Chebyshev Functions and their use for two-dimensional electrostatic problems in elliptic coordinates

RAUL PEREZ-ENRIQUEZ[1], IVAN MARIN-ENRIQUEZ[2], J. L. MARIN[2] AND R. RIERA[2]

[1]Departamento de Fisica
Universidad de Sonora
Apdo. Postal 1620
83000 Hermosillo, Son. MÉXICO

[2]Departamento de Investigación en Fisica
Universidad de Sonora Apdo. Postal 5-088
83190 Hermosillo, Son. MÉXICO

Abstract: Separation of the two-dimensional Laplace equation in elliptic coordinates leads to a Chebyshev-like differential equation for both the "angular" and "radial" variables, namely (η,ξ); in the case of η the well behaved solution in [-1,1] (its range of definition), are the usual first class Chebyshev polynomials. However, since ξ is defined in $[1,\infty)$, there is a need to construct another solution by, for example, a Frobenius series representation. Using these functions, the complete solution of two-dimensional Laplace's equation in this coordinate system can then be constructed accordingly, and could be used to study a variety of boundary-value electrostatic problems involving infinite conductors and lines of charge. Moreover, the corresponding Green's function for the Laplace operator can also be readily obtained using this procedure, a matter that can be useful in the study of many problems in solid state physics which involve energy levels and/or optical properties of hydrogenic impurities within nanostructures of elliptic shape. These subjects are afforded and discussed in the present communication, some useful trends regarding applications of the result are also given.

Keywords: Chebyshev functions, Chebyshev differential equation, Laplace operator, Elliptic coordinates, nanostructures with elliptic shape, Frobenius method

1 Introduction

Laplace equation plays a fundamental role in potential theory since many two-dimensional boundary-value problems are of crucial importance for both, physics and mathematics. This is the case, for instance, in electrostatics, fluid flow through obstacles, conformal mapping and so on.

The solution of this equation for a specific boundary-value problem in electrostatics, can give information that a *priori* is unknown; namely, when an initially isolated conductor (charged or raised to a given potential) is perturbed by a charge distribution, the charge on the conductor's surface after the perturbation redistributes to an unknown distribution, then the conventional solution for the potential as an integral involving the surface charge cannot be used. In those cases, the general solution of Laplace equation becomes an important tool to obtain the new potential.

In most electrostatic problems, a given charge distribution is usually involved and one must solve instead the Poisson equation, but either in this case the general solution of Laplace equation is still important since it can be used to construct an auxiliary function, the Green's Function, which allows one to find the particular solution of Poisson equation that satisfies all the boundary conditions.

The construction of the general solution of two-dimensional Laplace equation involves its separability in a given coordinate system, its is separable, for instance, in rectangular, polar, parabolic, elliptic and other less common coordinate systems (See for Ref.[1]). In the specific case of elliptic coordinates, its separation leads to a Chebyshev-type ordinary differential equation for both "angular" (η) and "radial" (ξ) coordinates. The solution associated to the angular variable are the well known first-class Chebyshev polynomials but in the case of the radial one, they are not longer useful because this coordinate is defined in $[1,\infty)$ and clearly the polynomials diverge at infinity.

This fact implies that we need to find a different solution which must be properly behaved in this interval; once such a solution is known, the construction of the Green's Function associated to the Laplace operator in this coordinate system can be readily done.

The knowledge of both, the general solution and the Green's Function for the Laplace operator can used to solve a variety of electrostatic boundary-value problems which involve infinite conductors and infinite charged lines in elliptic coordinates.

In addition, the two-dimensional Green's function representation allows one to find the two-dimensional Coulomb potential, a matter that can be useful to study many properties of solid state physics systems which involves hydrogenic impurities in nanostructured materials of elliptic shape in a similar way as it has been done for other shapes [2,3,4].

The same potential in the moment space was studied by Ditrich [5]. Other authors, as Furman [6], have treated elliptical charge configurations.

The aim of this work is to stress at both, academic and research levels, the importance inherent to the knowledge of the general solution of the Laplace equation and the wide possibilities of applications.

For the sake of clarity, this communication has been structured as follows: In section 2, we discuss the form of the two-dimensional Coulomb potential and its relation with the well known form of the Green Function, as reported in [7,8]; the general solution of Laplace equation in elliptic coordinates is discussed in section 3; a representation of the Green function in this coordinates is constructed in section 4 and finally, in section 5, we made some conclusion and discussion on the possible applications of the results presented here-in.

2 Two-dimensional Coulomb potential

The two-dimensional Green function, as known in textbooks (see for instance, Ref [7]) is of the form:

$$G(\boldsymbol{\rho},\boldsymbol{\rho}') = -\frac{1}{2\pi}\ln|\boldsymbol{\rho}-\boldsymbol{\rho}'|, \qquad (1)$$

which can be interpreted as the electrostatic potential at $\boldsymbol{\rho}$ due to an infinite line of charge, with unit charge per length, located at $\boldsymbol{\rho}'$ and it is solution of the equation:

$$\nabla^2 G(\boldsymbol{\rho},\boldsymbol{\rho}') = -\delta(\boldsymbol{\rho}-\boldsymbol{\rho}') \qquad (2)$$

where $\delta(\boldsymbol{\rho}-\boldsymbol{\rho}')$ is the Dirac delta function.

