N electrons in a quantum dot: two-point Padé 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 = $ (effective rydberg/effective dot energy)$^{1/6}$. Two-point Padé 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% over the entire interval $0 \leqslant \beta < \infty$.

1. Introduction

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

For 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 = $ (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 Padé approximants interpolating from $\beta = 0$ to $\beta \to \infty$. We give results for two, three, four, and five electrons.

To our knowledge, there are only a few alternative analytical ways to obtain the energy of certain levels over the entire interval $0 \leqslant \beta < \infty$. 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 the idea of improving the perturbative series by using the asymptotics for $\beta \to \infty$ [5]. We see 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 Padé approximants for states with $|J| = 0, 1, 2$, for which the methods of [2, 4] do not work.

2. Two-point Padé approximants

The construction of approximants follows the idea of [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 following sections) when $\beta \to 0$ and $\beta \to \infty$:

$$\epsilon|_{\beta \to 0} = \sum_{k=0}^{s} b_k \beta^k + \mathcal{O}(\beta^{s+1}) \tag{1}$$

$$\epsilon|_{\beta \to \infty} = \beta^2 \left\{ \sum_{k=0}^{t} a_k/\beta^k + \mathcal{O}(1/\beta^{t+1}) \right\}. \tag{2}$$

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

A two-point Padé approximant is a rational function:

$$P(\beta) = \sum_{k=0}^{L} p_k \beta^k \Big/ \sum_{k=0}^{K} q_k \beta^k \tag{3}$$

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 the number of coefficients in the expansions (1) and (2) to the number of unknowns in (3), we obtain

$$s + t = 2K + 1. \tag{4}$$

At a given K, there is a set of possible pairs s, t. We will attach indices 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. $s \approx t$. For example, at $K = 3$ the best one, whose coefficients are computed almost trivially, is $P_{4,3}$.

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

$$p_k = q_0 b_k + q_1 b_{k-1} + \cdots + q_k b_0 \qquad\qquad 0 \leqslant k \leqslant \text{Min}(s, K+2) \tag{5}$$

$$p_k = q_K a_{K+2-k} + q_{K-1} a_{K+1-k} + \cdots + q_{k-2} a_0 \qquad K + 2 - \text{Min}(K+2, t) \leqslant k \leqslant K + 2. \tag{6}$$

On eliminating the overlapping p_k, i.e. k in the interval $\text{Max}(0, s + 1 - K) \leqslant k \leqslant \text{Min}(s, K+2)$, a system of linear equations for the coefficients q_k are obtained. We assume that s is in the interval $K - 1 \leqslant s \leqslant K + 2$, so 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:

$$P_{4,3}(\beta) = b_0 + \frac{b_3 \beta^3}{1 + q_1 \beta + q_2 \beta^2 + q_3 \beta^3} + a_0 \beta^2 \left\{ 1 - \frac{1 + q_1 \beta}{1 + q_1 \beta + q_2 \beta^2 + q_3 \beta^3} \right\} \tag{7}$$

where

$$q_2 = a_0/(b_0 - a_2) \qquad q_1 = a_0 q_2/b_3 \qquad q_3 = (a_0 q_1 - b_3)/(b_0 - a_2).$$

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 (centre-of-mass motion is excluded) is written in dimensionless variables as

$$\frac{H}{\hbar\Omega} = h + \frac{\omega_c}{2\Omega} J + \frac{g\omega_c}{2\Omega} S_z \tag{8}$$

where ω_c is the cyclotron 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 gyromagnetic factor, and

$$
\begin{aligned}
h = &- \sum_{k=1}^{N-1}\left(\frac{\partial^2}{\partial\rho_k^2} + \frac{1}{\rho_k}\frac{\partial}{\partial\rho_k}\right) - \sum_{k=1}^{N-2}\left(\frac{1}{\rho_k^2} + \frac{1}{\rho_{k+1}^2}\right)\frac{\partial^2}{\partial\theta_k^2} \\
&+ 2\sum_{k=1}^{N-3}\frac{1}{\rho_{k+1}^2}\frac{\partial^2}{\partial\theta_k\,\partial\theta_{k+1}} + \frac{2\mathrm{i}J}{N-1}\sum_{k=1}^{N-2}\left(\frac{1}{\rho_k^2} - \frac{1}{\rho_{k+1}^2}\right)\frac{\partial}{\partial\theta_k} \\
&+ \sum_{k=1}^{N-1}\left(\frac{J^2}{(N-1)^2}\frac{1}{\rho_k^2} + \frac{1}{4}\rho_k^2\right) + \beta^3\sum_{k<l}\frac{1}{r_{kl}}.
\end{aligned}
\tag{9}
$$

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

$$
\boldsymbol{\rho}_k = \sqrt{\frac{\mu_k}{\mu_1}}\left\{\mathbf{r}_{k+1} - \frac{1}{k}\sum_{j=1}^{k}\mathbf{r}_j\right\} \qquad k = 1, \ldots, N-1
\tag{10}
$$

and the angles between $\boldsymbol{\rho}_k$ and $\boldsymbol{\rho}_{k+1}$, denoted by θ_k. The dimensionless reduced masses are $\mu_k = k/(k+1)$. The steps towards obtaining equation (9) are the following. First, write the kinetic energy in terms of the Jacobi vectors. Then change to polar coordinates (ρ_k, α_k), where α_k is the angle associated with $\boldsymbol{\rho}_k$. After that, introduce the angles $\theta_k = \alpha_{k+1} - \alpha_k$, and $\Xi = (\alpha_1 + \cdots + \alpha_{N-1})/(N-1)$. Ξ is the canonical conjugate to the total angular momentum, J.

