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LETTER TO THE EDITOR

Ground-state energy of a particle in a polygonal box

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Abstract. We find the ground-state energy of a particle enclosed in a regular polygon of n sides by perturbing about the equivalent circle and thereby setting up a n^{-1} expansion. The first correction is $O(n^{-3})$ and hence a two-term answer is very accurate for polygons with many sides.

The ground-state energy of a quantum particle confined in a two-dimensional regular polygonal box can be solved exactly only in the special cases of the triangle, square and the limiting case of the circle. While the determination of the ground-state energy for the circle and square is an elementary exercise the solution to the triangle problem is more formidable (Krishnamurthy *et al* 1982). The corresponding problems in classical physics are the flow through a pipe of polygonal cross section, the torsion of a cylinder of polygonal cross section or the electrostatic energy of an uniformly charged cylinder of similar geometry. The classical problems like their quantum counterpart can be solved for the circle, square and triangle. It was shown some time ago (Ferrell and Bray 1976) that for the classical problem the solution for a regular polygon of n sides can be obtained by perturbing the solution for the circle in powers of n^{-1} and thereby setting up a n^{-1} expansion, which is pretty accurate at low orders. In this letter we point out that the ground-state energy of a particle in a regular polygon of n sides can be obtained in a perturbation expansion in n^{-1} and a low-order result can be accurate for large n and reasonable for $n=3$.

We consider a polygonal box of n sides and of area A. A circle of equal area and centred at the centre of the regular polygon is considered and as the zeroth-order approximation the particle is confined in the equivalent circle of radius a. Clearly

$$a^2 = A/\pi. \tag{1}$$

The ground-state energy of the particle in this circular box is

$$E_0 = \frac{\hbar^2}{m}\frac{\xi_0^2}{a^2} \simeq \frac{\hbar^2}{2m}\frac{(2.41)^2}{a^2} = \frac{\hbar^2}{2m}\frac{\pi}{A}(2.41)^2 \tag{2}$$

where ξ_0 is the first zero of the zeroth-order Bessel function and is known to be $\xi_0 \simeq 2.41$. If we use this energy to find the ground state of the square box, then we underestimate by 8%, while for a triangular box we underestimate by 21%. Considering the crudeness of the approximation this is already somewhat remarkable.

We now proceed to obtain the first correction to the circle. We focus on one of the n sectors produced by the polygon, i.e. $-\pi/n \leqslant \theta \leqslant \pi/n$. The radius r of a point on the polygon is now a function of θ and the deviation from the radius 'a' of the circle of equal area can be written as (using small-angle approximations and to the lowest order in n^{-1})

$$\Delta r/a = (r(\theta)-a)/a \simeq \tfrac{1}{2}\theta^2 - \tfrac{1}{6}(\pi/n)^2$$

$$= \sum_{\nu=1}^{\infty} c_{\nu n}\cos n\nu\theta \qquad c_{\nu n} = 2(-1)^{\nu}/n^2\nu^2 \tag{3}$$

with $c_{0n}=0$, as the areas of the circle and polygon are equal. The wavefunction at this order can be written as

$$\psi(r) = J_0(k_0 r) + \sum d_{\nu n}(r)\cos n\nu\theta = J_0(k_0 r) + \psi_1(r,\theta) \tag{4}$$

where $k_0^2 = 2mE_0/\hbar^2$ and we must have at first order of smallness (i.e. first order in $c_{\nu n}$)

$$-\frac{\hbar^2}{2m}\nabla^2\psi_1 = E_0\psi_1 + E_1\psi_0 \tag{5}$$

and the boundary condition

$$0 = \psi(a-\Delta r) = J_0(k_0 a) - k_0\Delta r J_0'(k_0 a) + \psi_1(a,\theta)$$

$$= -k_0 J_0'(k_0 a)\sum_{\nu} c_{\nu n}\cos n\nu\theta + \sum d_{\nu n}(a)\cos n\nu\theta.$$

Clearly,

$$d_{\nu n}(a) = k_0 J_0'(k_0 a) c_{\nu n} \tag{6}$$

and

$$d_0(a) = 0. \tag{7}$$

From (4) and (5) it is clear that $d_n(r) = J_n(k_0 r)$, and $d_0(r) = J_0(k_0 r)$, which forces $E_1 = 0$ and a complete solution of the problem is obtained to this order as

$$E = E_0 \tag{8}$$

$$\psi(r) = J_0(k_0 r) + \sum_{\nu} c_{\nu n}\frac{J_n(k_0 r)}{J_n(k_0 a)} k_0 J_0'(k_0 a)\cos \nu n\theta. \tag{9}$$

