$N$ electrons in a quantum dot: Two-point Pade approximants

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Abstract

We present analytic estimates for the energy levels of $N$ electrons ($N = 2 - 5$) in a two-dimensional parabolic quantum dot. A magnetic field is applied perpendicularly to the confinement plane. The relevant scaled energy is shown to be a smooth function of the parameter $\beta = (\text{effective Rydberg/effective dot energy})^{1/6}$. Two-point Pade approximants are obtained from the series expansions of the energy near the oscillator ($\beta \to 0$) and Wigner ($\beta \to \infty$) limits. The approximants are expected to work with an error not greater than 2.5% in the entire interval $0 \leq \beta < \infty$.

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1 Introduction

The problem of $N$ electrons in quantum dots and magnetic fields has been widely considered in recent years [1].

Concerning the energy levels of $N$ electrons in model two-dimensional parabolic quantum dots, the actual magnitude to compute is a scaled energy which depends only on one parameter, $\beta=(\text{effective Rydberg/effective dot energy})^{1/6}$. When $\beta \to 0$ (very high magnetic fields, for example), we may use perturbation theory to compute the energy levels. In the opposite limit, $\beta \to \infty$, a strong coupling expansion may be used to obtain the energy. The idea of the present paper is to construct two-point Pade approximants interpolating from $\beta = 0$ to $\beta \to \infty$. We show results for 2, 3, 4, and 5 electrons.

To our knowledge, there are only a few alternative analytical ways to obtain the energy of certain levels in the entire interval $0 \leq \beta < \infty$. Semiclassical [2] and $1/|J|$-expansions [3, 4], both working for states with high angular momentum, $J$, are available. Besides these expansions, there is also an idea of improving the perturbative series by using the asymptotics at $\beta \to \infty$ [5]. We understand the present paper as a useful complement to the results of [2 - 5]. We will see, for example, that it is very simple to find Pade approximants for states with $|J| = 0, 1, 2$, for which the methods of [2, 4] do not work.

2 Two-point Pade approximants

The construction of approximants follows the idea of paper [6], in which the hydrogenic energy levels in a magnetic field were obtained.

Let us consider the expansions of the scaled energy (to be computed in the next sections) when $\beta \to 0$ and $\beta \to \infty$,

\begin{align*}
\epsilon|_{\beta \to 0} & = \sum_{k=0}^{s} b_k \beta^k + \mathcal{O}(\beta^{s+1}), \\
\epsilon|_{\beta \to \infty} & = \beta^2 \left\{ \sum_{k=0}^{t} a_k / \beta^k + \mathcal{O}(1/\beta^{t+1}) \right\}.
\end{align*}

(1) (2)
Many of the coefficients entering (1, 2) are zero. For example, all the \( b_k \) with \( k \neq 0 \) \( \mod 3 \), \( a_1, a_3 \), etc.

A two-point Padé approximant is a rational function,

\[
P(\beta) = \frac{\sum_{k=0}^{L} p_k \beta^k}{\sum_{k=0}^{K} q_k \beta^k},
\]

reproducing the expansions (1) and (2). \( q_0 \) may be fixed to one. The asymptotics when \( \beta \to \infty \) forces \( L \) to be equal to \( K + 2 \). Equating number of coefficients in the expansions (1) and (2) to number of unknowns in (3), we obtain,

\[
s + t = 2K + 1.
\]

At a given \( K \), there is a set of possible pairs \( s, t \). We will attach indexes \( s \) and \( t \) to the approximant, \( P_{s,t} \). Among the possible \( P_{s,t} \), the best one takes nearly the same number of terms in the expansions (1) and (2) [6], i.e. \( s \approx t \).

Let us consider the equations fulfilled by the \( p_k \) and the \( q_k \). Equating (3) to (1) and (2), we obtain,

\[
\begin{align*}
p_k &= q_0 b_k + q_1 b_{k-1} + \ldots + q_k b_0, \quad 0 \leq k \leq \text{Min}(s, K + 2), \\
p_k &= q_K a_{K+2-k} + q_{K-1} a_{K+1-k} + \ldots + q_{K-2} a_0, \\
&\quad K + 2 - \text{Min}(K + 2, t) \leq k \leq K + 2.
\end{align*}
\]

Eliminating the overlapping \( p_k \), i.e. \( k \) in the interval \( \text{Max}(0, s + 1 - K) \leq k \leq \text{Min}(s, K + 2) \), a system of linear equations for the coefficients \( q_k \) arise. We assume that \( s \) is in the interval \( K - 1 \leq s \leq K + 2 \), such that this system contains \( K \) equations. Let us write explicitly, for example, the approximant \( P_{4,3} \). The coefficients \( b_1, b_2, b_4, a_1 \) and \( a_3 \) are assumed to be zero. The result is the following,

\[
P_{4,3}(\beta) = b_0 + \frac{b_3 \beta^3}{1 + q_1 \beta + q_2 \beta^2 + q_3 \beta^3} + a_0 \beta^2 \left\{ 1 - \frac{1 + q_1 \beta}{1 + q_1 \beta + q_2 \beta^2 + q_3 \beta^3} \right\},
\]

where \( q_2 = a_0/(b_0 - a_2) \), \( q_1 = a_0 q_2/b_3 \), \( q_3 = (a_0 q_1 - b_3)/(b_0 - a_2) \).
Formula (7), or similar expressions for higher approximants (see Appendix 1), is to be used throughout the paper. Let us indicate the way to compute the $b_k$ and the $a_k$.

