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A Note on the Theory of Vibration-Rotation Interaction

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Attempts to treat the differential equation for the radial component of the *Eigenfunktion* of a rotating harmonic oscillator by the W.K.B. or alternative methods, have encountered difficulties because of the nature of the equation. The interval from $r=0$ to $r=\infty$, on which the equation has to be considered, includes both a singular point and a turning point. About these points the Stokes' phenomenon is involved, and the elementary asymptotic solutions fail to remain valid. Known theory which is applicable to the equation in intervals which contain such critical points is here called upon to yield an equation for the *Eigenwerte*, and to produce descriptions of the solutions over the complete range of the variable.

I. INTRODUCTION

THE equation for the radial component F of the *Eigenfunktion* of a rotating harmonic oscillator is, with a suitable choice of units and in familiar notation,

$$(d^2F/dr^2)+[(E-V/B_e)-(l(l+1)/r^2)]F=0,$$ [1]

with

$$V=(\omega^2/4B_e)(r-1)^2.$$

In terms of the symbols

$$\lambda=(E/\omega_e)-\tfrac{1}{2},\quad \alpha=B_e/\omega_e,$$

it assumes the form

$$(d^2F/dr^2)-[((r-1)^2/4\alpha^2)-(2\lambda+1/2\alpha)+(l(l+1)/r^2)]F=0. \quad (1.1)$$

The value of the constant α is small—generally very small—and Eq. (1.1) therefore involves the "large parameter," $1/\alpha$. The point $r=1$ at which the coefficient of the highest power of this parameter becomes zero in a *turning point* for the equation, and is therefore critical, as is also the point $r=0$ at which the equation is singular. The problem to be considered is that of determining the characteristic λ-values for which the equation admits of a solution that vanishes both at $r=0$ and at $r=\infty$, and of describing the characteristic solutions which have that property.[2]

II. THE SOLUTION AROUND $r=0$

Since the function sought is to vanish at $r=0$, we begin by a consideration of Eq. (1.1) in an interval abutting this point. At $r=0$ the equation is singular (except when $l=0$) and has the exponents $(l+1)$ and $-l$. A solution of the type sought thus always exists, and is unique except for an arbitrary multiplicative factor independent of r.

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[1] Cf. J. E. Rosenthal and L. Motz, "Application of a new mathematical method to vibration rotation interaction," Proc. Nat. Acad. Sci. **23**, 259–265 (1937). We have chosen to depart from the notation of this paper by writing r and l in the place of ρ and J, in order to avoid a later confusion of symbols.

[2] This paper was written after a reading of that by Rosenthal and Motz cited in reference 1. The authors of that paper attempted the solution of the problem here considered by a procedure which may be briefly described as follows: With v any non-negative integer, the function Y is taken to be a solution of the equation

$$(d^2Y/dr^2)-\{((r-1)^2/4\alpha^2)-(2v+1/2\alpha)\}Y=0,$$

which vanishes at $r=\infty$. The differences $(\lambda-v)$ and $(\log F-\log Y)$ are then assumed to be expressible as power series in α. Recurrence formulas for the coefficients of these series are obtained by substituting the assumed forms of λ and F into Eq. (1.1), and by taking suitable regard of the boundary conditions the coefficients are formally determined. The calculations are laborious and, unfortunately, generally futile, since the results are divergent by virtue of their involving infinite discontinuities. No reason is advanced to support any presumption that the method ever yields a usuable result, for even in the exceptional case in which the most glaring cause of failure does not manifest itself, only formal manipulations are described and no consideration is given to the rather essential matter of validity. That such a method of attack upon this problem was foredoomed to failure might well have been predicted. For, in the first place, the comparison of a solution F of an equation which is singular at $r=0$ with a solution Y of a non-singular equation might well have been appraised as unpromising. In the second place, asymptotic representations, such as the assumed power series in α would in this case be, familiarly fail to maintain their validity over intervals that contain a turning point. In the light of these facts, the title of the paper in question might well be regarded as a bit naive, rather bombastic, and, what is worst, wholly misleading.