You most notice that this function is also solution of the Laplace equation in charge-free two-dimensional space, i.e., when $\boldsymbol{\rho}\neq\boldsymbol{\rho}'$.

In two dimensions, the electrostatic potential does not coincide with the usual Coulomb potential, since the former is associated with an infinite line of charge (or an infinite charged conducting cylinder) while the later is associated with the interaction of two *point* charges, a matter which sometimes causes confusion. Anyway, the Coulomb potential for a unit *point* charge in two dimensions can be readily related with the two-dimensional Green's function from Eq. (1), as:

$$\frac{1}{|\boldsymbol{\rho}-\boldsymbol{\rho}'|} = \exp\left[2\pi G(\boldsymbol{\rho},\boldsymbol{\rho}')\right] \qquad (3)$$

In this way, a two-dimensional problem which involves Coulomb potential can be afforded by firstly constructing the general solution and the Green's function associated with the Laplace operator in the system of coordinates adequately selected for the specific geometry or shape of the object or system under study.

In the next sections, we shall describe how this can be done in the specific case of elliptic coordinates, but it can be readily adapted to other orthogonal coordinate system in which Laplace equation is separable or, at least, partially separable.

3 General Solution for Laplace's Equation in elliptic coordinates

In this section, we will develop Laplace's operator in two dimensions using an elliptic coordinate system. This analysis becomes apparent when we are analyzing the problem of a line of charge parallel to an elliptic-cylindrical conductor because we can look for a solution by considering the bidimensional problem of obtaining Green's function, which is solution to Poisson's equation

$$\nabla^2 G(\boldsymbol{\rho},\boldsymbol{\rho}') = -\delta(\boldsymbol{\rho},\boldsymbol{\rho}'). \qquad (4)$$

We already know that it can be developed by a harmonic expansion of functions which are solutions to Laplace's equation

$$\nabla^2\phi(\boldsymbol{\rho}) = 0. \qquad (5)$$

The points considered are those points different from those of the source ($\boldsymbol{\rho}\neq\boldsymbol{\rho}'$). Our first step towards the solution will be to consider the transformation of Laplace's operator from Cartesian coordinates to an elliptic system. Using the transformation equations

$$\begin{aligned} &x = a\xi\eta; \quad \xi\in[1,\infty); \\ &y = a(\xi^2-1)^{1/2}(1-\eta^2)^{1/2}; \quad \eta\in[-1,1) \end{aligned} \qquad (6)$$

The scale factors related to this transformation are

$$h_\xi = \left[\left(\frac{\partial x}{\partial \xi}\right)^2 + \left(\frac{\partial y}{\partial \xi}\right)^2\right]^{1/2} = a\left[\frac{\xi^2-\eta^2}{\xi^2-1}\right]^{1/2} \quad (7)$$

and

$$h_\eta = \left[\left(\frac{\partial x}{\partial \eta}\right)^2 + \left(\frac{\partial y}{\partial \eta}\right)^2\right]^{1/2} = a\left[\frac{\xi^2-\eta^2}{1-\eta^2}\right]^{1/2}. \quad (8)$$

3.1 Laplacian operator

The scale factors that has been previously calculated will allow us to construct the Laplacian operator, which will have the form

$$\nabla^2 = \frac{1}{h_\xi h_\eta}\left\{\frac{\partial}{\partial \xi}\left[\frac{h_\eta}{h_\xi}\frac{\partial}{\partial \xi}\right] + \frac{\partial}{\partial \eta}\left[\frac{h_\xi}{h_\eta}\frac{\partial}{\partial \eta}\right]\right\} \quad (9)$$

we can obtain

$$\begin{aligned}\nabla^2 = {}& \frac{(\xi^2-1)^{1/2}(1-\eta^2)^{1/2}}{a^2(\xi^2-\eta^2)}\left\{\frac{\partial}{\partial \xi}\left[a\frac{(\xi^2-\eta^2)^{1/2}}{(1-\eta^2)^{1/2}}\right.\right. \\ & \left.\times\frac{1}{a}\frac{(\xi^2-1)^{1/2}}{(\xi^2-\eta^2)^{1/2}}\frac{\partial}{\partial \xi}\right] + \frac{\partial}{\partial \eta}\left[a\frac{(\xi^2-\eta^2)^{1/2}}{(\xi^2-1)^{1/2}}\right. \quad (10) \\ & \left.\times\frac{1}{a}\frac{(1-\eta^2)^{1/2}}{(\xi^2-\eta^2)^{1/2}}\frac{\partial}{\partial \eta}\right]\end{aligned}$$

or

$$\begin{aligned}\nabla^2 = {}& \frac{1}{a^2(\xi^2-\eta^2)}\left\{(\xi^2-1)^{1/2}\frac{\partial}{\partial \xi}\left[(\xi^2-1)^{1/2}\frac{\partial}{\partial \xi}\right]\right. \\ & \left.+(1-\eta^2)^{1/2}\frac{\partial}{\partial \eta}\left[(1-\eta^2)^{1/2}\frac{\partial}{\partial \eta}\right]\right\}. \end{aligned} \quad (11)$$

This is the expression for the Laplace operator in elliptic coordinates.

