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# The Theory of Quantum Dots in External Magnetic Field

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A method of intermediate problems, which provides convergent improvable lower bound estimates for eigenvalues of linear half-bound Hermitian operators in Hilbert space, is applied to investigation of the energy spectrum and eigenstates of a two-electron two-dimensional quantum dot (QD) formed by a parabolic confining potential in the presence of external magnetic field. It is shown that this method, being supplemented with conventional Rayleigh–Ritz variational method and stochastic variational method, provides an efficient tool for precise calculation of the energy spectrum of various models of quantum dots and helps to verify results obtained so far by various analytical and numerical methods being of current usage in numerous theoretical studies of quantum dots.

**Keywords:** Energy Spectrum, Quantum Dot, Magnetic Field.

## 1. INTRODUCTION

Among nano-sized and low-dimensional systems of various kinds, quantum dots (QD's) are thought to be potentially fit for numerous present and future applications and currently accounted as promising building blocks for novel electronic, spintronic and optoelectronic devices. The properties of QD's are shown to be greatly influenced by electron–electron interaction and correlation effects.[1–3] Precise estimation of the energy spectrum and eigenstates of a quantum dot is a typical goal of nearly any theoretical study because their properties crucially stipulates relevant physical characteristics of the quantum dot as standing alone as being a part of electric circuits or interacting with environment through its various interfaces.

Thus, it is very important to have reliable methods to solve many-electron QD eigenstate and eigenvalue problem and investigate QD's internal electron structure.[4] As a consequence, nearly all the mathematical methods, developed within the domain of quantum mechanics so far, have already been used on various particular necessities, though on a varying scale, in the theory of quantum dots. Among them one can mention "exact" numerical diagonalization,[1,2] quantum Monte Carlo numerical simulation techniques[5] and Hartree–Fock calculations.[1,6–8] The series expansion method[9,10] as well as the newly developed semiclassical perturbation theory in D-dimensions[11] have been employed in the QD studies too.

Despite all the differencies as in approach, power and complexity, all the most frequently applicable methods of approximate calculation of eigenvalues and eigenstates of realistic physical models of low-dimensional quantum systems, quantum dots among them, share one unfavorable feature: they allow either direct calculation of the magnitudes in question without proper error estimates or, at best, provides one with nonincreasing or even convergent upper bounds for the eigenvalues as, for example, the widely applicable Rayleigh–Ritz method does, but, again, without error estimates.

To control the error of the approximations provided by the upper bounds for some quantity it would be enough to derive corresponding lower bounds which are highly desirable to be convergent too. Therefore, development of regular methods to construct such bounds bears a lot of theoretical and practical significance but represents much more challenging task than derivation of the upper bounds. As to various models of quantum dots, the most suitable, to our knowledge, ground to achieve this goal would be the method of intermediate problems ascending in its basic idea to the maximum-minimum characterization of eigenvalues of half-bounded Hermitian operators in Hilbert space introduced by Weyl[12] and elaborated later by numerous contributors[13,14] with regard to problems of classical and quantum mechanics. Being supplemented with regular Rayleigh–Ritz or newly developed stochastic variational method,[15] the method of intermediate problems may serve as a powerful tool for investigation of the energy spectrum of few-body quantum systems with prescribed or controllable precision and provides an opportunity to verify results obtained by other numerical and analytical methods.[16] A stochastic variational method can also be developed on its basis[17] allowing, in principle, construction