The eigenfunctions of H are $\mathrm{e}^{\mathrm{i}J\Xi}\psi$, where Ξ accounts for global rotations, and the ψ are the eigenfunctions of h. The eigenvalues of H are trivially obtained from the eigenvalues of h, which will be called ϵ. We will obtain Padé approximants to ϵ.

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

$$
\epsilon|_{\beta\to 0} = b_0 + b_3\beta^3 + b_6\beta^6 + \cdots
\tag{11}
$$

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

$$
\begin{aligned}
\frac{h}{\beta^2} = &\frac{1}{4}\sum_{k=1}^{N-1}\rho_k^2 + \sum_{k<l}\frac{1}{r_{kl}} + \frac{J^2}{(N-1)^2\beta^4}\sum_{k=1}^{N-1}\frac{1}{\rho_k^2} \\
&- \frac{1}{\beta^4}\left\{\sum_{k=1}^{N-1}\left(\frac{\partial^2}{\partial\rho_k^2} + \frac{1}{\rho_k}\frac{\partial}{\partial\rho_k}\right) + \sum_{k=1}^{N-2}\left(\frac{1}{\rho_k^2} + \frac{1}{\rho_{k+1}^2}\right)\frac{\partial^2}{\partial\theta_k^2}\right\} \\
&+ \frac{2}{\beta^4}\left\{\sum_{k=1}^{N-3}\frac{1}{\rho_{k+1}^2}\frac{\partial^2}{\partial\theta_k\,\partial\theta_{k+1}} + \frac{\mathrm{i}J}{N-1}\sum_{k=1}^{N-2}\left(\frac{1}{\rho_k^2} - \frac{1}{\rho_{k+1}^2}\right)\frac{\partial}{\partial\theta_k}\right\}.
\end{aligned}
\tag{12}
$$

In the leading approximation, $\beta \to \infty$, we shall minimize the classical potential energy entering the r.h.s. of (12). When $N \leqslant 5$, it is found that the electrons sit at the corners of a regular polygon. This is a few-body version of the Wigner solid. In these configurations,

the classical energy (harmonic plus Coulomb potentials) becomes a function of one variable, namely ρ_1:

$$U = \frac{N\rho_1^2}{8\sin^2 \pi/N} + \frac{\sin \pi/N}{\rho_1} \sum \frac{1}{|\sin \theta_{kl}/2|} \tag{13}$$

where θ_{kl} is the angle between particles k and l, measured from the c.m. The minimization of U leads to an equilibrium value of ρ_1, i.e. ρ_{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 writing $\rho_k = \rho_{k0} + z_k/\beta$, $k = 1, \ldots, N-1$, $\theta_k = \theta_{k0} + z_{N-1+k}/\beta$, $k = 1, \ldots, N-2$, and expanding the Hamiltonian:

$$h/\beta^2 = U(\rho_{10}) + h_2/\beta^2 + h_3/\beta^3 + \cdots. \tag{14}$$

If we write

$$\psi = \psi_0 + \psi_1/\beta + \psi_2/\beta^2 + \cdots \tag{15}$$
$$\epsilon/\beta^2 = a_0 + a_2/\beta^2 + a_3/\beta^3 + \cdots \tag{16}$$

then the Schrödinger equation, $h\psi = \epsilon\psi$, is split into the set of uncoupled equations

$$a_0 = U(\rho_{10}) \tag{17}$$
$$h_2\psi_0 = a_2\psi_0 \qquad \text{etc.} \tag{18}$$

The Hamiltonian h_2 describes harmonic oscillations around the Wigner structure. The expression for a_2 is thus

$$a_2 = \sum_{k=1}^{2N-3} \omega_k(n_k + 1/2) \tag{19}$$

where the ω_k are the normal frequencies. Higher corrections are obtained by considering h_3, h_4, etc, as perturbations to h_2.

Below, we present results for two, three, four, and five 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, Ξ changes by π, and ψ does not change. Thus, the even $|J|$ are related to antisymmetric spin functions, $S = 0$, and the odd $|J|$ are related to states with spin $S = 1$.

Let ϕ_k be the eigenfunctions of h at $\beta = 0$:

$$\phi_k = C_k\rho_1^{|J|}L_k^{|J|}(\rho_1^2/2)e^{-\rho_1^2/4} \tag{20}$$

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

$$b_0 = 2k + |J| + 1. \tag{21}$$

We take a fixed k as the unperturbed level—say, n_1. Higher coefficients of the expansion are computed from

$$b_3 = \langle n_1|\frac{1}{\rho_1}|n_1\rangle \tag{22}$$

$$b_6 = \frac{1}{2}\sum_{k\neq n_1} \frac{|\langle n_1|1/\rho_1|k\rangle|^2}{(n_1 - k)} \qquad \text{etc.} \tag{23}$$

Table 1. The first non-zero coefficients b_k and a_k for a set of two-electron states.

