

Analytic Solutions for Hindered Rotation Quantum Problem

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How to cite this paper: Ragni, M. (2024) Analytic Solutions for Hindered Rotation Quantum Problem. *Applied Mathematics*, 15, 709-718.

<https://doi.org/10.4236/am.2024.1510041>

Received: July 2, 2024

Accepted: October 8, 2024

Published: October 11, 2024

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Abstract

Normalizable analytic solutions of the quantum rotor problem with divergent potential are presented here as solution of the Schrödinger equation. These solutions, unknown to the literature, represent a mathematical advance in the description of physical phenomena described by the second derivative operator associated with a divergent interaction potential and, being analytical, guarantee the optimal interpretation of such phenomena.

Keywords

Analytics Solutions, Schrodinger Equation, Interaction Potential

1. Introduction

The hindered rotations are of crucial relevance in quantum mechanics due to the ability to describe phenomena ranging from the behavior of molecules, through the inversion of chirality and arriving at the coupling of angular momenta and their applications in quantum composition [1]-[11]. Despite the fact that the rotation operator, or the second derivative operator on a cyclic coordinate, is closely linked to the principles of physics and their interpretation, the only analytical solutions known in the literature are those with constant potential [12]-[19]. In other words, we have a single basis set to expand the solutions of physics equations such as Schrödinger's. Consequently, for non-constant rotation potentials, the only possible approach is that which leads to numerical solutions of the problem addressed.

As is well known, numerical solutions make the process of understanding the physics of the problem an even greater challenge and, when the solutions represent the starting point of other problems as in the case of the study of chemical reactions, the complexity of the numerical treatment, together with the propagation

of the error, with a certain frequency they give results without significance. It is with this problem in mind that, in this article, the analytical solutions of the rotational quantum mechanical problem with divergent potential at $+\infty$ for a specific value of the angle that describes the rotation are described.

The article is divided as it follows. In the next section, the problem is mathematically formalized and the solutions are calculated by dividing them into even and odd types. The section “Remarks and perspectives” continues the article presenting some important observations. Appendixes “ c coefficients” and “ $s_{i,m}$ ” conclude the paper offering useful information for the reader that wants to build up the solutions of the problem.

2. Theory

The Schrödinger equation solved here is defined mathematically by the free rotor operator

$$-\frac{d^2\Phi_i(\phi)}{d\phi^2} \quad (1)$$

plus an interaction potential $V(\phi)$ appropriately chosen to represent the hindered rotation. Following, this potential is presented and the eigenfunctions analytically calculated.

2.1. Hindered Rotational Potential

Being able to encounter square-integrable analytical wavefunctions for the Schrödinger Equation presented above is strictly dependent on the mathematical expression used to represent Hindered Rotational Potential. Thinking about a generalization of the free-rotor quantum problem, the chosen function is so that the Schrödinger Equation becomes:

$$-\frac{d^2\Phi_i(\phi)}{d\phi^2} + \left(\frac{\cos(\phi)}{1 - \cos(\phi)} - \lambda_i \right) \Phi_i(\phi) = 0. \quad (2)$$

A graphical representation of this potential is given in **Figure 1**. Let's observe that the square-integrable zero nodes wave-function $\Phi_0(\phi) = 1 - \cos(\phi)$ is eigenfunction of Eq. (2) with eigenvalue 0. Due to the fact that it has no nodes, it can be stated that it is the eigenfunction associated with the smallest eigenvalue of the Equation.

It's convenient to search the remaining eigenfunctions in the form $\Phi_i(\phi) = \Phi_0(\phi)P_i(\phi)$ and expanding $P_i(\phi)$ in sum of sine and cosine functions (See next two subsections). Substituting so defined $\Phi_i(\phi)$ into Eq.(2), and dividing it by $\Phi_0(\phi)$, it is found that

$$-\frac{d^2P_i(\phi)}{d\phi^2} - \frac{2\sin(\phi)}{1 - \cos(\phi)} \frac{dP_i(\phi)}{d\phi} - \lambda_i P_i(\phi) = 0. \quad (3)$$

As well know, the symmetry in variable ϕ expressed by Eq. (2) and Eq. (3) permits to demonstrate that the searched eigenfunctions are of two types: the symmetric or (even ones), expressible as sum of cosine functions, and the anti-symmetric (or odd) ones, expressible as sum of sine functions. Analytic expression

and associated eigenvalues are given in the next two subsection, respectively.

