EIGENVALUE PROBLEM IN TWO DIMENSIONS FOR AN IRREGULAR BOUNDARY

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An analytical perturbative method is suggested for determining the eigenvalues of the Helmholtz equation $(\nabla^2 + k^2)\psi = 0$ in two dimensions where $\psi$ vanishes on an irregular closed curve. We can thus find the energy levels of a quantum mechanical particle confined in an infinitely deep potential well in two dimensions having an irregular boundary or the vibration frequencies of a membrane whose edge is an irregular closed curve. The method is tested by calculating the energy levels for an elliptical and a supercircular boundary and comparing with the results obtained numerically. Further, the phenomenon of level crossing due to shape variation is also discussed.

I. INTRODUCTION

The energy levels of a quantum particle confined in a 2D regular box can be solved exactly only in the cases of a square and a triangle and in the limiting case of a circle. While the determination of the energy levels for the circular or the square boundary is a trivial exercise, the problem of the triangular boundary is more formidable [1]. The corresponding problems in the classical regime can be the flow of liquid through a pipe of polygonal cross-section or the free vibration of a membrane (with a fixed boundary) of polygonal shape. The classical problems, like their quantum counterparts, are amenable to simple analytical treatments only in the cases of a circle, a square and a triangle. The problem of a regular polygonal box has been solved by perturbing about the equivalent circle and the results have been quite accurate [2]. The same problem has been solved by Cureton and Kuttler [3] in the context of vibration of membranes. Here we address the problem of finding out the energy eigenvalues when the boundary has no simple geometric shape. The Schroedinger equation for a particle of mass $m$ and energy $E$ confined in an infinitely deep 2D potential well is

$$\frac{-\hbar^2}{2m} \nabla^2 \psi = E \psi \quad (1a)$$

which can be recast as

$$(\nabla^2 + k^2)\psi = 0 \quad (1b)$$

where $k = \sqrt{\frac{2mE}{\hbar^2}}$. Thus the problem boils down to solving the Helmholtz equation with the Dirichlet condition $\psi = 0$ on the ‘irregular’ boundary. Exact solutions can be obtained only in a few special cases. The standard procedure is to choose a curvilinear coordinate system suited to the geometry of the problem and employ the method of separation of variables. For a boundary having an irregular shape no particular coordinate system will be useful. Hence, we resort to perturbative methods to solve the problem. Here we will perturb the boundary about a circle so that in our problem solutions can be obtained in the form of corrections to the solutions for the circular boundary. Till now, most of the efforts at finding out the eigenvalues of the Helmholtz equation for an irregular boundary have been numerical. Mazumdar [4, 5, 6] reviews the approximate methods invoked for this problem. In addition to the extensive summary of theoretical results, Kuttler and Sigillito [7] also gives a comprehensive review of the different numerical methods employed. More recently, Amore [8] gives a numerical recipe using a collocation approach based on little sinc functions. As far as analytical works are concerned, Rayleigh [9] and also Fetter and Walecka [10] finds the ground state energy eigenvalues for a vibrating membrane. A general formalism has been suggested by Morse and Feshbach [11] using the Green functions. Parker and Mote [12] have put forward a perturbative method for finding the eigenvalues and the eigenfunctions through fifth order. A similar method has been proposed by Nayfeh [13]. However, the eigenvalues are found out only to the first order. Read [14] has also suggested a general analytical approach to the problem. Bera et al [15] have proposed a perturbative approach to the problem but failed to express the solutions in a closed form. Our approach is similar in spirit to that of Bera. Here we present a closed form solution to the problem in a more systematic and efficient manner. The method is tested by comparing the analytical results with those obtained numerically for a supercircu-
lar and an elliptical boundary. Further, the phenomenon of energy level crossing as induced by the shape variation is also dealt with for both the boundaries. In section II we set up our general scheme and in section III we apply it to the case of a supercircle and an ellipse. A short conclusion is presented in section IV.

II. PERTURBATION ABOUT THE EQUIVALENT CIRCLE

Given any $r(\theta)$ defining the boundary in 2D enclosing an area $A$ we first construct a circle of radius $R_0$ such that

$$A = \pi R_0^2$$ (2)

We can then expand $r(\theta)$ about $R_0$ in terms of Fourier series at different orders of smallness (denoted by $\lambda$) as,

$$r(\theta) = R_0 \left[ 1 + \sum_{\nu=1}^{\infty} \lambda^\nu f^{(\nu)}(\theta) \right]$$ (3)

where,

$$f^{(\nu)}(\theta) = \sum_{n} \left( C_n^{(\nu)} \cos n\theta + S_n^{(\nu)} \sin n\theta \right)$$ (4)

Here, for simplicity, we have considered only a one parameter dependence of $r(\theta)$, which thus represents a family of curves which reduce to the equation for a circle in the limiting case $\lambda \to 0$. $\lambda$ should be much smaller than unity which ensures that the variation of $r(\theta)$ with $\theta$ is small enough to permit the use of perturbative methods.

