad \text{and} \quad \frac{d^2E_{k,l}^{(-2)}}{dq_o^2} > 0. \quad (26)$$

Equation (26) in turn gives, with $\bar{l} = \sqrt{Q}$,

$$l_D - \beta = \sqrt{q_o^3V''(q_o)}. \quad (27)$$

The shifting parameter $\beta$ is determined by choosing $\bar{l}E_{k,l}^{(-1)} = 0$. Hence

$$\beta = -\left[ \frac{1}{2} + (k + \frac{1}{2})\Omega \right], \quad \Omega = \sqrt{3 + \frac{q_o V''(q_o)}{V'(q_o)}} \quad (28)$$
where primes of $V(q_0)$ denote derivatives with respect to $q_0$. Then equation (17) reduces to

$$
\left[ -\frac{1}{2} \frac{d^2}{dx^2} + \sum_{n=0}^{\infty} v^{(n)} \bar{l}^{-n/2} \right] \Psi_{k,l}(x) = \left[ \sum_{n=1}^{\infty} q_0^2 E_{k,l}^{(n-1)} \bar{l}^{-n} \right] \Psi_{k,l}(x).
$$

Setting the wave functions with any number of nodes $k$ as

$$
\Psi_{k,l}(x(q)) = F_{k,l}(x) \exp(U_{k,l}(x)),
$$

equation (29) readily transforms into the following Riccati equation:

$$
F_{k,l}(x) \left[ -\frac{1}{2} \left( U_{k,l}''(x) + U_{k,l}'(x)U_{k,l}'(x) \right) + \sum_{n=0}^{\infty} v^{(n)}(x) \bar{l}^{-n/2} 
- \sum_{n=1}^{\infty} q_0^2 E_{k,l}^{(n-1)} \bar{l}^{-n} 
- F_{k,l}'(x)U_{k,l}'(x) - \frac{1}{2} F_{k,l}''(x) \right] = 0,
$$

where the primes denote derivatives with respect to $x$. It is evident that this equation admits solution of the form

$$
U_{k,l}'(x) = \sum_{n=0}^{\infty} U_k^{(n)}(x) \bar{l}^{-n/2} + \sum_{n=0}^{\infty} G_k^{(n)}(x) \bar{l}^{-(n+1)/2},
$$

$$
F_{k,l}(x) = x^k + \sum_{n=0}^{\infty} \sum_{p=0}^{k-1} a_{p,k}^{(n)} x^p \bar{l}^{-n/2},
$$

where
$$U_k^{(n)}(x) = \sum_{m=0}^{n+1} D_{m,n,k} x^{2m-1}; \quad D_{0,n,k} = 0, \quad (34)$$

$$G_k^{(n)}(x) = \sum_{m=0}^{n+1} C_{m,n,k} x^{2m}. \quad (35)$$

Substituting equations (32) - (35) into equation (29) implies

$$F_{k,l}(x) \left[ -\frac{1}{2} \sum_{n=0}^{\infty} \left( U_k^{(n)} \bar{l}^{-(n+1)/2} + G_k^{(n)} \bar{l}^{-(n+1)/2} \right) 
- \frac{1}{2} \sum_{n=0}^{\infty} \sum_{m=0}^{n} \left( U_k^{(m)} U_k^{(n-m)} \bar{l}^{-n/2} + G_k^{(m)} G_k^{(n-m)} \bar{l}^{-(n+2)/2} \right) 
+ 2U_k^{(m)} G_k^{(n-m)} \bar{l}^{-(n+1)/2} + \sum_{n=0}^{\infty} v^{(n)} \bar{l}^{-n/2} - \sum_{n=1}^{\infty} q_0 E_k^{(n-1)} \bar{l}^{-(n+1)} \right] 
- F_{k,l}'(x) \left[ \sum_{n=0}^{\infty} \left( U_k^{(n)} \bar{l}^{-n/2} + G_k^{(n)} \bar{l}^{-(n+1)/2} \right) \right] - \frac{1}{2} F_{k,l}''(x) = 0 \quad (36)$$

The solution of equation (36) follows from the uniqueness of power series representation. Therefore, for a given $k$ we equate the coefficients of the same powers of $\bar{l}$ and $x$, respectively. One can then calculate the energy eigenvalues and eigenfunctions from the knowledge of $C_{m,n,k}$, $D_{m,n,k}$, and $a_{p,k}^{(n)}$ in a hierarchical manner. Nevertheless, the procedure just described is suitable for a software package such as MAPLE to determine the energy eigenvalue and eigenfunction corrections up to any order of the pseudoperturbation series (23).