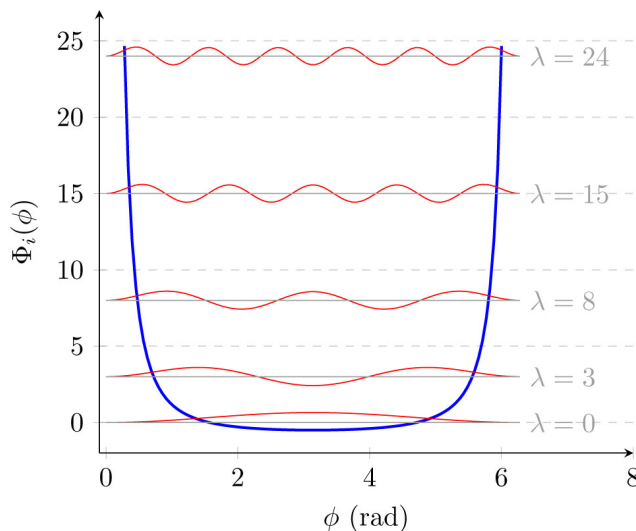


Figure 1. Hindered Rotation Wave-functions. Blue curve represents the potential $\cos(\phi)/(1-\cos(\phi))$ while red and dark-green curves represent the first even eigenfunctions.

2.2. Even Solutions

Even solutions are searched in the form $P_{Even,i} = \sum_{m=0}^{M_{\max}} c_{i,m} \cos(m\phi)$. Substituting in Eq. (3), it is obtained

$$2 \sin \phi \sum_{m=0}^{M_{\max}} [m c_{i,m} \sin(m\phi)] + (1 - \cos(\phi)) \sum_{m=0}^{M_{\max}} [(m^2 - \lambda_i) c_{i,m} \cos(m\phi)] = 0. \quad (4)$$

Employing some trigonometric equalities, the above equation can be conveniently rewritten as

$$0 = \sum_{m=0}^{M_{\max}} c_{i,m} (C_+(m) + C(m) + C_-(m)), \quad (5)$$

$$C_+(m) = (\lambda_i - m(m+2)) \cos((m+1)\phi), \quad (6)$$

$$C(m) = 2(m^2 - \lambda_i) \cos(m\phi), \quad (7)$$

$$C_-(m) = (\lambda_i - m(m-2)) \cos((m-1)\phi). \quad (8)$$

Observing these equations, and, in particular, Eq. (6), it can be seen that the series can be interrupted for a positive (integer) value of $M_{\max} = i$. Doing this, equation presents the term $\cos((i+1)\phi)$ multiplied by $C_+ = \lambda_i - i(i+2)$. To make this term equals to zero, the only way is to assume $\lambda_i = i(i+2)$. At this step, the coefficients $c_{i,m}$ are determinable following the standard procedure described in **Appendix A** where the indetermination on $c_{i,0}$ is resolved considering the normalization $|\Phi_i(\phi)|^2 = 1$.

The first five normalized even eigenfunctions are reported in **Table 1** and plotted in **Figure 1**. Finally, it follows the three-term recurrence relationship.

$$2((2n+1)(2n+3)\cos(x)+2)P_{Even,i} = (2n+1)^{3/2}\sqrt{2n+5}P_{Even,i+1} + (2n+3)^{3/2}\sqrt{2n-1}P_{Even,i-1}. \tag{9}$$

Table 1. Normalized explicit expressions for the first five even solutions of Eq. (2).