Now, we can consider the Laplace's equation given in Eq. (5). This can be rewritten using Eq. (11) as

$$\begin{aligned}\nabla^2\psi(\xi,\eta) = {}& \frac{1}{a^2(\xi^2-\eta^2)}\left\{(\xi^2-1)^{1/2}\frac{\partial}{\partial \xi}\right. \\ & \times\left[(\xi^2-1)^{1/2}\frac{\partial}{\partial \xi}\right] + (1-\eta^2)^{1/2}\frac{\partial}{\partial \eta} \quad (12) \\ & \left.\times\left[(1-\eta^2)^{1/2}\frac{\partial}{\partial \eta}\right]\right\}\psi(\xi,\eta),\end{aligned}$$

and then solved by the variable separation method. So, we introduce

$$\psi(\xi,\eta) = S(\xi)H(\eta), \quad (13)$$

and rearrange to obtain

$$\begin{aligned}& \frac{(1-\eta^2)^{1/2}}{H(\eta)}\frac{d}{d\eta}\left[(1-\eta^2)^{1/2}\frac{dH(\eta)}{d\eta}\right] \\ & = -\frac{(\xi^2-1)^{1/2}}{S(\xi)}\frac{d}{d\xi}\left[(\xi^2-1)^{1/2}\frac{dS(\xi)}{d\xi}\right] \quad (14) \\ & = const.\end{aligned}$$

3.2 Angular equation: Chebyshev polynomials

The effect of variable separation allows us to define a constant. Assuming that $const. = m^2$, from the left term of Eq. (14), we obtain the well known Chebyshev equation

$$(1-\eta^2)^{1/2}\frac{d}{d\eta}\left[(1-\eta^2)^{1/2}\frac{dH}{d\eta}\right] + m^2 H = 0 \quad (15)$$

which has solutions for $m = 0, 1, 2, \cdots$, valid for $\eta \in [-1, 1]$:

$$H(\eta) = T_m(\eta), \quad (16)$$

known simply as the Chebyshev polynomials.
These polynomials are orthogonal and satisfy the following condition

$$\int_{-1}^{1}\frac{T_m(\eta)T_{m'}(\eta)}{(1-\eta^2)^{1/2}}d\eta = a_m\delta_{m,m'}. \quad (17)$$

Their general expression is

$$T_m(\eta) = \cos(m\cos^{-1}\eta). \quad (18)$$

3.3 Radial equation: second solution to Chebyshev's equation

From the right hand term of Eq. (14), and with the constant of separation already defined, one can obtain

$$(\xi^2-1)^{1/2}\frac{d}{d\xi}\left[(\xi^2-1)^{1/2}\frac{dS}{d\xi}\right] - m^2 S = 0, \quad (19)$$

that must be solved in the $[1, \infty)$ interval. We can recognize it as the Chebyshev equation of second class. In this range, the Chebyshev polynomials remain to be a valid solution, but they are irregular at infinity, so we will need another linearly independent solution for this equation, in order to completely describe an electrostatic problem such as the one we are interested in.

We have to decide how to obtain the second solution to Chebyshev's equation, as there are several ways to obtain it; one of them will be discussed here.

3.3.1 Second solution by the Frobenius' method

In order to obtain the solution using the Frobenius method, we have used the traditional way, as it is shown in the Appendix. The functions obtained have the following form and properties:

$$S_m(\xi) = \begin{cases} a_0 \ln\left(\xi + \sqrt{\xi^2 - 1}\right) & m = 0 \\ a_0 \xi^{-m} \left[1 + m\sum_{l=1}^{\infty} a_l \xi^{-2l}\right], & m \geq 1 \end{cases} \quad (20)$$

where $a_0 \neq 0$, $\xi \in [1,\infty)$ and

$$a_l = \frac{\Gamma(m+2l)4^{-l}}{\Gamma(m+l+1)\Gamma(l+1)}.$$

They decay very fast as ξ grows and have a finite value in $\xi = 1$. Those functions, in conjunction with Chebyshev's polynomials are a complete set of functions that will allow us to develop the Green's function corresponding to a singular point in the elliptic coordinate system.

4 Green's Function

With the aid of the functions $T_m(\eta)$ for the angular function, and the functions $T_m(\xi)$ and $S_m(\xi)$ for the radial variable, we can construct the Green's function in the two-dimensional space.