Although the energy series, equation (23), could appear divergent, or, at best, asymptotic for small $\bar{l}$, one can still calculate the eigenenergies to a very good accuracy by forming the sophisticated Padé approximation [22-24,26,32]
\[ P^M_N(1/\bar{l}) = (P_0 + P_1/\bar{l} + \cdots + P_M/\bar{l}^M)/(1 + q_1/\bar{l} + \cdots + q_N/\bar{l}^N) \] (37)

to the energy series (23). The energy series is calculated up to \( E^{(18)}_{k,l}/\bar{l}^{18} \) by
\[ E_{k,l} = \bar{l}^2 E^{(-2)}_{k,l} + E^{(0)}_{k,l} + \cdots + E^{(18)}_{k,l}/\bar{l}^{18} + O(1/\bar{l}^{19}), \] (38)

and with the \( P_{10}^9(1/\bar{l}) \) Padé approximant it becomes
\[ E_{k,l}[10,9] = \bar{l}^2 E^{(-2)}_{k,l} + P_{10}^9(1/\bar{l}). \] (39)

Our recipe is therefore well prescribed.

3 Results and discussion

It is obvious, to a scaling factor, that Hamiltonians (3) and (7) bear the same form of a hybrid of a repulsive Coulomb and oscillator potentials
\[ V(q) = b^2 q^2/2 + 2/q. \] (40)

Hence, equation (28) yields
\[ \Omega = \sqrt{\frac{4 b^2 q_o^3 - 2}{b^2 q_o^3 - 2}}, \] (41)

and, in turn, equation (27) reads
\[ l_D + \frac{1}{2} \left( 1 + (2k + 1) \sqrt{\frac{4 b^2 q_o^3 - 2}{b^2 q_o^3 - 2}} \right) = \sqrt{b^2 q_o^4 - 2 q_o}. \] (42)
Once \( q_o \) is determined (often numerically) the coefficients \( C_{m,n,k} \), \( D_{m,n,k} \), and \( a_{p,k}^{(n)} \) are obtained in a sequential manner. Then the eigenvalues and eigenfunctions are calculated in one batch for each value of \( k \), \( D \), \( l \), and \( b \).

In order to make remediable analysis of our results we have calculated the first twenty terms of our energy series. We have also computed the corresponding sequence of Padé approximants \( P_1^1(1/\bar{l}) \), \( P_2^2(1/\bar{l}) \), \( \cdots \), \( P_9^9(1/\bar{l}) \) and observed their effects on the leading energy term \( \bar{l}^2 E_{k,l}^{(-2)} \). Moreover, the twofold effect of the first term in the effective potential

\[
V_{\text{eff}}(q) = \frac{m^2 - 1/4}{q^2} + V(q)
\]

should be in point. That is, for \( |m| = 0 \) it represents an attractive core that strengthens the confinement, whereas for \( |m| \geq 1 \) it represents a repulsive core and strengthens the Coulomb repulsion.

### 3.1 Ion - electron interaction effect

In table 1 we display the energies of an electron in parabolic QDs, including ion - electron interaction, in a magnetic field for \( \gamma_d = 0.2 \). They compare excellently with those reported by Zhu et al. in figures 1(a) and 1(b) of [6]. In addition we report PSLET results for 4d\(^-\), 4p\(^-\), 5d\(^-\), and 6f\(^-\) states.

In figure 1 we plot the energies of an electron in such QDs (with \( \gamma_d = 0.2 \)) versus \( \gamma \), excluding ion - electron interaction. Clearly, it shows that whilst the magnetic field completely lifts the well known confinement degeneracy, \( (2k + |m| + 1)\gamma_d \), as \( \gamma \) increases from zero, it eventually introduces Landau degeneracy as \( \gamma \rightarrow \infty \). And, at \( \gamma = \infty \) only \( s \) - states are feasible and degenerate. That is, a state \( (k', m') \) would cluster at an \( s \)-state \( (k, 0) \) through
the prescription

\[ 2(k' - k) = -|m'| - m'. \] (44)