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of improvable lower bounds for energy eigenvalues of realistic models of quantum dots confining relatively large number of excess electrons. Numerical studies of the latter systems proved to be especially difficult and time-consuming if undertaken by means of direct numerical solution of the underlying Schrödinger equation leading to highly multidimensional grids, or by regular variational approaches resulting in prohibitively large sets of basis states. It is worth noticing, that whenever a particular algorithm based on the method of intermediate problems is applied in order to get lower bound estimates for energy eigenvalues, the corresponding eigenstates would result immediately as a concomitant outcome of the calculations. Error estimates for the so derived eigenstates can also be obtained but, what appears to be more practical, such error estimates can also be derived instead for the approximate eigenstates calculated within the frame of the Rayleigh–Ritz regular or stochastic variational method[15] provided that the lower bound estimates for the corresponding energy eigenvalues are known.[18–20] Equally, under the same premises, expectation values (matrix elements) of physically relevant operator variables (dipole or quadruple moments of a quantum dot, for example) calculated with respect to these Rayleigh–Ritz approximate eigenstates can be given their respective error bound estimates too. In addition, mathematically rigorous methods of low-dimensional system investigation can provide an opportunity for verification of the methods of analytical and numerical analysis being of current usage.

## 2. TWO-DIMENSIONAL TWO-ELECTRON QD IN EXTERNAL MAGNETIC FIELD

Two-electron quantum dots confined in a parabolic potential represent an example of one of the simplest QD system revealing the influence of the electron–electron correlations on the QD properties. For most practical purposes the parabolic confinement potential, seen by electrons in a QD, characterizes the low-lying part of the dot energy spectrum correctly. Hence, in what follows, we consider a two-electron dot in two dimensions described by the Hamiltonian

$$H = \sum_{i=1,2} \frac{1}{2m_e^*}\left(\hat{\mathbf{p}}_i + \frac{e}{c}\hat{\mathbf{A}}(\mathbf{r}_i)\right)^2 + \frac{1}{2}m_e^*\omega_0^2(\mathbf{r}_1^2+\mathbf{r}_2^2) + \frac{e^2}{\varepsilon|\mathbf{r}_1-\mathbf{r}_2|} + \sum_{i=1,2}\frac{g^*\mu_B}{\hbar}\mathbf{B}\cdot\hat{\mathbf{S}}_i \quad (1)$$

where $m^*$ is the conduction-band effective mass of each of the two electrons moving in a medium with dielectric constant $\varepsilon$, $e$ is the absolute value of the electron charge, $g^*$ is the effective $g$ factor and $\omega_0$ is the frequency of a harmonic confining potential. For two-dimensional (2D) quantum dots $r_i = |\mathbf{r_i}|$, where $\mathbf{r_i} = (x_i, y_i)$. The vector potential $\hat{\mathbf{A}}(\mathbf{r})$, $(\mathbf{B} = \mathrm{rot}\mathbf{A})$ is introduced in the symmetric gauge, $\hat{\mathbf{A}}(\mathbf{r}) = B/2(-y, x, 0)$. The Hamiltonian (1) can also be written down as

$$H = \sum_{i=1,2}\left(-\frac{\hbar^2}{2m_e^*}\nabla_i^2 + \frac{\omega_c}{2}L_{z,i} + \frac{m_e^*\Omega_0^2}{2}r_i^2\right) + \frac{e^2}{\varepsilon|\mathbf{r}_1-\mathbf{r}_2|} + \sum_{i=1,2}\frac{g^*\mu_B}{\hbar}\mathbf{B}\cdot\hat{\mathbf{S}}_i \quad (2)$$

where $\Omega_0^2 = \omega_0^2 + \omega_c^2/4$, $\omega_c = eB/m_e^*c$ is the cyclotron frequency, and $L_z$ is the $z$-component of the angular momentum operator. Further on, due to the parabolic form of the confining potential, the Hamiltonian of Eq. (2) can be presented as a sum of center-of-mass and relative motion term

$$H = H_R + H_r + H_s \quad (3)$$

with

$$H_R = -\frac{\hbar^2}{4m_e^*}\nabla_R{}^2 + \frac{\omega_c}{2}L_{z,cm} + m_e^*\Omega_0^2R^2 \quad (4)$$

$$H_r = -\frac{\hbar^2}{m_e^*}\nabla_{\mathbf{r}}{}^2 + \frac{\omega_c}{2}L_{z,rel} + \frac{1}{4}m_e^*\Omega_0^2r^2 + \frac{e^2}{\varepsilon r} \quad (5)$$