As mentioned before, we need to solve Poisson's equation for a linear distribution of charge, located at $\boldsymbol{\rho}' = (\xi', \eta')$, which is

$$\begin{aligned} \nabla^2 G(\boldsymbol{\rho}, \boldsymbol{\rho}') &= -\delta(\boldsymbol{\rho} - \boldsymbol{\rho}') \\ &= -\frac{1}{h_\xi h_\eta}\delta(\xi - \xi')\delta(\eta - \eta'), \end{aligned} \quad (21)$$

where ∇^2 is given by Eq. (11).

Because the $\{T_m(\eta)\}$ polynomials constitute a complete set of basis functions in [-1,1], i.e. in the angular coordinate, Dirac's delta function can be expressed as a linear combination of them, in the form

$$\delta(\eta - \eta') = \sum_{m=0}^{\infty} \frac{T_m(\eta)T_m(\eta')}{(1-\eta^2)^{1/2}}. \quad (22)$$

Furthermore, the delta function can be used to define a function by the means of

$$\int_{-1}^{1} \delta(\eta - \eta')T_{m'}(\eta)d\eta = T_{m'}(\eta') \quad (23)$$

then, using Eq. (22) we have

$$\begin{aligned} T_{m'}(\eta') &= \sum_m A_m T_m(\eta') \int \frac{T_{m'}(\eta)T_m(\eta)}{(1-\eta^2)^{1/2}} d\eta \\ &= \sum_m A_m a_m \delta_{m,m'} T_m(\eta'). \end{aligned}$$

That is,

$$T_{m'}(\eta') = A_{m'} a_{m'} T_{m'}(\eta') \quad \Rightarrow \quad A_{m'} = \frac{1}{a_{m'}}. \quad (24)$$

Thus, we have Eq. (22) as

$$\delta(\eta - \eta') = \sum_{m=0}^{\infty} \frac{1}{a_m} \frac{T_m(\eta)T_m(\eta')}{(1-\eta^2)^{1/2}}. \quad (25)$$

Using this result and the definition of the scale factors for elliptical coordinates, we can return to our differential equation for Green's function

$$\begin{aligned} \nabla^2 G(\xi,\eta;\xi',\eta') &= -\frac{(\xi^2-1)^{1/2}(1-\eta^2)^{1/2}}{a^2(\xi^2-\eta^2)} \\ &\times \delta(\xi - \xi') \sum_{m=0}^{\infty} \frac{1}{a_m} \frac{T_m(\eta)T_m(\eta')}{(1-\eta^2)^{1/2}} \\ &= -\frac{(\xi^2-1)^{1/2}}{a^2(\xi^2-\eta^2)} \delta(\xi-\xi') \sum_m \frac{1}{a_m} T_m(\eta)T_m(\eta') \end{aligned} \quad (26)$$

or, assuming that Green's function can be separated as a product of functions of the base space, i.e., if

$$\begin{aligned} G(\boldsymbol{\rho}, \boldsymbol{\rho}') &= G(\xi,\eta;\xi',\eta') \\ &= \sum_m B_m(\xi',\eta') g_m(\xi) T_m(\eta) \end{aligned} \quad (27)$$

then

$$\begin{aligned} &\frac{1}{a^2(\xi^2-\eta^2)} \left\{ (\xi^2-1)^{1/2} \frac{d}{d\xi} (\xi^2-1)^{1/2} \frac{d}{d\xi} \right. \\ &\left. + (1-\eta^2)^{1/2} \frac{d}{d\eta} (1-\eta^2)^{1/2} \frac{d}{d\eta} \right\} \\ &\times \sum_m B_m g_m(\xi) T_m(\eta) \\ &= -\frac{(\xi^2-1)^{1/2}\delta(\xi-\xi')}{a^2(\xi^2-\eta^2)} \sum_m \frac{T_m(\eta)T_m(\eta')}{a_m}. \end{aligned} \quad (28)$$

Regrouping and using the results of Eq. (15), we have

$$\begin{aligned} &\sum_m \left\{ B_m \left[(\xi^2-1)^{1/2} \frac{d}{d\xi} (\xi^2-1)^{1/2} \frac{dg_m}{d\xi} - m^2 g_m \right] \right. \\ &\left. + (\xi^2-1)^{1/2} \delta(\xi-\xi') \frac{T_m(\eta')}{a_m} \right\} T_m(\eta) = 0 \end{aligned} \quad (29)$$

But we already know that the $\{T_m(\eta)\}$ set is linearly independent, thus we have

$$\begin{aligned} &(\xi^2-1)^{1/2} \frac{d}{d\xi} (\xi^2-1)^{1/2} \frac{dg_m}{d\xi} - m^2 g_m = \\ &\quad -\frac{(\xi^2-1)^{1/2}\delta(\xi-\xi')T_m(\eta')}{a_m B_m(\xi',\eta')} \end{aligned} \quad (30)$$