In the range of small \( \gamma \) (namely, \( 0 < \gamma < 0.4 \)), one clearly observes that there are minima for states with negative \( m \), whereas for states with positive \( m \) and s-states \((m = 0)\) increase monotonically. This should be attributed to the following: (i) For \( m = 0 \), the effective potential does not support a minimum and the Zeeman term has no effect on these states, hence s-states increase monotonically. (ii) For \( |m| \geq 1 \), the effective potential supports minima and the Zeeman term \( m\gamma \) refines them for negative value of \( m \) or shifts them up for positive \( m \). However, in the range of large \( \gamma \) the magnetic field \((\text{in } \sim \Gamma^2 q^2)\) dominates over the Zeeman term and the leading term in the effective potential, hence all energy levels increase monotonically in this range of \( \gamma \). As a result of (i) and (ii) one observes the energy levels crossings between different states in the range of small \( \gamma \) in Figure 1.

The inclusion of the ion-electron interaction (figures 2-4) significantly changes the spectral properties mentioned above. At \( \gamma = 0 \) (see figures 2-4), one notices that all energies are shifted up. For example, the 1s-states is shifted \((\text{in } R\gamma^*\text{ units})\) by 0.6162, 2p\(^-\) and 2p\(^+\) by 0.4666, 3d\(^-\) and 3d\(^+\) by 0.3829, 4f\(^-\) and 4f\(^+\) by 0.3305, etc. This shift decreases as \(|m|\) increases. For higher levels \((\text{larger } |m|)\) \( q \) increases and the Coulomb repulsion \( \sim 1/q \) decreases, a characteristic which is reflected upon the energy shift-ups in figures 2-4. As \( \gamma \) increases from zero, figures 2-4 clearly show that the ion-electron interaction \textit{completely} lifts Landau degeneracy and results in change in levels ordering. Consequently, energy crossings occur and odd-even parity oscillations are manifested \((2p^+ \text{ crosses with } 4d^-, 4d^- \text{ crosses with } 4f^+, 3d^+\) in figure 3). Figure 1(b) of Zhu et al.[6] also bear this out.

To explain energy crossings, we consider the energy shift-ups as a result
of the ion-electron interaction. At $\gamma = 0.4$ (energy crossings occur in the range $0 < \gamma < 0.4$) for example, the 1s-state is shifted (in Ry$^*$ units) by $\sim 1.03$, 2p$^-$ and 2p$^+$ by $\sim 0.73$, 3d$^-$ and 3d$^+$ by $\sim 0.59$, 4f$^-$ and 4f$^+$ by $\sim 0.50$, and so on. Obviously the ion-electron interaction does not distinguish between positive and negative $m$ values. Moreover, the shift-ups decrease as $|m|$ increase for a given $k$, or for a given $|m|$ as $k$ increases (because of the Coulomb repulsion characteristic mentioned above). This in fact explains why the energy ladder of the lower batch, say, of energy levels in figure 1 is turned up-side-down in figure 2. Similar scenarios could be also developed for figures 3 and 4.

### 3.2 Electron - electron interaction effect

Next, we calculate the e$^-$ - e$^-$ interaction energies $E_{ee}(n_r, m)$ for two electrons in QDs and compare them, in tables 2 and 3, with those reported by Zhu et al.[6]. They are in almost exact accord. We also display PSLET results for 4s, 4p, 5d, 4f, and 5g states. Figure 5 shows that $E_{ee}(n_r, m)$ increases with $\gamma$ and the levels ordering is $E_{ee}(0, 0) > E_{ee}(1, 0) > E_{ee}(2, 0) > \cdots > E_{ee}(0, 1) > E_{ee}(1, 1) > E_{ee}(2, 1) > \cdots > E_{ee}(0, 2) > E_{ee}(1, 2) > \cdots$, etc.

Before we proceed any further let us study the quantum size effect on the two-electron spectra. Table 4 shows the quantum levels of two electrons in QDs with different values of $\gamma_d(\gamma_d^{-1/2})$, hence showing the quantum size effect, when $\gamma = 0$. It documents changes in the levels ordering (consequently, energy crossings and singlet-triplet spin oscillations occur) as $\gamma_d(\gamma_d^{-1/2})$ decreases (increases) from 1(1). Hereby, it should be noted that Zhu’s [6] result $E(1, 0; 0, 1; 0)$ for $\gamma_d = 0.2$ is now corrected from 1.4402 to 1.4413 in accordance with his finding in table 1 of [6]. The levels orderings for $\gamma_d = 0.05$ are changed from (h) (e) to (e) (h) and from (k) (n) to (n) (k) in accordance with our findings, based on the stability of, at least, the last five terms of
the Padé sequence (a signal of convergence to the exact results) mentioned above.

