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Method of intermediate problems in the theory of Gaussian quantum dots placed in a magnetic field

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Applicability of the method of intermediate problems to the investigation of the energy eigenvalues and eigenstates of a quantum dot (QD) formed by a Gaussian confining potential in the presence of an external magnetic field is discussed. Being smooth at the QD boundaries and of finite depth and range, this potential can only confine a finite number of excess electrons thus forming a realistic model of a QD with smooth interface between the QD and its embedding environment. It is argued that the method of intermediate problems, which provides convergent improvable lower bound estimates for eigenvalues of linear half-bound Hermitian operators in Hilbert space, can be fused with the classical Rayleigh-Ritz variational method and stochastic variational method thus resulting in an efficient tool for analytical and numerical studies of the energy spectrum and eigenstates of the Gaussian quantum dots, confining small-to-medium number of excess electrons, with controllable or prescribed precision.

Key words: *quantum dots, eigenvalues, eigenstates, upper and lower bounds*

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1. Introduction

Various theoretical and experimental aspects of the physics of nano-sized and low-dimensional systems have been under steady uninterrupted development for decades, but only in the last ten-fifteen years of research activities in the field, considerable extra momentum has been gained which can be partly ascribed to the progress in nanofabrication of these systems, partly to the development of new experimental techniques but, most of all, to a general continuous trend and desire to diminish the size of components of integrated electronic circuits down to the so-called mesoscopic scale. Among low-dimensional systems of various kinds, quantum dots are potentially fit for many practical applications and are currently thought to be promising building blocks for novel electronic, spintronic and optoelectronic devices.

Reliable estimation of the energy spectrum and eigenstates of a quantum dot is a typical purpose of almost every theoretical study because their properties crucially stipulate the relevant physical characteristics of the quantum dot standing alone as a part of electric circuits or interacting with the environment through its various interfaces.

As a matter of fact, nearly all the mathematical methods, developed within the domain of quantum mechanics so far, have already been employed in the theory of quantum dots in various specific applications though on a varying scale. 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, are various numerical methods which permit either direct calculations of the magnitudes in question without proper error estimates or, at best, provide the calculations with nonincreasing or even convergent upper bounds for the eigenvalues. The widely applicable Rayleigh-Ritz method does it 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 the corresponding lower bounds which are highly desirable to be convergent. Therefore, the development of regular methods to construct such bounds bears a lot of theoretical and practical significance but represents a much more challenging task than derivation of the upper bounds. As to various models of quantum dots, the most suitable ground to fulfill this task 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 H. Weyl [1] and elaborated later by numerous contributors [2,3] with regard to the problems of classical and quantum mechanics. Being supplemented with regular Rayleigh-Ritz or newly developed stochastic variational method [4], 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 would permit to verify the results obtained by other numerical and analytical methods [5]. A stochastic variational method can also be developed on its basis [6] permitting, in principle, the construction of improvable lower bounds for energy eigenvalues of realistic models of quantum dots confining a 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 noting, 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, which appears to be more effective, such error estimates can also be derived for the approximate eigenstates calculated within the framework of the Rayleigh-Ritz regular or stochastic variational method [4] provided that the lower bound estimates for the corresponding energy eigenvalues are known. 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.

2. Quantum dot formed by a Gaussian confining potential

In what follows, a model of a quantum dot confined by a Gaussian potential in an external uniform magnetic field **B** will be considered

$$H = \sum_{i=1}^{N} \frac{1}{2m_{\mathrm{e}}^{*}} \left(\hat{\mathbf{p}}_i + \frac{e}{c}\hat{\mathbf{A}}(\mathbf{r}_i)\right)^2 + \sum_{i=1}^{N} \hat{V}(r_i) + \sum_{i<j}^{N} \frac{\mathrm{e}^2}{\varepsilon \hat{r}_{ij}} + \sum_{i=1}^{N} \frac{g^{*}\mu_{\mathrm{B}}}{\hbar}\mathbf{B}\cdot\hat{\mathbf{S}}_i\,. \tag{2.1}$$