3 The coefficients $b_k$ and $a_k$

Let us consider the two dimensional motion of $N$ electrons in a parabolic quantum dot of energy $\hbar \omega_0$. A magnetic field is applied normally to the plane of motion. The Hamiltonian governing the internal motion (center of mass motion is excluded) is written in dimensionless variables as

$$
\frac{H}{\hbar \Omega} = h + \frac{\omega_c}{2\Omega} J + \frac{g \omega_c}{2\Omega} S_z,
$$

(8)

where $\omega_c$ is the cyclotronic frequency, $\Omega = \sqrt{\omega_0^2 + \omega_c^2/4}$ is the effective dot frequency, $J$ is the total (internal) angular momentum (along the $z$ axis), $S_z$ is the $z$-projection of the total spin, $g$ is the effective giromagnetic factor, and

$$
h = - \sum_{k=1}^{N-1} \left( \frac{\partial^2}{\partial \rho_k^2} + \frac{1}{\rho_k} \frac{\partial}{\partial \rho_k} \right) - \sum_{k=1}^{N-2} \left( \frac{1}{\rho_k^2} + \frac{1}{\rho_{k+1}^2} \right) \frac{\partial^2}{\partial \theta_k^2}
$$

$$
+ 2 \sum_{k=1}^{N-3} \frac{1}{\rho_{k+1}^2} \frac{\partial^2}{\partial \rho_k \partial \theta_{k+1}} + \frac{2iJ}{N-1} \sum_{k=1}^{N-2} \left( \frac{1}{\rho_k^2} - \frac{1}{\rho_{k+1}^2} \right) \frac{\partial}{\partial \theta_k}
$$

$$
+ \sum_{k=1}^{N-1} \left( \frac{J^2}{(N-1)^2} \frac{1}{\rho_k^2} \frac{1}{4 \rho_{k+1}^2} + \beta^3 \sum_{k<l} \frac{1}{r_{kl}} \right)
$$

(9)

Notice that $h$ depends only on one parameter, $\beta^3 = \sqrt{\frac{\mu e^4}{\kappa^2 h^2}} \sqrt{\hbar \Omega}$, where $\mu$ is the effective electron mass, and $\kappa$ - the relative dielectric constant. The coordinates entering $h$ are the moduli of the Jacobi vectors,

$$
\bar{\rho}_k = \sqrt{\frac{\mu_k}{\mu_1}} \left\{ \bar{r}_{k+1} - \frac{1}{k} \sum_{j=1}^{k} \bar{r}_j \right\}, \quad k = 1, \ldots, N - 1,
$$

(10)

and the angles between $\bar{\rho}_k$ and $\bar{\rho}_{k+1}$, denoted by $\theta_k$. The dimensionless reduced masses are $\mu_k = k/(k + 1)$. 

4
The eigenfunctions of $H$ are $e^{iJ\Xi}\psi$, where $\Xi$ accounts for global rotations, and $\psi$ are the eigenfunctions of $h$. The eigenvalues of $H$ are trivially obtained from the eigenvalues of $h$, which will be called $\epsilon$. We will obtain Pade approximants to $\epsilon$.

In the $\beta \to 0$ (oscillator) limit, perturbation theory may be applied to obtain $\epsilon$. The resulting series is the following

$$\epsilon|_{\beta \to 0} = b_0 + b_3\beta^3 + b_6\beta^6 + \ldots,$$

(11)

where $b_0 = N - 1 + |J| + 2n$, $n$ is the total number of oscillator quanta, $b_3 = \langle \phi | \sum_{k<l} r_{kl}^{-1} | \phi \rangle$, etc. In systems with more than two electrons, sometimes degenerate perturbation theory shall be used to compute $b_3$, $b_6$, etc.

On the other hand, when $\beta \to \infty$ a strong coupling expansion may be applied. Distances are scaled according to $\rho \to \beta \rho$. The hamiltonian $h$ takes the form

$$\frac{\hbar}{\beta^2} = \frac{1}{4} \sum_{k=1}^{N-1} \rho_k^2 + \frac{1}{\rho_{kl}} + \frac{J^2}{(N-1)^2 \beta^4} \sum_{k=1}^{N-1} \frac{1}{\rho_k^2}$$

$$- \frac{1}{\beta^4} \left\{ \sum_{k=1}^{N-1} \left( \frac{\partial^2}{\partial \rho_k^2} + \frac{1}{\rho_k} \frac{\partial}{\partial \rho_k} \right) + \sum_{k=1}^{N-2} \left( \frac{1}{\rho_k^2} + \frac{1}{\rho_{k+1}^2} \right) \frac{\partial^2}{\partial \theta_k^2} \right\}$$

$$+ \frac{2}{\beta^4} \left\{ \sum_{k=1}^{N-3} \frac{1}{\rho_{k+1}^2} \frac{\partial^2}{\partial \theta_k \partial \theta_{k+1}} + \frac{iJ}{N-1} \sum_{k=1}^{N-2} \left( \frac{1}{\rho_k^2} - \frac{1}{\rho_{k+1}^2} \right) \frac{\partial}{\partial \theta_k} \right\}. \quad (12)$$

In the leading approximation, $\beta \to \infty$, we shall minimize the classical potential energy entering the r.h.s. of (12). It is found that the electrons sit at the corners of a regular polygon. This is a few-body version of the Wigner solid. The classical energy becomes a function of one variable, $\rho_1$,

$$U = \frac{N \rho_1^2}{8 \sin^2 \pi/N} + \frac{\sin \pi/N}{\rho_1} \sum_{k=1}^{N-1} \frac{1}{|\sin \theta_{kl}/2|},$$

(13)

where $\theta_{kl}$ is the angle between particles $k$ and $l$, measured from the c.m. The minimization of $U$ leads to the equilibrium value of $\rho_1$, $\rho_{10}$. The equilibrium values of the other coordinates are obtained from geometric considerations. The energy in this approximation is given by $U(\rho_{10})$. Corrections to this value are obtained by writting $\rho_k = \rho_{k0} + z_k/\beta$, $k = 1,\ldots,N-1$, $\theta_k = \theta_{k0} + z_{N-1+k}/\beta$, $k = 1,\ldots,N-2$, and expanding
\( h/\beta^2 = U(\rho_{10}) + h_2/\beta^2 + h_3/\beta^3 + \ldots, \) \hspace{1cm} (14)  
\[ \psi = \psi_0 + \psi_1/\beta + \psi_2/\beta^2 + \ldots, \] \hspace{1cm} (15)  
\[ \epsilon/\beta^2 = a_0 + a_2/\beta^2 + a_3/\beta^3 + \ldots. \] \hspace{1cm} (16)

The Schrodinger equation is split into the set of uncoupled equations

\[ a_0 = U(\rho_{10}), \] \hspace{1cm} (17)
\[ h_2\psi_0 = a_2\psi_0, \text{ etc.} \] \hspace{1cm} (18)

The hamiltonian \( h_2 \) describes harmonic oscillations around the Wigner structure. The expression for \( a_2 \) is thus

\[ a_2 = \sum_{k=1}^{2N-3} \omega_k(n_k + 1/2), \] \hspace{1cm} (19)

where the \( \omega_k \) are the normal frequencies. Higher corrections are obtained by considering \( h_3, h_4, \text{ etc} \) as perturbations to \( h_2 \).