To study the $e^-e^-$ interaction effect on the spectra, we plot the energy levels $E(k, m; K, M; s)$ of two-electron QDs with $\gamma_d = 0.2$ and at different values of $\gamma$ are plotted in figure 6 (excluding the $e^- - e^-$ interaction) and figure 7 (including $e^- - e^-$ interaction). Figure 6 clearly shows that the magnetic field partially lifts the well known confinement degeneracy as $\gamma$ increases from zero and induces Landau degeneracy as $\gamma \to \infty$. Again, one observes the clustering of the quantum levels around $E(k, 0; K, 0; 0)$ states as $\gamma \to \infty$, following a similar trend as that of (44).

The inclusion of the $e^- - e^-$ interaction completely lifts the confinement and Landau degeneracies and changes the levels ordering. Consequently, energy crossings occur, at which singlet - triplet spin oscillations obtain, at specific magnetic fields. Figures 6 and 7 bear these out. One could follow a similar scenario as that in section 3-1 to explain the energy crossings, since the $e^- - e^-$ interaction is effectively a repulsive Coulomb term.

In table 5 we display our results for two interacting electrons in QDs in a magnetic field at different values of $\gamma$, and for $\gamma_d = 0.2$. When plotted with the same scale, our results excellently agree with those of Zhu, figure 2(b) in [6]. However, it should be mentioned that the quantum levels classified in figure 2(b) of Zhu [6] as a, b, c, · · · do not bear positive values of $m$ and $M$ but rather negative ones, classified in table 5 of this text.

4 Concluding remarks

In this paper we have used our recently developed PSLET theory [22-27] to study the magnetic fingerprints on the spectra of an electron in parabolic QDs with negatively charged ion, and on two interacting electrons in such QDs.
We have also emphasized the effect of the symmetry of the problem (marked in the leading term of the effective potential in (43)) on the confinement and Coulomb repulsive terms. The comparison of PSLET results with those of Zhu et al.[6] is readily very satisfactory.

Although we have started with the central force Schrödinger equation and augmented the orbital angular momentum by $l \rightarrow l_D = l + (D - 3)/2$, to incorporate interdimensional degeneracies, we have only considered the $D = 2$ with $l = |m|$ case for the attendant problems.

A general observation concerning the method used by Zhu et al.[6] is in order. We have already mentioned that the series solution method used by Zhu et al.[6] is based upon the asymptotically physical grounds of the wave functions in the regions $0 < r$ and $r < \infty$ (i.e. $r \rightarrow 0$ and $r \rightarrow \infty$, respectively). Effectively and obviously, the authors used the asymptotic behaviours of the wave functions at weak and strong magnetic field limits implicitly. In the weak field limit the wave function is dominated by a Coulombic character (hence Coulombic like basis are used in equation (12) of [6]) and in the strong field limit its dominated by a harmonic oscillator character (hence harmonic oscillator like basis are used in equation (14) of [6]). In fact, this is the only explanation, we could think of, as to why our results do not exactly agree with those of Zhu in table 2, for $\Gamma = 0.4$.

The conceptual soundness of our PSLET is obvious. It avoids troublesome questions pertaining to the nature of small parameter expansions (weak or strong field limits), and trend of convergence to the exact results. On the computational and practical methodical sides, it offers (beyond its promise as being quite handy) a useful pseudoperturbation prescription where the zeroth order approximation $\tilde{\mathcal{P}}^2 E_{k,l}^{(-2)}$ inherits a substantial amount (more than 90% for the above problems) of the total energy.

Finally, PSLET theory could be applied to two electrons in an external
oscillator potential in $D = 3$ space [33], QD lattices [34], 3 - electron QDs [35], 2 - dimensional hydrogenic donor states in a magnetic field [36-39], etc.
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Figures captions

**Fig.1:** $E_i(k,m)$ versus $\gamma$ for the ion - electron in QDs with $\gamma_d = 0.2$, excluding the ion - electron interaction.

