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On the ground state of regular polygonal billiards

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Abstract. The Helmholtz equation for regular polygons is investigated by means of the conformal mapping from the circle, which provides an expansion parameter for the approximate evaluation of the lowest eigenvalue and the corresponding eigenvector.

1. Introduction

The Helmholtz equation with Dirichlet boundary conditions for regular polygons, here written in complex coordinates

$$-4\frac{\partial^2}{\partial z \partial z^*}\psi(z,z^*) = \epsilon^2 \psi(z,z^*) \tag{1}$$

has a simple analytical solution only for the square and the limit case of the circle. The case of the equilateral triangle was solved by Lamé [1] long ago, and then rediscussed by various authors. Standing as the eigenvalue equation for a quantum particle in a billiard with reflecting walls, the corresponding classical dynamics is integrable in the sense of the theorem by Arnold precisely in the three mentioned cases, the Hamiltonian flow taking place on an invariant surface with the topology of a torus. Regular polygons with number of sides n > 4 have invariant surfaces with higher but finite genus, and are called 'pseudo-integrable'. After this picture of the classical dynamics, which more generally was drawn for polygonal billiards, Richens and Berry [2] computed the action-angle variables for the equilateral triangle and obtained the quantum spectrum by using the Bohr–Sommerfeld rules.

A detailed account of the properties of classical polygonal billiards is given by Gutkin [3].

The triangular billiard also has an interpretation as a model for the dynamics of three hard point particles in a segment. For the case of equal masses, Jung [4] gave the solution for the equilateral triangle with an approach based on symmetries.

Integrability is a consequence of the property of the triangle and the square to tessellate the plane. Any trajectory can be unfolded to a straight line by a sequence of reflections of the polygon about the sides hit by the particle. For regular polygons with n > 4, including hexagons, reflections require more than one sheet. On the quantum side, the property of integrability is linked to the simplicity of the solutions of the eigenvalue problem. The following lemma by Amar *et al* [5], states that a solution to equation (1) in terms of a finite sum

$$\psi(z, z^*) = \sum_{k}^{\ell} c_k \mathrm{e}^{\frac{1}{2}(\alpha_k z^* - \alpha_k^* z)} \qquad |\alpha_k| = \epsilon \tag{2}$$

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that vanishes on a segment, has the property $\psi(z, z^*) = -\psi(z', z'^*)$, where z' is the point symmetric to z with respect to the straight line containing the segment. In particular, ψ vanishes on the whole straight line. This implies that, among regular polygons, only the cases n = 3, 4 allow a solution of this type. However, a part of the spectrum of the hexagon is inherited from the equilateral triangle, due to the relationship among the two lattices. Expansions more general than (2) were shown to be not allowed for the non-integrable cases [6].

Choosing the polygons inscribed in the unit circle, with vertices at the roots of unity, the lowest value ϵ_n for the triangle, the square and the circle are:

$$\epsilon_3 = 4\pi/3 \qquad \epsilon_4 = \pi \qquad \epsilon_\infty = j_{0,1} \tag{3}$$

where $j_{0,1}$ is the first zero of Bessel's function J_0 . It is instructive to write the ground states for n = 3, 4 in polar coordinates, as Neumann series of Bessel functions:

$$\psi_n(r,\theta) = J_0(\epsilon_n r) \cos\left(\frac{\pi}{2n}\right) + 2\sum_{k=1}^{\infty} \cos\left(kn\frac{\pi}{2} + \frac{\pi}{2n}\right) J_{nk}(\epsilon_n r) \cos(nk\theta).$$
(4)

A proof is given in the appendix. Unfortunately, this expression cannot be generalized to all values of n, because it always corresponds to a finite sum of trigonometric functions. However, it is reasonable to conjecture the following general expression for the ground state of regular polygons

$$\psi_n(r,\theta) = J_0(\epsilon_n r) + 2\sum_{k=1}^{\infty} h_k J_{nk}(\epsilon_n r) \cos(nk\theta).$$
(5)

The function is symmetric under mirror transformations of the polygon; it is then sufficient to require vanishing on the boundary segment in the sector $0 \le \theta \le \pi/n$.