i	λ	Explicit expression
0	0	$(1 - \cos(\phi))/\sqrt{3\pi}$
1	3	$2\Phi_0(3\cos(\phi)+2)/\sqrt{5}$
2	8	$\sqrt{3}\Phi_0(10\cos(2\phi)+16\cos(\phi)+9)/\sqrt{35}$
3	15	$2\Phi_0(7\cos(3\phi)+12\cos(2\phi)+15\cos(\phi)+8)/\sqrt{21}$
4	24	$\Phi_0(18\cos(4\phi)+32\cos(3\phi)+42\cos(2\phi)+48\cos(\phi)+25)/\sqrt{33}$

2.3. Odd Solutions

Similar to the even eigenfunctions, the odd solution are expanded in sums of sine functions defining $P_{Odd,i} = \sum_{m=1}^{\infty} s_{i,m} \sin(m\phi)$. Consequently, we have

$$0 = 2\sin(\phi) \sum_{m=1}^{\infty} [ms_{i,m} \cos(m\phi)] - (1 - \cos(\phi)) \sum_{m=1}^{\infty} [(m^2 - \lambda_i)s_{i,m} \sin(m\phi)] \tag{10}$$

that, with trigonometric manipulations, becomes

$$0 = \sum_{m=1}^{\infty} s_{i,m} [S_+(m) + S(m) + S_-(m)], \tag{11}$$

$$S_+(m) = (\lambda_i - m(m+2))\sin((m+1)\phi), \tag{12}$$

$$S(m) = 2(m^2 - \lambda_i)\sin(m\phi), \tag{13}$$

$$S_-(m) = (\lambda_i - m(m-2))\sin((m-1)\phi). \tag{14}$$

Apparently, this problem is similar to the one about of the even solutions and that the expansion $P_{Odd,i}$ can be stopped for a particular value of m . But there is a crucial difference in the sums. The odd ones start with $m=1$, while the even ones start with $m=0$. Its because $\sin(0\phi)=0$ and no contribution to the expansion is given. In other words, $s_{i,0}$ is 0 and this has consequences on the rest of the coefficients, as it can be seen stopping the series to $m=1$:

$$s_{i,1}(\lambda_i - 3)\sin(2\phi) + 2s_{i,1}(1 - \lambda_i)\sin(\phi) = 0. \tag{15}$$

As it will be evident, the absence of $s_{i,0}$ in the multiplicative coefficient of $\sin(\phi)$ makes the equation inconsistent. Similar results are obtained considering other values for the maximum value of m . This means that the series cannot be stopped and that the odd eigenfunctions are expressed by a sum of infinite weighted terms of the type $\sin(m\phi)$.

With some tedious but not impossible mathematical steps, Eq.(11) is rewrite as

$$\sum_{m=1}^{\infty} [(m^2 - 1 - \lambda_i)(s_{i,m+1} + s_{i,m-1}) + 2(\lambda_i - m^2)s_{i,m}] \sin(m\phi) = 0 \tag{16}$$

where, as observed above, $s_{i,0} = 0$. The Three Terms Recurrence Relationship

$(m^2 - 1 - \lambda_i)(s_{i,m+1} + s_{i,m-1}) + 2(\lambda_i - m^2)s_{i,m} = 0$ establishes the role for the convergence of the expansion $P_{Odd,i}$ that is obviously strictly dependent on the value of λ_i . In particular, the equation

$$\frac{s_{i,m+1} + s_{i,m-1}}{2s_{i,m}} = \frac{m^2 - \lambda_i}{m^2 - \lambda_i - 1} = 1 + \frac{1}{m^2 - \lambda_i - 1} \quad (17)$$

must be true for each value of m . Conveniently, λ is here replaced with $i(i+2)$, expression that was encountered in the subsection above, obtaining

$$\frac{s_{i,m+1} + s_{i,m-1}}{2s_{i,m}} = \frac{m^2 - i(i+2)}{(m+i+1)(m-i-1)} = 1 + \frac{1}{(m+i+1)(m-i-1)}. \quad (18)$$