$$H_s = \sum_{i=1,2}\frac{g^*\mu_B}{\hbar}\mathbf{B}\cdot\hat{\mathbf{S}}_i \quad (6)$$

where $\mathbf{R} = (\mathbf{r}_1 + \mathbf{r}_2)/2$, $\nabla_{\mathbf{R}} = \nabla_1 + \nabla_2$, $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$ and $\nabla_r = (\nabla_1 - \nabla_2)/2$. Due to this separation, the two-particle wave functions can be written in polar coordinates in the form $\Phi(\mathbf{R})\psi(r)\exp(-im\phi)$ with azimuthal quantum number $m = 0, \pm1, \pm2, \ldots$ of the relative motion. Therefore, because of the Pauli exclusion principle the total quantum state must be spin singlet ($s = 0$) and triplet ($s = 1$) for even and odd $m$, respectively. Because of the separation of variables in the Hamiltonian (3), its eigenvalues $E$ are a sum $E = E_{cm} + E_{rel} + E_s$ of the center-of-mass energy $E_{cm}$, the relative motion energy $E_{rel}$ and the spin-field interaction energy $E_s$. The eigenvalues of the center-of-mass motion Hamiltonian (4) are essentially the ones of a two-dimensional harmonic oscillator in external magnetic field

$$E_{cm}(N, M) = \hbar\Omega_0(2N + |M| + 1) - \hbar\omega_c\frac{M}{2} \quad (7)$$

with radial ($N = 0, 1, 2, \ldots$) and azimuthal ($M = 0, \pm1, \pm2, \ldots$) quantum numbers. In what follows, we will omit energy contributions belonging to the center-of-mass motion energy $E_{cm}$ and spin-field interaction energy $E_s$ because of their trivial and manifestly additive role.

To obtain the eigenvalues of the relative motion Hamiltonian (5) the time-independent Schrödinger equation

$$H_r[\psi(r)\exp(-im\phi)] = E_n(m)[\psi(r)\exp(-im\phi)] \quad (8)$$

must be solved. At this point, it is convenient to introduce new dimensionless variables for energies and distances by measuring them in natural units of $\hbar\Omega_0$ and $l = \sqrt{\hbar/m_e^*\Omega_0}$ respectively, i.e., $E_n'(m) = E_n(m)/\hbar\Omega_0$ and $r' = r/l$. Further on, we will omit the prime sign "′" at $r'$ for convenience. Hence, Eq. (8) can be reduced to the equation for the radial function $\psi(r)$ only

$$-\frac{d^2\psi}{dr^2} - \frac{1}{r}\frac{d\psi}{dr} + \left(\frac{m^2}{r^2} + \frac{1}{4}r^2 + \frac{\gamma}{r} - \frac{m}{2}\frac{\omega_c}{\Omega_0} - E_n'(m)\right)\psi = 0 \quad (9)$$

where the effective Bohr radius $a_B = (\hbar^2/m_e^*)(\varepsilon/e^2)$ and the dimensionless parameter $\gamma = l/a_B$ describes the relative magnitude of the Coulombic energy and confinement energy scales. In its turn, Eq. (8) allows interpretation in terms of the time-independent Schrödinger equation with some effective Hamiltonian $H_{\mathrm{eff}}$

$$H_{\mathrm{eff}}\psi(r) = (H^0 + H')\psi(r) = E_n''(m)\psi(r) \quad (10)$$

with

$$H^0 = -\frac{d^2\psi}{dr^2} - \frac{1}{r}\frac{d\psi}{dr} + \left(\frac{m^2}{r^2} + \frac{1}{4}r^2\right) \quad (11)$$

and

$$H' = \frac{\gamma}{r} \tag{12}$$

with $E_n''(m) = E_n'(m) + (m/2)(\omega_c/\Omega_0)$.

