

# Energy levels of a particle confined in a super-circular box

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**Abstract.** We find the energy levels of a free particle confined in a two dimensional infinite potential well having super-circular boundary ( $|x|^n + |y|^n = a^n$  where  $n$  is a rational number and  $a$  is a positive real number) by perturbing about the equivalent circle ( $n = 2$ ). The ground state energies are very accurate over a wide range of  $n$  and can be improved further by introducing a phenomenological constant determined from the knowledge of exact results available for diamond ( $n = 1$ ). For excited states, we find that the shape effect can cause parametric resonance which can lead to singlet-triplet crossing.

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## 1 Introduction

The energy levels of a quantum free particle confined in a two-dimensional box can be determined exactly only in the special cases of the triangle, square (rectangle) and the limiting case of the circle. Solutions are quite simple for square and circle but for the triangle, the problem is more involved [1]. The problem of the regular polygonal box has been solved by perturbing about the equivalent circle and the results have been very accurate [2]. Here we address the problem of finding out the energy eigen-values of a particle confined in a two dimensional infinite potential well having super-circular boundary. This is a particularly nice instance of obtaining a solution by perturbing a boundary for which the problem is soluble. This is of relevance because it is becoming possible to confine particles in regions of various shapes. Two dimensional quantum dots are generally taken to have circular symmetry. However, a circular symmetry cannot be guaranteed in practice. Accordingly probes have been constructed to determine the shape of the dots [3–5]. In this context, the study of shape dependence of energy levels ought to be useful.

Quantitative definition of aromaticity has been proposed using  $\pi$  molecular orbital (MO) theories as the simple Hückel and Pariser-Parr-Pople and its related methods. The difference in energy between an annulene and its reference linear polyene has been used to judge the extent of aromaticity of a compound. However mathematical relationship between the Hückel theory and free electron model has been probed in various ways which

confirms that the Hückel MO theory and particle in a box (PIAB) model are simply different ways of solving the same Schrödinger equation [6]. Consequently, PIAB model correctly reproduce the  $4n + 2$  or  $4n$  rule for aromaticity and anti-aromaticity respectively by just calculating the difference of energies of the molecule treating it as a linear one and the cyclic one. But the regular circular structure is not guaranteed for various kind of cyclic conjugated polyenes. In these cases certain variants of shape are encouraged which will give the correct description of the molecule. Again the allowed or forbidden pathways of certain pericyclic reactions (cycloaddition reactions, electrocyclic reactions and sigmatropic rearrangements) can be judged by looking at the aromatic nature of the transition states (TS) [7]. As the TS may be of various geometries, the study of shape dependent energy levels would be of immense interest.

Super-circle is a special case of super-ellipse, popularly known as Piet Hein super-ellipse [8] after the name of Piet Hein, a famous Danish architect, poet and scientist. The equation of a super-ellipse is given by the Lamé equation [9],

$$\frac{|x|^n}{a^n} + \frac{|y|^n}{b^n} = 1 \quad (1.1)$$

with  $n > 0$  and rational. The constants  $a$  and  $b$  are positive real numbers. Super-ellipses are also known as Lamé curves or Lamé ovals [10]. They can be parametrically described as

$$\begin{aligned} x &= a \cos^{\frac{2}{n}}(t) \\ y &= b \sin^{\frac{2}{n}}(t). \end{aligned} \quad (1.2)$$

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**Table 1.** Different closed curves.

$n$	curve ( $a = b$ )
$<1$	asteroid
1	diamond
2	circle
$>2$	super-circle
$\infty$	square

For  $n$  greater than 2, we take only the real positive values of  $\cos^{\frac{2}{n}}(t)$  and  $\sin^{\frac{2}{n}}(t)$  in equation (1.2) for  $0 \leq t \leq \frac{\pi}{2}$  and use the symmetry of the figure to continue to the other quadrants. If  $n$  is a rational number, then the super-ellipse is algebraic. However for irrational  $n$ , it is transcendental. For even integer, the curve becomes closer to a rectangle as  $n$  increases. Gielis [11] has considered the further generalization of the super-ellipse given in polar coordinates by,

$$r(\theta) = \left[ \left| \frac{\cos(\frac{1}{4}m\theta)}{a} \right|^{n_2} + \left| \frac{\sin(\frac{1}{4}m\theta)}{a} \right|^{n_3} \right]^{-\frac{1}{n_1}}. \quad (1.3)$$

Introduction of the parameter  $m$  and use of polar coordinates give rise to curves with  $m$ -fold rotational symmetry,  $n_1, n_2, n_3$  and  $n_4$  are positive and rational.

We will treat these patterns or shapes as systematic variants on the circular shape. When  $a = b$ , we get a super-circle. For different values of  $n$  we get different closed curves as shown in Table 1. Confining a particle in a super-circle gives rise to a super-circular billiard. The classical dynamics of a particle confined in such a billiard [14–16] is an interesting problem which has been extensively studied for certain shapes, but not yet been systematically studied. For  $n < 1$ , i.e. for asteroidal shapes, the dynamics is expected to be strongly chaotic and the corresponding quantum problems should be of interest in the study of quantum chaos.

The Schrödinger equation for an infinite potential well is

$$\frac{\hbar^2}{2m} \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) \psi + E\psi = 0. \quad (1.4)$$

So the problem reduces to solving the Helmholtz equation [17,18] with the Dirichlet condition  $\psi = 0$  on the boundary of the super-circular region. Exact solutions can be obtained for some special cases and the usual procedure for finding an exact solution is to find a curvilinear coordinate [19,20] system where the locus of one of the coordinates is a super-circle, and the wave-function is separable for that particular coordinate system. The special case for which exact solutions can be obtained are the square [21] ( $n = \infty$ , using Cartesian coordinate system), the circle [23] ( $n = 2$ , using polar coordinate system) and the diamond ( $n = 1$ , using Cartesian coordinate system, diamond can be obtained from square by a  $45^\circ$  rotation). In the case of the circle we write  $\Psi(r, \theta) = R(r)\Phi(\theta)$ , where  $R(r)$  is the radial part of the wavefunction and  $\Phi(\theta)$  is the corresponding angular part which depends on  $\theta$ . Separation of variable gives the radial function  $R(r)$  to be

solutions of Bessel's function [17], given by

$$\frac{d^2 R}{d\rho^2} + \frac{1}{\rho} \frac{dR}{d\rho} + \left( 1 - \frac{\nu^2}{\rho^2} \right) R = 0 \quad (1.5)$$

where  $\rho = kr$ ,  $k = \sqrt{\frac{2mE}{\hbar^2}}$  and  $\nu$  is an integer which appears in the angular part of the wave functions. The restriction to integer is a consequence of the requirement of single-valuedness for  $\phi$  where

$$\Phi(\phi) = e^{\pm i\nu\phi}. \quad (1.6)$$

The circular symmetry of the problem demands only a circular symmetric ground state as the solution of the Schrödinger equation. Hence we take  $\nu = 0$ , which means that the solutions are given by Bessel's functions of zero order. The value of  $k$  is determined from the boundary condition and is given by roots of  $J_0(\rho)$  for circular boundary of radius  $R$ . Consequently the ground state energy is given by

$$\begin{aligned} E_0 &= \frac{\hbar^2}{2m} \left( \frac{2.4048}{R} \right)^2 \\ &= \frac{\hbar^2}{2mR^2} 5.783. \end{aligned} \quad (1.7)$$