$|J|, n$	b_0	b_3	b_6	a_0	a_2	a_4
0, 0	1	1.253 314	−0.345 655	1.190 551	0.866 025	−0.034 998
0, 1	3	0.939 986	−0.087 406	1.190 551	2.598 076	0.174 989
0, 2	5	0.802 904	−0.041 161	1.190 551	4.330 127	0.594 963
1, 0	2	0.626 657	−0.032 762	1.190 551	0.866 025	0.594 963
1, 1	4	0.548 325	−0.016 339	1.190 551	2.598 076	0.804 950
1, 2	6	0.499 367	−0.010 112	1.190 551	4.330 127	1.224 924
2, 0	3	0.469 993	−0.011 153	1.190 551	0.866 025	2.484 844
2, 1	5	0.430 827	−0.007 016	1.190 551	2.598 076	2.694 831
2, 2	7	0.402 676	−0.004 920	1.190 551	4.330 127	3.114 805
3, 0	4	0.391 661	−0.005 533	1.190 551	0.866 025	5.634 647
3, 1	6	0.367 182	−0.003 911	1.190 551	2.598 076	5.844 634
3, 2	8	0.348 211	−0.002 950	1.190 551	4.330 127	6.264 608

We show in table 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 ρ_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

$$h_2 = -\frac{\partial^2}{\partial z_1^2} + \frac{3}{4}z_1^2 \tag{24}$$

$$h_k = \frac{(-1)^k}{\rho_{10}^{k+1}}z_1^k - \frac{(-1)^{k-3}}{\rho_{10}^{k-2}}z_1^{k-3}\frac{\partial}{\partial z_1} + \frac{J^2(-1)^{k-4}(k-3)}{\rho_{10}^{k-2}}z_1^{k-4} \qquad k \geqslant 3. \tag{25}$$

Notice that the h_k with odd (even) k contain only odd (even) numbers of creation and annihilation operators. Thus, as can be easily verified, all of the coefficients a_k with odd k will be zero. Computation of the matrix elements of h_k is a trivial task. Finally, we obtain

$$a_2 = \omega_1(n_1 + 1/2) \tag{26}$$

$$a_4 = 2^{-2/3}\left\{(n_1^2 + n_1 + 7/6)/6 + J^2 - 1/4\right\} \qquad \text{etc} \tag{27}$$

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 for $\beta \to \infty$. As level crossings cannot occur in a sector with fixed J because there are no more conserved quantities in the problem, 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 table 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 figure 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 figure 2, we compare the approximants in the sequence $P_{K+1,K}$. The same state as in figure 1 is studied. The relative differences between consecutive approximants are shown. The β-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 that the approximant $P_{6,5}$ (the
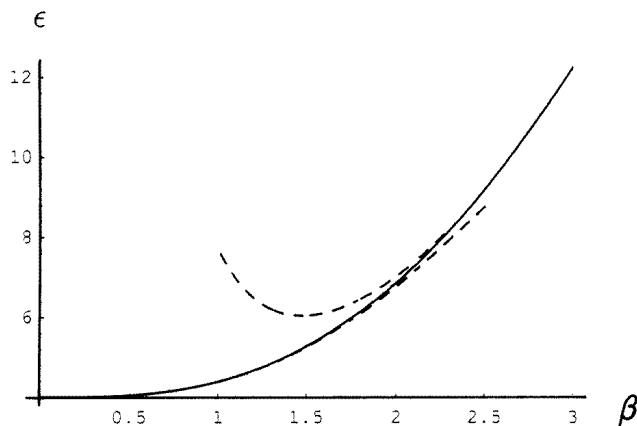
Figure 1. Weak- and strong-coupling expansions (dashed lines), and the approximant $P_{6,5}$ (solid line) for two electrons in a state with $|J| = 3$, $n_1 = 0$.
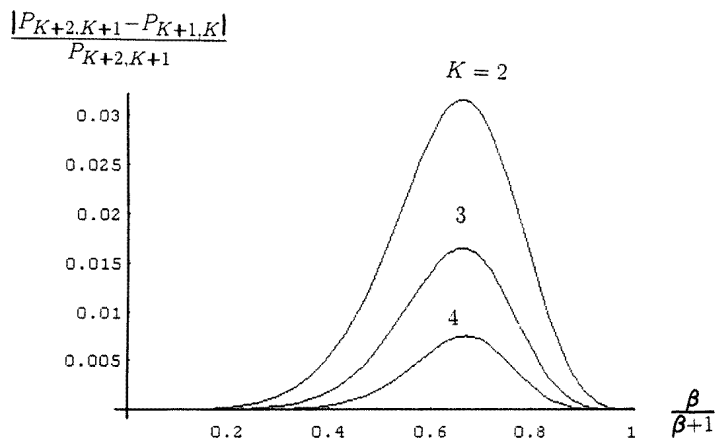

Figure 2. Relative differences between consecutive approximants in the sequence $P_{K+1,K}$. The state with $|J| = 3$, $n_1 = 0$ is shown.

highest that we computed) is 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 regime (see figure 1).

Similar results are obtained for the other states in table 1. When $J = 0$, however, the relative differences between the approximants increase to 2%, and some approximants cannot 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 figure 3 the convergence of the sequence $P_{K+1,K}$ at particular β-values, at which exact solutions are available [8]. It can be easily shown, for example, that