The eigenvalue problem

$$H^0\psi_n^0(r) = E^0(n,m)\psi_n^0(r) \tag{13}$$

can be solved explicitly for each $m$ with the corresponding eigenstates

$$\psi_n^0(r) = \sqrt{\left(\frac{1}{2}\right)^{|m|+1}\frac{2n!}{(n+|m|)!}}\, r^{|m|} \times \exp(-r^2/4)L_n^{|m|}(r^2/2) \tag{14}$$

where $L_n^\alpha(x)$ are generalized Laguerre polynomials

$$L_n^\alpha(x) = \frac{1}{n!}e^x x^{-\alpha}\frac{d^n}{dx^n}(e^{-x}x^{n+\alpha}) \tag{15}$$

and eigenvalues

$$E^0(n,m) = 2(2n+|m|+1) \tag{16}$$

where $n = 0, 1, 2, \ldots$ is the radial quantum number.

## 3. BASICS OF THE METHOD OF INTERMEDIATE PROBLEMS

To make this proceeding self-contained, some technicalities of the method of intermediate problems are outlined here in brief. The starting point of the method is the standard time-independent Schrödinger equation

$$H\psi = E\psi \tag{17}$$

where $H$ is some Hermitian operator with respect to the inner product $(\phi, \psi) = \int \phi^*\psi\, d\tau$ in Hilbert space. It is assumed that all continuous energy levels of $H$ are higher than the lowest discrete energy levels of one's interest. Let us assume, too, that these discrete eigenvalues of $H$ can be ordered in a nondecreasing sequence,

$$E_1 \le E_2 \le \ldots \tag{18}$$

in which each degenerate eigenvalue, if any happens to be among others, appears the number of times of its multiplicity. Eigenstates $\psi_i$, corresponding to the eigenvalues $E_i$, satisfy the equation

$$H\psi_i = E_i\psi_i \tag{19}$$

and are assumed to be orthonormalized, so that

$$(\psi_i, \psi_j) = \delta_{ij} \tag{20}$$

where $\delta_{ij}$ is Kronecker's delta. It is further assumed that the Hamiltonian $H$ can be decomposed as

$$H = H^0 + H' \tag{21}$$

where $H^0$ has known eigenvalues and eigenstates and $H'$ is an arbitrary Hermitian operator which is to be positive definite in the sense that

$$(\psi, H'\psi) = \int \psi^* H'\psi\, d\tau > 0 \quad (\psi \neq 0) \tag{22}$$

for every $\psi$ in the domain of $H$. Hereafter, it is assumed that the lowest part of the discrete spectrum of $H^0$ is below its continuous spectrum and that the corresponding discrete eigenvalues can be ordered in the same manner (18) as those ones belonging to the total Hamiltonian $H$

$$E_1^0 \le E_2^0 \le \ldots \tag{23}$$

with the degenerate eigenvalues appearing the number of times of their multiplicity. The corresponding orthonormalized eigenstates $\psi_i^0$ satisfy the equation

$$H^0\psi_i^0 = E_i^0\psi_i^0, \quad (\psi_i^0, \psi_j^0) = \delta_{ij} \tag{24}$$

Because $H^0 \le H$ in the sense of inequality

$$(\psi, H^0\psi) \le (\psi, H\psi) \tag{25}$$

for every $\psi$ in the domain of $H$, it follows from the Weyl comparison theorem[12] that

$$E_i^0 \le E_i \quad (i = 1, 2, \ldots) \tag{26}$$

Therefore, the eigenvalues of $H^0$ already provide rough lower bound to the eigenvalues of $H$. The Hamiltonian $H^0$ is called the base Hamiltonian as usual. It is worth noticing that the decomposition (21) is not unique and can be tailored to meet the requirements of a particular problem in question.