No curvilinear coordinate system can be found where the locus of one of the coordinates is any super-circle for arbitrary values of  $n$ . A non-curvilinear coordinate system will yield a partial differential equation which would be difficult to solve by separation of variables. Hence we use a variant of the standard perturbative technique [21] to solve this problem. In the problems of practical interest (quantum dot), the deviation from the circular shape will be small. The result that we obtain can be used as a diagnostic for determining how “circular” a circular dot is. Variants from the circular shape will lead to change in the frequency spectrum. In fact, the effect can be dramatic in the case of parametric resonance.

Perturbation theory is a common tool in the study of eigenvalue problems. A classic case of an eigenvalue problem is the time-independent Schrödinger equation, which can be written as

$$H\psi = -\frac{\hbar^2}{2m} \nabla^2 \psi + V\psi = E\psi \quad (1.8)$$

where  $H$  is called the Hamiltonian,  $m$  is the mass of the particle whose wave functions are given by  $\psi(\mathbf{r})$  and whose eigen-energy is  $E$ . The problem is to find the allowed energies  $E_n$  and the corresponding wave-functions  $\psi_n$ . The energies  $E_n$  are generally discrete and forced by boundary conditions of the problem. There are very few situations where  $E$  and  $\psi$  can be exactly determined. Primary among them are the cases of (i) particle confined in a box, (ii) particle confined by a harmonic potential and (iii) particle confined by Coulomb potential. The shape-invariant potentials [22] for which exact solutions can be found are certain variations on the above set. If we denote the Hamiltonian for which an exact solution can be found by  $H_0$ ,

**Table 2.** Calculated ground state.

$n$	$(E_0)_n$ ( $n = 2$ approx)	$E$ (numerical)	$E$ (perturbative)	% error
0.8	2.0340	2.3288	2.3645	1.5
1.0	1.5715	1.6927	1.7080	0.9
1.2	1.3334	1.3863	1.3894	0.2
1.4	1.1969	1.2148	1.2181	0.3
1.6	1.1075	1.1103	1.1141	0.3
1.8	1.0468	1.0427	1.0481	0.5
2.0	1.0000	0.9967	1.0000	0.3
2.5	0.9296	0.9314	0.9331	0.2
3.0	0.8891	0.8997	0.9022	0.3
5.0	0.8270	0.8621	0.8551	-0.8
10.0	0.7970	0.8597	0.8434	-1.9
20.0	0.7887	0.8517	0.8452	-0.8
50.0	0.7862	0.8516	0.8495	-0.2
100.0	0.7858	0.8516	0.8511	0.1

then an arbitrary Hamiltonian  $H$ , can be written as

$$H = H_0 + \lambda H' \quad (1.9)$$

where  $\lambda$  is a parameter and  $H'$  is called the perturbing Hamiltonian. In this case if the eigenvalue of  $H_0$  be denoted by  $E_n^{(0)}$  and the eigen functions by  $\psi_n^{(0)}$  then the eigenvalues  $E_n$  of  $H$  can be written in a power series expansion as

$$E_n = E_n^{(0)} + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + \dots \quad (1.10)$$

$$E_n^{(1)} = \langle \psi_n^{(0)} | H' | \psi_n^{(0)} \rangle \quad (1.11)$$

$$E_n^{(2)} = \sum_{l \neq n} \frac{|\langle \psi_n^{(0)} | H' | \psi_l^{(0)} \rangle|^2}{E_n^{(0)} - E_l^{(0)}} \quad (1.12)$$

and so on. These expressions are valid when the state  $\psi_n^{(0)}$  is non-degenerate which is always true for the ground state of the circle. In our case, it is not the Hamiltonian that is perturbed. Rather it is the boundary conditions which are being changed. We cannot cast our problem as a calculation of the matrix elements of  $H'$ . We can always resort to numerical integrations to obtain the energy eigenvalues in this case. The standard algorithm for the solution of a partial differential equation (PDE) with the finite element method (FEM) [24,25] involves three main steps. First, the domain, on which the PDE should be solved, is discretized into finite elements. The solutions of the PDE are approximated by piecewise continuous polynomials and the PDE is thereby discretized and split into a finite number of algebraic equations. The aim is to determine the unknown coefficients of these polynomials in such a way, that the distance (which is defined by the norm in a suitable vector space) from the exact solution becomes a minimum. Therefore, the finite element method is essentially a minimization technique for variational problems. Since the number of elements is finite, the problem is reduced to calculating a finite number of coefficients of the polynomials instead of finding a continuous solution for PDE.

The algorithm followed to solve this problem is different from the standard one and this was necessitated by

the nature of the problem. In our boundary value problem, the wavefunction vanishes at the boundary. So, the set of algebraic equations obtained by using the standard finite element method do not have any constant term in them and therefore it is possible to get non-trivial values for the wavefunction in the region inside the infinite potential well. This means one should put some constraints on the values, the wave function can take. The obvious choice is the normalization condition. Hence the algorithm used in this case involves the following steps:

1. calculation of the finite difference replacement of the Hamiltonian (in this case the two dimensional Laplacian),
2. discretization of the region using square grids,
3. compilation of the set of finite difference equations corresponding to the Schrödinger equation for an infinite potential well in two dimension,
4. calculation of the matrix representation of the Hamiltonian operator from the set of algebraic equations,
5. calculation of the eigenvalues and normalized eigenvectors of the matrix.

A point to be noted regarding the above algorithm. A square grid was used for simplicity of computation. A triangular grid may yield better results. The numerical results for the ground state energy for various values of  $n$  are exhibited in the appropriate column of Table 2.