A convenient way to deal with the difficulty of boundary conditions is to map the polygon conformally onto the unit disk $|z| \leq 1$. The conformal map giving the one-to-one correspondence of points z in the unit disk with points w(z) in the polygon, is the Schwarz-Christoffel transform [7],

$$w(z) = C_n \int_0^z \mathrm{d}s \, (1 - s^n)^{-2/n} \qquad C_n = \frac{\Gamma(1 - 1/n)}{\Gamma(1 + 1/n)\Gamma(1 - 2/n)} \tag{6}$$

where the value of the scale factor C_n assures that the corners of the polygon, given by the roots of the equation $z^n = 1$, are fixed points of the mapping. The Helmholtz equation for the polygon is mapped into

$$-4\frac{\partial^2}{\partial z \partial z^*}\psi(z, z^*) = \epsilon^2 |w'(z)|^2 \psi(z, z^*)$$
(7)

with the simple boundary condition $\psi = 0$ for |z| = 1. The weight function is the generator of Gegenbauer's polynomials:

$$|w'(re^{i\theta})|^2 = C_n (1 + r^{2n} - 2r^n \cos n\theta)^{-2/n} = C_n \sum_{k=0}^{\infty} r^{kn} C_k^{2/n} (\cos n\theta).$$
(8)

The mapping technique has already been used to compute zeta functions $\zeta(s)$, sums of negative integer powers of eigenvalues, for regular polygons. As shown by Itzykson *et al* [8], they may be obtained by integrating products of the Green's function of the Laplace operator in the polygon, which is related in a simple way to that of the circle. The approximate evaluation of zeta functions for regular polygons was done by Kvitsinsky [9] to first order in ϵ , where $|w'(z)|^2 = C_n^2 [1 + \epsilon(z, z^*)]$. Aurell and Salomonson [10] have

studied the functional determinant of the Laplacian in polygons, $\exp\{-\zeta'(0)\}$, by means of conformal mappings.

Integral (6) for the analytic function w(z) can be evaluated by a power expansion in z to give a hypergeometric series:

$$w(z) = C_n z_2 F_1\left(\frac{2}{n}, \frac{1}{n}; 1 + \frac{1}{n}; z^n\right) = C_n z \sum_{k=0}^{\infty} f_k z^{nk}$$
(9a)

$$f_0 = 1$$
 $f_k = \frac{1}{k!(nk+1)} \left(\frac{2}{n}\right) \left(\frac{2}{n}+1\right) \dots \left(\frac{2}{n}+k-1\right).$ (9b)

Note the periodicity property $w(e^{i2\pi/n}z) = e^{i2\pi/n}w(z)$, and the action of complex conjugation: $w(z)^* = w(z^*)$.

Since, obviously, w(z) = z when *n* goes to infinity, it is natural to search an approximate solution of equation (7) in the form of a 1/n expansion, starting from the known solutions of the circle. To improve the result even for low *n*, in this paper the ground state ϵ_n and the corresponding eigenfunction ψ_n for regular polygons are calculated in the form of λ expansions, where the fictitious parameter λ is introduced at the level of the hypergeometric series:

$$w(z) = C_n z [1 + \lambda f(z)]$$
 $f(z) = \sum_{k=1}^{\infty} f_k z^{kn}$ (10)

and is put equal to unity at the end. The expansion scheme differs from that used by Kvitsinsky, making, in this case, computations simpler. I explicitly evaluate up to the third-order term for ϵ_n , and the second-order term for the eigenfunction. The eigenfunction has the form given in equation (5). The effectiveness of the expansion can be tested against the cases n = 3, 4 where convergence is expected to be worse and, on the other hand, exact results are available.

By writing the expansion for the eigenvalue

$$\epsilon_n = \frac{1}{C_n} \epsilon_0 [1 - \lambda \delta_1 - \lambda^2 \delta_2 - \lambda^3 \delta_3 + \ldots]$$
(11*a*)

one obtains $\epsilon_0 = j_{0,1}$, $\delta_1 = 0$ and

$$\delta_{2} = \frac{\epsilon_{0}}{2} \sum_{k=1}^{\infty} f_{k}^{2} \frac{J_{kn+1}(\epsilon_{0})}{J_{kn}(\epsilon_{0})}$$
(11b)