If we now calculate the area using (3),(4) and equate it with (2) then the following constraint relations among the Fourier coefficients are arrived at,

$$\sum_{\nu=0}^{\infty} \sum_{\nu=0}^{\nu=1} \left[ C_n^{(\nu)} C_n^{(\sigma-\nu)} + 2 C_0^{(\nu)} C_0^{(\sigma-\nu)} + S_n^{(\nu)} S_n^{(\sigma-\nu)} \right]$$

$$= -4C_0^{(\sigma)}$$ (5a)

In particular we have,

$$C_0^{(1)} = 0$$ (5b)

$$4C_0^{(2)} = -\sum_{n=1}^{\infty} [C_n^{(1)2} + S_n^{(1)2}]$$ (5c)

Now, as a first approximation, the energy $E_o$ of the particle confined by $r(\theta)$ will be that of a particle enclosed in a circle of radius $R_0$

$$E_o = \frac{h^2 \rho_{m,n}}{2m R_0^2}$$ (6)

with $\rho_{m,n} = k_{m,n} R_0$ being the $n$th node of the $m$th order Bessel function. The next step is to improve upon the ‘equal area’ approximation by perturbing the equivalent circle and finding out the first and the second order corrections to the eigenvalues.

We expand $\psi$ and $E$ as

$$\psi = \psi_0 + \lambda \psi_1 + \lambda^2 \psi_2 + ...$$ (7a)

$$E = E_0 + \lambda E_1 + \lambda^2 E_2 + ...$$ (7b)

Using (5a), (7b) in (1a), equating the coefficients of different powers of $\lambda$ to 0 and after some rearrangement we arrive at the set of equations,

$$\nabla^2 \psi_0 = -\frac{2mE_0}{\hbar^2} \psi_0$$ (8a)

$$(\nabla^2 + k_0^2)\psi_1 = -\frac{2mE_1}{\hbar^2} \psi_0$$ (8b)

$$(\nabla^2 + k_0^2)\psi_2 = -\frac{2m}{\hbar^2} (E_1 \psi_1 + E_2 \psi_0)$$ (8c)

(8a) can readily be identified as the equation for the circular boundary with $\psi_0$ as the eigenfunction corresponding to energy $E_0$.

The boundary condition is

$$\psi(R_0 + \lambda R_0 f^{(1)} + \lambda^2 R_0 f^{(2)} + ...) = 0$$

Taylor expansion about $r = R_0$, use of (8a) and equating the coefficients of different powers of $\lambda$ to 0 yields

$$\psi_0(R_0) = 0$$ (9a)

$$\psi_1(R_0) + R_0 f^{(1)} \psi_0'(R_0) = 0$$ (9b)

$$\psi_2(R_0) + R_0 f^{(1)} \psi_1'(R_0) + R_0 f^{(2)} \psi_0'(R_0) = 0$$ (9c)

We discuss separately the cases $l = 0$ and $l \neq 0$. 
A. Calculation of Energy for $l = 0$ State

For the $l=0$ state,

$$\psi_0 = N J_0(\rho)$$

(10)

where $J_0$ is the 0th order Bessel function, and $N$ is the normalisation constant. $E_0$ is obtained from (6) with $m = 0$, and an appropriate $n$.

The first order correction to the wavefunction obtained as a solution to (8b) is,

$$\psi_1 = \sum_{p=1}^{\infty} (a_p \cos p\theta + \bar{a}_p \sin p\theta) J_p + a_0 J_0 - \frac{\rho E_1}{2 E_0} N J_1$$

(11)

where the last term is the particular integral to (8b). Incorporating (11) in (9b) and separately matching the cosine and sine terms we have

$$a_p = -\rho_0, n NC_p^{(1)} \frac{J_p'(\rho_0, n)}{J_p(\rho_0, n)}$$

(12a)

$$\bar{a}_p = -\rho_0, n NS_p^{(1)} \frac{J_p'(\rho_0, n)}{J_p(\rho_0, n)}$$

(12b)

$$E_1 = 0$$

(12c)

The remaining constant $a_0$ can be found out by normalising the corrected wavefunction over the enclosed area. However, that is not required right now for our purpose. (12c) implies that there cannot be any correction to the energy in the first order. So any possible correction to the energy can only come from the second or higher orders.