Here m_{e}^{*} is the electron conduction-band mass, e is the absolute value of the electron charge, g^{*} is the effective g factor and indices i, j label the electrons. The Coulomb interaction between the excess electrons is assumed to be proportional to the inverse effective dielectric constant of the bulk material ε and an the inverse interelectron distance $r_{ij} = |\mathbf{r}_i - \mathbf{r}_j|$. The vector potential $\hat{\mathbf{A}}(\mathbf{r})$, $(\mathbf{B} = \mathrm{rot}\mathbf{A})$ is introduced in the symmetric gauge, $\hat{\mathbf{A}}(\mathbf{r}) = B/2(-y, x, 0)$, and $\hat{V}(r)$ is the attractive Gaussian potential

$$\hat{V}(r) = -V_0 \exp(-r^2/2R^2) \tag{2.2}$$

with the depth of the potential well $V_0 > 0$ and the range R, and $r = |\mathbf{r}|$, where $\mathbf{r} = (x, y)$ for 2D quantum dots and $\mathbf{r} = (x, y, z)$ for 3D quantum dots.

For the sake of simplicity and clarity, we limited our present research to the case of two-dimensional quantum dots, though, as will be seen later, generalization of the outlined approach for the case of three-dimensional spherical quantum dots embedded into a supporting matrix is straightforward.

The usage of a Gaussian potential is advantageous in comparison with other commonly employed types of potentials. This potential possesses the finite depth and range so that it can confine only a finite number of the excess electrons, which fact mimics the actual experimental situation properly. In the vicinity of the dot center this potential can be approximated by the parabolic potential routinely applicable in countless dot model studies so far. Therefore, the whole body of the theoretical results obtained for parabolic potentials presently would hold at least approximately for Gaussian potentials for some range of model parameters.

3. The one-electron eigenvalue problem

3.1. The one-electron Gaussian quantum dot model

To our knowledge, no analytical solutions have been obtained so far for the one-electron eigenvalue problem set by the Hamiltonian

$$\hat{H}(i) = \frac{1}{2m_{\mathrm{e}}^{*}}\left(\hat{\mathbf{p}}_i + \frac{\mathrm{e}}{c}\hat{\mathbf{A}}(\mathbf{r}_i)\right)^2 + \hat{V}(r_i) + \frac{g^{*}\mu_{\mathrm{B}}}{\hbar}\mathbf{B}\cdot\hat{\mathbf{S}}_i \tag{3.1}$$

with the attractive Gaussian potential (2.2) even without an external magnetic field though several attempts have been undertaken to solve this problem for the latter case approximately [7–11] due to the role the potentials of this type play in nuclear physics describing the scattering of complex nuclei [12]. Contrariwise, normalized eigenstates of the Hamiltonian

$$\hat{H}_0(i) = \hat{H}_{i0} + \hat{H}_{si0} = \frac{1}{2m_{\mathrm{e}}^{*}}\left(\hat{\mathbf{p}}_i + \frac{\mathrm{e}}{c}\hat{\mathbf{A}}(\mathbf{r}_i)\right)^2 + \frac{g^{*}\mu_{\mathrm{B}}}{\hbar}\mathbf{B}\cdot\hat{\mathbf{S}}_i \tag{3.2}$$

are well known [13] and can be presented as

$$\Psi_{nm\sigma}(r,\phi,s) = \psi_{nm}(r,\phi)\chi_{\sigma}(s) = \frac{1}{\sqrt{2\pi}}\mathrm{e}^{\mathrm{i}m\phi}R_{nm}\left(\frac{r^2}{2a_0^2}\right)\chi_{\sigma}(s), \tag{3.3}$$

where $\chi_{\sigma}(s)$ is a spin function and the radial part is given by

$$R_{nm}(x) = \frac{1}{a_0}\sqrt{\frac{n!}{(n+|m|)!}}\exp\left(-\frac{x}{2}\right)x^{\frac{|m|}{2}}L_n^{|m|}(x), \tag{3.4}$$

where $L_n^{|m|}(x)$ is a generalized Laguerre polynomial. The corresponding eigenvalues are

