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LETTER TO THE EDITOR

Explicit asymptotic formulae for the spheroidal angular eigenvalues

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Abstract. Asymptotic formulae for the angular spheroidal eigenvalues are found using the Bohr–Sommerfeld quantization rule and pertubation theory. Approximate calculations for the separation between two consecutive eigenvalues are obtained.

The solution of the spheroidal wave equation has long been a subject of interest in many areas of physics. For instance, it plays an important role in the study of light scattering in optics [1–3], the nuclear shell model [4], theoretical cosmological models [5], and atomic and molecular physics [6]. In all these topics, the related physical system has spheroidal symmetry, so that in these cases it is suitable to use a spheroidal coordinate system, the natural coordinate system for describing a revolution ellipsoid. Using the method of separation variables in this coordinates system, the full wave equation solution can be written as products of radial and angular solutions wave equations [7, 8]. The radial solution is always associated with a specified potential on each particular case, but the angular solution is general. In this letter we are interested in calculating the eigenvalues of regular prolate spheroidal angle functions, which are the regular solutions of the following differential equation [7, 8]:

$$\frac{\mathrm{d}}{\mathrm{d}\eta}\left[(1-\eta^2)\frac{\mathrm{d}}{\mathrm{d}\eta}S_{\ell,m}\right]+\left[\left(\lambda_\ell^m\right)^2-c^2\eta^2-\frac{m^2}{1-\eta^2}\right]S_{\ell,m}=0 \qquad -1\leqslant\eta\leqslant 1. \tag{1}$$

Here c is the deformation parameter proportional to semifocal distance of the ellipse, ℓ is a positive integer ($\ell=0,1,\ldots$), the integer m defined in the range $-\ell\leqslant m\leqslant\ell$, is the L_z angular momentum eigenvalue (in units of $\hbar=1$), and the number $\left(\lambda_\ell^m(c)\right)^2$ is the prolate spheroidal angular eigenvalue. We can observe from (1), the simplest case of $c=0$, the function $S_{\ell,m}$ reduces to the associated Legendre function and $\left(\lambda_\ell^m(0)\right)^2=\ell(\ell+1)$ is its eigenvalue. For general c values, $\lambda_\ell^m(c)$ are the roots of an infinite continued fraction transcendental equation [7, 8]. For small c and ℓ values, the $\left(\lambda_\ell^m\right)^2$ Taylor expansion series is a satisfactory approximation to the exact eigenvalue problem [7, 8]. Nevertheless, many practical situations such as scattering cross section calculations, need to use λ_ℓ^m with large ℓ values. Unfortunately, in this regime trying to obtain λ_ℓ^m by solving the exact transcendental equation is impracticable, because for large ℓ values this transcendental equation presents many numerical instabilities [8, 9]. Eu and Sink [10–12] presented the pioneering work that calculated for large ℓ the spheroidal angular functions and their eigenvalues with some

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accuracy. To that end, they applied semiclassical methods to (1), defined in a finite domain $-1 \leqslant \eta \leqslant 1$. In the case of the eigenvalue calculations, they used the semiclassical Bohr–Sommerfeld quantization rule subject to a parametric Langer modification, obtained by numerical interpolation. In the present investigation, we will develop for large ℓ explicit asymptotic approximations for λ_ℓ^m based on semiclassical methods and perturbation theory. In order to apply semiclassical methods to (1) it is necessary to perform the variable change $\eta \equiv tgh(x)$, mapping the finite interval $(-1, 1)$ into the infinite one $(-\infty, \infty)$ and (1) can be rewritten as

$$-\frac{d^2}{dx^2}S_{\ell,m} + V(x)S_{\ell,m} = -m^2 S_{\ell,m} \qquad -\infty \leqslant x \leqslant \infty. \tag{2}$$

The above equation is analogous to a one-dimensional time-independent Schrödinger equation (in units such that $\hbar = 2m = 1$) with *energy-like* parameter the negative integers $-m^2$ and subject to an *effective potential* $V(x)$ (see figure 1). The effective potential $V(x)$ is written in the following manner:

$$V(x) \equiv -\left(\left(\lambda_\ell^m\right)^2 - c^2\right)\mathrm{sech}^2(x) + c^2\mathrm{sech}^4(x). \tag{3}$$