Below, we present results for 2, 3, 4, and 5 electrons.

4 Two electrons

As mentioned above, the eigenfunctions of \( H \) are written as \( e^{iJ\Xi}\psi(\rho_1) \). Under a permutation of particles, \( \Xi \) changes by \( \pi \), and \( \psi \) does not change. Thus, even \( |J| \) are related to antisymmetric spin functions, \( S = 0 \), and odd \( |J| \) are related to states with spin \( S = 1 \).

Let \( \phi_k \) be the eigenfunctions of \( h \) at \( \beta = 0 \),

\[ \phi_k = C_k \rho_1^{0J} L_k^{0J}(\rho_1^2/2)e^{-\rho_1^2/4}, \] \hspace{1cm} (20)

where \( C_k = (2^{0J}(k+|J|)!/k!)^{-1/2} \), and \( L_k^{0J} \) are generalized Laguerre polynomials. The corresponding eigenvalues are

\[ b_0 = 2k + |J| + 1. \] \hspace{1cm} (21)

We take a fixed \( k \) as the unperturbed level, let us say, \( n_1 \). Higher coefficients of the expansion are computed from
\[ b_3 = < n_1 | \frac{1}{\rho_1} | n_1 >, \quad (22) \]
\[ b_6 = \frac{1}{2} \sum_{k \neq n_1} \frac{| < n_1 | 1/\rho_1 | k > |^2}{(n_1 - k)}, \quad \text{etc.} \quad (23) \]

We show in Tab. 1 the coefficients \( b_3 \) and \( b_6 \) for a set of two-electron states.

Let us consider now the opposite limit, \( \beta \to \infty \). The equilibrium value of \( \rho_1 \) (scaled) is \( \rho_{10} = 2^{1/3} \). The coefficient \( a_0 \) is thus \( a_0 = 3/2^{4/3} \). Then, we write \( \rho_1 = \rho_{10} + z_1/\beta \), and expand the hamiltonian. The results are

\[ h_2 = -\frac{\partial^2}{\partial z_1^2} + \frac{3}{4} z_1^2, \quad (24) \]
\[ h_k = \frac{(-1)^k}{\rho_{10}^{k+1}} z_1^{k} - \frac{(-1)^{k-3}}{\rho_{10}^{k-2}} z_1^{k-3} \frac{\partial}{\partial z_1} + \frac{J^2 (-1)^{k-4} (k-3)}{\rho_{10}^{k-2}} z_1^{k-4}, \quad k \geq 3 \quad (25) \]

Notice that the \( h_k \) with odd \( k \) contain an odd number of creation and annihilation operators. Thus, all the \( a_k \) with odd \( k \) will be zero. Computation of the matrix elements of \( h_k \) is a trivial task. Finally, we obtain

\[ a_2 = \omega_1 (n_1 + 1/2), \quad (26) \]
\[ a_4 = 2^{-2/3} \left\{ (n_1^2 + n_1 + 7/6)/6 + J^2 - 1/4 \right\}, \quad \text{etc} \quad (27) \]

where \( \omega_1 = \sqrt{3} \), i.e. the classical result [7]. Note that we have used the same number, \( n_1 \), to label the state at \( \beta = 0 \) and \( \beta \to \infty \). As level crossings can not occur, the first state at \( \beta = 0 \) should be the first when \( \beta \to \infty \), and so on. Note also that \( J \) appears for the first time in \( a_4 \).

The coefficients \( a_2 \) and \( a_4 \) are also shown in Tab. 1 for a set of states. From this Table and formulae contained in Appendix 1, we may construct Padé approximants for the energy levels.

We show in Fig. 1 the three curves \( \epsilon |_{\beta \to 0} = b_0 + b_3 \beta^3 + b_6 \beta^6 \), \( \epsilon |_{\beta \to \infty} = a_0 \beta^2 + a_2 + a_4 / \beta^2 \), and \( P_{6,5}(\beta) \) for the first state with quantum numbers \( |J| = 3, n_1 = 0 \). This is the typical behaviour of the approximants.
In Fig. 2, we compare the approximants in the sequence $P_{K+1,K}$. The same state as in Fig. 1 is studied. The relative differences between consecutive approximants are shown. The $\beta$ axis is compressed to $(0,1)$. We see that the maximal difference reduces by a factor of two when $K$ is increased by one. These results suggest the $P_{6,5}$ approximant (the highest we computed) to be accurate to about three parts in $10^3$ or better. Notice that the maxima are reached at $\beta \approx 2$, i.e. in the region where the approximants jump from the weak-coupling to the strong-coupling regimes (see Fig. 1).

Similar results are obtained for the other states in Tab. 1. When $J = 0$, however, relative differences between approximants increase up to 2%, and some approximants can not be used as they exhibit a pole. So, the best of our Padé estimates are expected to work with an error not greater than 2% in the worst situation.

We show in Fig. 3 the convergence of the sequence $P_{K+1,K}$ at particular $\beta$ values, at which exact solutions are available [8]. It can be easily shown, for example, that

$$\psi = \rho_1^{\lfloor J \rfloor} \left( 1 + \rho_1 / \sqrt{2|J| + 1} \right) e^{-\rho_1^2}, \quad (28)$$

are eigenfunctions of $h$ at $\beta = (2|J| + 1)^{1/6}$, with eigenvalues $\epsilon = |J| + 2$. The corresponding $n_1$ are zero. When $0 \leq |J| \leq 3$, $\beta$ is in the interval $1 \leq \beta \leq 1.38$, well outside the exactly solvable limits. The relative error of the $P_{6,5}$ approximant is lower than 2 % at $J = 0$, and less than 0.2 % at $|J| = 3$.