$$E_{nm\sigma} = E_{nm} + E_{\sigma} = \hbar\omega_c\left(n + \frac{|m|+m}{2} + \frac{1}{2}\right) + \frac{g^{*}\mu_{\mathrm{B}}}{\hbar}B\sigma, \tag{3.5}$$

where $\sigma = \pm 1/2$, $n = 0, 1, \ldots$, $m = 0, \pm 1, \ldots$ and μ_{B} is the Bohr magneton. It is seen that the magnitudes $\hbar\omega_c = (\hbar\mathrm{e}B)/(m_{\mathrm{e}}^{*}c)$ and $a_0 = \sqrt{(\hbar c)/(\mathrm{e}B)}$ provide natural characteristic energy and length scales. The energy eigenvalues (3.5) are infinitely degenerate and form the so-called Landau levels. Due to this feature, the method of the intermediate problems cannot be applied directly to this type of models. At the same time, the total angular momentum component $\sum_i \hat{L}_z^i$ is preserved for the models (2.1) and (3.1) as well as the total spin component $\sum_i \hat{S}_z^i$. Therefore, instead of the model (3.2) with infinitely degenerate energy spectrum (3.5) as well as instead of the model (3.1) one can consider a sequence of models reduced to subspaces labeled with the angular momentum quantum number m and the spin quantum number σ. The energy contribution of the spin part of the Hamiltonian (3.2) is trivially accountable and thus can be omitted. Therefore, further studies can be limited to the treatment of the reduced Hamiltonian

$$\hat{H}_i(m) = \sum_{n,n'=0}^{\infty} |nm\rangle\langle nm|\left(\hat{H}_{i0} + \hat{\hat{V}}(r_i) - V_0\right)|n'm\rangle\langle n'm| \tag{3.6}$$

using the method of intermediate problems. Here an identity transformation of the Gaussian potential was introduced

$$\hat{V}(r) \equiv V_0\left(1 - \exp(-r^2/2R^2)\right) - V_0 \equiv \hat{\hat{V}}(r) - V_0\,, \tag{3.7}$$

where the addition energy V_0 can be currently dropped and then restored only upon the completion of all the calculations. As will be seen in the next section, the necessity of this transformation stems from the positivity condition (3.13).

3.2. 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

$$H\psi = E\psi, \tag{3.8}$$

where H is some Hermitian operator with respect to the inner product $(\phi, \psi) = \int \phi^* \psi \mathrm{d}\tau$ 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 also assume that these discrete eigenvalues of H can be ordered in a nondecreasing sequence,

$$E_1 \leqslant E_2 \leqslant \cdots . \tag{3.9}$$

Eigenstates ψ_i, corresponding to the eigenvalues E_i, satisfy the equation

$$H\psi_i = E_i\psi_i\,, \tag{3.10}$$

and are assumed to be orthonormalized, so that

$$(\psi_i, \psi_j) = \delta_{ij}\,, \tag{3.11}$$

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

$$H = H^0 + H', \tag{3.12}$$

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

$$(\psi, H'\psi) = \int \psi^* H' \psi \mathrm{d}\tau > 0, \qquad (\psi \neq 0) \tag{3.13}$$

for every ψ 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 (3.9) as the ones belonging to the total Hamiltonian H

$$E_1^0 \leqslant E_2^0 \leqslant \cdots . \tag{3.14}$$

The corresponding orthonormalized eigenstates ψ_i^0 satisfy the equation

$$H^0\psi_i^0 = E_i^0\psi_i^0\,, \qquad (\psi_i^0, \psi_j^0) = \delta_{ij}\,. \tag{3.15}$$

Since $H^0 \leqslant H$ in the sense of inequality

$$(\psi, H^0\psi) \leqslant (\psi, H\psi) \tag{3.16}$$

for every ψ in the domain of H, it follows from the Weyl comparison theorem [1] that

$$E_i^0 \leqslant E_i, \qquad (i = 1, 2, \dots). \tag{3.17}$$

Therefore,the eigenvalues of H^0 already provide a rough lower bound to the eigenvalues of H. The Hamiltonian H^0 is called the base Hamiltonian as usual. It is worth noting that the decomposition (3.12) 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 $H^{l,k}$. These Hamiltonians are to be constructed to satisfy the inequalities

$$H^{l,k} \leqslant H^{l+1,k} \leqslant H^k \leqslant H, \qquad (l, k = 1, 2, \dots), \tag{3.18}$$

$$H^{l,k} \leqslant H^{l,k+1} \leqslant H, \qquad (l, k = 1, 2, \dots). \tag{3.19}$$