In Section 2, we calculate the ground state energy for the particle in a super-circular box by considering the equivalent circle of equal area. This already yields a ground state energy within 10% of the exact answer for all values of  $n$  ranging from  $n = 1$  to  $n = \infty$  (Tab. 2). Consequently it makes sense to consider a perturbation in shape around the equivalent circle i.e. around  $n = 2$ . For the ground state, we can supplement the perturbation theory with added information from the diamond ( $n = 1$ ). Hence, we can arrive at a formula which allows a good description for the ground state energy for all values of  $n$ . We treat the excited states in Section 3. For the excited states, we can only use perturbation theory without the additional constraints. Hence we can discuss the shapes

for which  $n \simeq 2$ . However, the excited states bring in a new element — the possibility of parametric resonance. This allows the level crossing for shapes which are close to  $n = 2$  and hence should be experimentally observable for confinement in quantum dots where shapes are slightly deviant from the circle. A discussion of the results follows in Section 4.

The equivalent circle or square is a figure which has an area equal to that of the super-circle. The super-circle covers the area

$$A_n = 4 \int_0^a (a^n - x^n)^{\frac{1}{n}} dx = \frac{2a^2 [\Gamma(\frac{1}{n})]^2}{n [\Gamma(\frac{2}{n})]}. \quad (1.13)$$

A circle, which covers the same area  $A_n$ , has a radius  $R_n$  following from  $\pi R_n^2 = A_n$  or

$$R_n = a \sqrt{\frac{2}{\pi n}} \frac{\Gamma(\frac{1}{n})}{\sqrt{\Gamma(\frac{2}{n})}}. \quad (1.14)$$

The ground state energy equation (1.7) of a circle ( $c$ ) of radius  $R_n$  of equation (1.14) is

$$E_{0,n}^c = \frac{\pi n}{2} \frac{\Gamma(\frac{2}{n})}{[\Gamma(\frac{1}{n})]^2} \frac{K}{a^2}, \quad K = \frac{\hbar^2}{2m} (2.4048)^2. \quad (1.15)$$

This constitutes the first approximation to the ground state energy for all values of  $n$ . The efficacy of this approximation is shown in Table 2, where the numerical value of the ground state energy are shown in the second column. The results for  $E_{0,n}^c$  are given in the first column of Table 2. We note that  $E_{0,n}^c$  is exact for  $n = 2$  as expected, while for  $n = 3$ , it yields  $E_{0,3}^c = 0.8891$  as opposed to the numerical value of 0.8997. The closeness suggests that a perturbative treatment around  $n = 2$  should improve the agreement. We note from Table 2, that the ground state energy decreases continuously with increasing value of  $n$ . This can be understood from equation (1.13), where we see that the confining area becomes larger for increasing  $n$ . Increasing the area allows us to decrease the mean square momentum fluctuations and thus the energy decreases.

## 2 Perturbation about the equivalent circle for the ground state

The super-circle is given in polar coordinates by

$$r = \frac{a}{(\cos^n(\theta) + \sin^n(\theta))^{\frac{1}{n}}}. \quad (2.1)$$

For  $\Delta r = r - R$ , it results in

$$\frac{\Delta r}{R} = \left[ \frac{\sqrt{n\pi} [\Gamma(\frac{2}{n})]^{\frac{1}{2}}}{2} \frac{1}{[\Gamma(\frac{1}{n})] [\cos^n(\theta) + \sin^n(\theta)]^{\frac{1}{n}}} \right] - 1. \quad (2.2)$$

Here  $R$  is the radius of the equivalent circle. Now we want to perturb the problem around  $n = 2$ . Writing the terms

of equation (2.2) in a power series of  $\epsilon$  ( $\epsilon = n - 2$ ) and collecting terms up to first order, we get

$$\begin{aligned} \frac{\Delta r}{R} &= \frac{\epsilon}{4} \left[ \Psi\left(\frac{1}{2}\right) + 1 - \Psi(1) \right] \\ &\quad - \frac{\epsilon}{4} [\cos^2(\theta) \log(\cos^2(\theta)) + \sin^2(\theta) \log(\sin^2(\theta))]. \end{aligned} \quad (2.3)$$

Now we need to express the above equation in terms of a Fourier series as

$$\frac{\Delta r}{R} = \sum_{l=0}^{\infty} C_l \cos(l\theta), \quad (2.4)$$

where  $C_0 = 0$  as the areas of the circle and the super-circle are equal. Non-zero values of  $C_l$  exist when  $l$  is a integral multiple of 4 such as  $C_4 = -\frac{\epsilon}{12}$ ,  $C_8 = -\frac{\epsilon}{120}$ ,  $C_{12} = -\frac{\epsilon}{420}$ ,  $C_{16} = -\frac{\epsilon}{1008}$ ,  $C_{20} = -\frac{\epsilon}{1980}$ ,  $C_{24} = -\frac{\epsilon}{3432}$ , and so on.

The shape of the boundary now depends on the polar angle  $\theta$  and hence an isotropic ground state is not admissible, since it cannot vanish everywhere on the boundary. Accordingly, the first correction to the  $n = 2$  wave function will have an angular dependence which can be expanded as the trigonometric basis set to write

$$\begin{aligned} \psi(r) &= J_0(k_0 r) + \sum_{l=0}^{\infty} D_l(r) \cos(l\theta) \\ &= J_0(k_0 r) + \psi_1(r, \theta), \end{aligned} \quad (2.5)$$

where  $\psi_1(r, \theta) = \sum_{l=0}^{\infty} D_l(r) \cos(l\theta)$  is the first order correction to the wave-function,  $k_0^2 = \frac{2mE_0}{\hbar^2}$  and  $E_0$  is the ground state energy of the circle. From the normalization of  $\psi(r)$  and  $\psi_0(r)$ , we can easily see that  $D_0(0) = 0$  identically. The first order Schrödinger equation now can be written as

$$-\frac{\hbar^2}{2m} \nabla^2 \psi_1 = E_0 \psi_1 + E_1 \psi_0 \quad (2.6)$$

and the boundary condition

$$\psi(R + \Delta r) = 0. \quad (2.7)$$

Expanding in Taylor series up to the first order in  $C_l$

$$J_0(k_0 R) + k_0 R \frac{\Delta r}{R} J_0'(k_0 R) + \psi_1(R, \theta) = 0. \quad (2.8)$$

Now  $J_0(k_0 R) = 0$ , as it is the solution of the circle. Hence, using the expression of  $\psi_1$

$$\sum_{l=0}^{\infty} D_l(R) \cos(l\theta) = -k_0 R J_0'(k_0 R) \sum_{l=1}^{\infty} C_l \cos(l\theta). \quad (2.9)$$