The basic idea of the method of intermediate problems is to approximate the original Hamiltonian $H$ from below by a non-decreasing sequence of the so-called truncated intermediate Hamiltonians $H^k$. These Hamiltonians are to be constructed to satisfy the inequalities

$$H^k \le H^{k+1} \le H \quad (k = 1, 2, \ldots) \tag{27}$$

Therefore, the Hamiltonian $H^k$ increases if the index $k$ is increased and thus must give improvable lower bounds for the lowest eigenvalues of the original Hamiltonian $H$. It was shown[21,22] that the truncated Hamiltonians $H^k$ can be represented in a general form

$$H^k = H^0 + H'P^k \quad (k = 1, 2, \ldots) \tag{28}$$

The operator $P^k$ defines a projection of an arbitrary vector $\phi$ in the domain of $H$ onto the subspace formed by a sequence of vectors $p_1, p_2, \ldots, p_k$:

$$P^k\phi = \sum_{i=1}^{k}\alpha_i p_i \tag{29}$$

where constants $\alpha_i$ must satisfy the equations

$$[p_j, P^k\phi] = [p_j, \phi] = \sum_{i=1}^{k}\alpha_i[p_j, p_i] \quad (j = 1, 2, \ldots, k) \tag{30}$$

Here an auxiliary inner product with respect to the metric operator $H'$ was introduced as

$$[\psi, \phi] = (\psi, H'\phi) = \int \psi^* H'\phi\, d\tau \tag{31}$$

for every pair of vectors $\psi$, $\phi$ for which $H'\psi$ and $H'\phi$ are defined. Vectors $p_1, p_2, \ldots, p_k$ are to be chosen linearly independent in the vector space with inner product (31). These vectors are to be normalizable but their explicit normalization is not required.

Projections $P^k$ become larger with the increase of the number $k$ of the elements $p_i$ in the sense that the following inequality holds

$$0 \le [\phi, P^k\phi] \le [\phi, P^{k+1}\phi] \le [\phi, \phi], \quad (k = 1, 2, \ldots) \tag{32}$$

which in original vector space reads as

$$0 \le (\phi, H'P^k\phi) \le (\phi, H'P^{k+1}\phi) \le (\phi, H'\phi) \quad (k = 1, 2, \ldots) \tag{33}$$

From Eqs. (29) and (30) it follows that

$$H'P^k\phi = \sum_{i,j=1}^{k} (H'p_i, \phi) b_{ij} H'p_j \tag{34}$$

where $b_{ij}$ are the elements of the matrix inverse to the matrix with terms $[p_j, p_i]$. As a consequence of Eq. (33)

$$H'P^k \le H'P^{k+1} \le H' \quad (k = 1, 2, \ldots) \tag{35}$$

and the intermediate truncated Hamiltonians $H^k$ defined as

$$H^k = H^0 + H'P^k \quad (k = 1, 2, \ldots) \tag{36}$$

satisfy inequalities

$$H^k \le H^{k+1} \le H \tag{37}$$

by construction if inequalities (35) are taken into account. Therefore, the lowest ordered eigenvalues $E_i^k$ of $H^k$ must satisfy inequalities

$$E_i^k \le E_i^{k+1} \le E_i \quad (i, l, k = 1, 2, \ldots) \tag{38}$$

thus providing improvable lower bounds for the original eigenvalues $E_i$ of the Hamiltonian $H$.

It is not a trivial problem to find the eigenstates and eigenvalues of the Hamiltonian $H^k$ in the case of arbitrary set of vectors $\{p_i\}$. However, for a proper choice of these vectors the task can be simplified significantly. One of such choices was proposed in Ref. [21] where each vector $p_i$ was defined by the equation

$$H'p_i = \psi_i^0, \quad i = 1, 2, \ldots, k \tag{39}$$

or, equivalently,

$$p_i = (H')^{-1}\psi_i^0, \quad i = 1, 2, \ldots, k \tag{40}$$

which holds due to existence of the inverse operator $(H')^{-1}$ for positive definite operator $H'$. With so chosen set of vectors $\{p_i\}$ substituted into (34) the Hamiltonian $H^k$ now acts as

$$H'\phi = H^0\phi + \sum_{i,j=1}^{k} (\psi_i^0, \phi) b_{ij} \psi_j^0 \tag{41}$$