**Fig.2:** Same as figure 1 including the ion - electron interaction for 1s, 2p$^-$, 3d$^-$, and 4f$^-$ states.

**Fig.3:** Same as figure 2 for 2s, 3d$^+$, 4f$^+$, 3p$^-$, 2p$^+$, and 4d$^-$ states.

**Fig.4:** Same as figure 2 for 3s, 3p$^+$, 4p$^-$, 5d$^-$, and 6f$^-$ states.

**Fig.5:** Electron - electron interaction energies $E_{ee}(k,m)$ versus $\Gamma$ for the states reported in tables 2 and 3.

**Fig.6:** $E(k,m;K,M)$ versus $\gamma$ for two electrons in QDs with $\gamma_d = 0.2$ excluding the e$^-$ - e$^-$ interaction.

**Fig.7:** Same as figure 6 including the e$^-$ - e$^-$ interaction.
Table 1: \( E_i(k, m) \) with the ion - electron interaction for \( \gamma_d = 0.2 \) and different values of \( \gamma \)

| \( \gamma \) | 0   | 0.1 | 0.2  | 0.3  | 0.4  |
|--------------|-----|-----|------|------|------|
| \( E_i(0, 0) \) (1s) | 0.8162 | 0.8860 | 1.0537 | 1.2617 | 1.4816 |
| \( E_i(0, -1) \) (2\( p^- \)) | 0.8666 | 0.8445 | 0.9339 | 1.0724 | 1.2282 |
| \( E_i(0, -2) \) (3\( d^- \)) | 0.9829 | 0.8775 | 0.9100 | 1.0070 | 1.1307 |
| \( E_i(0, -3) \) (4\( f^- \)) | 1.1305 | 0.9449 | 0.9278 | 0.9922 | 1.0922 |
| \( E_i(0, 1) \) (2\( p^+ \)) | 0.8666 | 1.0445 | 1.3339 | 1.6724 | 2.0288 |
| \( E_i(0, 2) \) (3\( d^+ \)) | 0.9829 | 1.2775 | 1.7100 | 2.2070 | 2.7307 |
| \( E_i(0, 3) \) (4\( f^+ \)) | 1.1305 | 1.5449 | 2.1278 | 2.7922 | 3.4922 |
| \( E_i(1, 0) \) (2s) | 1.1741 | 1.2864 | 1.5612 | 1.9097 | 2.2867 |
| \( E_i(1, -1) \) (3\( p^- \)) | 1.2336 | 1.2557 | 1.4563 | 1.7415 | 2.0623 |
| \( E_i(1, -2) \) (4\( d^- \)) | 1.3599 | 1.2999 | 1.4466 | 1.6940 | 1.9860 |

| \( \gamma \) | 0   | 0.05 | 0.1 | 0.15 | 0.2 |
|--------------|-----|------|-----|------|-----|
| \( E_i(1, 1) \) (3\( p^+ \)) | 1.2336 | 1.3156 | 1.4557 | 1.6405 | 1.8563 |
| \( E_i(2, 2) \) (3s) | 1.5406 | 1.5815 | 1.6967 | 1.8692 | 2.0814 |
| \( E_i(2, -1) \) (4\( p^- \)) | 1.6077 | 1.6014 | 1.6748 | 1.8101 | 1.9888 |
| \( E_i(2, -2) \) (5\( d^- \)) | 1.7415 | 1.6900 | 1.7273 | 1.8339 | 1.9893 |
| \( E_i(2, -3) \) (6\( f^- \)) | 1.9002 | 1.8042 | 1.8069 | 1.8869 | 2.0218 |
Table 2: Electron - electron interaction energies $E_{ee}(k, m)$ at different values of $\Gamma$. The values in brackets are reported by Zhu et al.[6].