Clearly

$$D_l(R) = -k_0 R J_0'(k_0 R) C_l. \quad (2.10)$$

From equations (2.5), (2.6), we can write

$$-\frac{\hbar^2}{2m} \left[ \sum_{l=0}^{\infty} \frac{d^2 D_l(r)}{dr^2} \cos(l\theta) + \sum_{l=0}^{\infty} \frac{1}{r} \frac{dD_l(r)}{dr} \cos(l\theta) - \sum_{l=0}^{\infty} \frac{l^2}{r^2} D_l(r) \cos(l\theta) \right] = E_0 \sum_{l=0}^{\infty} D_l(r) \cos(l\theta) + E_1 J_0(k_0 r). \quad (2.11)$$

For  $l = 0$

$$-\frac{\hbar^2}{2m} \left[ \frac{d^2 D_0(r)}{dr^2} + \frac{1}{r} \frac{dD_0(r)}{dr} \right] = E_0 D_0(r) + E_1 J_0(k_0 r), \quad (2.12)$$

while for  $l \neq 0$

$$-\frac{\hbar^2}{2m} \left[ \frac{d^2 D_l(r)}{dr^2} + \frac{1}{r} \frac{dD_l(r)}{dr} - \frac{l^2}{r^2} D_l(r) \right] = E_0 D_l(r). \quad (2.13)$$

The solution of equation (2.13)

$$D_l(r) = A_l J_l(k_0 r), \quad (2.14)$$

where  $A_l$  is a constant, fixed by the boundary condition in equation (2.10). As for equation (2.12) we note that the complementary function in the solution is  $J_0(k_0)$ . This vanishes on the boundary  $r = R$ . Hence the particular integral has to vanish at  $r = R$ . This makes  $E_1 = 0$ . The first correction  $E_1$  will be nonzero for a few selected cases — these are the parametric resonance caused by the shape variation. Thus at the first order, the ground state energy is unchanged while the wave function becomes

$$\begin{aligned} \psi(r) &= J_0(k_0 r) + \sum_{l=0}^{\infty} D_l(r) \cos(l\theta) \\ &= J_0(k_0 r) - \sum_{l \neq 0}^{\infty} A_l J_l(k_0 r) \cos(l\theta) \\ &= J_0(k_0 r) - \sum_{l \neq 0}^{\infty} C_l \frac{J_l(k_0 r)}{J_l(k_0 R)} k_0 R J_0'(k_0 R) \cos(l\theta). \end{aligned} \quad (2.15)$$

The reasonability of the wave function is discussed in Section 4.

To get the first correction to the energy we need to proceed to the second order. The wave function to this order can be written as

$$\psi(r) = J_0(k_0 r) + \sum_{l=0}^{\infty} C_l \frac{J_l(k_0 r)}{J_l(k_0 R)} k_0 J_0'(k_0 R) \cos(l\theta) + \sum_{l=0}^{\infty} G_l(r) \cos(l\theta). \quad (2.16)$$

To determine the energy correction  $E_2$ , we need  $G_0(R)$  alone. This can be seen from the fact that to satisfy the

Schrödinger equation to the second order of smallness,

$$-\frac{\hbar^2}{2m} \nabla^2 \psi_2 = E_0 \psi_2 + E_2 \psi_0 \quad (2.17)$$

and the only part which involves the energy  $E_2$  is the purely  $r$ -dependent part of  $\psi_2$  which is given by  $G_0(r)$ . Thus  $G_0(r)$  satisfies the equation

$$(\nabla^2 + k_0^2) G_0(r) = -\frac{2mE_2}{\hbar^2} \psi_0 \quad (2.18)$$

or,

$$\left( \frac{d^2}{d\rho^2} + \frac{1}{\rho} \frac{d}{d\rho} + 1 \right) G_0(\rho) = -\frac{E_2}{E_0} J_0(\rho), \quad (2.19)$$

where  $\rho = k_0 r$ . The boundary condition on  $G_0(\rho)$  is obtained from equation (2.17). The boundary condition needs to be satisfied to order  $C_l^2$  and the Taylor series expansion to the required order gives

$$\begin{aligned} \sum_{l=0}^{\infty} G_l(r) \cos(l\theta) &= (k_0 R)^2 J_0'(k_0 R) \sum_{l=0}^{\infty} C_l^2 \frac{J_l'(k_0 R)}{J_l(k_0 R)} \cos^2(l\theta) \\ &\quad - \frac{(k_0 R)^2}{2} J_0''(k_0 R) \sum_{l=0}^{\infty} C_l^2 \cos^2(l\theta). \end{aligned} \quad (2.20)$$

Using the identity

$$J_0''(k_0 R) = -\frac{J_0'(k_0 R)}{(k_0 R)}, \quad (2.21)$$

when  $J_0(k_0 R) = 0$ , we can reduce equation (2.20) to

$$\begin{aligned} \sum_{l=0}^{\infty} G_l(r) \cos(l\theta) &= \\ &= \frac{(k_0 R)^2}{2} J_0'(k_0 R) \sum_{l=0}^{\infty} C_l^2 \frac{J_l'(k_0 R)}{J_l(k_0 R)} (1 + \cos(2l\theta)) \\ &\quad + \frac{(k_0 R)}{4} J_0'(k_0 R) \sum_{l=0}^{\infty} C_l^2 (1 + \cos(2l\theta)). \end{aligned} \quad (2.22)$$

Equating the  $\theta$  independent terms, we get,

$$G_0(k_0 R) = \frac{(k_0 R)^2}{4} \left[ \sum_{l=0}^{\infty} C_l^2 \left( \frac{2J_l'(k_0 R)}{J_l(k_0 R)} + \frac{1}{k_0 R} \right) J_0'(k_0 R) \right]. \quad (2.23)$$

For large  $l$ ,  $\frac{J_l'(k_0 R)}{J_l(k_0 R)} = \frac{l}{k_0 R}$  and to leading order in  $l$

$$\begin{aligned} G_0(k_0 R) &= \frac{(k_0 R)^2}{2} \frac{J_0'(k_0 R)}{k_0 R} \sum_{l=0}^{\infty} l C_l^2 \\ &= -\frac{(k_0 R)}{2} J_1(k_0 R) \sum_{l=0}^{\infty} l C_l^2, \end{aligned} \quad (2.24)$$

as  $J'_0(k_0R) = -J_1(k_0R)$ . We now need to solve equation (2.19). The homogeneous solution has to be  $J_0(k_0R)$ , the other linearly independent solution being ill behaved at  $r = 0$  and is not acceptable. Denoting the particular integral by  $P(k_0r)$ , we can write

$$G_0(\rho) = AJ_0(\rho) + P(\rho), \quad (2.25)$$

where the constant  $A$  can be determined by requiring  $G_0(\rho)$  to be orthogonal to the zeroth order solution  $J_0(\rho)$  over the original circle. The boundary condition of equation (2.24) gives

$$P(k_0R) = -\frac{(k_0R)}{2}J_1(k_0R) \sum_{l=0}^{\infty} lC_l^2. \quad (2.26)$$