$$\delta_{3} = \frac{\epsilon_{0}^{2}}{4} \sum_{k=2}^{\infty} f_{k} \sum_{s=1}^{k-1} f_{k-s} f_{s} \frac{J_{sn+1}(\epsilon_{0})}{J_{sn}(\epsilon_{0})} \left[2 \frac{J_{kn+1}(\epsilon_{0})}{J_{kn}(\epsilon_{0})} + \frac{J_{(k-s)n+1}(\epsilon_{0})}{J_{(k-s)n}(\epsilon_{0})} \right]$$
$$- \frac{\epsilon_{0}^{2}}{4} \sum_{k=2}^{\infty} f_{k} \frac{J_{kn+2}(\epsilon_{0})}{J_{kn}(\epsilon_{0})} \sum_{s=1}^{k-1} f_{s} f_{k-s}.$$
(11c)

The approximate values ϵ_n given by the expansion are computed numerically and listed in table 1. The lowest order is given by a simple rescaling and provides a fair approximation; the factors δ_2 and δ_3 rapidly vanish with increasing *n*. A 1/n expansion would have given less satisfactory results and involved in any case the need of numerical computations to produce numbers; the present approach corresponds to a partial resummation of terms of the 1/n expansion.

Table 1.

Ground state							
n —	$j_{0,1}/C_n$	δ_2	δ_3	ϵ_n	Exact		
3	4.248 4580	0.012 858 3	0.000 985 20	4.189 644	4.188 790		
4	3.152 7955	0.003 435 97	0.000 100 10	3.141 647	3.141 593		
5	2.824 3478	0.001 224 88	0.00001722	2.820840			
6	2.676 3608	0.000 523 64	0.000 004 10	2.674948			
8	2.546 8987	0.000 135 14	0.000 000 43	2.546 553			
∞	—	—	—	—	2.404 826		

2. The λ expansion

The most obvious approach would be to use the standard perturbation theory to solve the eigenvalue equation (7), written in the form

$$(\hat{H}_0\psi)(r,\theta) = (C_n\epsilon_n)^2 |1+\lambda\sum_{k=1}^{\infty} f_k(kn+1)(r\mathrm{e}^{\mathrm{i}\theta})^{kn}|^2\psi(r,\theta)$$
(12)

where $-\hat{H}_0$ is the Laplace operator in the unit disk. The eigenfunctions of \hat{H}_0 are the Fourier–Bessel basis

$$u_{m,s}(r,\theta) = \frac{1}{\sqrt{\pi}} \frac{J_m(j_{m,s}r)}{J_{m+1}(j_{m,s})} e^{\pm im\theta} \qquad m = 0, 1, \dots, s = 1, 2 \dots$$
(13)

Difficulties arise starting from the lowest order because of integrations of products of Bessel functions, and summations over zeros.

An equivalent but computationally much more convenient approach is to represent the solution of the equation in the integral form

$$\psi(z, z^*) = \frac{1}{2\pi} \int_0^{2\pi} d\alpha \, h(\alpha) e^{\frac{1}{2} \epsilon [e^{i\alpha} w(z^*) - e^{-i\alpha} w(z)]}$$
(14)

where the index *n* in ψ and ϵ is omitted. Both the eigenvalue ϵ and the function $h(\alpha)$ are obtained by imposing the boundary condition on the circle for all angles θ :

$$0 = \frac{1}{2\pi} \int_0^{2\pi} d\alpha \, h(\alpha) e^{\frac{1}{2} \epsilon [e^{i\alpha} w(e^{-i\theta}) - e^{-i\alpha} w(e^{i\theta})]}.$$
 (15)

Once they are found, the eigenfunction of the polygon, solving equation (1), is obtained by entering them into expression (14), with the variable z replacing the mapping function w(z). By introducing the Fourier components of the periodic function $h(\alpha)$

$$h(\alpha) = \sum_{k=-\infty}^{\infty} h_k e^{ik\alpha}$$
(16)

we obtain the following representation of the eigenfunction for the polygon:

$$\psi(r,\theta) = \sum_{k} h_{k} \mathrm{e}^{\mathrm{i}k\theta} J_{-k}(\epsilon r).$$
(17)

In particular, for the circle, the requirement of vanishing on the boundary leads to the Bessel–Fourier basis $u_{m,s}$.