We are going to analyze this equation in the region of the singularity, i.e. the region where $\xi \neq \xi'$. In this case, we have Eq. (28) and it will have two different solutions: one regular at infinity, and other regular and finite at $\xi = 1$. Those functions will be used to construct Green's function, which has to be continuous at $\xi = \xi'$. They are:

$$g_m(\xi) = \begin{cases} BT_m(\xi) & 1 < \xi < \xi' \\ AS_m(\xi) & 1 < \xi' < \xi < \infty \end{cases} \quad (31)$$

where A and B are coefficients that need to be calculated. Integrating Eq. (30) around $\xi=\xi'$, we have

$$\lim_{\varepsilon\to\infty}\left[\int_{\xi'-\varepsilon}^{\xi'+\varepsilon}\frac{d}{d\xi}(\xi^2-1)^{1/2}\frac{dg_m}{d\xi}d\xi-m^2\int_{\xi'-\varepsilon}^{\xi'+\varepsilon}g_m d\xi\right] =-\lim_{\varepsilon\to\infty}\int_{\xi'-\varepsilon}^{\xi'+\varepsilon}\frac{\delta(\xi-\xi')T_m(\eta')d\xi}{a_m B_m(\xi',\eta')} \tag{32}$$

The second integral in the left-hand side of Eq. (32) vanishes, while the first one and that of the right hand side simplify to the functions evaluated at $\xi=\xi'$; then we have

$$(\xi^2-1)^{1/2}\frac{dg_m}{d\xi}\Bigg|_{\xi'-}^{\xi'+}=-\frac{T_m(\eta')}{a_m B_m(\xi',\eta')} \tag{33}$$

Assuming that

$$B_m(\xi',\eta')=B'_m(\xi')T_m(\eta'), \tag{34}$$

and considering Eq. (31), we can rewrite Eq. (33) as

$$(\xi'^2-1)^{1/2}AS'_m(\xi')-(\xi'^2-1)^{1/2}BT'_m(\xi')=-\frac{1}{a_m B'_m(\xi')} \tag{35}$$

But the continuity of Green's function puts the condition

$$AS_m(\xi')=BT_m(\xi') \quad\Rightarrow\quad \frac{A}{B}=\frac{T_m(\xi')}{S_m(\xi')}; \tag{36}$$

then, from Eq. (35),

$$(\xi'^2-1)^{1/2}B\left[T_m(\xi')\frac{S'_m(\xi')}{S_m(\xi')}-T'_m(\xi')\right]=-\frac{1}{a_m B'_m(\xi')},$$

or

$$(\xi'^2-1)^{1/2}BW\{S_m,T_m\}=-\frac{S_m(\xi')}{a_m B'_m(\xi')} \tag{37}$$

where $W\{S_m,T_m\}$ is the Wronskian between these pair of functions, and is precisely

$$W\{S_m,T_m\}=-\frac{1}{(\xi'^2-1)^{1/2}}; \tag{38}$$

then, the coefficient of the B'_m is

$$BB'_m(\xi')=\frac{S_m(\xi')}{a_m} \quad\Rightarrow\quad AB'_m=\frac{T_m(\xi')}{a_m}, \tag{39}$$

when we use Eq. (36). With these factors we can construct the functions for the regions above and below ξ', i.e.

$$\begin{aligned} g_m^+(\xi')&=AB'_m(\xi')=\frac{T_m(\xi')}{a_m}\\ g_m^-(\xi')&=BB'_m(\xi')=\frac{S_m(\xi')}{a_m}. \end{aligned} \tag{40}$$

Finally, we arrive to the expression for Green's function using Eqs. (27), (34) and (40), to have

$$G(\boldsymbol{\rho},\boldsymbol{\rho}')=\sum_{m=0}^{\infty}\frac{T_m(\eta)T_m(\eta')f_m(\xi,\xi')}{a_m}, \tag{41}$$

where

$$f_m(\xi,\xi')=\begin{cases}S_m(\xi')T_m(\xi), & 1<\xi<\xi'\\ T_m(\xi')S_m(\xi), & 1<\xi'<\xi\end{cases} \tag{42}$$

and

$$a_m=\begin{cases}\pi, & m=0\\ \dfrac{\pi}{2}, & m\neq 0\end{cases} \tag{43}$$

This function has the required properties and the condition of being symmetrical respect to the exchange between variables.

Using Eq. (3) and (41), we obtain an expression for the Coulomb potential:

$$\frac{1}{|\boldsymbol{\rho}-\boldsymbol{\rho}'|}=\prod_{m=0}^{\infty}\exp\left[\frac{2\pi T_m(\eta)T_m(\eta')f_m(\xi,\xi')}{a_m}\right] \tag{44}$$

This form of the Coulomb potential can be implemented in a numerical approach.

5 Conclusion

In this communication we have obtained the general solution of Laplace equation and its corresponding Green's Function in elliptic coordinates. In addition, a representation of the two-dimensional Coulomb potential was given. The reported expressions for these functions can be used to study an interesting class of two-dimensional problems which range from purely electrostatic to actual solid state physics problems. In the former case, we can mention, for instance, the boundary-value problem of an elliptic conducting cylinder, with a given potential or surface charge, and a charged line; in the latter, the study of hydrogenic impurities in bidimensional nanostructured quantum dots of elliptic shape.