Now putting the values of coefficients  $C_l$ , and  $k_0R = 2.4048$ , we get

$$P(k_0R) = -0.01745\epsilon^2. \quad (2.27)$$

To find the particular integral, the simplest procedure is to try a power series expansion

$$P(\rho) = \sum_{l=1}^{\infty} a_l \rho^{2l}. \quad (2.28)$$

Expanding  $J_0(\rho)$  and  $P(\rho)$  up to the tenth power of  $\rho$  and putting  $\rho = k_0R$ , we get

$$P(k_0R) = -\frac{E_2}{E_0} \left[ 0.25(k_0R)^2 - 0.03125(k_0R)^4 + (1.302 \times 10^{-3})(k_0R)^6 - (2.7125 \times 10^{-5})(k_0R)^8 + (3.3907 \times 10^{-7})(k_0R)^{10} \right]. \quad (2.29)$$

Inserting the value of  $(k_0R) = 2.4048$  in equation (2.29), we find

$$P(k_0R) = -\frac{E_2}{E_0} 0.62421. \quad (2.30)$$

From equations (2.27) and (2.30)

$$\frac{E_2}{E_0} = 0.027955\epsilon^2 \quad (2.31)$$

and the total energy up to second order correction

$$\begin{aligned} E &= E_0 + E_1 + E_2 \\ E &= E_0(1 + 0.027955\epsilon^2) \end{aligned} \quad (2.32)$$

as  $E_1 = 0$ . Hence the ground state energy for the ground state of the super-circle up to second order correction is,

$$E = \frac{\hbar^2}{2m} \frac{(2.4048)^2}{R^2} (1 + 0.027955\epsilon^2). \quad (2.33)$$

When  $\epsilon = n - 2$  is negative, we have incorporated the next correction empirically by introducing a phenomenological  $\epsilon^4$  term which is designed in such a way that it will

give exact answer at  $n = 1$ . Hence the energy expression becomes

$$E = \frac{\hbar^2}{2m} \frac{(2.4048)^2}{R^2} (1 + 0.027955\epsilon^2 + 0.0577\epsilon^4), \quad \epsilon < 0. \quad (2.34)$$

For  $\epsilon > 0$  i.e.  $n > 2$ , we need to go as far as  $n = \infty$ . Perturbation theory may appear useless, but we can use a form of duality. For  $n > 2$ , we define a fraction  $m$  ( $1 \leq m \leq 2$ ) such that  $\frac{1}{m} + \frac{1}{n} = 1$ . Using equation (1.15), we now arrive at

$$\frac{E^{(n)}}{E^{(m)}} = (n-1) \frac{\Gamma(\frac{2}{n})}{\Gamma(2-\frac{2}{n})} \left[ \frac{\Gamma(1-\frac{1}{n})}{\Gamma(\frac{1}{n})} \right]^2, \quad (2.35)$$

which leads to

$$\begin{aligned} E^{(n)} &= n \frac{\Gamma(\frac{2}{n})}{[\Gamma(\frac{1}{n})]^2} \frac{\hbar^2}{2m} (2.4048)^2 \frac{\pi}{2} \\ &\times \left[ 1 + 0.027955 \left( \frac{n-2}{n-1} \right)^2 + 0.0577 \left( \frac{n-2}{n-1} \right)^4 \right]. \end{aligned} \quad (2.36)$$

The results from equations (2.35, 2.36) are shown in Table 2. For excited states, we cannot exploit the benefit of ‘‘exact’’ results but the interest there lies in the fact that for very small values of  $\epsilon$  i.e. within the realm of perturbation theory, parametric resonance can induce large scale changes. We note in passing that the three dimensional cylindrical box with a super-circular cross section and of height  $L$  can be easily handled because the problem would be separable in the  $Z$ -coordinate and the  $X-Y$  plane. While the  $X-Y$  plane problem is to be treated as discussed, the energy formula of equations (2.34 and 2.35) will have an additional contribution of  $\frac{\pi^2 \hbar^2}{2mL^2}$  from the confinement in the  $Z$ -direction.

### 3 Perturbation theory for the excited states and parametric resonance

In this section we would like to develop the perturbation theory for the excited states. The excited states come in two varieties—degenerate ( $l \neq 0$ ) and nondegenerate ( $l = 0$ ). We begin with the states with finite value of  $l$ . The unperturbed energy for such a state can be written as

$$E = \frac{\hbar^2 k_{ln}^2}{2m}, \quad (3.1)$$

where  $k_{ln}$  is obtained from the  $n$ th zero of  $J_l(kr)$ . The degenerate wave-functions at this order can be written as  $A_l J_l(k_{ln}r) \cos(l\theta)$  and  $B_l J_l(k_{ln}r) \sin(l\theta)$ , where  $A_l$  and  $B_l$  can be found from the normalization condition. Since our shape variation can be expressed as a series in cosines alone, the sine solution will be unaffected. It is the cosine solution that will be subjected to perturbation. The first

order correction,  $\psi_1(r, \theta)$  and  $E_1$  to the wave-function and energy respectively, satisfy

$$-\frac{\hbar^2}{2m}\nabla^2\psi_1(r, \theta) = E_0\psi_1(r, \theta) + E_1\psi_0(r, \theta). \quad (3.2)$$

In  $(r, \theta)$  coordinate

$$\left[ \frac{\partial^2}{\partial r^2} + \frac{1}{r} \frac{\partial}{\partial r} + \frac{1}{r^2} \frac{\partial^2}{\partial \theta^2} \right] \psi_1(r, \theta) = -\frac{2mE_1}{\hbar^2} \psi_0(r, \theta). \quad (3.3)$$

We now expand

$$\psi_1(r, \theta) = \sum_p \phi_p(r) \cos(p\theta), \quad (3.4)$$

whence

$$\sum_p \left[ \frac{\partial^2 \phi_p}{\partial r^2} + \frac{1}{r} \frac{\partial \phi_p}{\partial r} + \left( k_{ln}^2 - \frac{p^2}{r^2} \right) \phi_p \right] \cos(p\theta) = -A_1 \frac{2mE_1}{\hbar^2} J_l(k_{ln}r) \cos(l\theta). \quad (3.5)$$