To start the perturbative scheme, let us expand in λ the weight function $h(\alpha)$ and, correspondingly, its Fourier components:

$$h(\alpha) = h^{(0)}(\alpha) + \lambda h^{(1)}(\alpha) + \lambda^2 h^{(2)}(\alpha) + \cdots \qquad h_k = h_k^{(0)} + \lambda h_k^{(1)} + \lambda^2 h_k^{(2)} + \cdots$$
(18)

and insert it, together with the λ expansion (11*a*) of the exact eigenvalue, into the boundary equation (15) and solve it at the various orders in λ .

At zero order in λ , we get the equation

$$0 = \sum_{k} h_k^{(0)} \mathrm{e}^{-\mathrm{i}k\theta} J_k(\epsilon_0) \tag{19}$$

which, for the ground state of polygons, is solved by setting

$$h_k^{(0)} = \delta_{0,k} \qquad \epsilon_0 = j_{0,1}.$$
 (20)

Different zeros $j_{0,s}$ of J_0 would provide other eigenvalues of the polygon, with the same expansions (11a)–(11c).

The equation for the *first order*, after simple integrations and use of the symmetry relation $J_{-n}(x) = (-1)^n J_n(x)$, reads

$$0 = \frac{1}{2\pi} \int_0^{2\pi} d\alpha h^{(1)}(\alpha) e^{i\epsilon_0 \sin(\alpha-\theta)} + \epsilon_0 \delta_1 J_1(\epsilon_0) - \epsilon_0 J_1(\epsilon_0) \frac{1}{2} [f(e^{i\theta}) + f(e^{-i\theta})].$$
(21)

By taking the integral in the variable θ one obtains the result $\delta_1 = 0$. By introducing the Fourier expansion of the function $h^{(1)}(\alpha)$ all integrals can be evaluated. The requirement of vanishing for all θ gives

$$h_{\pm nk}^{(1)} = \frac{\epsilon_0}{2} \frac{J_1(\epsilon_0)}{J_{\pm kn}(\epsilon_0)} f_k \qquad k = 1, 2 \dots$$

$$(22)$$

all other coefficients being zero. As it normally occurs in perturbation theory, the component $h_0^{(1)}$ is not provided by the equation, due to the condition $J_0(\epsilon_0) = 0$; the freedom in choosing the phase of ψ allows us to put $h_0^{(1)} = 0$.

The equation for the second order, after all simple integrations, is:

$$0 = \frac{1}{2\pi} \int_{0}^{2\pi} d\alpha h^{(2)}(\alpha) e^{i\epsilon_0 \sin(\alpha-\theta)} + \epsilon_0 \delta_2 J_1(\epsilon_0) + \frac{1}{8} \epsilon_0^2 J_2(\epsilon_0) [f(e^{i\theta})^2 + f(e^{-i\theta})^2] + \frac{1}{2} \epsilon_0 \sum_{k=-\infty}^{\infty} h_{kn}^{(1)} e^{ikn\theta} [f(e^{-i\theta}) J_{-kn-1}(\epsilon_0) - f(e^{i\theta}) J_{-kn+1}(\epsilon_0)].$$
(23)

Again, we are allowed to put $h_0^{(2)} = 0$. The condition of vanishing for all θ gives the value δ_2 given in equation (11*b*), and

$$h_{\pm n}^{(2)} = \frac{J_{1}(\epsilon_{0})}{J_{\mp n}(\epsilon_{0})} \frac{\epsilon_{0}^{2}}{4} \sum_{s=1}^{\infty} f_{s+1} f_{s} \left[\frac{J_{(s+1)n+1}(\epsilon_{0})}{J_{(s+1)n}(\epsilon_{0})} + \frac{J_{sn+1}(\epsilon_{0})}{J_{sn}(\epsilon_{0})} \right]$$

$$h_{\pm nk}^{(2)} = \frac{J_{1}(\epsilon_{0})}{J_{\mp kn}(\epsilon_{0})} \frac{\epsilon_{0}^{2}}{4} \sum_{s=1}^{\infty} f_{k+s} f_{s} \left[\frac{J_{(k+s)n+1}(\epsilon_{0})}{J_{(k+s)n}(\epsilon_{0})} + \frac{J_{sn+1}(\epsilon_{0})}{J_{sn}(\epsilon_{0})} \right]$$