It is seen from Eq. (41) that if $(\psi_i^0, \phi) = 0$, $i = 1, 2, \ldots, k$ then $H^k\psi = H^0\psi$. Therefore, each eigenstate $\psi_j^0$ which was not used in the definition (40) is an eigenstate of $H^k$ with the original persistent eigenvalue $E_j^0$. It was proved in a similar way[23] that the continuous spectrum of $H^k$ is identical with that of $H^0$. Hence, the remaining eigenstates of $H^k$ can be represented in the form

$$\psi = \sum_{\nu=1}^{k} \gamma_\nu \psi_\nu^0 \tag{42}$$

and the Schrödinger time-independent equation $H^k\psi = E\psi$ results into the equivalent system of linear algebraic equation with respect to $\gamma_i$

$$\sum_{i=1}^{k} \gamma_i [(E_j^0 - E)\delta_{ij} + b_{ij}] = 0, \quad 1 \le i \le k \tag{43}$$

The eigenvalues of the intermediate Hamiltonian $H^k$ are the roots of the equation

$$|(E_i^0 - E)\delta_{ij} + b_{ij}| = 0, \quad 1 \le i, j \le k \tag{44}$$

but they are not the $k$ lowest eigenvalues of the Hamiltonian $H^k$ in general case. Therefore, these eigenvalues must be united with those unperturbed eigenvalues $E_j^0$ whose corresponding eigenstates were not employed in the definition (40) of the $\{p_i\}$ vectors. Then, the whole set of the thus obtained eigenvalues $\{E_i^k\}$ of the Hamiltonian $H^k$ must be rearranged into a nondecreasing sequence $E_1^k \le E_2^k \le E_3^k \le \ldots$ thus leading to the lower bound inequalities of the kind

$$E_i^0 \le E_i^k \le E_i^{k+t} \le E_i, \quad 1 \le i, k, t \tag{45}$$

## 4. RESULTS

Finally, we calculated the low-lying energy spectrum $E_n''(m)$ for the effective Hamiltonian model (10) for small values of the azimuthal quantum number $m = 0, m = \pm 1$ and two strongly different values of the parameter $\gamma = 1$ and $\gamma = 0.05$. Due to conservation of the orbital momentum, in all of the cases considered the original Hamiltonian (1) as well as the effective Hamiltonian (10) were reduced to a subspace characterized by the particular value of the azimuthal quantum number $m$ and the ensuing reduced eigenvalue problem was treated by means of the lower bound estimate formalism outlined in the Section 3. In the course of the calculations the reduced Hamiltonian (11) served as the base problem Hamiltonian $H^0$ while the interaction Hamiltonian (12) stood for the operator $H'$ in the decomposition (21). The eigenstates (14) were employed as the eigenstates of the base problem $\psi_i^0$. Totally, 200 such eigenstates were employed in calculations. The results are listed in the Tables I and II correspondingly. Regular Rayleigh–Ritz method with the base formed

**Table I. Upper $E''_{n,\mathrm{upp}}(m)$ and lower $E''_{n,\mathrm{low}}(m)$ bounds for energy eigenvalues $E''_n(m)$: $\gamma = 1.0$.**