This last equation shows that for the odd solution i cannot assume integer values. Moreover, the value of first odd eigenvalue is between those of the firsts two consecutive even eigenvalues for which $i=0$ and $i=1$, respectively. Therefore, $0 < i < 1$. Observing that

$$\frac{s_{i,m+1}}{s_{i,m}} = 2 \frac{m^2 - \lambda}{m^2 - \lambda - 1} - \frac{s_{i,m-1}}{s_{i,m}} \quad (19)$$

and that to guarantee the convergence of P_{odd} series it must be

$$\left| \frac{s_{i,m+1}}{s_{i,m}} \right| < 1 \quad (20)$$

for $m \rightarrow \infty$, it is deduced that

$$-1 < 2 \frac{m^2 - \lambda}{m^2 - \lambda - 1} - \frac{s_{i,m-1}}{s_{i,m}} < 1. \quad (21)$$

With some algebraic manipulations, this last equation becomes

$$3 + \frac{2}{m^2 - \lambda - 1} > \frac{s_{m-1}}{s_m} > 1 + \frac{2}{m^2 - \lambda - 1} \quad (22)$$

or

$$3 + \frac{2}{(m+i+1)(m-i-1)} > \frac{s_{m-1}}{s_m} > 1 + \frac{2}{(m+i+1)(m-i-1)}. \quad (23)$$

Resuming, from a certain value of m onward, the sequence of s_m is positive-defined if $s_1 > 0$ or negative-defined if $s_1 < 0$. Numerical tests confirm this result. Moreover, it is obtained that the sequences of $s_{\lambda,m}$ are positive or negative defined for each value of m .

The symmetrization obtained in Eq. (18) demonstrates that the expression $\lambda_i = i(i+2)$ describes the metric of the eigenvalues space. For this reason, i takes on the role of a quantum number and must take on equally spaced values. Considering the values of i that provides the even solutions, the odds ones are obtained with not negative half-integer values ($i = 1/2, 3/2, 5/2, 7/2, \dots$).

3. Remarks and Perspectives

Analytic eigenfunctions for a hindered potential applied to a quantum rotor

problem were found. Even functions are expressed by finite weighted sums of $\cos(m\phi)$ functions while for the odd ones the weighted sums are over infinite terms $\sin(m\phi)$. In both cases, the coefficients of the expansions are here determined analytically and the eigenvalues λ_i for the given potential are calculated as $i(i+2)$, where i is not negative integer or half-integer for even and odd solutions, respectively.

The eigenproblem described here represents the first step for a generalization of the free rotation quantum problem to a hindered one. The second step is represented by the introduction of a more general potential given by the expression

$$V(\phi) = \frac{a \cos(n\phi)}{1 - a \cos(n\phi)}. \quad (24)$$

The behavior of the Schrödinger equation under the action of this potential is under study and more investigations are, at the present moment, necessary. However, it is possible to anticipate that, for values of $a = \pm 1$ and n positive integer, $\lambda_i = i(i+2n)$.

But the main challenge is to make a vary in the open interval $(-1, 1)$ because the resulting potential presents one or more finite barriers (It depends on the value of n) and eigenvalues with energies below the barriers. Consequently, the eigenfunctions represent a set of orthogonal functions completely new compared to those encountered in the literature that are never solutions of potentials with finite barriers.

Such a cyclic potential can be used to describe a variety of physical systems ranging from the roto-torsions of molecules, through the inversion of chirality, and arriving at the description of confined atoms and entangled coordinates predicted in field theories with more than four dimensions.

Conflicts of Interest

The author declares no conflicts of interest regarding the publication of this paper.