Therefore, the Hamiltonians $H^{l,k}$ increase whatever index k or l is increased and thus should give improvable lower bounds for the lowest eigenvalues of the original Hamiltonian H. It was shown [15] that the truncated Hamiltonians $H^{l,k}$ can be represented in a general form

$$H^{l,k} = H^{l,0} + H'P^k, \qquad (l, k = 1, 2, \dots). \tag{3.20}$$

Here the Hamiltonian $H^{l,0}$ is a truncation of the base Hamiltonian H^0 of the order l defined as

$$H^{l,0}\psi = \sum_{i=1}^{l} \left(\psi_i^0, \psi\right) E_i^0 \psi_i^0 + E_{l+1}^0 \left[\psi - \sum_{i=1}^{l} \left(\psi_i^0, \psi\right) \psi_i^0\right], \qquad (l = 1, 2, \dots), \tag{3.21}$$

or, alternatively, in Dirac's more transparent bra and ket notations

$$H^{l,0} = \sum_{i=1}^{l} E_i^0 |E_i^0\rangle\langle E_i^0| + E_{l+1}^0 \left[\hat{I} - \sum_{i=1}^{l} |E_i^0\rangle\langle E_i^0|\right], \quad (l = 1, 2, \dots), \tag{3.22}$$

where $\hat{I}$ stands for the identity operator. Truncations of H^0 satisfy the inequalities

$$H^{l,0} \leqslant H^{l+1,0} \leqslant H^0, \qquad (l = 1, 2, \dots), \tag{3.23}$$

which were proved in general case in [17].

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

$$P^k\phi = \sum_{i=1}^{k} \alpha_i p_i \,, \tag{3.24}$$

where constants α_i should satisfy the equations

$$\left[p_j, P^k\phi\right] = \left[p_j, \phi\right] = \sum_{i=1}^{k} \alpha_i \left[p_j, p_i\right], \qquad (j = 1, 2, \dots, k). \tag{3.25}$$

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

$$[\psi, \phi] = (\psi, H'\phi) = \int \psi^* H' \phi \,\mathrm{d}\tau \tag{3.26}$$

for every pair of vectors ψ, ϕ for which $H'\psi$ and $H'\phi$ are defined. Vectors $p_1, p_2, \dots, p_k$ are to be chosen linearly independent in the vector space with an inner product (3.26). 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 involved. As a consequence, the following inequality holds

$$0 \leqslant [\phi, P^k\phi] \leqslant [\phi, P^{k+1}\phi] \leqslant [\phi, \phi], \qquad (k = 1, 2, \dots), \tag{3.27}$$

which in the original vector space reads as

$$0 \leqslant (\phi, H'P^k\phi) \leqslant (\phi, H'P^{k+1}\phi) \leqslant (\phi, H'\phi), \qquad (k = 1, 2, \dots). \tag{3.28}$$

From equations (3.24, 3.25) it follows that

$$H'P^k\phi = \sum_{i,j=1}^{k} (H'p_i, \phi) b_{ij} H'p_j \,, \tag{3.29}$$

where b_{ij} are the elements of the matrix inverse to the matrix with terms $[p_j, p_i]$. As a consequence of equation (3.28)

$$H'P^k \leqslant H'P^{k+1} \leqslant H', \qquad (k = 1, 2, \dots), \tag{3.30}$$

and the intermediate truncated Hamiltonians H^k defined as

$$H^k = H^0 + H'P^k, \qquad (k = 1, 2, \dots) \tag{3.31}$$

satisfy inequalities

$$H^k \leqslant H^{k+1} \leqslant H \tag{3.32}$$

by construction if inequalities (3.30) are taken into account.