$$\psi = \rho_1^{|J|}(1 + \rho_1/\sqrt{2|J| + 1})e^{-\rho_1^2} \tag{28}$$

are eigenfunctions of h at $\beta = (2|J| + 1)^{1/6}$, with eigenvalues $\epsilon = |J| + 2$. The corresponding n_1 are zero. When $0 \leqslant |J| \leqslant 3$, β is in the interval $1 \leqslant \beta \leqslant 1.38$, well outside
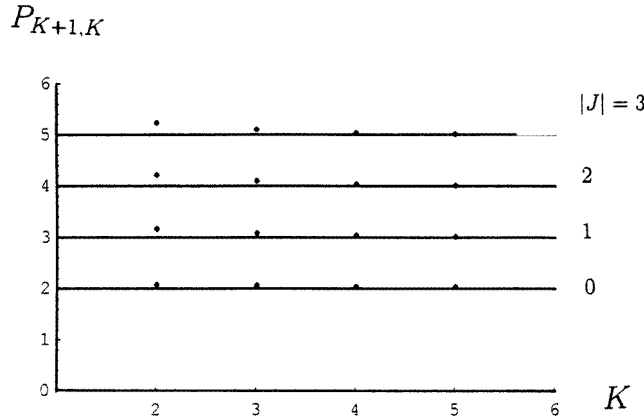
$P_{K+1,K}$

Figure 3. Convergence of the Padé 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].

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

$$a_0 = \frac{3^{5/3}}{2}. \tag{29}$$

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 at

$$h_2 = -\left(\frac{\partial^2}{\partial u^2} + \frac{\partial^2}{\partial v^2} + \frac{\partial^2}{\partial z^2}\right) + \frac{3}{4}u^2 + \frac{3}{8}(v^2 + z^2) \tag{30}$$

$$h_3 = \frac{1}{16\sqrt{2}\rho_{10}}\left\{-32\frac{\partial}{\partial u} + 32u\frac{\partial^2}{\partial z^2} - 8u^3 - 6uv^2 - 5v^3 - 6uz^2 + 15vz^2\right\} \tag{31}$$

$$h_4 = \frac{1}{\rho_{10}^2}\left\{\frac{J^2}{2} + u\frac{\partial}{\partial u} - \frac{3}{2}u^2\frac{\partial^2}{\partial z^2} + \frac{1}{4}u^4 + v\frac{\partial}{\partial v} - 2iJv\frac{\partial}{\partial z} - \frac{3}{2}v^2\frac{\partial^2}{\partial z^2} + \frac{3}{8}u^2v^2 + \frac{5}{8}uv^3\right.$$
$$\left. + \frac{9}{256}v^4 + \frac{3}{16}u^2z^2 - \frac{15}{16}uvz^2 - \frac{3}{128}v^2z^2 + \frac{41}{256}z^4\right\} \qquad \text{etc.} \tag{32}$$

u, v, 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

$$\psi = \chi_{n_1}(u)\chi_{n_2}(v)\chi_{n_3}(z)e^{iJ\Xi} \tag{33}$$

where the χ are oscillator functions, i.e. Hermite polynomials multiplied by gaussians. A function ψ that can be antisymmetrized is related to a spin-polarized state ($S = 3/2$) of three electrons. On the other hand, a mixed-symmetry ψ is related to a spin-half state.

Let us consider the lowest state with a given J, i.e. that 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

$$a_2 = \sqrt{3}(n_1 + 1/2) + \sqrt{3/2}(n_1 + n_2 + 1). \tag{34}$$

Higher corrections are computed from perturbation theory around h_2. For the same reason as for two particles, a_3 and a_5 are equal to zero. The next non-zero coefficient is

$$a_4 = \langle n_1, n_2, n_3 | h_4 | n_1, n_2, n_3 \rangle$$
$$+ \sum_{(k_1,k_2,k_3) \neq (n_1,n_2,n_3)} \frac{\langle n_1, n_2, n_3 | h_3 | k_1, k_2, k_3 \rangle \langle k_1, k_2, k_3 | h_3 | n_1, n_2, n_3 \rangle}{\sqrt{3}(n_1 - k_1) + \sqrt{3/2}(n_1 + n_2 - k_1 - k_2)}. \tag{35}$$

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

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

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 tunnelling 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 arising 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 constructed as indicated in [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 for $\beta \to \infty$ 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 for $\beta \to \infty$, 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 (1, 0, 0). At $|J| = 1$, (3, M) goes to (0, 0, 0), and (5, A) goes to a state with $n_1 = 0, n_2 + n_3 = 1$. At $|J| = 2$, (4, M) goes to (0, 0, 0), and (6, A) goes to a state with $n_1 = 0, n_2 + n_3 = 1$. At $|J| = 3$, (5, A) goes to (0, 0, 0), and (5, M) to a state with $n_1 = 0, n_2 + n_3 = 1$.

Let us write out explicitly the wave functions needed at $\beta = 0$ (up to normalizations). In the case of mixed symmetry, only one representative of the doublet is given.

For $J = 0$:

$$\phi_{4,A} = \rho_1\rho_2 \sin\theta_1 \, e^{-(\rho_1^2 + \rho_2^2)/4} \tag{37}$$

$$\phi_{4,M} = (\rho_1^2 - \rho_2^2)e^{-(\rho_1^2 + \rho_2^2)/4} \tag{38}$$

$$\phi_{6,A} = \rho_1\rho_2 \sin\theta_1 (\rho_1^2 + \rho_2^2 - 8)e^{-(\rho_1^2 + \rho_2^2)/4}. \tag{39}$$

For $J = 1$:

$$\phi_{3,M} = \rho_1 e^{-i\theta_1/2} e^{-(\rho_1^2 + \rho_2^2)/4} \tag{40}$$

$$\phi_{5,A} = \left\{ (-2\rho_1\rho_2^2 + \rho_1^3) e^{-i\theta_1/2} - \rho_1\rho_2^2 e^{3i\theta_1/2} \right\} e^{-(\rho_1^2 + \rho_2^2)/4}. \tag{41}$$