In a similar fashion the second correction to the wavefunction as a solution to (8c) with $E_1 = 0$ is found out to be,

$$\psi_2 = \sum_{p=1}^{\infty} (b_p \cos p\theta + \bar{b}_p \sin p\theta) J_p + b_0 J_0 - \frac{\rho E_2}{2 E_0} N J_1$$

(13)

which, when introduced in (8c), now yields,

$$E_2 = E_0 \left[ \sum_{p=1}^{\infty} (C_p^{(1)})^2 + S_p^{(1)})^2 \right] \left[ \frac{J_p'(\rho_0, n)}{J_p(\rho_0, n)} + \frac{1}{2} - 2C_0^{(2)} \right]$$

(14a)

$$b_k = -\rho_0, n J_0 [NC_k^{(2)} + a_0 C_k^{(1)}] + \frac{\rho_0, n J_0 N}{2} \left( \frac{1}{2} + \frac{\rho_0, n J_p}{2 J_p} \right)$$

(14b)

As before, the remaining constant $b_0$ can be determined by normalising the wavefunction up to the order of $\lambda^2$.

B. Calculation of Energy for $l \neq 0$ state

The $l \neq 0$ states come in 2 varieties,

$$\psi_0 = N_l J_l(\rho) \left( \frac{\cos l\theta}{\sin l\theta} \right)$$

(15)

For simplicity, we assume that $S_n^{(\sigma)} = 0$ for all $\sigma$. We will work with

$$\psi_0 = N_l J_l(\rho) \cos l\theta$$

(16)

The result for the other case will be similar. The first correction to the wavefunction obtained as a solution to (8d) is,

$$\psi_1 = \sum_{p=1}^{\infty} a_p J_p \cos p\theta + \left( a_1 J_1 - \frac{E_1}{E_0} \frac{\rho}{2 N_l J_{l+1}} \right) \cos l\theta$$

(17)

Following a similar procedure as that for the ground state we now have,

$$E_1 = -C_{2l}^{(1)} E_0$$

(18a)

$$a_p = -\frac{\rho_{l,j}}{2} N_l J_l(J_{l+1} + C^{(1)}_{l+1})$$

(18b)

$$a_0 = -\frac{\rho_{l,j}}{2} N_l J_0(J_{l+1} + C^{(1)}_{l+1})$$

(18c)

with $a_l$ being obtained from the normalisation condition. The second order corrections yield,

$$\psi_2 = \sum_{m=0}^{\infty} b_m J_m - \frac{\rho E_1}{E_0} a_m J_{m+1} \cos m\theta$$
The constants $b_n$ present purpose. For the case of the ground state. However, that is not needed for our present purpose. For the case,

$$\psi_0 = N_l J_l(\rho) \sin \theta$$

(20)

similar calculations result in,

$$\psi_1 = \sum_{p=1, p \neq l}^{\infty} \bar{a}_p J_p \sin \rho \theta + \left( \bar{a}_l J_l - \frac{E_1}{E_0} \frac{p \rho l_n J_n}{2 J_n(\rho_{l,j})} \right) \sin \theta$$

(21a)

$$E_1 = C_{2l}^{(1)} E_0$$

(21b)

$$\bar{a}_p = \frac{p \rho l_n J_n}{2 J_n(\rho_{l,j})} (C_{p+l}^{(1)} - C_{|p-l|}^{(1)}) \quad \text{for } p \neq 0, l$$

(21c)

$$\bar{a}_0 = 0$$

(21d)

$$\psi_2 = \sum_{m=1}^{\infty} \left[ \bar{b}_m J_m - \frac{p \rho l_n}{2 E_0} \bar{a}_m J_{m+1} \right] \sin m \theta$$

$$+ \left[ C_{2l}^{(1)} \rho J_{l+2} - \frac{E_2}{E_0} J_{l+1} \right] N_l \rho \sin \theta$$

(21e)

$$E_2 = \frac{C_{2l}^{(1)} 2}{2} + \frac{1}{4} \sum_{n=1}^{\infty} C_n^{(1)} (2 C_n^{(1)} - C_{2l+n}^{(1)} - C_{2l-n}^{(1)}) - 2 C_0^{(2)}$$

$$+ C_2^{(2)} + \sum_{n=0, n \neq l}^{\infty} \left( C_n^{(1)} - C_l^{(1)} \right)^2 \frac{p \rho l_n J_n(\rho_{l,j})}{2 J_n(\rho_{l,j})}$$

(19a)

III. APPLICATION TO SIMPLE CASES

A. Introduction

The general formalism having been outlined above we now estimate the energy levels of a supercircle and an ellipse where direct comparison with the numerical results can be made.