If  $p = l$

$$\left[ \frac{\partial^2 \phi_l}{\partial r^2} + \frac{1}{r} \frac{\partial \phi_l}{\partial r} + \left( k_{ln}^2 - \frac{l^2}{r^2} \right) \phi_l \right] = -A_1 \frac{2mE_1}{\hbar^2} J_l(k_{ln}r) \quad (3.6)$$

and if  $p \neq l$

$$\left[ \frac{\partial^2 \phi_p}{\partial r^2} + \frac{1}{r} \frac{\partial \phi_p}{\partial r} + \left( k_{ln}^2 - \frac{p^2}{r^2} \right) \phi_p \right] = 0. \quad (3.7)$$

The boundary condition for the first order of correction in  $\Delta r$  can be written as

$$\begin{aligned} 0 &= \psi_0 \left( R + \epsilon R \sum_m C_m \cos(m\theta) \right) + \psi_1(R) \\ &= \psi_0(R) + \epsilon R \sum_m C_m \cos(m\theta) \psi_0'(R) + \psi_1(R) \\ &= A_l \epsilon R \sum_m C_m \cos(m\theta) J_l'(k_{ln}R) k_{ln} \cos(l\theta) + \psi_1(R) \\ &= \frac{1}{2} A_l \epsilon R J_l'(k_{ln}R) k_{ln} \sum_m C_m [\cos(m+l)\theta \\ &\quad + \cos(m-l)\theta] + \sum_p \phi_p(R) \cos(p\theta), \end{aligned} \quad (3.8)$$

leading to

$$\phi_p(R) = -\frac{1}{2} A_l \epsilon R J_l'(k_{ln}R) k_{ln} [C_{p-l} + C_{p+l}]. \quad (3.9)$$

For  $p \neq l$ , the solution  $\phi_p(r)$  is seen to be  $B_p J_p(k_{ln}r)$  and the boundary condition of equation (3.9) fixes the constant  $B_p$  as

$$B_p = -\frac{1}{2} A_l \epsilon R k_{ln} \frac{J_l'(k_{ln}R)}{J_p(k_{ln}R)} [C_{p-l} + C_{p+l}]. \quad (3.10)$$

For  $p = l$ , on the other hand, the solution

$$\phi_l = B_l J_l(k_{ln}r) + P_l(k_{ln}r),$$

where  $P_l(k_{ln}r)$  is the particular integral of equation (3.6). Writing  $X = k_{ln}r$ , we need to find the particular integral of

$$\left[ \frac{\partial^2 P_l}{\partial X^2} + \frac{1}{X} \frac{\partial P_l}{\partial X} + \left( 1 - \frac{l^2}{X^2} \right) P_l \right] = -A_1 \frac{2mE_1}{\hbar^2} \frac{1}{k_{ln}^2} J_l(X). \quad (3.11)$$

Writing

$$P_l(X) = -\frac{E_1}{E_0} A_l \sum_s b_s X^s = -\frac{E_1}{E_0} A_l \xi(X),$$

the boundary condition at  $X = k_{ln}R$  fixes  $E_1$  as

$$-\frac{E_1}{E_0} \xi(X) = -\frac{\epsilon}{2} C_{2l} k_{ln} R J_l'(k_{ln}R), \quad (3.12)$$

since  $C_0 = 0$ . Thus, there will be a correction at the first order in  $\epsilon$ , provided  $l$  is such that  $C_{2l} \neq 0$ . From our listing of  $C_{2l}$  we find that this will happen whenever  $l$  is an even integer. Hence  $E_1 \neq 0$  for  $l = 2, 4, 6$ , etc. This is the case of parametric resonance. For these selected values of  $l$ , the energy acquires a first order correction. This correction is very strong and will interfere with the neighboring levels which differ by unity. That level will not have a first order correction. This is what can lead to level crossing in a single particle non-circular quantum dot. Two electron quantum dots show level crossing due to the coulomb repulsion. Here a single quantum dot is capable of showing the same effect due to change of boundary. The sensitivity to boundaries also occurs in classical dynamics of a particle confined in a billiard.

The wave-function to this order is

$$\psi(r, \theta) = A_l J_l(k_{ln}r) \cos(l\theta) + \sum_{m \neq l} B_m J_m(k_{ln}r) \cos(m\theta) + P_l(k_{ln}r) \cos(l\theta). \quad (3.13)$$

Note that we do not have a problem with normalization at this order because

$$\int J_l(X) P_l(X) X dX = 0.$$

Turning to the second order, we have

$$\begin{aligned} -\frac{\hbar^2}{2m} \left[ \frac{\partial^2}{\partial r^2} + \frac{1}{r} \frac{\partial}{\partial r} + \frac{1}{r^2} \frac{\partial^2}{\partial \theta^2} \right] \psi_2(r, \theta) = \\ E_0 \psi_2(r, \theta) + E_1 \psi_1(r, \theta) + E_2 \psi_0(r, \theta). \end{aligned} \quad (3.14)$$

As before, we expand

$$\psi_2(r, \theta) = \sum_m \chi_m(r) \cos(m\theta),$$

and inserting in equation (3.14)

$$\begin{aligned} \sum_m \left[ \frac{\partial^2}{\partial r^2} + \frac{1}{r} \frac{\partial}{\partial r} + k_{ln}^2 - \frac{m^2}{r^2} \right] \chi_m(r) = \\ - \frac{2mE_1}{\hbar^2} \left[ \sum_{m \neq l} B_m J_m(k_{ln}r) \cos(m\theta) + P_l(k_{ln}r) \cos(l\theta) \right] \\ - \frac{2mE_2}{\hbar^2} A_l J_l(k_{ln}r) \cos(l\theta). \quad (3.15) \end{aligned}$$

To find the energy shift  $E_2$  at the second order, we need to concentrate on the  $m = l$  case alone. In this case

$$\begin{aligned} \left[ \frac{\partial^2}{\partial X^2} + \frac{1}{X} \frac{\partial}{\partial X} + 1 - \frac{l^2}{X^2} \right] \chi_l(X) = \\ - \frac{E_1}{E_0} P_l(X) - \frac{E_2}{E_0} A_l J_l(X). \quad (3.16) \end{aligned}$$