For $J = 2$:

$$\phi_{4,M} = \rho_1\rho_2 e^{-(\rho_1^2 + \rho_2^2)/4} \tag{42}$$

$$\phi_{6,A} = \rho_1\rho_2 \sin\theta_1 (\rho_1^2 e^{-i\theta_1} + \rho_2^2 e^{i\theta_1}) e^{-(\rho_1^2 + \rho_2^2)/4}. \tag{43}$$

For $J = 3$:

$$\phi_{5,A} = \left\{ \rho_1^3 e^{-3i\theta_1/2} - 3\rho_1\rho_2^2 e^{i\theta_1/2} \right\} e^{-(\rho_1^2 + \rho_2^2)/4} \tag{44}$$

$$\phi_{5,M} = \left\{ \rho_1^3 e^{-3i\theta_1/2} + \rho_1\rho_2^2 e^{i\theta_1/2} \right\} e^{-(\rho_1^2 + \rho_2^2)/4}. \tag{45}$$

Table 2. The first non-zero coefficients b_k and a_k for certain three-electron states.

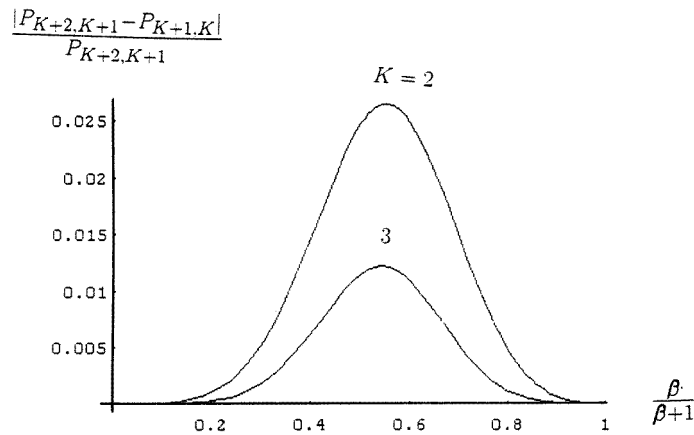| $|J|$, symmetry	b_0	b_3	a_0	a_2	a_4
0, A	4	1.879 97	3.120 13	2.090 77	0.035 8156
0, M	4	2.584 96	3.120 13	3.315 52	−0.061 9104
0, A	6	1.762 47	3.120 13	3.822 82	0.200 926
1, M	3	2.819 96	3.120 13	2.090 77	0.276 191
1, A	5	1.821 22	3.120 13	3.315 52	0.178 464
2, M	4	2.232 47	3.120 13	2.090 77	0.997 315
2, A	6	1.586 23	3.120 13	3.315 52	0.899 589
3, A	5	1.703 72	3.120 13	2.090 77	2.199 19
3, M	5	2.261 84	3.120 13	3.315 52	2.101 46

Figure 4. As figure 2, but for the first antisymmetric state of three electrons with $|J| = 3$.

The computation of b_3 is thus a trivial task. We grouped all of 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 Padé sequence $P_{K+1,K}$ is shown in figure 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 six parts in 10^3 or better over the entire interval $0 \leqslant \beta < \infty$. 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 $\rho_{20} = \sqrt{5/3}\,\rho_{10}$, $\rho_{30} = 2\rho_{10}/\sqrt{3}$, $\theta_{10} = \arctan 2$, and $\theta_{20} = 3\pi/4 - \theta_{10}$. a_0 is given by

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

Expanding around the equilibrium geometry, we obtain the quadratic Hamiltonian

$$
\begin{aligned}
h_2 = &-\left(\frac{\partial^2}{\partial z_1^2} + \frac{\partial^2}{\partial z_2^2} + \frac{\partial^2}{\partial z_3^2}\right) - \left(\frac{1}{\rho_{10}^2} + \frac{1}{\rho_{20}^2}\right)\frac{\partial^2}{\partial z_4^2} \\
&- \left(\frac{1}{\rho_{20}^2} + \frac{1}{\rho_{30}^2}\right)\frac{\partial^2}{\partial z_5^2} + \frac{2}{\rho_{20}^2}\frac{\partial}{\partial z_4}\frac{\partial}{\partial z_5} + V_2
\end{aligned}
\tag{47}
$$

where

$$
\begin{aligned}
V_2 = &\, 0.543\,374\,z_1^2 + 0.157\,283\,z_1 z_2 + 0.520\,305\,z_2^2 + 0.182\,039\,z_1 z_3 + 0.377\,402\,z_2 z_3 \\
&+ 0.460\,201\,z_3^2 + 0.171\,862\,z_2 z_4 + 0.192\,148\,z_3 z_4 + 0.517\,308\,z_4^2 \\
&+ 0.110\,937\,z_1 z_5 + 0.085\,931\,z_2 z_5 + 0.562\,904\,z_4 z_5 + 0.853\,613\,z_5^2.
\end{aligned}
\tag{48}
$$

The normal frequencies are easily found:

$$
\begin{aligned}
\omega_1 &= 1.049\,69 \\
\omega_2 &= 1.139\,11 \\
\omega_3 &= 1.362\,27 \\
\omega_4 &= 1.462\,01 \\
\omega_5 &= 1.756\,40
\end{aligned}
\tag{49}
$$

and, thus, the coefficient a_2 is given by

$$a_2 = \sum_{k=1}^{5} \omega_k (n_k + 1/2). \tag{50}$$

Notice that the frequency corresponding to the breathing mode, ω_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 antisymmetrized only when $|J|$ takes certain values. The allowed values are $|J| = 2, 6, 10, \ldots$. These are polarized spin states, i.e. with total spin $S = 2$. The excitations of the ω_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, tunnelling effects become more and more important.