## 5 Three electrons

First, let us consider the computation of the coefficients $a_k$ up to $a_5$. The Wigner configuration is a triangle with side $\rho_{10} = 3^{1/3}$ (scaled). The leading approximation to the energy is

$$a_0 = \frac{3^{5/3}}{2}. \quad (29)$$

Then, we write $\rho_1 = \rho_{10} + (u + v) / (\sqrt{2}\beta)$, $\rho_2 = \rho_{10} + (u - v) / (\sqrt{2}\beta)$, $\theta_1 = \pi/2 + \sqrt{2}z / (\rho_{10}\beta)$. Expanding the hamiltonian $h$, we arrive to
\[
\begin{align*}
    h_2 &= - \left( \frac{\partial^2}{\partial u^2} + \frac{\partial^2}{\partial v^2} + \frac{\partial^2}{\partial z^2} \right) + \frac{3}{4} u^2 + \frac{3}{8}(v^2 + z^2), \\
    h_3 &= \frac{1}{16\sqrt{2}\rho_{10}} \left\{ -32 \frac{\partial}{\partial u} + 32u \frac{\partial^2}{\partial z^2} - 8u^3 - 6uv^2 - 5v^3 - 6uz^2 \\
    &\quad + 15vz^2 \right\}, \\
    h_4 &= \frac{1}{\rho_{10}} \left\{ \frac{J^2}{2} + u \frac{\partial}{\partial u} - \frac{3}{2} u^2 \frac{\partial^2}{\partial z^2} + \frac{1}{4} u^4 + v \frac{\partial}{\partial v} - 2iJv \frac{\partial}{\partial z} \\
    &\quad - \frac{3}{2} v^2 \frac{\partial^2}{\partial z^2} + \frac{3}{8} u^2v^2 + \frac{5}{8} uv^3 + \frac{9}{256} v^4 + \frac{3}{16} u^2z^2 \\
    &\quad - \frac{15}{16} uvz^2 - \frac{3}{128} v^2z^2 + \frac{41}{256} z^4 \right\}, \text{ etc.}
\end{align*}
\]

\(u, v, \text{ and } z\) are normal coordinates. \(u\) corresponds to a symmetric oscillation (breathing) with frequency \(\omega_1 = \sqrt{3}\), whereas \(v\) and \(z\) correspond to a mixed oscillation of the Wigner structure, with frequency \(\omega_2 = \sqrt{3}/2\). In the harmonic approximation, the spatial wave function is written as
\[
\psi = \chi_{n_1}(u)\chi_{n_2}(v)\chi_{n_3}(z)e^{iJz},
\]
where the \(\chi\) are oscillator functions, i.e. Hermite polynomials multiplied by gaussians. A function \(\psi\) that can be antisymmetrized is related to a spin-polarized state \((S = 3/2)\) of three electrons. On the other hand, a mixed-symmetry \(\psi\) is related to a spin one half state.

Let us consider the lowest state with a given \(J\), i.e. that one with numbers \(n_1 = n_2 = n_3 = 0\). This state may be spatially antisymmetrized only when \(J = 3k\), with \(k\) - an integer. The argument goes along the lines sketched in [9]: a cyclical permutation of electrons in the triangle, leaving the wave function invariant, is equivalent to a \(2\pi/3\) rotation, which multiplies it by \(e^{iJ2\pi/3}\), thus \(e^{iJ2\pi/3} = 1\). The excitations with \(n_2 = n_3 = 0\) correspond also to antisymmetric states. The \(n_2 + n_3 = 1\) states correspond to mixed-symmetry doublets, etc. On the other hand, when \(J \neq 3k\) the lowest state and the excitations with \(n_2 = n_3 = 0\) have mixed symmetry. An antisymmetric and a mixed-symmetry state appear at \(n_2 + n_3 = 1\), etc. We will restrict the analysis to the lowest state and the first excitations.

The coefficient \(a_2\) is thus given by
\[ a_2 = \sqrt{3}(n_1 + 1/2) + \sqrt{3/2}(n_1 + n_2 + 1). \] (34)

Higher corrections are computed from perturbation theory around \( h_2 \). By the same reason as for two particles, \( a_3 \) and \( a_5 \) are equal to zero. The next nonzero coefficient is

\[
a_4 = < n_1, n_2, n_3 | h_4 | n_1, n_2, n_3 > + \sum_{(k_1, k_2, k_3) \neq (n_1, n_2, n_3)} \frac{< n_1, n_2, n_3 | h_3 | k_1, k_2, k_3 > < k_1, k_2, k_3 | h_3 | n_1, n_2, n_3 >}{\sqrt{3}(n_1 - k_1) + \sqrt{3/2}(n_1 + n_2 -k_1 - k_2)}. \] (35)

The computation of matrix elements entering (35) is trivial, leading to

\[
a_4 = \frac{1}{144 \rho^2_{10}} \left\{ -2 + 9\sqrt{2} + 72J^2 + (12 + 18\sqrt{2})n_1 + 12n_1^2 \right. \\
+ \left. (36 + 9\sqrt{2} + 18\sqrt{2}n_1)(n_2 + n_3) + 228n_2n_3 - 78(n_2^2 + n_3^2) \right\}. \] (36)

Let us stress that we expanded the hamiltonian around a structure with \( \theta_1 = \pi/2 \). There is an equivalent configuration with \( \theta_1 = -\pi/2 \). In the expansion (16), we have neglected tunneling between the two equivalent configurations. The same comment holds for systems with more than three electrons. Notice also that the second local minimum of \( U \), the linear structure (second “Lagrange” solution), is at a distance 0.36\( \beta^2 \) above the lowest state. We can disregard any effect coming from this structure when \( \beta^2 \gg a_2/0.36 \).

The computation of the coefficient \( b_3 \) requires the wave functions at \( \beta = 0 \). They may be explicitly written with the help of the indications of paper [10]. We will compute \( b_3 \) for a set of states with \( |J| = 0, 1, 2, \) and 3. In all of these states, the corresponding quantum numbers at \( \beta \to \infty \) can be specified.

For example, when \( J = 0 \), the first antisymmetric (A) state at \( \beta = 0 \), which starts from \( b_0 = 4 \) (it will be labelled \( (4,A) \)), goes to the first A at \( \beta \to \infty \), i.e. \( (n_1, n_2, n_3) = (0,0,0) \). The first mixed state, \( (4,M) \), goes to the first doublet with \( n_1 = 0, n_2 + n_3 = 1 \). The second antisymmetric state, \( (6,A) \), goes to the \( (1,0,0) \). At \( |J| = 1 \), the \( (3,M) \) goes to the \( (0,0,0) \), the \( (5,A) \) goes to a state with \( n_1 = 0, n_2 + n_3 = 1 \). At \( |J| = 2 \), the \( (4,M) \) goes to the
(0,0,0), and the (6,A) – to a state with $n_1 = 0$, $n_2 + n_3 = 1$. At $|J| = 3$, the (5,A) goes to the (0,0,0), and the (5,M) to a state with $n_1 = 0$, $n_2 + n_3 = 1$.