We now need to find boundary condition on  $\chi_l(r)$  at  $r = R$ . This reads

$$\begin{aligned} 0 = \psi_0 \left( R + \epsilon R \sum_m C_m \cos(m\theta) \right) \\ + \psi_1 \left( R + \epsilon R \sum_m C_m \cos(m\theta) \right) + \psi_2(R) \\ = \psi_0(R) + \epsilon R \sum_m C_m \cos(m\theta) \psi_0'(R) \\ + \frac{\epsilon^2 R^2}{2} \sum_{m_1} C_{m_1} \cos(m_1\theta) \sum_{m_2} C_{m_2} \cos(m_2\theta) \psi_0''(R) \\ + \psi_1(R) + \epsilon R \sum_{m_1} C_{m_1} \cos(m_1\theta) \psi_1'(R) + \psi_2(R) \\ = \frac{\epsilon^2 R^2}{2} \sum_{m_1, m_2} C_{m_1} C_{m_2} \cos(m_1\theta) \cos(m_2\theta) \\ \times A_l J_l''(k_{ln}R) k_{ln}^2 \cos(l\theta) \\ + \epsilon R k_{ln} \sum_{m_1} C_{m_1} \cos(m_1\theta) \\ \times \sum_{m_2} B_{m_2} J_{m_2}'(k_{ln}R) \cos(m_2\theta) \\ + \epsilon R k_{ln} \sum_m C_m \cos(m\theta) P_l'(k_{ln}R) \cos(l\theta) \\ + \chi(R) \cos(l\theta). \quad (3.17) \end{aligned}$$

Hence,

$$\begin{aligned} \chi(R) = - \frac{\epsilon R}{2} k_{ln} P_l'(k_{ln}R) C_{2l} \\ - \frac{\epsilon R}{2} k_{ln} \sum_{m_1} C_{m_1} B_{l-m_1} J_{l-m_1}'(k_{ln}R) \\ - \frac{\epsilon R}{2} k_{ln} \sum_{m_1} C_{m_1} B_{l+m_1} J_{l+m_1}'(k_{ln}R) \\ - \frac{\epsilon^2 R^2}{8} k_{ln}^2 R^2 J_l''(k_{ln}R) A_l \\ \times \sum_{m_1} [C_{m_1}^2 + C_{m_1} C_{2l-m_1} + C_{m_1} C_{2l+m_1}]. \quad (3.18) \end{aligned}$$

From equation (3.16), we note that solution  $\chi_l(r)$  can be written as

$$\chi_l(r) = C J_l(r) + Q_l(r), \quad (3.19)$$

where the particular integral  $Q_l(r)$  is to be found as a power series expansion

$$\begin{aligned} Q_l(r) = -A_l \frac{E_2}{E_0} \sum_s c_s r^s - \frac{E_1}{E_0} \sum_s d_s r^s \\ = -A_l \frac{E_2}{E_0} \zeta_1(r) - \frac{E_1}{E_0} \zeta_2(r). \quad (3.20) \end{aligned}$$

The boundary condition of equation (3.18), now fixes the second order shift as

$$\begin{aligned} - \frac{E_2}{E_0} \zeta_1(k_{ln}R) - \frac{1}{A_l} \frac{E_1}{E_0} \zeta_2(k_{ln}R) = \frac{\epsilon^2}{4} C_{2l}^2 (k_{ln}R)^2 \\ \times \left[ \frac{J_l'(k_{ln}R)}{k_{ln}R} + J_l''(k_{ln}R) \right] \\ + \frac{\epsilon^2}{4} (k_{ln}R)^2 \sum_{m_1} (C_{m_1}^2 + C_{m_1} C_{2l+m_1}) \\ \times \left[ \frac{J_l'(k_{ln}R) J_{l+m_1}'(k_{ln}R)}{J_{l+m_1}(k_{ln}R)} - \frac{J_l''(k_{ln}R)}{2} \right] \\ + \frac{\epsilon^2}{4} (k_{ln}R)^2 \sum_{m_1} C_{m_1} C_{2l-m_1} \\ \times \left[ \frac{J_l'(k_{ln}R) J_{l-m_1}'(k_{ln}R)}{J_{l-m_1}(k_{ln}R)} - \frac{J_l''(k_{ln}R)}{2} \right]. \quad (3.21) \end{aligned}$$



Using equation (3.21), we have computed the first four energy levels as

$$\begin{aligned}
 E_{00} &= \frac{\hbar^2}{2ma^2} (2.4048)^2 \left(\frac{\pi n}{2}\right) \frac{\Gamma(\frac{2}{n})}{[\Gamma(\frac{1}{n})]^2} \\
 &\quad \times [1 + 0.027955(n-2)^2], \\
 E_{10} &= \frac{\hbar^2}{2ma^2} (3.382)^2 \left(\frac{\pi n}{2}\right) \frac{\Gamma(\frac{2}{n})}{[\Gamma(\frac{1}{n})]^2} \\
 &\quad \times \left[\Gamma\left(\frac{1}{n}\right)\right]^2 [1 + 0.062766(n-2)^2], \\
 E_{20} &= \frac{\hbar^2}{2ma^2} (5.135)^2 \left(\frac{\pi n}{2}\right) \frac{\Gamma(\frac{2}{n})}{[\Gamma(\frac{1}{n})]^2} [1 - 2.1856923(n-2) \\
 &\quad + 0.0540083(n-2)^2] \text{ [parametric resonance]}, \\
 E_{01} &= \frac{\hbar^2}{2ma^2} (5.52)^2 \left(\frac{\pi n}{2}\right) \frac{\Gamma(\frac{2}{n})}{[\Gamma(\frac{1}{n})]^2} \\
 &\quad \times [1 + 0.00594753(n-2)^2]. \tag{3.22}
 \end{aligned}$$

## 4 Results and conclusion

### 4.1 Ground state energy and wave function

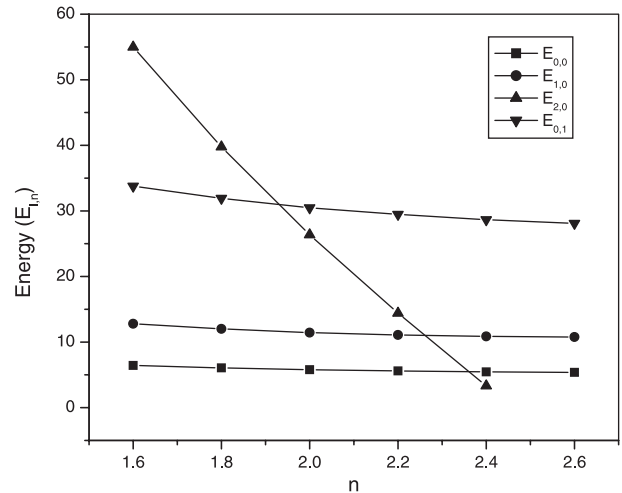
Using the expressions of equations (2.34) and (2.35), we exhibit the calculated ground state energies in Table 2 indicating the efficacy of our approximations.