In what follows, we restrict the analysis to the lowest spin-polarized 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 β. Indeed, as $\beta \to 0$, this state becomes an oscillator state with $b_0 = 7$, i.e. (7, A) in the terminology used above. There is a second state (7, A), with $J = 0$. However, according to Hund's rule, this state has a higher energy for $\beta \ll 1$. 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

$$b_3 = 6 \frac{\langle \phi_{7,A} | 1/\rho_1 | \phi_{7,A} \rangle}{\langle \phi_{7,A} | \phi_{7,A} \rangle} = \frac{91}{64} \sqrt{2\pi}. \tag{51}$$
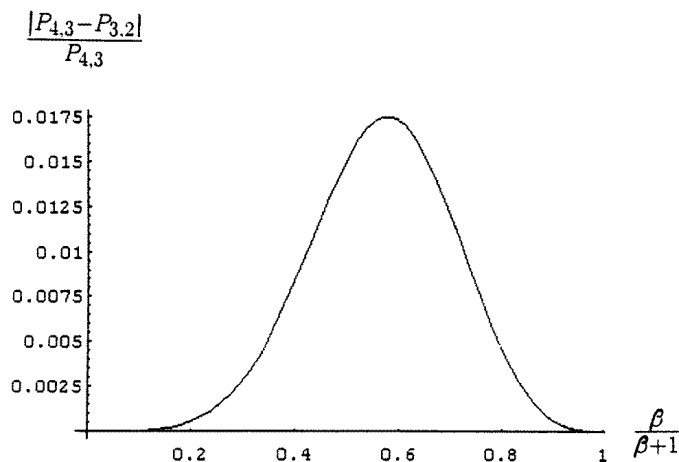

Figure 5. The relative difference between $P_{4,3}$ and $P_{3,2}$ for the lowest antisymmetric state of four electrons ($|J| = 2$).

Once we have 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 difference between $P_{3,2}$ and $P_{4,3}$ is shown in figure 5, suggesting that $P_{4,3}$ may estimate the energy with an error not greater than 2% at intermediate values of β.

Padé 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 $\rho_{10} = 1.307\,66$ (scaled). The equilibrium values of the other coordinates are as follows: $\rho_{20}/\rho_{10} = 1.441\,77$, $\rho_{30}/\rho_{10} = 1.532\,44$, $\rho_{40}/\rho_{10} = 1.345\,00$, $\theta_{10} = 0.865\,925$ rad, $\theta_{20} = 1.744\,28$ rad, and $\theta_{30} = -1.039\,41$ rad. a_0 is given by

$$a_0 = 9.280\,13. \tag{52}$$

Expanding around the equilibrium configuration, we obtain the Hamiltonian h_2,

$$h_2 = -\left(\frac{\partial^2}{\partial z_1^2} + \frac{\partial^2}{\partial z_2^2} + \frac{\partial^2}{\partial z_3^2} + \frac{\partial^2}{\partial z_4^2}\right) - \left(\frac{1}{\rho_{10}^2} + \frac{1}{\rho_{20}^2}\right)\frac{\partial^2}{\partial z_5^2} - \left(\frac{1}{\rho_{20}^2} + \frac{1}{\rho_{30}^2}\right)\frac{\partial^2}{\partial z_6^2}$$

$$- \left(\frac{1}{\rho_{30}^2} + \frac{1}{\rho_{40}^2}\right)\frac{\partial^2}{\partial z_7^2} + \frac{2}{\rho_{20}^2}\frac{\partial}{\partial z_5}\frac{\partial}{\partial z_6} + \frac{2}{\rho_{30}^2}\frac{\partial}{\partial z_6}\frac{\partial}{\partial z_7} + V_2 \tag{53}$$

where

$$
\begin{aligned}
V_2 = {} & 0.624\,037\,z_1^2 - 0.007\,988\,z_1z_2 + 0.514\,889\,z_2^2 + 0.107\,324\,z_1z_3 \\
& + 0.231\,789\,z_2z_3 + 0.438\,330\,z_3^2 + 0.073\,587\,z_1z_4 + 0.245\,901\,z_2z_4 \\
& + 0.381\,949\,z_3z_4 + 0.373\,258\,z_4^2 + 0.315\,672\,z_2z_5 - 0.296\,995\,z_3z_5 \\
& + 0.451\,706\,z_5^2 + 0.313\,498\,z_1z_6 - 0.217\,440\,z_2z_6 - 0.286\,484\,z_3z_6 \\
& + 0.326\,409\,z_4z_6 + 0.765\,563\,z_5z_6 + 1.438\,39\,z_6^2 - 0.126\,796\,z_2z_7 \\
& + 0.119\,294\,z_3z_7 + 0.169\,244\,z_5z_7 + 1.378\,49\,z_6z_7 + 1.460\,79\,z_7^2.
\end{aligned} \tag{54}
$$

The normal frequencies following from the eigenvalue problem for h_2 are

$$
\begin{aligned}
\omega_1 &= 0.727\,516 \\
\omega_2 &= 0.804\,763 \\
\omega_3 &= 1.371\,85 \\
\omega_4 &= 1.525\,05 \\
\omega_5 &= 1.688\,99 \\
\omega_6 &= 1.732\,05 \\
\omega_7 &= 1.743\,75
\end{aligned} \tag{55}
$$

and the coefficient a_2 is given by

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

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 changes to a $(10, A)$ state as $\beta \to 0$. It is not, however, the lowest of all antisymmetric levels for $\beta \ll 1$, because a second $(10, A)$ state with $|J| = 2$ minimizes the Coulomb repulsion.