To get the first correction to energy we need to proceed to the next order. The wavefunction ψ to this order can be written as

$$\psi(r) = J_0(k_0 r) + k_0 J_0'(k_0 a)\sum_{\nu} c_{n\nu}\frac{J_n(k_0 r)}{J_n(k_0 a)}\cos n\nu\theta + \sum_{\nu} g_{\nu n}(r)\cos n\nu\theta. \tag{10}$$

The boundary condition needs to be satisfied to order $c_{\nu n}^2$ and Taylor expanding to the required order we can find $g_{\nu n}(a)$. 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

$$-\frac{\hbar^2}{2m}\nabla^2\psi_2 = E_0\psi_2 + E_2\psi_0 \tag{11}$$

and the only part which involves the energy E_2 is the purely r-dependent part of ψ_2 which is given by $g_0(r)$. Thus $g_0(r)$ satisfies the equation

$$(\nabla^2 + k_0^2)g_0(r) = -\frac{2mE_2}{\hbar^2}\psi_0$$

or

$$\left(\frac{d^2}{dx^2}+\frac{1}{x}\frac{d}{dx}+1\right)g_0(x)=-\frac{E_2}{E_0}J_0(x) \tag{12}$$

where $x=k_0r$. The boundary condition on $g_0(x)$ is obtained from (10) by working to second order. We find

$$g_0(k_0a)=\frac{(k_0a)^2}{4}\left[\sum c_{\nu n}^2\left(\frac{2J_n'(k_0a)}{J_n(k_0a)}+\frac{1}{k_0a}\right)J_0'(k_0a)\right]. \tag{13}$$

For large n, $J_{\nu n}'(k_0a)/J_{\nu n}(k_0a)=n\nu/k_0a$ and hence, to leading order in n, (13) is

$$g_0(k_0a)=\frac{(k_0a)^2}{4}\frac{J_0'(k_0a)}{k_0a}\sum_\nu\frac{8}{n^3\nu^3}=-\frac{2(k_0a)^2}{n^3}J_1(k_0a)\zeta(3) \tag{14}$$

where $\zeta(z)$ is the Riemann zeta function.

We now need to solve equation (12). The homogeneous solution has to be $J_0(k_0r)$, the other linearly independent solution being ill behaved at $r=0$ and hence not admissible. Denoting the particular integral by $P(k_0r)$, we can write

$$g_0(x)=AJ_0(x)+P(x) \tag{15}$$

where the constant A can be determined by requiring $g_0(x)$ to be orthogonal to the zeroth-order solution $J_0(x)$ over the original circle. The boundary condition of (14) now requires

$$P(k_0a)=-\frac{2(k_0a)^2}{n^3}\pi_1(k_0a)\zeta(3) \tag{16}$$

since $J_0(k_0a)=0$. To find the particular integral the simplest procedure is to try a power series expansion

$$P(x)=\sum_{n=1}a_nx^{2n}. \tag{17}$$

A five-term expansion gives $P(k_0a)=-0.62E_2/E_0$, leading to

$$\frac{E_2}{E_0}\simeq\frac{9.3\zeta(3)}{n^3}\simeq\frac{10.8}{n^3}. \tag{18}$$

Thus, with the first correction included

$$E=\frac{\hbar^2}{2m}\frac{\pi}{A}(2.41)^2\left(1+\frac{10.8}{n^3}\right)+O\left(\frac{1}{n^4}\right). \tag{19}$$

For $n=3$, this formula yields a 10% overestimate, while for $n=4$ it overestimates by 7.5%. For boxes with larger n the formula is expected to be extremely accurate.

We conclude by noting that equation (18) can be improved by adding a phenomenological n^{-4} term which is designed to give the exact answer at $n=3$. This leads to (note that the actual expansion would have n^{-4} as the next order term, see (13))

$$E=\frac{\hbar^2}{2m}\frac{\pi}{A}(2.41)^2\left(1+\frac{10.8}{n^3}-\frac{10.5}{n^4}\right) \tag{20}$$

the overshoot at $n=4$ being 4%.

References

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