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Appendix A. c Coefficients

In this appendix, Eq.(5) is used to find the coefficients of the expansion given at the beginning of section 2.2. Using Eq. (3) and considering the case of $M_{\max} = i = 4$, the condition to be respected is expressed by

$$\begin{aligned}
 & c_{4,4}(\lambda_4 - 24)\cos(5\phi) \\
 & + ((c_{4,3} - 2c_{4,4})\lambda_4 + 32c_{4,4} - 15c_{4,3})\cos(4\phi) \\
 & + ((c_{4,4} - 2c_{4,3} + c_{4,2})\lambda_4 - 8c_{4,4} + 18c_{4,3} - 8c_{4,2})\cos(3\phi) \\
 & + ((c_{4,3} - 2c_{4,2} + c_{4,1})\lambda_4 - 3c_{4,3} + 8c_{4,2} - 3c_{4,1})\cos(2\phi) \\
 & + ((c_{4,2} - 2c_{4,1} + 2c_{4,0})\lambda_4 + 2c_{4,1})\cos(\phi) \\
 & + (c_{4,1} - 2c_{4,0})\lambda_4 + c_{4,1} = 0.
 \end{aligned} \tag{A1}$$

Observe that the coefficient of $\cos(5\phi)$ is automatically zero because $\lambda_4 = 4(4 + 2) = 24$. Consequently the equation above is reduced to

$$\begin{aligned}
 & (9c_{4,3} - 16c_{4,4})\cos(4\phi) \\
 & + (16c_{4,4} - 30c_{4,3} + 16c_{4,2})\cos(3\phi) \\
 & + (21c_{4,3} - 40c_{4,2} + 21c_{4,1})\cos(2\phi) \\
 & + (24c_{4,2} - 46c_{4,1} + 48c_{4,0})\cos(\phi) \\
 & + 25c_{4,1} - 48c_{4,0} = 0
 \end{aligned} \tag{A2}$$

that is verified if

$$\begin{aligned}
 & (9c_{4,3} - 16c_{4,4}) = 0 \\
 & (16c_{4,4} - 30c_{4,3} + 16c_{4,2}) = 0 \\
 & (21c_{4,3} - 40c_{4,2} + 21c_{4,1}) = 0 \\
 & (24c_{4,2} - 46c_{4,1} + 48c_{4,0}) = 0 \\
 & 25c_{4,1} - 48c_{4,0} = 0.
 \end{aligned} \tag{A3}$$

Apparently, it is a system of five linear equations and five unknown coefficients $c_{4,m=0,\dots,4}$, but this is not correct because one of these is redundant. This can be demonstrated imposing (for convenience) $c_{4,0} = 25$ so that, to respect the last of Eq.(A3), $c_{4,2} = 48$. Consequently

$$\begin{aligned}
 & (9c_{4,3} - 16c_{4,4}) = 0 \\
 & (16c_{4,4} - 30c_{4,3} + 16c_{4,2}) = 0 \\
 & (21c_{4,3} - 40c_{4,2} + 1008) = 0 \\
 & (24c_{4,2} - 1008) = 0.
 \end{aligned} \tag{A4}$$

Doing $c_{4,2} = 42$:

$$\begin{aligned}
 & (9c_{4,3} - 16c_{4,4}) = 0 \\
 & (16c_{4,4} - 30c_{4,3} + 672) = 0
 \end{aligned}$$

$$(21c_{4,3} - 40c_{4,2} - 672) = 0. \quad (\text{A5})$$

Doing $c_{4,2} = 42$:

$$\begin{aligned} (9c_{4,3} - 16c_{4,4}) &= 0 \\ (16c_{4,4} - 30c_{4,3} + 672) &= 0 \\ (21c_{4,3} - 672) &= 0. \end{aligned} \quad (\text{A6})$$

Doing $c_{4,3} = 32$:

$$\begin{aligned} (288 - 16c_{4,4}) &= 0 \\ (16c_{4,4} - 288) &= 0 \end{aligned} \quad (\text{A7})$$

and this demonstrates the redundancy because the two conditions are identical and $c_{4,4} = 18$. To uniquely define $\Phi_4(\phi)$ the just found coefficients $c_{4,m=0,\dots,4}$ have to be scaled by a normalization factor so that $\int_0^{2\pi} |\Phi_4(\phi)|^2 d\phi = 1$.