The wave function of the $J = 0$ state is given in appendix 2. Calculations may also be performed analytically, leading to

$$b_3 = \frac{149}{64}\sqrt{2\pi}. \tag{57}$$

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

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

8. Concluding remarks

We have studied systems of two to five 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 ϵ on the coupling constant β. This
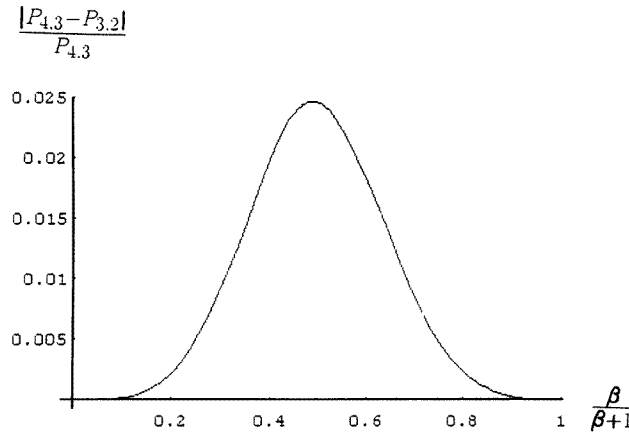
$$\frac{|P_{4,3}-P_{3,2}|}{P_{4,3}}$$

Figure 6. As figure 5, but for the lowest antisymmetric state of five electrons with angular momentum $J = 0$.

fact is graphically represented in figure 1, where it is seen that the 'regions of convergence' of the perturbative and the strong-coupling series 'intersect' one another.

The degrees of homogeneity of the potentials are also important factors contributing towards the smoothness of ϵ. They lead to expansion series containing only powers of β^3 for $\beta \to 0$, and inverse powers of β^2 for $\beta \to \infty$. From the calculational point of view, this 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 of a fifth-order polynomial and a third-order polynomial in β. These approximants are exact in both the $\beta \to 0$ 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.

Acknowledgments

Appendix 1. The approximants used in the paper

$$P_{3,2}(\beta) = b_0 + a_0\beta^2 \left\{1 - (1 + b_3\beta/a_0 + a_0\beta^2/(b_0 - a_2))^{-1}\right\}. \tag{A1}$$

$P_{4,3}$ is given by equation (7).

$$P_{5,4}(\beta) = b_0 + \frac{b_3\beta^3}{1 + q_1\beta + \cdots + q_4\beta^4} - \frac{(b_0 - a_2)q_4\beta^4}{1 + q_1\beta + \cdots + q_4\beta^4}$$
$$+ a_0\beta^2 \left\{1 - \frac{1 + q_1\beta}{1 + q_1\beta + \cdots + q_4\beta^4}\right\} \tag{A2}$$

where

$$q_2 = a_0 q_3 / b_3 \qquad q_1 = \frac{1}{a_0} \{b_3 + (b_0 - a_2) q_3\}$$

$$q_4 = \frac{a_0}{a_4} \left\{ -1 + \frac{b_0 - a_2}{b_3} q_3 \right\} \tag{A3}$$

and q_3 is determined from the equation

$$-b_3 q_1 + a_0 q_2 - (b_0 - a_2) q_4 = 0. \tag{A4}$$

We also have

$$P_{6,5}(\beta) = b_0 + \frac{b_3 \beta^3}{1 + q_1 \beta + \cdots + q_5 \beta^5} - \frac{(b_0 - a_2)\{q_4 \beta^4 + q_5 \beta^5\}}{1 + q_1 \beta + \cdots + q_5 \beta^5}$$

$$+ a_0 \beta^2 \left\{ 1 - \frac{1 + q_1 \beta}{1 + q_1 \beta + \cdots + q_5 \beta^5} \right\} \tag{A5}$$

where

$$q_3 = \frac{1}{b_3} \{a_0 q_4 - b_6\} \qquad q_2 = \frac{1}{b_0 - a_2} \{a_0 + a_4 q_4\}$$