As a collateral result, the solution of the Chebyshev differential equation in $[1,\infty)$ was constructed using the Frobenius method, which allowed us to define the Second Chebyshev Functions, and to construct both the Green's function and the Coulomb potential in this coordinate system.

The formalism followed here-in to obtain these results can be extended to any two-dimensional coordinate system in which the Laplace equation is separable or, at least, partially separable.

Work is in progress to apply some of the results to specific systems and will be published elsewhere.

References:

[1] Ley-Koo E. and Góngora A. Desarrollos armónicos del potencial Coulombiano en coordenadas cilíndricas, parabólicas y esferoidales. *Rev. Mex. Fis.* Vol. 39, No. 5, 1993, pp. 785-793

[2] Marin J. L. and Cruz S. A. Enclosed quantum systems: use of the Direct Variational Method. *J. of Phys. B: At. Mol. Opt. Phys.* Vol. 24, pp. 2899, 1991

[3] Cruz S. A., Ley-Koo E., Marin J. L. and Taylor-Armitage A. Variational Calculation for the hydrogen atom confined in space with paraboloidal and spheroidal boundaries. *Int. J. of Quantum Chem.* Vol. 54, pp. 3, 1995

[4] Marin J. L., Riera R. Confined systems and nanostructured materials, in *Handbook of advanced electronic and photonic materials and devices* V. 6, Ed. Nalwa H. S., Academic Press, 2001

[5] Ditrich W. The Coulomb Green's function in two dimensions. *Am. J. Phys.* Vol. 67, No. 9 (1999) pp. 768-775

[6] Furman M. A. Compact complex expressions for the electric field of two-dimensional elliptical charge distributions. *Am. J. Phys.* Vol. 62, No. 12, 1999, pp. 1134-1140

[7] Arfken G. and Weber H. J. *Mathematical Methods for Physicists.* Academic Press, 2001

[8] Kellogg O. D. *Foundations of Potential Theory.* Dover Publications, 1953

[9] Marin J. L. and Cruz S. A. On the use of Direct Variational methods to study confined quantum systems. *Am. J. Phys.* Vol 59, pp. 931, 1991

[10] Boyd John P. *Chebyshev and Fourier Spectral Methods*. Dover Publications, 2001

Aknowledgements: Raúl Pérez-Enríquez and Ivan Marín-Enríquez are PhD students at Departamento de Inv. En Fisica (Universidad de Sonora) and are supported by CONACyT and UNISON. This work has been done under project CONACyT-40629 and 47682.

Appendix

The Chebyshev's differential equation outside the [-1, 1] interval can be expressed as follows:

$$(\xi^2-1)\frac{d^2H}{d\xi^2}+\xi\frac{dH}{d\xi}-n^2H(\xi)=0 \qquad (45)$$

where, H has a removable singularity in $\xi=1$ and is regular at $\xi=\infty$. In order to find a solution, we will use the Frobenius method; in doing so, we suggest the following form for the function

$$H(\xi)=\sum_{l=0}^{\infty}a_l\,\xi^{k-l} \qquad (46)$$

Then the first and second derivatives will be

$$H'(\xi)=\sum_{l=0}^{\infty}(k-l)a_l\,\xi^{k-l-1} \qquad (47)$$

and

$$H''(\xi)=\sum_{l=0}^{\infty}(k-l)(k-l-1)a_l\,\xi^{k-l-2} \qquad (48)$$

Making the substitution of those expressions in Eq. (45), we will have

$$\begin{aligned}&(\xi^2-1)\cdot\sum_{l=0}^{\infty}(k-l)(k-l-1)a_l\xi^{k-l-2}\\&+\xi\cdot\sum_{l=0}^{\infty}(k-l)a_l\xi^{k-l-1}-n^2\cdot\sum_{l=0}^{\infty}a_l\xi^{k-l}=0,\end{aligned} \qquad (49)$$

i.e.,

$$\begin{aligned}&\sum_{l=0}^{\infty}a_{-l}\left[(k-l)(k-l-1)+(k-l)-n^2\right]\xi^{k-l}\\&-\sum_{l=0}^{\infty}(k-l)(k-l-1)a_{-l}\,\xi^{k-l-2}=0\end{aligned} \qquad (50)$$

After replacing the index in the second summation ($l\to l-2$), while we simplify the first one, we will obtain

$$\begin{aligned}&\sum_{l=0}^{\infty}a_{-l}\left[(k-l)^2-n^2\right]\xi^{k-l}\\&-\sum_{l=2}^{\infty}(k-l+2)(k-l+1)a_{-l+2}\xi^{k-l}=0,\end{aligned} \qquad (51)$$

and from it, the recurrence relations for the coefficients will appear:

$$a_0(k^2-n^2)=0 \qquad (52)$$

$$a_{-1}[(k-1)^2-n^2]=0 \qquad (53)$$

$$a_{-l}[(k-l)^2-n^2]=(k-l+2)(k-l+1)a_{-l+2} \quad \text{for} \quad l\geq 2 \qquad (54)$$