Using this quantum-mechanical point of view, we can re-interpret the solutions of (2) as eigenstates of the effective well potential $V(x)$. However, in this particular case, the effective potential has explicit dependence with eigenvalue. Figure 1 shows that λ_ℓ^m satisfies the inequality $\lambda_\ell^m > |m| \geqslant 0$, the spectrum for a given ℓ has $\ell + 1$ bound states, which are doubly degenerate because (2) is invariant under the discrete symmetry $m \to -m$. The *ground-state* is characterized by the limit $|m| = \ell$ and behaves as $\lambda_\ell^m \sim O(m)$, and on the other hand, for most *excited states* the spectrum behaves as $\lambda_\ell^m \sim O(\ell) \gg |m|$. For given ℓ, m and c, the classical forbidden region is delimited by the inequality $|x| > x_0$ (see figure 1), where $x_0 = x_0(\ell; m; c)$ is the classical turning point. The larger separations between the two turning points x_0 and $-x_0$ occur when $|m|$ has small values as compared to ℓ. In this situation the Bohr–Sommerfeld quantization rule can be applied with accuracy [13, 14],

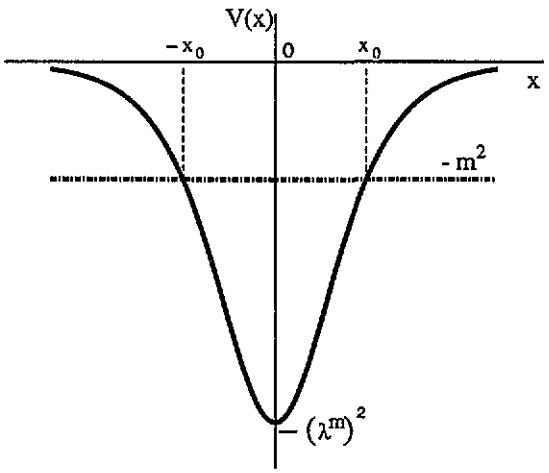

Figure 1. Shows the effective potential $V(x)$ (full curve), that has explicit dependence with eigenvalue, $V(x)$ is an even function that has at the origin the minimum value $-\left(\lambda_\ell^m\right)^2$. The negative integer $-m^2$ plays the role of *energy* (chain curve) and the x_0 and $-x_0$ are the two *classical turning points*.

namely

$$\int_{-x_0}^{x_0} \mathrm{d}x\sqrt{|m^2+V(x)|} = \left(\ell+\tfrac{1}{2}-|m|\right)\pi\,. \tag{4}$$

The above integral can be mapped into an elliptical integral and solved numerically. However, for large ℓ values compared to $|m|$, equation (4) can be solved asymptotically. The result for $m=0$ is

$$\lambda_\ell^0 \sim \left(\ell+\tfrac{1}{2}\right)+\frac{c^2}{4\lambda_\ell^0}+\frac{3}{64}\frac{c^4}{\left(\lambda_\ell^0\right)^3}+\frac{5}{256}\frac{c^6}{\left(\lambda_\ell^0\right)^5}+\mathrm{O}(c^8/(\lambda_\ell^0)^7)\,. \tag{5}$$

In the above asymptotic transcendental equation, the first term in the brackets corresponds to the usual Langer modification. Besides, (5) shows that λ_ℓ^0 is an increasing function of c, so that more sharp spheroidal symmetry systems have greater λ_ℓ^0 values. Equation (5) has the same accuracy of the Bohr–Sommerfeld quantization rule $\mathrm{O}(1/\ell^2)$, and can be solved using a numerical method. In the present work we use Newton's method to solve transcendental equations. This procedure converges rapidly to the desired λ_ℓ^0 value, the typical values for the number of iterations being less than 10 steps. Table 1 shows and compares these results with results obtained by Eu and Sink [10]. The error with present results is a decreasing ℓ function, so that this theory for large ℓ values has great accuracy. In the case of the *ground-state*, the two turning points are very close, consequently the use of the Bohr–Sommerfeld quantization rule is not suitable. On the other hand, the effective potential $V(x)$ is an even function whose Taylor expansion in the neighbourhood of the origin behaves as

$$V(x) \sim [-(\lambda_\ell^m)^2+((\lambda_\ell^m)^2+c^2)x^2]-(5c^2+2(\lambda_\ell^m)^2)\frac{x^4}{3} \equiv V_{ho}(x)+W(x)\,. \tag{6}$$