Let us write explicitly the needed wave functions at $\beta = 0$ (up to nor-

malisations). In the case of mixed symmetry, only one representative of the

doublet is given.

$J = 0$

\[
\begin{align*}
\phi_{4,A} &= \rho_1 \rho_2 \sin \theta_1 \ e^{-(\rho_1^2 + \rho_2^2)/4}, \\
\phi_{4,M} &= (\rho_1^2 - \rho_2^2) \ e^{-(\rho_1^2 + \rho_2^2)/4}, \\
\phi_{6,A} &= \rho_1 \rho_2 \sin \theta_1 \left( \rho_1^2 + \rho_2^2 - 8 \right) \ e^{-(\rho_1^2 + \rho_2^2)/4}.
\end{align*}
\]

$J = 1$

\[
\begin{align*}
\phi_{3,M} &= \rho_1 \ e^{-i\theta_1/2} \ e^{-(\rho_1^2 + \rho_2^2)/4}, \\
\phi_{5,A} &= \left\{ (-2\rho_1^3 \rho_2^2 + \rho_1^3) \ e^{-i\theta_1/2} - \rho_1 \rho_2^2 \ e^{3i\theta_1/2} \right\} \ e^{-(\rho_1^2 + \rho_2^2)/4}.
\end{align*}
\]

$J = 2$

\[
\begin{align*}
\phi_{4,M} &= \rho_1 \rho_2 \ e^{-(\rho_1^2 + \rho_2^2)/4}, \\
\phi_{6,A} &= \rho_1 \rho_2 \sin \theta_1 \left( \rho_1^2 e^{-i\theta_1} + \rho_2^2 e^{i\theta_1} \right) \ e^{-(\rho_1^2 + \rho_2^2)/4}.
\end{align*}
\]

$J = 3$

\[
\begin{align*}
\phi_{5,A} &= \left\{ \rho_1^3 e^{-3i\theta_1/2} - 3\rho_1 \rho_2^2 e^{i\theta_1/2} \right\} \ e^{-(\rho_1^2 + \rho_2^2)/4}, \\
\phi_{5,M} &= \left\{ \rho_1^3 e^{-3i\theta_1/2} + \rho_1 \rho_2^2 e^{i\theta_1/2} \right\} \ e^{-(\rho_1^2 + \rho_2^2)/4}.
\end{align*}
\]

The computation of $b_3$ is thus a trivial task. We grouped all the results together in Table 2. With these coefficients, we construct the approximants $P_{3,2}$, $P_{4,3}$, and $P_{5,4}$.

The convergence analysis of the Pade sequence $P_{K+1,K}$ is shown in Fig. 4 for the lowest antisymmetric state with $|J| = 3$. As in the two-electron problem, convergence is strong, suggesting the $P_{5,4}$ interpolant to be accurate to about 6 parts in $10^3$ or better in the entire interval $0 \leq \beta < \infty$. Similar results are obtained for the lowest states with $|J| = 2$, and 1. The excited states and the states with $J = 0$ show a slower convergence. The relative error is estimated as 2%.
6 Four electrons

First, let us compute the coefficients $a_0$ and $a_2$. As in previous cases, $a_1 = a_3 = 0$.

The equilibrium configuration at $\beta \to \infty$ is a square with side $\rho_{10} = (2 + \sqrt{2}/2)^{1/3}$ (scaled). The equilibrium values of the other coordinates are $\rho_{20} = \sqrt{5}/3 \rho_{10}$, $\rho_{30} = 2\rho_{10}/\sqrt{3}$, $\theta_{10} = \arctan 2$, $\theta_{20} = 3\pi/4 - \theta_{10}$. $a_0$ is given by

$$a_0 = 3(2 + \sqrt{2}/2)^{1/3}. \quad (46)$$

Expanding around the equilibrium geometry, we obtain the quadratic hamiltonian,

$$h_2 = -\left( \frac{\partial^2}{\partial z_1^2} + \frac{\partial^2}{\partial z_2^2} + \frac{\partial^2}{\partial z_3^2} \right) - \left( \frac{1}{\rho_{10}^2} + \frac{1}{\rho_{20}^2} \right) \frac{\partial^2}{\partial z_4^2}$$

$$- \left( \frac{1}{\rho_{20}^2} + \frac{1}{\rho_{30}^2} \right) \frac{\partial^2}{\partial z_5^2} + 2 \frac{\partial}{\partial z_4} \frac{\partial}{\partial z_5} + V_2, \quad (47)$$

where

$$V_2 = 0.543374 z_1^2 + 0.157283 z_1 z_2 + 0.520305 z_2^2 + 0.182039 z_1 z_3$$
$$+ 0.377402 z_2 z_3 + 0.460201 z_3^2 + 0.171862 z_2 z_4 + 0.192148 z_3 z_4$$
$$+ 0.517308 z_4^2 + 0.110937 z_1 z_5 + 0.085931 z_2 z_5 + 0.562904 z_4 z_5$$
$$+ 0.853613 z_5^2. \quad (48)$$

The normal frequencies are easily found, resulting in

$$\omega_1 = 1.04969,$$
$$\omega_2 = 1.13911,$$
$$\omega_3 = 1.36227,$$
$$\omega_4 = 1.46201,$$
$$\omega_5 = 1.75640, \quad (49)$$

and, thus, the coefficient $a_2$ is given by
\[ a_2 = \sum_{k=1}^{5} \omega_k (n_k + 1/2). \] (50)

Notice that the frequency corresponding to the breathing mode, \( \omega_5 \), is close to the classical value \( \sqrt{3} \), but it does not exactly coincide with \( \sqrt{3} \).