| $\Gamma$ | 0.05 | 0.1 | 0.2 | 0.4 |
|----------|------|-----|-----|-----|
| $E_{ee}(0, 0)$ (1s) | 0.1963 | 0.3081 | 0.4816 | 0.7479 |
| (0.1963) | (0.3081) | (0.4816) | (0.7494) |
| $E_{ee}(1, 0)$ (2s) | 0.1853 | 0.2871 | 0.4413 | 0.6716 |
| (0.1853) | (0.2871) | (0.4413) | (0.6723) |
| $E_{ee}(2, 0)$ (3s) | 0.1763 | 0.2703 | 0.4106 | 0.6164 |
| (0.1763) | (0.2703) | (0.4106) | (0.6000) |
| $E_{ee}(3, 0)$ (4s) | 0.1686 | 0.2565 | 0.3863 | 0.5742 |
| $E_{ee}(0, 1)$ (2p) | 0.1562 | 0.2333 | 0.3451 | 0.5057 |
| (0.1562) | (0.2333) | (0.3451) | (0.5066) |
| $E_{ee}(1, 1)$ (3p) | 0.1468 | 0.2168 | 0.3170 | 0.4597 |
| (0.1468) | (0.2168) | (0.3170) | (0.4637) |
| $E_{ee}(2, 1)$ (4p) | 0.1392 | 0.2039 | 0.2959 | 0.4265 |
| $E_{ee}(0, 2)$ (3d) | 0.1311 | 0.1915 | 0.2776 | 0.4000 |
| (0.1311) | (0.1915) | (0.2776) | (0.3998) |
| $E_{ee}(1, 2)$ (4d) | 0.1240 | 0.1799 | 0.2594 | 0.3720 |
| (0.1240) | (0.1799) | (0.2594) | (0.3784) |
| $E_{ee}(2, 2)$ (5d) | 0.1182 | 0.1707 | 0.2452 | 0.3505 |
| $E_{ee}(0, 3)$ (4f) | 0.1144 | 0.1652 | 0.2375 | 0.3399 |
| $E_{ee}(0, 4)$ (5g) | 0.1025 | 0.1472 | 0.2105 | 0.3002 |
Table 3: Same as table 2 for different values of $\Gamma$.

| $\Gamma$ | $E_{ee}(0, 0)$ (1s) | $E_{ee}(1, 0)$ (2s) | $E_{ee}(2, 0)$ (3s) | $E_{ee}(3, 0)$ (4s) | $E_{ee}(0, 1)$ (2p) | $E_{ee}(1, 1)$ (3p) | $E_{ee}(2, 1)$ (4p) | $E_{ee}(0, 2)$ (3d) | $E_{ee}(1, 2)$ (4d) | $E_{ee}(2, 2)$ (5d) | $E_{ee}(0, 3)$ (4f) | $E_{ee}(0, 4)$ (5g) |
|----------|---------------------|---------------------|---------------------|---------------------|---------------------|---------------------|---------------------|---------------------|---------------------|---------------------|---------------------|---------------------|
| 1        | 1.3196              | 1.1473              | 1.0333              | 0.9511              | 0.8279              | 0.7439              | 0.6860              | 0.6436              | 0.5957              | 0.5598              | 0.5432              | 0.4782              |
| 2.5      | 2.2807              | 1.9154              | 1.6966              | 1.5469              | 1.3404              | 1.1941              | 1.0964              | 1.0294              | 0.9496              | 0.8907              | 0.8650              | 0.7598              |
| 4        | 2.9934              | 2.4721              | 2.1744              | 1.9754              | 1.1707              | 1.5188              | 1.3922              | 1.3077              | 1.2047              | 1.1292              | 1.0969              | 0.9628              |
| 5        | 3.3992              | 2.7862              | 2.4435              | 2.2166              | 1.9195              | 1.7017              | 1.5589              | 1.4645              | 1.3485              | 1.2636              | 1.2277              | 1.0772              |
Table 4: $E(k, m; K, M; s)$ quantum levels of two electrons in QDs at different values of $\gamma_d(\gamma_d^{-1/2})$ for $\gamma = 0$, including electron - electron interaction. Zhu’s results [6] are obtained by replacing the last $j$ digits of our results with the $j$ digits in parentheses.