According to equations (3.23) and (3.30)

$$H^{l,k} \leqslant H^{l,k+1} \leqslant H^{l,0} + H' \leqslant H, \qquad (l, k = 1, 2, \dots). \tag{3.33}$$

Therefore, the lowest ordered eigenvalues $E_i^{l,k}$ of $H^{l,k}$ should satisfy the parallel inequalities

$$E_i^{l,k} \leqslant E_i^{l+1,k} \leqslant E_i^k \leqslant E_i, \qquad (i, l, k = 1, 2, \dots), \tag{3.34}$$

and

$$E_i^{l,k} \leqslant E_i^{l,k+1} \leqslant E_i, \quad (i, l, k = 1, 2, \dots), \tag{3.35}$$

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

As was proved in [17], the so constructed Hamiltonian $H^{l,k}$ can have no continuous spectrum and must have E_{l+1}^0 as an eigenvalue of infinite multiplicity. Therefore, only those eigenvalues of $H^{l,k}$ that are smaller or equal to E_{l+1}^0 can be considered as lower bound estimates for the eigenvalues of the initial Hamiltonian H.

The truncation procedure (3.21) can be significantly improved from the point of view of practical calculations if the original Hamiltonian H is formally decomposed as

$$H = H^{l,0} + (H^0 - H^{l,0}) + H' = H^{l,0} + H' + H'' = H^{l,0} + \tilde{H}', \qquad (l = 1, 2, \dots), \tag{3.36}$$

where the difference $\tilde{H}' = H - H^{l,0}$ is obviously positive and can play the role played before by the metric operator H'. In this case the positive contributions from the operator

$$H'' = H^0 - H^{l,0}, \quad (l = 1, 2, \dots) \tag{3.37}$$

to lower bound estimates are not simply neglected at will but rather carefully taken into consideration on common grounds with the contributions stemming from H', thus making these bounds higher than they might have been otherwise under the original truncation procedure (3.21).

3.3. Reduced linear algebraic problems for the one-electron model

The eigenvalues and eigenstates of the intermediate Hamiltonians $H^{l,k}$ of any order (i.e. for arbitrary magnitudes of the indices l and/or k) can be expressed analytically or calculated numerically in terms of the known eigenvalues and eigenstates of H^0 and an arbitrarily chosen set of linearly independent vectors p_i, $(i = 1, \dots, k)$. For numerical calculations it is especially convenient to follow the observation made by W. Börsch-Supan [15] that any intermediate Hamiltonian $H^{l,k}$ can be reduced to the finite-dimensional space $\mathcal{M}$ generated by the known eigenstates ψ_i^0, $(i = 1, \dots, l)$ of the base Hamiltonian H^0 and the vectors $H'p_i$, $(i = 1, \dots, k)$. This reduction makes it possible to determine the eigenstates of $H^{l,k}$ lying in $\mathcal{M}$ along with the corresponding eigenvalues from a linear algebraic problem of the order $l + k$ for one symmetric indefinite matrix relative to another. This problem can be formulated in terms of the system of equations with respect to γ_ν

$$\sum_{\nu=1}^{k+l} \gamma_\nu \left(C_{\mu\nu} - \left(E - E_{l+1}^0 \right) D_{\mu\nu} \right) = 0, \qquad (\mu = 1, 2, \dots, k + l)\,, \tag{3.38}$$

where

$$(C_{\mu\nu}) = \begin{pmatrix} \delta_{\mu\nu} & (\psi_\mu^0, H'p_{\nu-l}) \\ (H'p_{\mu-l}, \psi_\nu^0) & (H'p_{\mu-l}, H'p_{\nu-l} \end{pmatrix}, \tag{3.39}$$

and

$$(D_{\mu\nu}) = \begin{pmatrix} \delta_{\mu\nu}/(E_\nu^0 - E_{l+1}^0) & 0 \\ 0 & (H' p_{\mu-l}, p_{\nu-l}) \end{pmatrix}. \tag{3.40}$$

For the eigenvalues E which are not equal to E_{l+1}^0 the corresponding eigenstates of $H^{l,k}$ are given by

$$\psi(E) = \left(\sum_{\nu=1}^{l} \gamma_\nu \psi_\nu^0 + \sum_{\nu=l+1}^{l+k} \gamma_\nu H' p_{\nu-l} \right) \left(E - E_{l+1}^0 \right)^{-1}, \tag{3.41}$$

and E_{l+1}^0 is an eigenvalue of $H^{l,k}$ of infinite multiplicity.