As in the \( N = 3 \) problem, the lowest state with a given \( |J| \), i.e. \( n_k = 0 \), \( k = 1, \ldots, 5 \), can be spatially antisymmetrised only when \( |J| \) takes certain values. The allowed values are \( |J| = 2, 6, 10, \ldots \). These are polarised spin states, i.e. with total spin \( S = 2 \). The excitations of the \( \omega_5 \) mode have the symmetry of the ground state.

Let us stress that, as \( N \) increases, the number of equivalent configurations (geometries with the same \( a_0 \)) increases, and the energetic distance to other local minima of the classical energy decreases. Thus, tunelling effects become more and more important.

In what follows, we restrict the analysis to the lowest spin-polarised state, that is \( |J| = 2 \), and the \( n_k = 0 \). It seems that it is the lowest state of \( h \) in the sector with \( S = 2 \) at any \( \beta \). Indeed, as \( \beta \to 0 \), this state goes to an oscillator state with \( b_0 = 7 \), i.e. to the \((7,A)\) in the terminology used above. There is a second \((7,A)\) with \( J = 0 \). However, according to Hund’s rule, this state has a higher energy at \( \beta \ll 1 \). When \( \beta \to \infty \), the \( J = 0 \) state is also higher in energy because \( J = 0 \) is not compatible with \( n_k = 0 \), thus excitation quanta are needed.

Let us compute the coefficient \( b_3 \) for the \( |J| = 2 \) state. The wave function at \( \beta = 0 \) is given in Appendix 2. Calculations may be carried out analytically, leading to

\[ b_3 = 6 \frac{\langle \phi_{7,A} | \frac{1}{\rho_1} | \phi_{7,A} \rangle}{\langle \phi_{7,A} | \phi_{7,A} \rangle} = \frac{91}{64} \sqrt{2\pi}. \] (51)

Once computed \( a_0, a_2, b_0, \) and \( b_3 \), we may construct the approximants \( P_{3,2} \) and \( P_{4,3} \), which are the main results of this section. The relative error between \( P_{3,2} \) and \( P_{4,3} \) is shown in Fig. 5, suggesting that \( P_{4,3} \) may estimate the energy with an error not greater than 2% at intermediate values of \( \beta \).

Pade approximants to other levels may be constructed in the same way.
7 Five electrons

We follow the same programme as in the \( N = 4 \) problem, i.e. computation of \( a_0, a_2, b_0, \) and \( b_3 \) and, from them, construction of the approximants \( P_{3,2} \) and \( P_{4,3} \).

The equilibrium configuration at \( \beta \to \infty \) is a pentagon with side \( \rho_{10} = 1.30766 \) (scaled). The equilibrium values of the other coordinates are \( \rho_{20}/\rho_{10} = 1.44177, \rho_{30}/\rho_{10} = 1.53244, \rho_{40}/\rho_{10} = 1.34500, \theta_{10} = 0.865925 \) rad, \( \theta_{20} = 1.74428 \) rad, \( \theta_{30} = -1.03941 \) rad. \( a_0 \) is given by

\[
a_0 = 9.28013 .
\]  

Expanding around the equilibrium configuration, we obtain the hamiltonian \( h_2 \),

\[
h_2 = - \left( \frac{\partial^2}{\partial z_1^2} + \frac{\partial^2}{\partial z_2^2} + \frac{\partial^2}{\partial z_3^2} + \frac{\partial^2}{\partial z_4^2} \right) - \left( \frac{1}{\rho_{10}^2} + \frac{1}{\rho_{20}^2} \right) \frac{\partial^2}{\partial z_5^2} - \left( \frac{\partial^2}{\partial z_5^2} \right) - \left( \frac{\partial^2}{\partial z_6^2} \right) + \left( \frac{\partial^2}{\partial z_7^2} \right)
\]

\[
+ \frac{2}{\rho_{20}^2} \frac{\partial}{\partial z_5} \frac{\partial}{\partial z_6} + \frac{2}{\rho_{30}^2} \frac{\partial}{\partial z_6} \frac{\partial}{\partial z_7} + V_2 ,
\]

where

\[
V_2 = 0.624037 z_1^2 - 0.007988 z_1 z_2 + 0.514889 z_2^2 + 0.107324 z_1 z_3 \\
+ 0.231789 z_2 z_3 + 0.438330 z_3^2 + 0.073587 z_1 z_4 + 0.245901 z_2 z_4 \\
+ 0.381949 z_3 z_4 + 0.373258 z_4^2 + 0.315672 z_2 z_5 - 0.296995 z_3 z_5 \\
+ 0.451706 z_5^2 + 0.313498 z_1 z_6 - 0.217440 z_2 z_6 - 0.286484 z_3 z_6 \\
+ 0.326409 z_4 z_6 + 0.765563 z_5 z_6 + 1.43839 z_6^2 - 0.126796 z_2 z_7 \\
+ 0.119294 z_3 z_7 + 0.169244 z_5 z_7 + 1.37849 z_6 z_7 + 1.46079 z_7^2 .
\]

The normal frequencies following from the eigenvalue problem for \( h_2 \) are

\[
\omega_1 = 0.727516,
\]
\begin{align*}
\omega_2 &= 0.804763, \\
\omega_3 &= 1.37185, \\
\omega_4 &= 1.52505, \\
\omega_5 &= 1.68899, \\
\omega_6 &= 1.73205, \\
\omega_7 &= 1.74375,
\end{align*}

and the coefficient \( a_2 \) is given by

\begin{equation}
a_2 = \sum_{k=1}^{7} \omega_k (n_k + 1/2). \tag{56}
\end{equation}

The allowed values of \(|J|\) for antisymmetric states with \( n_k = 0 \) are \(|J| = 0, 5, 10, \ldots \). In these states the total spin is \( S = 5/2 \). In what follows, we consider the lowest state in this sequence, i.e. \( J = 0 \). This state goes to a (10,A) state as \( \beta \to 0 \). It is not, however, the lowest of all antisymmetric levels at \( \beta \ll 1 \) because a second (10,A) state with \(|J| = 2\) minimises the Coulomb repulsion.

The wave function of the \( J = 0 \) state is given in Appendix 2. Calculations may also be performed analytically, leading to

\begin{equation}
b_3 = \frac{149}{64} \sqrt{2\pi}. \tag{57}
\end{equation}

We show in Fig. 6 the relative difference between \( P_{3,2} \) and \( P_{4,3} \). This difference is not greater than 2.5%.