| $\gamma_d(\gamma_d^{-1/2})$ | 1(1)   | 0.4(1.5811) | 0.2(2.2361) | 0.05(4.4721) |
|-----------------------------|--------|-------------|-------------|-------------|
| a:(0,0;0,0;0)              | 3.3196 | 1.5479      | 0.8816      | 0.2963(2)   |
| b:(0,1;0,0;1)              | 3.8279(8) | 1.7057      | 0.9451(0)   | 0.3062      |
| c:(0,0;0,1;0)              | 4.3196 | 1.9479      | 1.0776      | 0.3311(0)   |
| d:(0,2;0,0;0)              | 4.6436 | 2.0000      | 1.0816      | 0.3463(2)   |
| e:(0,1;0,1;1)              | 4.8279(8) | 2.1057      | 1.1451(0)   | 0.3562      |
| f:(1,0;0,0;0)              | 5.1473(2) | 2.2716      | 1.2375(156) | 0.3644(476) |
| g:(0,0;1,0;0)              | 5.3196 | 2.3399      | 1.2413(02)  | 0.3811(0)   |
| h:(0,3;0,0;1)              | 5.5432(174) | 2.3479      | 1.2776      | 0.3853(4)   |
| i:(0,2;0,1;0)              | 5.6436 | 2.4000      | 1.2816      | 0.3963(2)   |
| j:(1,1;0,0;1)              | 5.7439(8) | 2.4597      | 1.3170      | 0.3968      |
| k:(0,1;1,0;1)              | 5.8279(8) | 2.5057      | 1.3451(0)   | 0.4025(66)  |
| l:(1,0;0,1;0)              | 6.1473(2) | 2.6716      | 1.4105(053) | 0.4062      |
| m:(0,0;1,1;0)              | 6.3196 | 2.7002      | 1.4413      | 0.4240      |
| n:(0,4;0,0;0)              | 6.4782(93) | 2.7479      | 1.4594      | 0.4311(0)   |
| o:(1,2;0,0;0)              | 6.5957(6) | 2.7720      | 1.4776      | 0.4353(4)   |
| p:(0,2;1,0;0)              | 6.6436 | 2.8000      | 1.4816      | 0.4463(2)   |
Table 5: $E(k, m; K, M; s)$ quantum levels of two electrons in QDs with different values of $\gamma$ and for $\gamma_d = 0.2$, including electron-electron interaction.

| $\gamma$ | 0  | 0.05 | 0.1  | 0.2  | 0.3  | 0.4  |
|-----------|----|------|------|------|------|------|
| A:(0,0;0,0;0) | 0.8816 | 0.9033 | 0.9644 | 1.1664 | 1.4217 | 1.6967 |
| B:(0,-1;0,0;1) | 0.9451 | 0.9194 | 0.9380 | 1.0667 | 1.2599 | 1.4790 |
| C:(0,0;0,-1;0) | 1.0816 | 1.0595 | 1.0880 | 1.2493 | 1.4822 | 1.7439 |
| D:(0,-2;0,0;0) | 1.0776 | 1.0067 | 0.9889 | 1.0648 | 1.2211 | 1.4129 |
| E:(0,-1;0,-1;1) | 1.1451 | 1.0756 | 1.0616 | 1.1496 | 1.3201 | 1.5262 |
| F:(0,-3;0,0;0) | 1.2375 | 1.1220 | 1.0697 | 1.0984 | 1.2249 | 1.3960 |
| G:(1,0;0,0;0) | 1.2413 | 1.2742 | 1.3670 | 1.6766 | 2.0734 | 2.5066 |
| H:(1,-1;0,0;1) | 1.3170 | 1.3030 | 1.3548 | 1.5963 | 1.9378 | 2.3238 |
| I:(1,0;0,-1;0) | 1.4413 | 1.4304 | 1.4906 | 1.7594 | 2.1339 | 2.5538 |
| J:(1,-2;0,0;0) | 1.4594 | 1.4004 | 1.4166 | 1.6078 | 1.9158 | 2.2773 |
| K:(1,-1;0,-1;1) | 1.5170 | 1.4592 | 1.4784 | 1.6792 | 1.9984 | 2.3710 |
Fig. 1

Fig. 2
Fig. 3

Energy (Ry)

γ = 0.2

Fig. 4

Energy (Ry)

γ = 0.2
Fig. 5

\( (n_r, m) \)

\( (0,0) \)

\( (1,0) \)

\( (2,0) \)

\( (3,0) \)

\( (0,1) \)

\( (1,1) \)

\( (2,1) \)

\( (0,2) \)

\( (1,2) \)

\( (2,2) \)

\( (0,3) \)

\( (0,4) \)

\( \gamma = 0.2 \)

Fig. 6

\( \gamma_d = 0.2 \)
Fig. 7

$\gamma_d = 0.2$

Energy (Ry) vs. $\gamma$. The graph shows the variation of energy with $\gamma$ for different curves labeled A to I.