B. Particle Enclosed in a Super circular Enclosure

Super circle is a special case of a super ellipse whose equation is given by the Lame equation,

$$\frac{|x|^n}{a^n} + \frac{|y|^n}{b^n} = 1$$

(22)

with $n > 0$ and rational, $a$ and $b$ being positive real numbers. They are also known as Lame curves or Lame ovals. Super ellipses can be parametrically described as,

$$x = a \cos^\frac{n}{2}(t)$$

(23)

$$y = b \sin^\frac{n}{2}(t)$$

(24)

Different values of $n$ gives us closed curves of different shapes. For $n > 2$ we consider only the real positive values of $\cos^\frac{n}{2}(t)$ and $\sin^\frac{n}{2}(t)$ for $0 \leq t \leq \frac{\pi}{2}$ and use the symmetry of the figure to continue to the other quadrants. We are interested in the case $a = b$ which corresponds to a supercircle. In polar coordinates the equation for the supercircle is,

$$r = \frac{a}{(\cos^\theta + \sin^\theta)^\frac{n}{2}}$$

(25)

and the radius of the equal area circle is,

$$R_0 = a\sqrt{\frac{2}{n\pi} \left| \frac{\Gamma(\frac{1}{n})}{\Gamma(\frac{2}{n})} \right|}$$

(26)

With the deformation parameter $\delta = 2 - n$ one arrives at after some rigorous calculation,

$$r = R_0 \left[ 1 + \sum_{n=1}^{\infty} C_{4n}^{(1)} \cos 4n\theta + \sum_{n=0}^{\infty} C_{4n}^{(2)} \cos 4n\theta \right]$$

(27)

where the Fourier coefficients are found to be

$$C_{4n}^{(1)} = -\frac{1}{4n(4n^2 - 1)}$$

$$C_{4n}^{(2)}$$

is given by (5c) to be .0070205 and $C_4^{(2)} = \frac{1}{32} \left( \frac{3\pi^2}{8} - \frac{21}{9} \right) = .0357983$. 

\[\text{C}_4^{(2)} \text{ is given by (5c) to be .0070205 and } C_4^{(2)} = \frac{1}{32} \left( \frac{3\pi^2}{8} - \frac{21}{9} \right) = .0357983.\]
Using these Fourier coefficients, the first few energy levels are calculated for the supercircular boundary in the range \(-1 \leq \delta \leq 1\), and compared with the numerically obtained values. This is shown in FIG.2.

where the numerical results are shown by discrete points and the analytical ones by the continuous lines. The fact that even for such a wide range of \(\delta\) the analytical results are in fairly good agreement with those obtained numerically does indeed justify the validity of our formalism. Furthermore, it is to be noted that the energy level corresponding to the unperturbed wavefunction \(\psi_0 = N_2 J_2 \cos 2\theta\) is strongly affected compared to the others and crosses over to its counterpart \(\psi_0 = N_2 J_2 \sin 2\theta\) at \(\delta = 0\). This crossing of energy levels is solely induced by the variation in the shape of the boundary of the potential well.

C. Particle Enclosed in an Elliptical Enclosure

The determination of the eigenvalues of the Helmholtz operator in 2D with an elliptical boundary has been investigated extensively. However, most of the efforts have been directed at the numerical estimation of the values [18, 19, 20]. An analytical method has been suggested by Wu and Shivakumar [21]. Here we propose a simpler approach to the problem. The equation for an ellipse with semiaxes \(a\) and \(b\), in polar coordinates is,

\[ r = \frac{b}{\sqrt{1 - (1 - \frac{b^2}{a^2}) \cos^2 \theta}} \]  

Defining the deformation parameter,

\[ \lambda = \frac{a - b}{a + b} \]

(28) can be recast as,

\[ r = R_0[1 + \lambda \cos 2\theta - \frac{1}{4} \lambda^2 + \frac{3}{4} \lambda^2 \cos 4\theta + \lambda^3 (\ldots) + ...] \]  

(30)

Comparing with our general Fourier series we observe that, \(C_2^{(1)} = 1\), \(C_0^{(2)} = -\frac{1}{4}\), \(C_4^{(2)} = \frac{3}{4}\). [12a], [14a], [18a], [19a], [21a], [21b], [21f] on using (5c) then gives,

\[ E_1 \left( \begin{array}{c} J_1 \cos l\theta \\ J_1 \sin l\theta \end{array} \right) = \left( - \right) E_0 \delta_{l1} \]  