Pade approximants to other levels may be constructed in the same way.

\section{Concluding Remarks}

We have studied systems of 2 - 5 electrons in a two-dimensional parabolic quantum dot. The potentials involved in this problem (harmonic plus Coulomb repulsion) are very gentle, and lead to a smooth dependence of the energy \( \epsilon \) on the coupling constant \( \beta \). This fact is graphically represented in Fig. 1, where it is seen that the “regions of convergence” of the perturbative and the strong-coupling series “intersect” with each other.
The degrees of homogeneity of the potentials are also important factors towards the smoothness of $\epsilon$. They lead to expansion series containing only powers of $\beta^3$ at $\beta \to 0$, and inverse powers of $\beta^2$ at $\beta \to \infty$. From the calculational point of view, it means that with the help of trivial computations, not beyond first order perturbation theory, we may construct approximants up to $P_{4,3}$, that is, a quotient between a 5th order and a 3rd order polynomial in $\beta$. These approximants are exact in both $\beta \to 0$ and $\beta \to \infty$ limits, leading to errors not greater than 2.5% in the small transition region where they jump from one expansion to the other. The accuracy may be improved by computing higher approximants, as shown for two and three electrons.

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10 Appendix 1. The approximants used in the paper

\[ P_{3,2}(\beta) = b_0 + a_0 \beta^2 \left\{ 1 - (1 + b_3 \beta^2 / a_0 + a_0 \beta^2 / (b_0 - a_2))^{-1} \right\}, \]  

(58)

\[ P_{4,3} \] is given in Eq. (7).

\[ P_{5,4}(\beta) = b_0 + \frac{b_3 \beta^3}{1 + q_1 \beta + \ldots + q_4 \beta^4} - \frac{(b_0 - a_2)q_4 \beta^4}{1 + q_1 \beta + \ldots + q_4 \beta^4} + a_0 \beta^2 \left\{ 1 - \frac{1 + q_1 \beta}{1 + q_1 \beta + \ldots + q_4 \beta^4} \right\}, \]  

(59)

where,

\[ q_2 = a_0 q_3 / b_3, \quad q_1 = \frac{1}{a_0} \{b_3 + (b_0 - a_2)q_3\}, \]

\[ q_4 = \frac{a_0}{a_4} \left\{ -1 + \frac{b_0 - a_2}{b_3} q_3 \right\}, \]  

(60)

and \( q_3 \) is determined from the equation

\[ -b_3 q_1 + a_0 q_2 - (b_0 - a_2) q_4 = 0. \]  

(61)

\[ P_{6,5}(\beta) = b_0 + \frac{b_3 \beta^3}{1 + q_1 \beta + \ldots + q_5 \beta^5} - \frac{(b_0 - a_2)\{q_4 \beta^4 + q_5 \beta^5\}}{1 + q_1 \beta + \ldots + q_5 \beta^5} + a_0 \beta^2 \left\{ 1 - \frac{1 + q_1 \beta}{1 + q_1 \beta + \ldots + q_5 \beta^5} \right\}, \]  

(62)

where,

\[ q_3 = \frac{1}{b_3} \{a_0 q_4 - b_0\}, \quad q_2 = \frac{1}{b_0 - a_2} \{a_0 + a_4 q_4\}, \]

\[ q_1 = \frac{1}{b_3} \{a_0 q_2 - (b_0 - a_2) q_4\}, \]

\[ q_5 = \frac{1}{a_4} \{b_3 + (b_0 - a_2) q_3 - a_0 q_1\}. \]  

(63)
and \( q_4 \) is found from
\[- b_3 q_2 + a_0 q_3 - (b_0 - a_2) q_5 = 0. \tag{64} \]

11 Appendix 2. Wave functions for 4 and 5 electrons at \( \beta = 0 \)

We show the explicit form of the functions \( \phi_{7,A}, N = 4 \), and \( \phi_{10,A}, N = 5 \). The \( \vec{r}_j \) are measured from the c. m., and \( (\vec{a} \times \vec{b})_z \) denotes the \( z \) component (normal to the plane) of the vectorial product.

\[
\phi_{7,A} = \left\{ [\vec{r}_3 \cdot \vec{r}_1 / \rho_3 + i(\vec{r}_3 \times \vec{r}_1)_z / \rho_3]^2 [\vec{r}_2 \times \vec{r}_3 + \vec{r}_4 \times \vec{r}_4 + \vec{r}_5 \times \vec{r}_2]_z \\
- [\vec{r}_3 \cdot \vec{r}_2 / \rho_3 + i(\vec{r}_3 \times \vec{r}_2)_z / \rho_3]^2 [\vec{r}_3 \times \vec{r}_4 + \vec{r}_4 \times \vec{r}_4 + \vec{r}_5 \times \vec{r}_3]_z \\
+ [\vec{r}_3 \cdot \vec{r}_3 / \rho_3 + i(\vec{r}_3 \times \vec{r}_3)_z / \rho_3]^2 [\vec{r}_4 \times \vec{r}_1 + \vec{r}_5 \times \vec{r}_2 + \vec{r}_2 \times \vec{r}_4]_z \\
- r_4^2 [\vec{r}_1 \times \vec{r}_2 + \vec{r}_2 \times \vec{r}_3 + \vec{r}_3 \times \vec{r}_1]_z \right\} e^{-(\rho_1^2 + \rho_3^2 + \rho_4^2)/4} e^{2i(\theta_1 + \theta_3)/3}. \tag{65} \]