Sometimes, another special choice for vectors p_i is possible

$$p_i = (H')^{-1} \psi_i^0, \qquad i = 1, 2, \dots, k. \tag{3.42}$$

As was shown in [14], k eigenvalues of the intermediate Hamiltonian H^k can be found by the solution of the matrix eigenvalue problem

$$\sum_{j=1}^{k} \left\{ [E_t^0 - E]\delta_{jt} + b_{jt} \right\} \gamma_j = 0, \qquad 1 \leqslant t \leqslant k, \tag{3.43}$$

where b_{ji} is the matrix inverse to that with elements

$$(\psi_i^0, p_j) = (\psi_i^0, (H')^{-1} \psi_j^0). \tag{3.44}$$

For the thus found eigenvalues E the corresponding eigenstates of H^k are given by

$$\psi(E) = \sum_{t=1}^{k} \gamma_t(E) \psi_t^0. \tag{3.45}$$

Moreover, if an eigenfunction ψ_t^0 of H^0 with an eigenvalue E_t^0 is not employed in forming any element p_i, then ψ_t^0 is also an eigenfunction of the intermediate Hamiltonian H^k with the same eigenvalue E_t^0. Unlike the Hamiltonian (3.20), the Hamiltonian H^k for the special choice of p_i vectors (3.42) may also possess a continuous spectrum which can be shown to be identical to that of H^0.

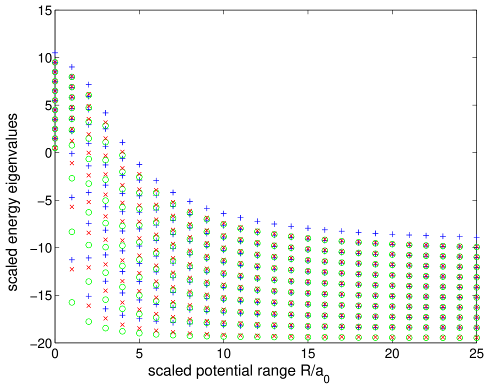

Figure 1. Scaled energy eigenvalues $E/\hbar w_c$ via scaled potential range R/a_0; circles o: m=0; crosses + : m=1; crosses x: m=-1; $V_0/\hbar w_c = 20$.

For the particular single electron model (3.6), the Hamiltonian H' in (3.12) can be identified with $\hat{\hat{V}}(r_i)$ thus satisfying the positivity condition (3.13). For any fixed angular quantum number m and any given order l of the intermediate Hamiltonian (3.20) the vectors ψ_i^0 must be identified with the first $l+1$ functions ψ_{nm}, $n = 0, 1, \dots, l$. Correspondingly, the eigenvalues $E_i^0, i = 1, \dots, l+1$ are E_{nm}, $n = 0, 1, \dots, l$ defined in equation (3.5). In our present numerical calculations the vectors p_i, $i = 1, \dots, k$ coincide with the first k eigenstates ψ_{nm}, $n = 1, \dots, k$. Actually, this choice ensures that the contribution to all the requisite matrix elements from the operator of the kind (3.37) is zero. What seems to be much more important is the fact that this choice made possible an analytical calculation of all matrix elements appearing in (3.38), thus increasing the precision of the results. For convenience, the condition $k = l$ was fulfilled throughout all the calculations. The upper bound estimates on the energy eigenvalues of the Hamiltonian (3.6) were obtained by the standard Rayleigh-Ritz method using a set of p eigenfunctions ψ_{nm} as the base set. The numbers l, k and p of the functions involved in all these calculations were chosen to ensure the coincidence of the corresponding upper and lower energy spectrum bound estimates up to the sixth digit. Exemplary results of these calculations are shown in figure 1 where ten lowest eigenvalues for each of the three different values of angular momentum $m = -1, m = 0$ and $m = 1$ are plotted via the Gaussian potential range R. It is seen that the originally degenerate at $R = 0$ eigenvalues become nondegenerate as the potential range R increases to the magnitudes comparable with the characteristic magnetic length a_0 and return to degeneracy again upon a further increase of the potential range, thus restoring the structure of Landau levels.