| State number | $E''_{n,\mathrm{low}}$ $(m = 0)$ | $E''_{n,\mathrm{upp}}$ $(m = 0)$ | $E''_{n,\mathrm{low}}$ $(m = \pm 1)$ | $E''_{n,\mathrm{upp}}$ $(m = \pm 1)$ |
|---|---|---|---|---|
| $n = 0$ | 3.98703 | 4.00047 | 5.19295 | 5.193 |
| $n = 1$ | 7.67122 | 7.69481 | 9.06465 | 9.06475 |
| $n = 2$ | 11.4768 | 11.5071 | 12.9783 | 12.9785 |
| $n = 3$ | 15.3421 | 15.3772 | 16.9145 | 16.9147 |
| $n = 4$ | 19.2415 | 19.2802 | 20.8645 | 20.8648 |
| $n = 5$ | 23.1626 | 23.2040 | 24.8238 | 24.8242 |
| $n = 6$ | 27.0984 | 27.1420 | 28.7897 | 28.7902 |
| $n = 7$ | 31.0447 | 31.0902 | 32.7605 | 32.7611 |
| $n = 8$ | 34.999 | 35.046 | 36.735 | 36.7357 |
| $n = 9$ | 38.9592 | 39.0076 | 40.7126 | 40.7134 |
| $n = 10$ | 42.9243 | 42.9739 | 44.6925 | 44.6934 |
| $n = 11$ | 46.8933 | 46.9439 | 48.6745 | 48.6755 |
| $n = 12$ | 50.8654 | 50.9169 | 52.6581 | 52.6592 |
| $n = 13$ | 54.8402 | 54.8926 | 56.6431 | 56.6443 |
| $n = 14$ | 58.8173 | 58.8704 | 60.6293 | 60.6306 |
| $n = 15$ | 62.7963 | 62.8501 | 64.6166 | 64.618 |

**Table II.** Upper $E''_{n,\mathrm{upp}}(m)$ and lower $E''_{n,\mathrm{low}}(m)$ bounds for energy eigenvalues $E''_n(m)$: $\gamma = 0.05$.

| State number | $E''_{n,\mathrm{low}}$ $(m=0)$ | $E''_{n,\mathrm{upp}}$ $(m=0)$ | $E''_{n,\mathrm{low}}$ $(m=\pm1)$ | $E''_{n,\mathrm{upp}}$ $(m=\pm1)$ |
|---|---|---|---|---|
| $n=0$ | 2.12069 | 2.12364 | 4.0625 | 4.06250 |
| $n=1$ | 6.0905 | 6.09356 | 8.05474 | 8.05475 |
| $n=2$ | 10.077 | 10.0801 | 12.0499 | 12.0499 |
| $n=3$ | 14.0687 | 14.0718 | 16.0464 | 16.0464 |
| $n=4$ | 18.0629 | 18.0661 | 20.0437 | 20.0437 |
| $n=5$ | 22.0586 | 22.0617 | 24.0416 | 24.0416 |
| $n=6$ | 26.0551 | 26.0583 | 28.0398 | 28.0398 |
| $n=7$ | 30.0523 | 30.0554 | 32.0383 | 32.0383 |
| $n=8$ | 34.0499 | 34.053 | 36.037 | 36.0370 |
| $n=9$ | 38.0478 | 38.051 | 40.0358 | 40.0359 |
| $n=10$ | 42.046 | 42.0492 | 44.0348 | 44.0348 |
| $n=11$ | 46.0444 | 46.0476 | 48.0339 | 48.0339 |
| $n=12$ | 50.043 | 50.0462 | 52.033 | 52.0331 |
| $n=13$ | 54.0417 | 54.0449 | 56.0323 | 56.0323 |
| $n=14$ | 58.0406 | 58.0438 | 60.0316 | 60.0316 |
| $n=15$ | 62.0395 | 62.0427 | 64.0309 | 64.031 |