$$+ \frac{J_{1}(\epsilon_{0})}{J_{\mp kn}(\epsilon_{0})} \left[\frac{\epsilon_{0}^{2}}{4} \sum_{s=1}^{k-1} f_{k-s} f_{s} \frac{J_{sn+1}(\epsilon_{0})}{J_{sn}(\epsilon_{0})} - \frac{\epsilon_{0}}{4} (kn+1) \sum_{s=1}^{k-1} f_{k-s} f_{s} \right]$$

$$k > 1.$$

$$(24b)$$

The equation for the *third order* is rather long:

$$0 = \sum_{k=-\infty}^{\infty} h_k^{(3)} e^{ik\theta} J_{-k}(\epsilon_0) + \frac{\epsilon_0}{2} \sum_{k=-\infty}^{\infty} h_{kn}^{(2)} e^{ikn\theta} [f(e^{-i\theta}) J_{-kn-1}(\epsilon_0) - f(e^{i\theta}) J_{kn+1}(\epsilon_0)] -\delta_2 \frac{\epsilon_0}{2} \sum_{k=-\infty}^{\infty} h_{kn}^{(1)} e^{ikn\theta} [J_{-kn-1}(\epsilon_0) - J_{-kn+1}(\epsilon_0)] + \delta_3 \epsilon_0 J_1(\epsilon_0) - \frac{\epsilon_0^3}{48} J_3(\epsilon_0)$$

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$$+\frac{\epsilon_{0}^{2}}{8}\sum_{k=-\infty}^{\infty}h_{kn}^{(1)}e^{ikn\theta}[f(e^{-i\theta})^{2}J_{-kn-2}(\epsilon_{0}) + f(e^{i\theta})^{2}J_{-kn+2}(\epsilon_{0})] -\frac{\epsilon_{0}^{3}}{16}J_{1}(\epsilon_{0})f(e^{-i\theta})f(e^{i\theta})[f(e^{-i\theta}) + f(e^{i\theta})].$$
(25)

By taking the integral in the variable θ , the term containing the unknown coefficients of the function $h^{(3)}$ vanishes because of $J_0(\epsilon_0) = 0$, and we obtain, with some labour, the term δ_3 , given in equation (11*c*).

The ground state of the polygon is obtained by entering the expansions of the Fourier coefficients into equation (17). By taking into account the found property $h_{-kn}^{(\ell)} = (-1)^{kn} h_{kn}^{(\ell)}$, one obtains the expression equation (5):

$$\psi_n(r,\theta) = J_0(\epsilon_n r) + 2\sum_{k=1}^{\infty} (h_{-nk}^{(1)} + h_{-kn}^{(2)} + \dots) J_{kn}(\epsilon_n r) \cos(kn\theta)$$
(26)

where the coefficients $h_{-kn}^{(1)}$ and $h_{-kn}^{(2)}$ are respectively given by equations (22) and (24).

3. Numerical evaluation

For the evaluation of the ground-state energy a numerical approach is necessary. In particular, one must compute ratios of consecutive Bessel functions with the same argument. To this end, for x smaller than all the zeros $j_{\nu,m}$ of J_{ν} , the expansion [11, 12]:

$$\frac{J_{\nu+1}(x)}{J_{\nu}(x)} = \frac{2}{x} \sum_{k=1}^{\infty} x^{2k} S_{\nu,2k} \qquad S_{\nu,2k} = \sum_{m=1}^{\infty} \frac{1}{j_{\nu,m}^{2k}}$$
(27)

is used, where the coefficients are obtainable through a recursive relation; a long list of values $S_{\nu,2k}$ is given in [13]. To achieve a good accuracy, terms up to k = 6 are used; for the triangle and the square, the first ratios $J_3/J_4, \ldots$ were obtained directly by means of the relation $zJ_{\nu+1}(z) + zJ_{\nu-1}(z) = 2\nu J_{\nu}(z)$.

The results of the calculations for the ground-state energies are collected in table 1, for some values of n.