Where $V_{ho}(x)$ is similar to a quadratic *harmonic oscillator* potential and $W(x)$ is an *anharmonic potential. For the ground state, λ_ℓ^m is $O(|m|)$ and $|V_{ho}| > |W|$ for $|x| < x_0$.* Using this fact and (6), we can re-interpret (2) as a harmonic oscillator Schrödinger equation subject to a perturbation potential $W(x)$. Then, using first-order perturbation theory, we find for the *ground state* that the spheroidal eigenvalue $\left(\lambda_\ell^m\right)^2$ with $|m|=\ell$ satisfies the following equation:

$$\left(\lambda_\ell^\ell\right)^2 \sim \ell^2+\sqrt{\left(\lambda_\ell^\ell\right)^2+c^2}-\frac{\left(2\left(\lambda_\ell^\ell\right)^2+5c^2\right)}{4\left(\left(\lambda_\ell^\ell\right)^2+c^2\right)}\,. \tag{7}$$

This transcendental equation can be numerically solved by Newton's method with great accuracy and fast convergence. For such, we use as initial guess the value

Table 1. Shows λ_ℓ^m, the square root of the angular spheroidal eigenvalues for $c=8$ and $m=0$ and compares the Eu work [10] (the second column) with the present results (the fifth column). Notice that the present calculations have a relative error of the order $\mathrm{O}(1/\ell^3)$, which decreases as ℓ increases, while the relative error associated with the results of [10] is a numerical interpolating error.

ℓ	Reference [10]	Error %	Exact	Equation (5)	Error %
5	8.1841	0.29	8.2076	8.0210	2.27
6	8.8045	0.20	8.8218	8.7244	1.10
7	9.5318	0.09	9.5232	9.4800	0.43
8	10.3223	0.25	10.2962	10.2782	0.17
9	11.1562	0.36	11.1165	11.1103	0.06

Table 2. Shows λ_ℓ^m, the square root of the angular spheroidal eigenvalues for $c = 8$ and $m = \ell$ and compares the Eu work [10] (the second column) with the present results (the fifth column). Notice that the present calculations have a relative error of the order 0.01%, while the relative error associated with the results of [10] is of the order 0.1%.

ℓ	Reference [10]	Error %	Exact	Equation (7)	Error %
5	5.8374	0.24	5.8234	5.8227	1.20×10^{-2}
6	6.7605	0.18	6.7484	6.7474	1.50×10^{-2}
7	7.7066	0.14	7.6959	7.6948	1.49×10^{-2}
8	8.6822	0.28	8.6580	8.6569	1.24×10^{-2}
9	9.6381	0.09	9.6297	9.6287	1.03×10^{-2}

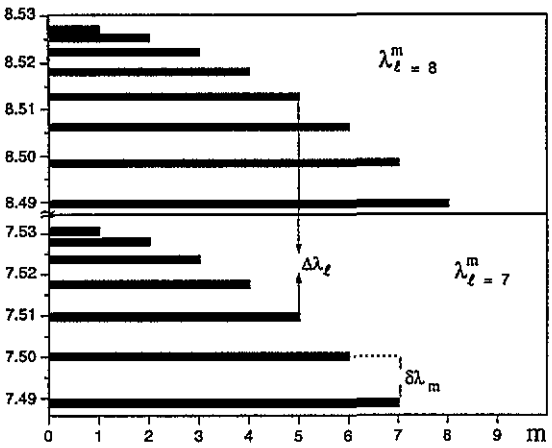

Figure 2. Shows for $c = 1.2$, the λ_ℓ^m levels diagram. The level separations are defined by $\Delta\lambda_\ell \equiv \lambda_{\ell+1}^m - \lambda_\ell^m$ and $\delta\lambda_m \equiv \lambda_\ell^{m+1} - \lambda_\ell^m$. We can observe that $\delta\lambda_m$ increases as m increases. Besides, $\Delta\lambda_\ell \gg |\delta\lambda_m|$, so that the λ_ℓ^m levels diagram is very similar to a band structure.