4. Two- and many-electron Gaussian quantum dots

In general, Gaussian quantum dots in a magnetic field containing two or more excess electrons can be treated using the method of intermediate problems in the same way as the simple one-electron quantum dot was treated above with the only difference that now the electron-electron interaction is to be taken into account. This interaction is repulsive and the additional interaction term $\sum_{i<j}^{N} \hat{V}(r_{ij})$ in H' satisfies the positivity condition (3.42). Therefore, all the prospected difficulties in applying the method would not be of conceptual but rather of technical nature due to cumbersome and laborious calculations. Of course, the Fermi statistics should be accounted for when constructing many-electron functions ψ_i^0 and p_i. Thus, the functions ψ_i^0 should be antisymmetric with respect to pairwise electron permutations eigenfunctions of the total angular and spin momentum built of the one-electron eigenstates (3.3). The amount of the required calculations drastically depends on the proper choice of the functions p_i. It is quite reasonable to anticipate that the stochastic variational method for the calculation of the lower bound estimates to eigenvalues, proposed in [6], will be useful in significantly cutting down the size of the $\{p_i\}$ sets.

For the two-electron quantum dot the special choice (3.42) of p_i functions looks advantageous. In this case

$$(H')^{-1} = (\hat{\hat{V}}(r_1) + \hat{\hat{V}}(r_2) + \hat{V}(r_{12}))^{-1} \tag{4.1}$$

and all matrix elements (3.44) can be reduced to calculating the three-dimensional integrals. Formally, further reduction to two-dimensional integrals is also possible but at the expense of elliptic functions showing up in the integrands. It was found that either three- or two-dimensional integrals can be calculated numerically by means of the Gauss-Kronrod adaptive method. The same choice (3.42) can be employed in general case of a quantum dot containing N electrons. The resulting matrix elements should be calculated by the methods of numerical multidimensional integration.

An alternative approach (3.38) can also be employed in the case of the two-electron Gaussian quantum dot. In this case it is convenient to choose the p_i functions in the form $p_i = r_{12}\psi_i^0$, but such a choice may be not optimal and can lead to prohibitively large sets of p_i functions. An expediency of using the correlated Gaussians [4,18], as a much more effective choice for p_i, is currently being investigated. This choice looks promising for Gaussian quantum dots containing small-to-medium number of electrons.

5. Conclusion

It was shown that the energy eigenvalues of practically important and realistic models of quantum dots formed by a Gaussian confining potential and placed in an external magnetic field can be estimated with arbitrarily prescribed precision by means of the standard Rayleigh-Ritz method, the method of intermediate problems being complementary to each other. Two-side improvable error bound estimates can be found for the eigenvalues while the corresponding eigenstates come out as a by-product of the applied methods together with their error bound estimates as well.

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Метод проміжних задач у теорії гаусових квантових точок, поміщених у магнітне поле

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Обговорюється застосовність методу проміжних задач до дослідження власних значень енергії та власних станів квантової точки (КТ), сформованої утримуючим Гаусовим потенціалом в присутності зовнішнього магнітного поля. Будучи гладким на границі КТ та маючи скінчені глибину та радіус взаємодії, цей потенціал може утримувати лише скінчене число надлишкових електронів, формуючи через це реалістичну модель КТ з гладкою границею розділу між КТ та її оточенням. Аргументується, що метод проміжних задач, що забезпечує збіжні покращені значення для нижньої границі власних значень лінійних напівзв'язаних Ермітових операторів у Гільбертовому просторі, може бути поєднаний з класичним варіаційним методом Релея-Рітца та стохастичним варіаційним методом, даючи в результаті ефективний засіб для аналітичних ти числових досліджень енергетичного спектру та власних станів гаусових квантових точок, що утримують від малого до середнього числа надлишкових електронів, з контрольованою та заданою точністю.

Ключові слова: *квантові точки, власні значення, власні стани, верхня та нижня границі*

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