The accuracy of our numerical scheme can be gauged by comparing the numerical results with the known exact results for  $n = 1, 2$  and  $\infty$ . In units of the exact ground state of the particle in a circular box, the ground state for  $n = 1$  is 1.7080 while the numerics yields 1.6927 — an error of 0.9%. At  $n = 2$ , the numerical result is 0.9967 as opposed to the exact result of 1.0000 (an error of 0.3%) while for  $n \rightarrow \infty$ , the numerical determination gives 0.8516 as compared to the exact answer of 0.8548 (error of 0.4%). The numerical result presented here are for a grid size of  $\frac{1}{10}$ . We have checked that for a grid size of  $\frac{1}{20}$  and  $\frac{1}{30}$  the numerical results for  $n = 2$  are 0.99913 and 0.99961 respectively and the corresponding errors are 0.087% and 0.04%. Thus by decreasing the grid size the computational error can be substantially reduced. We have not tried to go to an even smaller grid size because that is not wanted right now by the accuracy of the analytical work. This accuracy is sufficient for the purpose at hand, where we wanted to explore how far a straightforward perturbative calculation aided by constraints coming from known exact solutions at some values of  $n$  can take us. It is interesting to note that we can be within 2.5% of the true (numerical) answer for a wide range of  $n$  ( $0.5 < n < \infty$ ), with the accuracy close to or better than 1 percent over a significant part of that range.

The accuracy of the model has also to be tested on the wave-function by calculating the norm. The highest

**Table 3.** Calculated energy levels.

$n$	$E_{00}$	$E_{10}$	$E_{20}$	$E_{01}$
1.6	6.4332	12.7942	54.9842	33.7767
1.8	6.0653	12.0127	39.7592	31.9287
2.0	5.7831	11.4379	26.3682	30.4704
2.2	5.5976	11.0864	14.4046	29.4667
2.4	5.4599	10.8585	3.3300	28.6661



**Fig. 1.** Energy level diagram for a free particle confined in a super-circular box  $|x|^n + |y|^n = a^n$  (where  $n$  is a rational number and  $a$  is a positive real number) in the unit of  $\frac{\hbar^2}{2ma^2}$ . The level  $E_{2,0}$  shows parametric resonance that leads to level crossing.

deviation of the wave-function will occur when we go from the circle to the square. Hence we focus on  $n = 1$ . The first question to ask is has the wave-function vanishes on the boundary. We consider three points  $A, B, C$  on the square with  $(r, \theta)$  coordinates as  $(a, 0), (\frac{a}{\sqrt{2}}, 0), (a, \frac{\pi}{2})$ . The wave-functions are 0.011, 0.085 and 0.011 respectively. We take three other points in the interior of the square. These have the coordinates  $(\frac{a}{2}, 0), (\frac{a}{2\sqrt{2}}, \frac{\pi}{4}), (\frac{a}{2}, \frac{\pi}{2})$ . The norm of the wave-functions at these points are 0.539, 0.735 and 0.529 as compared to 0.564, 0.798 and 0.564 which are the exact values for the square. For these points the error are 6.2%, 7.9% and 6.2% respectively. The reasonability of this approach should provide an alternative window on certain problems in quantum chemistry which have been discussed in the introduction.

### 4.2 Excited state energies

Using the expressions of equation (3.22) we exhibit the calculated energy levels as (in the unit of  $\frac{\hbar^2}{2ma^2}$ ), see Table 3.

As stated in Section 3, the level  $E_{2,0}$  shows parametric resonance and is very strongly affected in comparison to the other levels shown. This raises the possibility of level crossing as shown in Figure 1. The observable effect will be in a significant change of the corresponding spectral lines.

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## References

1. H.R. Krishnamurthy, H.S. Mani, H.C. Verma, *J. Phys. A: Math. Gen.* **15**, 2131 (1982)
2. J.K. Bhattacharjee, K. Banerjee, *J. Phys. A: Math. Gen.* **20**, L759 (1987)
3. K. Lis, S. Bednarek, B. Szafran, J. Adamowski, *Physica E* **17**, 494 (2003)
4. P.S. Drouvelis, P. Schmelcher, F.K. Diakonov, *Phys. Rev. B* **69**, 155312 (2004)
5. I. Magnúsdóttir, V. Gudmundsson, *Phys. Rev. B* **60**, 16590 (1999)
6. H. Ichikawa, K. Sakata, *Intern. J. Quant. Chem.* **87**, 135 (2002) and references therein
7. S. Sakai, *J. Phys. Chem. A* **110**, 6339 (2006)
8. M. Gardner, "Piet Hein's Superellipse", in *Mathematical Carnival: A new Round-Up of Tantalizers and Puzzles from Scientific American* (Vintage, New York, 1977), Ch. 18, pp. 240–254
9. G. Lamé, *Examen des différentes méthodes employées pour résoudre les problèmes de géométrie* (Oxford University, 1818)
10. N.T. Gridgeman, *Math. Gaz.* **54**, 31 (1970)
11. J.A. Gielis, *Am. J. Bot.* **90**, 333 (2003)
12. I. Peterson, *Science News* **163**, 18 (2003)
13. J. Whitfield, *Nature Science Update* (April 2, 2003)
14. Y. Shimizu, *Chaos, Solitons Fractals* **5**, 1337 (1995)
15. M.V. Berry, *Eur. J. Phys.* **2**, 91 (1981)
16. I.M. Erham, H. Taseli, *J. Comput. Appl. Math.* **194**, 227 (2006)
17. *Handbook of Mathematical functions with Formulas, Graphs and Mathematical Tables*, edited by M. Abramowitz, I. Stegun, National Bureau of Standards, Washington, D.C. (1964)
18. K.F. Riley, M.P. Hobson, S.C. Bence, *Mathematical methods for physics and engineering* (Cambridge University Press, 2002), Ch. 19
19. M.R. Spiegel, *Vector Analysis* (Schaum's Outline Series, New York, 1959)
20. G. Arfken, *Mathematical Methods for Physicists* (Academy Press, 1995)
21. D.J. Griffiths, *Introduction to Quantum Mechanics*, 2nd edn. (Prentice Hall, 2004)
22. F. Cooper, A. Khare, U. Sukhatme, *Supersymmetry in Quantum Mechanics* (World Scientific, 2001)
23. W.D. Carl, Chemistry Education Material, University of Connecticut (2006)
24. S. Agmon, *Lectures on Elliptic Boundary Value Problems* (Van Nostrand, Princeton, N.J., 1965)
25. I. Babuška, U. Banerjee, J.E. Osborn, *Survey of meshless and generalized finite element methods: A unified approach* (Acta Numerica, 2003), pp. 1–125