\[
\phi_{10,A} = e^{-(\rho_1^2 + \rho_3^2 + \rho_4^2 + \rho_5^2)/4} \left\{ (\vec{r}_1 \cdot \vec{r}_2)(\vec{r}_1 \times \vec{r}_2)_z [\vec{r}_3 \times \vec{r}_4 + \vec{r}_4 \times \vec{r}_5 + \vec{r}_5 \times \vec{r}_3]_z \\
+ (\vec{r}_2 \cdot \vec{r}_3)(\vec{r}_2 \times \vec{r}_3)_z [\vec{r}_4 \times \vec{r}_5 + \vec{r}_5 \times \vec{r}_1 + \vec{r}_1 \times \vec{r}_4]_z \\
+ (\vec{r}_3 \cdot \vec{r}_4)(\vec{r}_3 \times \vec{r}_4)_z [\vec{r}_5 \times \vec{r}_1 + \vec{r}_1 \times \vec{r}_2 + \vec{r}_2 \times \vec{r}_5]_z \\
+ (\vec{r}_4 \cdot \vec{r}_5)(\vec{r}_4 \times \vec{r}_5)_z [\vec{r}_1 \times \vec{r}_2 + \vec{r}_2 \times \vec{r}_3 + \vec{r}_3 \times \vec{r}_1]_z \\
+ (\vec{r}_5 \cdot \vec{r}_1)(\vec{r}_5 \times \vec{r}_1)_z [\vec{r}_2 \times \vec{r}_3 + \vec{r}_3 \times \vec{r}_4 + \vec{r}_4 \times \vec{r}_2]_z \\
- (\vec{r}_1 \cdot \vec{r}_3)(\vec{r}_1 \times \vec{r}_3)_z [\vec{r}_4 \times \vec{r}_5 + \vec{r}_5 \times \vec{r}_2 + \vec{r}_2 \times \vec{r}_4]_z \\
- (\vec{r}_2 \cdot \vec{r}_4)(\vec{r}_2 \times \vec{r}_4)_z [\vec{r}_5 \times \vec{r}_1 + \vec{r}_1 \times \vec{r}_3 + \vec{r}_3 \times \vec{r}_5]_z \\
- (\vec{r}_3 \cdot \vec{r}_5)(\vec{r}_3 \times \vec{r}_5)_z [\vec{r}_1 \times \vec{r}_2 + \vec{r}_2 \times \vec{r}_4 + \vec{r}_4 \times \vec{r}_1]_z \\
+ (\vec{r}_1 \cdot \vec{r}_4)(\vec{r}_1 \times \vec{r}_4)_z [\vec{r}_5 \times \vec{r}_2 + \vec{r}_2 \times \vec{r}_3 + \vec{r}_3 \times \vec{r}_5]_z \\
+ (\vec{r}_2 \cdot \vec{r}_5)(\vec{r}_2 \times \vec{r}_5)_z [\vec{r}_1 \times \vec{r}_3 + \vec{r}_3 \times \vec{r}_4 + \vec{r}_4 \times \vec{r}_1]_z \right\}. \tag{66} \]
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Figure and Table Captions

Tab. 1. The first nonzero coefficients $b_k$ and $a_k$ for a set of two-electron states

Tab. 2. The first nonzero coefficients $b_k$ and $a_k$ for certain three-electron states

Fig. 1. Weak and strong-coupling expansions (dashed lines), and the $P_{6,5}$ approximant (solid line) for two electrons in a state with $|J| = 3, n_1 = 0$

Fig. 2. Relative differences between consecutive approximants in the sequence $P_{K+1,K}$, with $K$ ranging from 2 to 5. The state with $|J| = 3, n_1 = 0$ is shown

Fig. 3. Convergence of the Pade sequence $P_{K+1,K}$ at $\beta = (2|J| + 1)^{1/6}$. Two electrons in states with $n_1 = 0$ are considered. Solid lines represent the exact solutions found in [8]

Fig. 4. The same as in Fig. 2, now for the first antisymmetric state of three electrons with $|J| = 3$. $K$ ranges from 2 to 4

Fig. 5. Relative difference between $P_{4,3}$ and $P_{3,2}$ for the lowest antisymmetric state of four electrons ($|J| = 2$)

Fig. 6. The same as in Fig. 5, now for the lowest antisymmetric state of five electrons with angular momentum $J = 0$
Table 1

| $|J|$, $n$ | $b_0$ | $b_3$ | $b_6$ | $a_0$ | $a_2$ | $a_4$ |
|----------|-------|-------|-------|-------|-------|-------|
| 0, 0     | 1     | 1.253314 | -0.345655 | 1.190551 | 0.866025 | -0.034998 |
| 0, 1     | 3     | 0.939986 | -0.087406 | 1.190551 | 2.598076 | 0.174989 |
| 0, 2     | 5     | 0.802904 | -0.411161 | 1.190551 | 4.330127 | 0.594963 |
| 1, 0     | 2     | 0.626657 | -0.032762 | 1.190551 | 0.866025 | 0.594963 |
| 1, 1     | 4     | 0.548325 | -0.016339 | 1.190551 | 2.598076 | 0.804950 |
| 1, 2     | 6     | 0.499367 | -0.010112 | 1.190551 | 4.330127 | 1.224924 |
| 2, 0     | 3     | 0.469937 | -0.011153 | 1.190551 | 0.866025 | 2.484844 |
| 2, 1     | 5     | 0.430827 | -0.007016 | 1.190551 | 2.598076 | 2.694831 |
| 2, 2     | 7     | 0.402676 | -0.004920 | 1.190551 | 4.330127 | 3.114805 |
| 3, 0     | 4     | 0.391661 | -0.005533 | 1.190551 | 0.866025 | 5.634647 |
| 3, 1     | 6     | 0.367182 | -0.003911 | 1.190551 | 2.598076 | 5.844634 |
| 3, 2     | 8     | 0.348211 | -0.002950 | 1.190551 | 4.330127 | 6.264608 |

Table 2

| $|J|$, Symmetry | $b_0$ | $b_3$ | $a_0$ | $a_2$ | $a_4$ |
|---------------|-------|-------|-------|-------|-------|
| 0, A          | 4     | 1.87997 | 3.12013 | 2.09077 | 0.0358156 |
| 0, M          | 4     | 2.58496 | 3.12013 | 3.31552 | -0.0619104 |
| 0, A          | 6     | 1.76247 | 3.12013 | 3.82282 | 0.209926 |
| 1, M          | 3     | 2.81996 | 3.12013 | 2.09077 | 0.276191 |
| 1, A          | 5     | 1.82122 | 3.12013 | 3.31552 | 0.178464 |
| 2, M          | 4     | 2.23247 | 3.12013 | 2.09077 | 0.997315 |
| 2, A          | 6     | 1.58623 | 3.12013 | 3.31552 | 0.899589 |
| 3, A          | 5     | 1.70372 | 3.12013 | 2.09077 | 2.19919 |
| 3, M          | 5     | 2.26184 | 3.12013 | 3.31552 | 2.10146 |