From the secular equation (52) we will find the allowed values of *k*; if we assume that

$$a_0\neq 0,\quad a_1=0 \quad \text{then} \quad k^2-n^2=0 \quad \therefore \quad k=\pm n \qquad (55)$$

But the requirement for the function $H(\xi)$ to vanish as $\xi \to \infty$, makes the powers to be considered strictly negative; thus,

$$k = -n, \quad \text{with} \quad n > 0. \tag{56}$$

The recurrence relation (54) for the case $l \geq 2$ (even) and condition (56) will give

$$a_{-l} = \frac{(n+l-2)(n+l-1)}{l(l+2n)} a_{-l+2}, \tag{57}$$

a recurrence relation between coefficients that will allow us to find all coefficients as a function of a_0 that we assumed different from zero. In consequence,

$$\begin{aligned} a_{-2} &= \frac{n(n+1)}{2(2n+2)} a_0 = \frac{n(n+1)}{2 \cdot 2(n+1)} a_0 \\ &= \frac{n}{2 \cdot 2} a_0, \end{aligned} \tag{58}$$

$$\begin{aligned} a_{-4} &= \frac{(n+2)(n+3)}{4(4+2n)} a_{-2} = \frac{n(n+2)(n+3)}{2 \cdot 2 \cdot 4 \cdot 2(n+2)} a_0 \\ &= \frac{n(n+3)}{2^2 \cdot 4 \cdot 2} a_0, \end{aligned} \tag{59}$$

$$\begin{aligned} a_{-6} &= \frac{(n+4)(n+5)}{6(2n+6)} a_{-4} \\ &= \frac{n(n+3)(n+4)(n+5)}{2^3 \cdot 6 \cdot 4 \cdot 2(n+3)} a_0 \\ &= \frac{n(n+4)(n+5)}{2^3 6!!} a_0 \end{aligned} \tag{60}$$

Continuing this way, we will derive a compact expression for the coefficients,

$$a_{-2l} = \frac{n \cdot \prod_{s=l+1}^{2l-1} (n+s)}{2^{2l}\, l!} a_0, \quad \text{with} \quad l = 1, 2, 3, \cdots \tag{61}$$

Functions of well-defined parity will then be built with the aid of these coefficients:

$$H_n^{\pm}(\xi) = a_0 \left(\xi^{-n} + n \cdot \sum_{l=1}^{\infty} \frac{\prod_{s=l+1}^{2l-1} (n+s)}{2^{2l}\, l!} \xi^{-n-2l} \right), \tag{62}$$

where $+$ stands for n even and $-$ for n odd. In the special case where $n = 0$, the function $H_0(\xi)$ is solution to the differential equation

$$(\xi^2 - 1)^{1/2} \frac{d}{d\xi} (\xi^2 - 1)^{1/2} \frac{dH_0(\xi)}{d\xi} = 0, \tag{63}$$

where we have put Eq. (45) in self-adjoint form; this can be solved by direct integration, and yields the function

$$H_0(\xi) = C \ln\left(\xi + \sqrt{\xi^2 - 1}\right) \tag{64}$$

We call then this set of functions the Chebyshev functions of 2nd Class that are solution to Eq. (45), and are defined by

$$S_n(\xi) = \begin{cases} a_0 \ln\left(\xi + \sqrt{\xi^2 - 1}\right), & \text{for} \quad n = 0 \\ a_0 \xi^{-n} \left[1 + n \cdot \sum_{l=1}^{\infty} \frac{\Gamma(n+2l) \cdot (2\xi)^{-2l}}{\Gamma(n+l+1) \cdot \Gamma(l+1)} \right] & \text{for} \quad n \geq 1 \end{cases} \tag{65}$$

In Figs. 1 through 4 we show graphs of those functions for values of the index $n = 0, 1, 2, \cdots, 6$

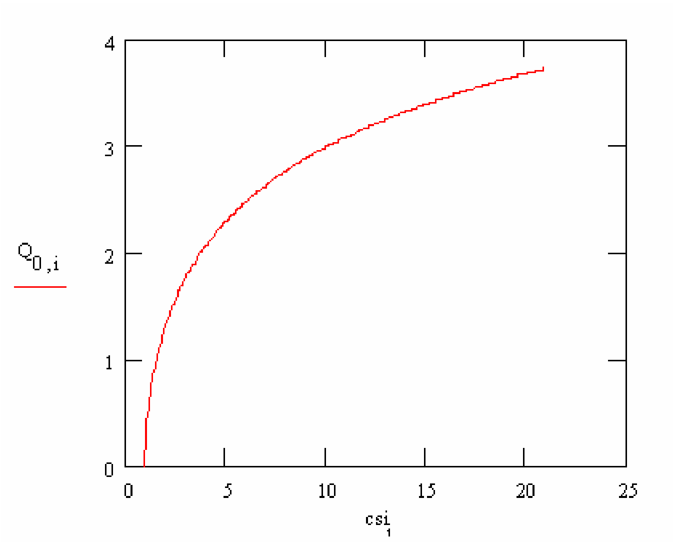

Fig. 1. Graph for the Chebyshev function of 2nd class, $S_0(\xi)$.