by the same number of unperturbed eigenstates $\psi_i^0$ was used to obtain the upper bound estimates for the energy eigenvalues of the Hamiltonian (10). It is seen that for both cases, i.e., $\gamma = 0.05$ and $\gamma = 1$, the gap between the lower and upper bounds is relatively small even for low lying eigenvalues. For the case of relatively strong interaction $\gamma = 1$ the gaps between the lower and upper bounds are larger than the gaps for the same eigenvalues by order in the case of weak interaction $\gamma = 0.05$. Also, in both cases, the gaps are larger for the low-lying eigenvalues than for the eigenvalues belonging to highly excited eigenstates. It is natural, because, as anticipated, the Coulomb repulsion interaction between the electrons must affect the system ground state as well as adjacent eigenstates to mush higher degree than the states belonging to the upper part of the spectrum. The gaps could be decreased if stricter lower and upper bounds would be obtained by boldly increasing the number $k$ of the base functions $\psi_i^0$ involved in the calculation though this approach being time-consuming. The reason for this is that the unperturbed eigenstates $\psi_i^0$ are no longer adequate for construction of the subspace $\{p_i\}$ and the usage of stochastic variational approach[15, 17] in order to get lower and upper bounds seems to be preferable instead. The same situation actually persists for weak interaction $\gamma = 0.05$ but the discrepancy between the upper and lower bounds is much less

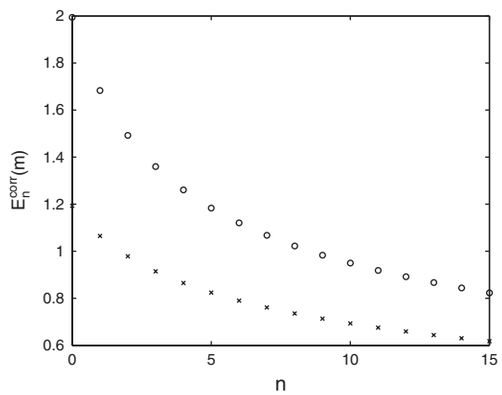


**Fig. 1.** Correlation energies $E_n^{\mathrm{corr}}(m)$; $\gamma = 1$; circles ∘: $m = 0$; crosses ×: $m = \pm1$.

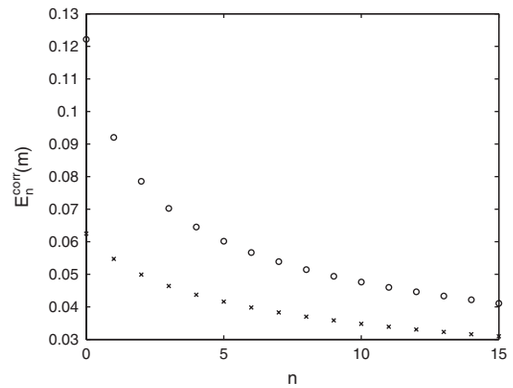


**Fig. 2.** Correlation energies $E_n^{\mathrm{corr}}(m)$; $\gamma = 0.05$; circles ∘: $m = 0$; crosses ×: $m = \pm1$.

pronounced in this case and much smaller sets of functions $\psi_i^0$ are required to reach the same degree of the upper and lower bound proximity. Coincidence between the lower and upper bounds is very good for $|m| = 1$ for both values of $\gamma$ thus indicating that the electrons being in these eigenstates must be staying far apart from each other. Correlation energies due to Coulomb interaction for the electron relative motion defined as

$$E_n^{\mathrm{corr}}(m) = \frac{E''_{n,\mathrm{upp}}(m) + E''_{n,\mathrm{low}}(m)}{2} - E^0(n,m) \qquad (46)$$

were calculated too and are presented in Figures 1 and 2.

## 5. SUMMARY

Applicability of the method of intermediate problems to investigation of the energy spectrum of two-dimensional two-electron quantum dots formed by a parabolic confining potential in the presence of constant uniform external magnetic field was discussed. It was shown that the method is able to provide improvable energy spectrum lower bound estimates for weak and relatively strong electron–electron interaction strength with prescribed or controllable precision at reasonable expense of computational time. Being supplemented with upper bound estimates computed by means of conventional regular or stochastic Rayleigh–Ritz variational method, this approach allows to find the energy spectrum with any desired precision and thus may help verify the results obtained so far by various approximate numerical and analytical approaches to the energy spectrum evaluation.

## References and Notes

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