The λ expansion could also have been carried out starting from a value $j_{0,k}$ with k > 1, and the formulae would be the same as indicated in the introduction. One could also start from an initial state of the circle J_p with $p \neq 0$. In this way, repeating the above computations, one obtains expansions for excited states, with the rule that p is not an integer multiple of n. To second order, writing the same expansion (11a), one obtains:

$$\delta_1 = 0 \qquad \delta_2 = \frac{\epsilon_0}{4} \sum_{k=1}^{\infty} f_k^2 \left(\frac{J_{kn+p+1}(\epsilon_0)}{J_{kn+p}(\epsilon_0)} + \frac{J_{kn-p+1}(\epsilon_0)}{J_{kn-p}(\epsilon_0)} \right)$$
(28)

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First excited state							
n	$j_{1,1}/C_n$	δ_2	$\epsilon_n^{(1)}$	Exact			
3	6.769 25	0.044 913	6.46516	6.398 48			
4	5.023 48	0.010230	4.97209	4.967 29			
5	4.500 15	0.003557	4.48469				
6	4.264 36	0.001 429	4.25828				
8	4.058 08	0.000358	4.05663				
∞	—	—	—	3.83171			

where ϵ_0 is now a zero of J_p . Note that δ_2 is independent of the sign of p, meaning that the doubly degenerate level of the circle evolves into a degenerate level of the polygon. For the first excited state, Liboff [14] proved that it is indeed doubly degenerate, with the nodal line given by a mirror symmetry of the polygon. A detailed discussion of degeneracies for n = 3, 4 is given in [15].

A few values for the first excited state of regular polygons are provided in table 2. For n = 3, 4 the accordance is rather poor, but the correction term for larger n indicates that the values become reliable.

Appendix

By using the integral representation of Bessel functions and the discrete representation of Dirac's delta function

$$J_{\nu}(t) = \frac{1}{2\pi} \int_{0}^{2\pi} d\varphi \, e^{it \sin \varphi - i\nu\varphi} \qquad \sum_{k=-\infty}^{\infty} e^{ik(\varphi-\theta)} = 2\pi(\varphi-\theta) \tag{A.1}$$

one can show the following identity, where n is an integer:

$$\sum_{k=-\infty}^{\infty} J_{\nu+kn}(t) \cos[(\nu+kn)\varphi+\beta] = \frac{1}{n} \sum_{\ell=0}^{n-1} \cos\left[t \sin\left(\frac{2\pi}{n}\ell\right)\cos\varphi-\nu\ell\frac{2\pi}{n}\right] \cos\left[t \cos\left(\frac{2\pi}{n}\ell\right)\sin\varphi+\beta\right].$$
(A.2)

In particular, for v = 0, $\varphi = \pi/2 - \theta$, $t = \epsilon r$, $\beta = \pi/(2n)$, $x = r \cos \theta$, $y = r \sin \theta$:

$$J_{0}(\epsilon r)\cos\left(\frac{\pi}{2n}\right) + 2\sum_{k=1}^{\infty} J_{kn}(\epsilon r)\cos\left[kn\frac{\pi}{2} + \frac{\pi}{2n}\right]\cos(kn\theta)$$
$$= \frac{1}{n}\sum_{\ell=0}^{n-1}\cos\left[\epsilon x\cos\left(\frac{2\pi}{n}\ell\right) + \frac{\pi}{2n}\right]\cos\left[\epsilon y\sin\left(\frac{2\pi}{n}\ell\right)\right].$$
(A.3)

For n = 3, 4 one obtains the first eigenstates of the equilateral triangle and the square:

$$\psi_{3}(x, y) = \frac{1}{2} \sin\left[\frac{4\pi}{3}\left(\frac{1}{2}x + \frac{\sqrt{3}}{2}y\right)\right] + \frac{1}{2} \sin\left[\frac{4\pi}{3}\left(\frac{1}{2}x - \frac{\sqrt{3}}{2}y\right)\right] \\ -\frac{1}{2} \sin\left(\frac{4\pi}{3}x\right) + \frac{\sqrt{3}}{2} \cos\left[\frac{4\pi}{3}\left(\frac{1}{2}x + \frac{\sqrt{3}}{2}y\right)\right] \\ + \frac{\sqrt{3}}{2} \cos\left[\frac{4\pi}{3}\left(\frac{1}{2}x - \frac{\sqrt{3}}{2}y\right)\right] + \frac{\sqrt{3}}{2} \cos\left(\frac{4\pi}{3}x\right)$$
(A.4)

 $\psi_4(x, y) = \cos(\pi x) + \cos(\pi y).$

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