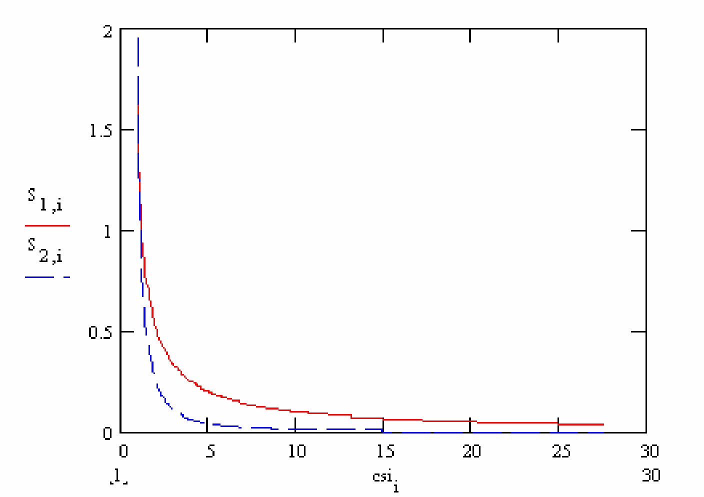

Fig. 2. Graphs for the Chebyshev functions of 2nd class for $n = 1, 2$.

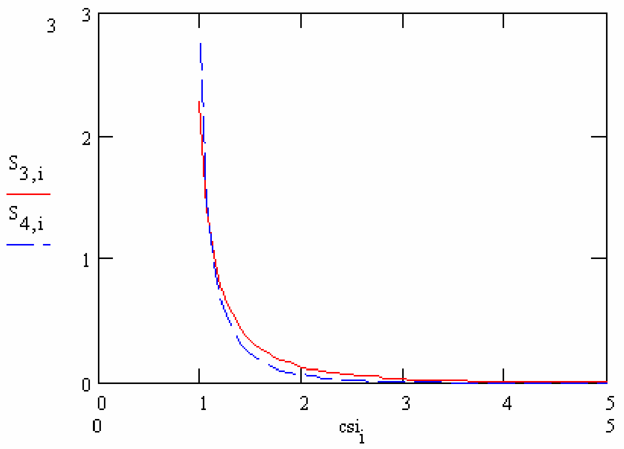

Fig. 3. Graphs for the Chebyshev functions of 2nd class for $n = 3, 4$.

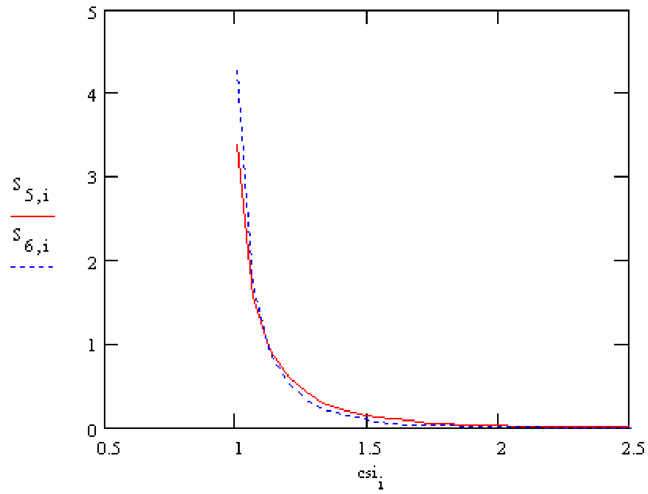

Fig. 4. Graphs for the Chebyshev functions of 2nd class for $n = 5, 6$.

Finally, we consider necessary to point out that this method to obtain Chebyshev Functions of 2nd class is not unique; an alternative way to build these functions would involve the direct evaluation form the Wronskian and the Chebyshev polynomials of 1st class as discussed by Arfken and Weber for the Legendre polynomials [7].

The closed form of those Chebyshev Functions of 2nd class would be expressed as

$$S_n(\xi) = T_n(\xi)\left\{ A_n + B_n \int_1^{\xi} \frac{dx}{(x^2-1)^{1/2}[T_n(x)]^2} \right\} \quad (66)$$

with A_n a constant to be determined and the $T_n(x)$, Chebyshev polynomials, evaluated in the interval of interest. The problem with this method is that we have to calculate them one by one. As an illustration, the three first ones are the following:

$$\begin{aligned} S_0(\xi) &= A_0 \ln\left[\xi + \sqrt{\xi^2 - 1}\right] \\ S_1(\xi) &= A_1\left[\xi - \sqrt{\xi^2-1}\right] \\ S_2(\xi) &= A_2\left[(2\xi^2-1) + 2\xi\sqrt{\xi^2-1}\right] \end{aligned} \quad (67)$$

Both representations are compatible when calculated for $\xi > 1+\varepsilon$, but the series form of functions $S_n(\xi)$ is easiest to implement in a numerical calculation as that of Green's function on elliptic coordinates.