Appendix B. $s_{i,m}$

Taking $s_{i,1} = 1/2$, they follow the expressions of the firsts eleven coefficients $s_{i,m}$.

$$s_{i,2} = \frac{\lambda_i - 1}{\prod_{j=0}^0 (\lambda_i - j(j+2))}, \quad (\text{B8})$$

$$s_{i,3} = \frac{3\lambda_i^2 - 17\lambda_i + 16}{2\prod_{j=0}^1 (\lambda_i - j(j+2))}, \quad (\text{B9})$$

$$s_{i,4} = \frac{2(\lambda_i - 5)(\lambda_i^2 - 11\lambda_i + 12)}{\prod_{j=0}^2 (\lambda_i - j(j+2))}, \quad (\text{B10})$$

$$s_{i,5} = \frac{5\lambda_i^4 - 170\lambda_i^3 + 1817\lambda_i^2 - 6648\lambda_i + 5760}{2\prod_{j=0}^3 (\lambda_i - j(j+2))}, \quad (\text{B11})$$

$$s_{i,6} = \frac{3\lambda_i^5 - 185\lambda_i^4 + 3965\lambda_i^3 - 35207\lambda_i^2 + 119040\lambda_i - 100800}{\prod_{j=0}^4 (\lambda_i - j(j+2))}, \quad (\text{B12})$$

$$s_{i,7} = \frac{7\lambda_i^6 - 707\lambda_i^5 + 26453\lambda_i^4 - 455137\lambda_i^3 + 3621696\lambda_i^2 - 11620800\lambda_i + 9676800}{2\prod_{j=0}^5 (\lambda_i - j(j+2))}, \quad (\text{B13})$$

$$\begin{aligned} s_{i,8} &= \frac{4(\lambda_i^7 - 154\lambda_i^6 + 9184\lambda_i^5 - 269058\lambda_i^4 + 4055247\lambda_i^3)}{\prod_{j=0}^6 (\lambda_i - j(j+2))} \\ &+ \frac{4(-29988756\lambda_i^2 + 92685600\lambda_i - 76204800)}{\prod_{j=0}^6 (\lambda_i - j(j+2))}, \end{aligned} \quad (\text{B14})$$

$$\begin{aligned} s_{i,9} &= \frac{3(3\lambda_i^8 - 668\lambda_i^7 + 59514\lambda_i^6 - 2726652\lambda_i^5 + 68754523\lambda_i^4)}{2\prod_{j=0}^7 (\lambda_i - j(j+2))} \\ &+ \frac{3(-947476560\lambda_i^3 + 6646620480\lambda_i^2 - 19971302400\lambda_i + 16257024000)}{2\prod_{j=0}^7 (\lambda_i - j(j+2))}, \end{aligned} \quad (\text{B15})$$

$$\begin{aligned}
s_{i,10} = & \frac{5\lambda_i^9 - 1545\lambda_i^8 + 195882\lambda_i^7 - 13207738\lambda_i^6 + 513568401\lambda_i^5}{\prod_{j=0}^8 (\lambda_i - j(j+2))} \\
& + \frac{-11686013181\lambda_i^4 + 150898575168\lambda_i^3 - 1017148380480\lambda_i^2}{\prod_{j=0}^8 (\lambda_i - j(j+2))} \quad (\text{B16}) \\
& + \frac{2989666713600\lambda_i - 2414168064000}{\prod_{j=0}^8 (\lambda_i - j(j+2))},
\end{aligned}$$

$$\begin{aligned}
s_{i,11} = & \frac{11\lambda_i^{10} - 4565\lambda_i^9 + 792990\lambda_i^8 - 75173098\lambda_i^7 + 4252840471\lambda_i^6}{2\prod_{j=0}^9 (\lambda_i - j(j+2))} \quad (\text{B17}) \\
& + \frac{-147622553073\lambda_i^5 + 3115657332432\lambda_i^4 - 38286831418560\lambda_i^3}{2\prod_{j=0}^9 (\lambda_i - j(j+2))} \\
& + \frac{250120955980800\lambda_i^2 - 722275190784000\lambda_i + 579400335360000}{2\prod_{j=0}^9 (\lambda_i - j(j+2))}.
\end{aligned}$$