$(\lambda_\ell^\ell)^2 \sim \ell^2 + 1/2 + \sqrt{\ell^2 + c^2}$. Table 2 shows and compares ours results with previous results given by Eu and Sink [10]. The error of the present theory is the specific error associated with perturbation theory, while the error related with Eu and Sink work [10] is an interpolating error. For large ℓ, typically $\ell > 20$ and small c compared to ℓ, this perturbation procedure can be used for the calculation of the first excited states with satisfactory accuracy.

In many quantum-mechanical problems, the calculation of the levels separation is of great interest. The levels separation is related to the density of states, whose calculation has many applications in quantum mechanics. In the present work we are motivated to calculate the levels separation by academic and numerical reasons. In other words, if we have explicit formulae for these separations we can use (5) or (7) to generate any λ_ℓ^m. We define the spheroidal eigenvalues separation for two consecutive ℓ and the same m values and for the same ℓ and consecutive m values respectively as $\Delta\lambda_\ell \equiv \lambda_{\ell+1}^m - \lambda_\ell^m$ and $\delta\lambda_m \equiv \lambda_\ell^{m+1} - \lambda_\ell^m$ (see figure 2). Using (4) λ_ℓ^m asymptotic solution formulae and perturbation theory [7, 8] we can obtain these separations, which for large ℓ values behave, respectively, as

$$\Delta\lambda_\ell \sim 1 - \left(\frac{c}{\lambda_\ell^m}\right)^2 + \frac{1}{12\pi}\left(\frac{m}{\lambda_\ell^m}\right)^3 \tag{8}$$

$$\delta\lambda_m \sim -\frac{c^2}{\lambda_\ell^m}\frac{(2m+1)}{(2\ell-1)(2\ell+3)}. \tag{9}$$

The above equations have less accuracy than (5) and (7), but we can apply these equations in order to obtain a good estimate for any λ_ℓ^m. For such, we iterate those formulae jointly with (8) and (9). On the other hand, equations (8) and (9) show that for large ℓ values the inequality $\Delta\lambda_\ell \gg |\delta\lambda_m|$ is valid. Consequently, the spheroidal eigenvalues $(\lambda_\ell^m)^2$ for the same ℓ value form a band structure (see figure 2). The minus signal in (9) implies that lower eigenvalues are associated with greater m values (see figure 2). Besides, equation (9) shows that the level separation with consecutive m values and the same ℓ value is m linearly increasing, then the separation between the first two levels is less than the two last levels (see figure 2).

Our final remarks are that in this letter, using a quantum-mechanical point of view, we can re-interpret the angular spheroidal eigenvalue problem as being the problem of finding the bound states of the effective potential $V(x)$. In this particular case, we have a non-trivial problem because the potential is related to the eigenvalue (see equation (3)). More precisely, we have to find the minimum potential value $V(0) = -(\lambda_\ell^m)^2$ for a given *energy-like* parameter $-m^2$ (see figure 1). This quantum-mechanical interpretation permits us to develop explicit formulae for the angular spheroidal eigenvalues (5), (7) and their separations (8), (9), respectively. We think that these results can be improved if we develop uniform asymptotic approximations for the spheroidal angular functions [15, 16]. These approximations have the disadvantage of using the transcendental Airy functions [16] that imply some numerical difficulties. Work on these issues is in progress, and planned to be reported briefly. The main results of this work can be applied in some problems related to deformation of spherical symmetry. For that purpose, there should be no need to use the usual perturbation form theory or any sophisticated numerical method [17].

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