(31a)

\[ E_2 \left( \begin{array}{c} J_1 \cos l\theta \\ J_1 \sin l\theta \end{array} \right) = E_0 \left( \delta_{l1} \frac{1}{2} + \frac{\rho_{l,j} J_0'(\rho_{l,j})}{2 J_0(\rho_{l,j})} \right) \]

\[ + \left( -\frac{1}{2} + \frac{\rho_{l,j} J_0'(\rho_{l,j})}{2 J_0(\rho_{l,j})} \right) E_0 \delta_{l2} \quad |p - l| = 2 \]  

(31b)

The results for the elliptical boundary are shown in FIG.2. From FIG.2 it is seen that as in the case of the supercircle here also the \(J_1 \cos \theta\) state is strongly affected by the boundary perturbation and crosses over to its counterpart \(J_1 \sin \theta\) at \(\delta = 0\). However, quite interestingly, the \(J_2\) states do not cross but are rather repelled by each other. They touch each other tangentially at \(\delta = 0\). While for one of these states the analytical method works quite well it has a restricted validity for the other one. In fact, we compared the energy levels for the first 10 states and found out the agreement between the analytical and the numerical results to be quite satisfactory except when the levels repel each other. This phenomenon of level repulsion, also goes by the name of “loici veering”. In case of level repulsion the validity of the perturbation theory is restricted to a small range in \(\delta\) (e.g. \(|\delta| \geq 0.08\)). This is in sharp contrast to the case where there is no repulsion in which case the agreement with the perturbation theory persists over a wide range.

IV. CONCLUSION

One of the principle virtues of the method proposed is its generality. With slight modification, the formalism can readily be adopted to study the shape dependence of the eigenvalues of a vibrating membrane with Dirichlet conditions on an irregular boundary. The approach can also be useful in studying the modes of propagation of electromagnetic waves in waveguides with irregular cross sections. Another potential area where this formalism might be useful is in the study of quantum dots. This field has been an area of vigorous research for the past few years. 2D quantum dots are generally taken to have a circular symmetry. However, in practice such a symmetry can not be strictly ensured. There is bound to be small deviations from exact circular symmetry. Hence, probes have been constructed to investigate the shape of the dots [22, 23, 24]. As shown in this paper the energy eigenvalues of a particle confined in 2D in an infinitely deep potential well will essentially depend upon the shape of the confining region. Hence a study of the shape dependence of the energy levels might prove to be useful in shedding light upon the actual shapes of the dots. Another significant aspect of our formalism is the use of the general Fourier series to express the deviation of the boundary from a circular one which allows us to treat any sort of boundary within the limit of small perturbation for which our formalism is valid. Further, the solutions are found out exactly in a closed form without any major approximations which is indeed remarkable. The case of the supercircular membrane shows that even for quite large perturbations the method yields satisfactory results. The accuracy of the method can be still improved by including higher order corrections. In fact, we have also found out the third order corrections, although the results are not included here. On the contrary, the case of the elliptical boundary points out to the failure of
the perturbation theory whenever the energy levels exhibit loci veering. This provides potential topics for future investigations. Another point which we want to emphasize here is that the success (and also the efficiency) of the formalism depends to a large extent upon the judicious choice of the deformation parameter $\lambda$. For the case of the ellipse we defined $\lambda$ to be $\lambda = \frac{a-b}{a+b}$ whereas the eccentricity $\epsilon$ would seem a more appropriate candidate for $\lambda$. For the elliptical boundary we have considered deformations up to the extent where $a:b = 2:1$ for which $\lambda = 0.333$. Had we formulated the problem in terms of the eccentricity the same deformation would have led to the value of $\epsilon = 0.866$. It can also be shown that in that case the deformation parameter would actually be $\epsilon^2$, so that for the same deformation we would have $\epsilon^2 = 0.75$ which is obviously much larger than the parameter which we have actually used here. Such a high value of the deformation parameter goes against the very essence of the perturbative nature of the method. This means that while we have terminated the Fourier series and also the eigenvalues at the second order of smallness when working with $\lambda = \frac{a-b}{a+b}$, for $\lambda = \epsilon^2$ we would have to consider higher order terms to get the same accuracy. Finally, we note that the same formalism can also be adopted by perturbing the boundary of a square or a rectangular membrane for which the results are exactly known.

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FIG. 1: Comparison of the energy eigenvalues obtained numerically and analytically for a particle enclosed in a supercircular boundary (in units of $\frac{\hbar^2}{2mR^2}$)
FIG. 2: Comparison of the energy eigenvalues obtained nu-