$$q_1 = \frac{1}{b_3} \{a_0 q_2 - (b_0 - a_2) q_4\} \tag{A6}$$

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

and q_4 is found from

$$-b_3 q_2 + a_0 q_3 - (b_0 - a_2) q_5 = 0. \tag{A7}$$

Appendix 2. Wave functions for four and five electrons at $\beta = 0$

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

$$\begin{aligned}
\phi_{7,A} = \Big\{ & \left[\boldsymbol{\rho}_3 \cdot \boldsymbol{r}_1 / \rho_3 + \mathrm{i}(\boldsymbol{\rho}_3 \times \boldsymbol{r}_1)_z / \rho_3 \right]^2 [\boldsymbol{r}_2 \times \boldsymbol{r}_3 + \boldsymbol{r}_3 \times \boldsymbol{r}_4 + \boldsymbol{r}_4 \times \boldsymbol{r}_2]_z \\
& - \left[\boldsymbol{\rho}_3 \cdot \boldsymbol{r}_2 / \rho_3 + \mathrm{i}(\boldsymbol{\rho}_3 \times \boldsymbol{r}_2)_z / \rho_3 \right]^2 [\boldsymbol{r}_3 \times \boldsymbol{r}_4 + \boldsymbol{r}_4 \times \boldsymbol{r}_1 + \boldsymbol{r}_1 \times \boldsymbol{r}_3]_z \\
& + \left[\boldsymbol{\rho}_3 \cdot \boldsymbol{r}_3 / \rho_3 + \mathrm{i}(\boldsymbol{\rho}_3 \times \boldsymbol{r}_3)_z / \rho_3 \right]^2 [\boldsymbol{r}_4 \times \boldsymbol{r}_1 + \boldsymbol{r}_1 \times \boldsymbol{r}_2 + \boldsymbol{r}_2 \times \boldsymbol{r}_4]_z \\
& - r_4^2 [\boldsymbol{r}_1 \times \boldsymbol{r}_2 + \boldsymbol{r}_2 \times \boldsymbol{r}_3 + \boldsymbol{r}_3 \times \boldsymbol{r}_1]_z \Big\} \mathrm{e}^{-(\rho_1^2 + \rho_2^2 + \rho_3^2)/4} \mathrm{e}^{2\mathrm{i}(\theta_1 + 2\theta_2)/3}.
\end{aligned} \tag{B1}$$

$$\begin{aligned}
\phi_{10,A} = \mathrm{e}^{-(\rho_1^2 + \rho_2^2 + \rho_3^2 + \rho_4^2)/4} \Big\{ & (\boldsymbol{r}_1 \cdot \boldsymbol{r}_2)(\boldsymbol{r}_1 \times \boldsymbol{r}_2)_z [\boldsymbol{r}_3 \times \boldsymbol{r}_4 + \boldsymbol{r}_4 \times \boldsymbol{r}_5 + \boldsymbol{r}_5 \times \boldsymbol{r}_3]_z \\
& + (\boldsymbol{r}_2 \cdot \boldsymbol{r}_3)(\boldsymbol{r}_2 \times \boldsymbol{r}_3)_z [\boldsymbol{r}_4 \times \boldsymbol{r}_5 + \boldsymbol{r}_5 \times \boldsymbol{r}_1 + \boldsymbol{r}_1 \times \boldsymbol{r}_4]_z \\
& + (\boldsymbol{r}_3 \cdot \boldsymbol{r}_4)(\boldsymbol{r}_3 \times \boldsymbol{r}_4)_z [\boldsymbol{r}_5 \times \boldsymbol{r}_1 + \boldsymbol{r}_1 \times \boldsymbol{r}_2 + \boldsymbol{r}_2 \times \boldsymbol{r}_5]_z \\
& + (\boldsymbol{r}_4 \cdot \boldsymbol{r}_5)(\boldsymbol{r}_4 \times \boldsymbol{r}_5)_z [\boldsymbol{r}_1 \times \boldsymbol{r}_2 + \boldsymbol{r}_2 \times \boldsymbol{r}_3 + \boldsymbol{r}_3 \times \boldsymbol{r}_1]_z \\
& + (\boldsymbol{r}_5 \cdot \boldsymbol{r}_1)(\boldsymbol{r}_5 \times \boldsymbol{r}_1)_z [\boldsymbol{r}_2 \times \boldsymbol{r}_3 + \boldsymbol{r}_3 \times \boldsymbol{r}_4 + \boldsymbol{r}_4 \times \boldsymbol{r}_2]_z \\
& - (\boldsymbol{r}_1 \cdot \boldsymbol{r}_3)(\boldsymbol{r}_1 \times \boldsymbol{r}_3)_z [\boldsymbol{r}_4 \times \boldsymbol{r}_5 + \boldsymbol{r}_5 \times \boldsymbol{r}_2 + \boldsymbol{r}_2 \times \boldsymbol{r}_4]_z \\
& - (\boldsymbol{r}_2 \cdot \boldsymbol{r}_4)(\boldsymbol{r}_2 \times \boldsymbol{r}_4)_z [\boldsymbol{r}_5 \times \boldsymbol{r}_1 + \boldsymbol{r}_1 \times \boldsymbol{r}_3 + \boldsymbol{r}_3 \times \boldsymbol{r}_5]_z \\
& - (\boldsymbol{r}_3 \cdot \boldsymbol{r}_5)(\boldsymbol{r}_3 \times \boldsymbol{r}_5)_z [\boldsymbol{r}_1 \times \boldsymbol{r}_2 + \boldsymbol{r}_2 \times \boldsymbol{r}_4 + \boldsymbol{r}_4 \times \boldsymbol{r}_1]_z \\
& + (\boldsymbol{r}_1 \cdot \boldsymbol{r}_4)(\boldsymbol{r}_1 \times \boldsymbol{r}_4)_z [\boldsymbol{r}_5 \times \boldsymbol{r}_2 + \boldsymbol{r}_2 \times \boldsymbol{r}_3 + \boldsymbol{r}_3 \times \boldsymbol{r}_5]_z \\
& + (\boldsymbol{r}_2 \cdot \boldsymbol{r}_5)(\boldsymbol{r}_2 \times \boldsymbol{r}_5)_z [\boldsymbol{r}_1 \times \boldsymbol{r}_3 + \boldsymbol{r}_3 \times \boldsymbol{r}_4 + \boldsymbol{r}_4 \times \boldsymbol{r}_1]_z \Big\}.
\end{aligned} \tag{B2}$$

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