Equation (1.1) near $r=0$ is of a type which has been considered by the author, and for which the forms of the solutions are accordingly known.[3] As it stands the equation is not of the normal form assumed in (L. '35). It may be normalized, however, by the change of variables

$$r=z^2/4, \quad F=z^{\frac{1}{2}}u, \tag{2.1}$$

which gives it the form

$$(d^2u/dz^2)+\{(z^2[(1-z^2/4)^2-2\alpha(2\lambda+1)]/-16\alpha^2)+(\tfrac{1}{4}-(2l+1)^2/z^2)\}u=0. \tag{2.2}$$

It is then of the type

$$(d^2u/dz^2)+\{\rho^2\varphi^2+(\tfrac{1}{4}-A^2/z^2)\}u=0,$$

which is basic to (L. '35), and conforms to it with

$$\begin{aligned}&\rho=i/4\alpha,\\&\varphi=z\{(1-(z^2/4))^2-2\alpha(2\lambda+1)\}^{\frac{1}{2}},\\&\mu=\tfrac{1}{4},\\&\beta=l+\tfrac{1}{2}.\end{aligned} \tag{2.3}$$

It is an essential hypothesis of (L. '35) that the function φ be bounded from zero except near $z=0$ on the interval concerned. This restricts the interval in the present instance to exclude the points at which

$$(1-(z^2/4))^2-2\alpha(2\lambda+1)=0,$$

namely, the points $r=1\pm(2\alpha(2\lambda+1))^{\frac{1}{2}}$. The results which may be taken from (L. '35) are accordingly valid for r on a range

$$0\leqq r\leqq b, \text{ with } b<1-(2\alpha(2\lambda+1))^{\frac{1}{2}}. \tag{2.4}$$

In terms of the functions

$$\xi=\rho\int_0^z\varphi dz,$$

namely, in this case,

$$\xi=(i/2\alpha)\int_0^r\{(1-r)^2-2\alpha(2\lambda+1)\}^{\frac{1}{2}}dr, \tag{2.5}$$

the paper (L. '35) describes a solution u_1 of Eq. (2.2), which vanishes at $z=0$, by the formulas

$$u_1=(\xi^{\beta+\frac{1}{2}}/\rho^{\frac{1}{2}}\varphi^{\frac{1}{2}})\{\xi^{-\beta}J_\beta(\xi)+(\xi/\rho)O(1)\}, \tag{2.6}$$

when $|\xi|$ is small or of moderate magnitude, and

$$u_1=(1/\rho^{\frac{1}{2}}\varphi^{\frac{1}{2}})\{c_1e^{i\xi}[1]+c_2e^{-i\xi}[1]\}, \tag{2.7}$$

when $|\xi|$ is large. As usual J_β denotes here the Bessel function of the first kind of the order β. The symbol $O(1)$ stands for a bounded function of r and ρ, and $[x]$ is intended to denote a quantity which differs from x by at most terms of the order of $1/\xi$ or of the order of $(\log\rho)/\rho$. When $\arg z=0$, as is the case when r is on the interval (2.4), the coefficients to be used in the formula (2.7) are

$$\begin{aligned}c_1&=(1/(2\pi)^{\frac{1}{2}})\exp(-(\beta+\tfrac{1}{2})\pi i/2),\\c_2&=(1/(2\pi)^{\frac{1}{2}})\exp((\beta+\tfrac{1}{2})\pi i/2).\end{aligned}$$

The formula (2.7) is explicit only to terms of the order of $(\log\rho)/\rho$, which means in the present instance terms of the order of $\alpha\log\alpha$. It is, therefore, clearly useless to retain in the symbols involved by it any terms of the order of α or its higher powers. We may therefore use as appropriate equivalents the following:

$$\begin{aligned}&\varphi\sim z(1-r),\\&\xi\sim i\{(1-(1-r)^2/4\alpha)+(\lambda+\tfrac{1}{2})\log(1-r)\},\\&(\xi/\rho)\sim\{1-(1-r)^2\}.\end{aligned} \tag{2.8}$$

The formula (2.7) thus becomes

$$\begin{aligned}z^{\frac{1}{2}}u_1=&(\exp((l+1)\pi i/2)/(2\pi)^{\frac{1}{2}}\rho^{\frac{1}{2}})\\&\times\{(-1)^{l+1}(1-r)^{-\lambda-1}\\&\times\exp(-1-(1-r)^2/4\alpha)[1]\\&+(1-r)^\lambda\exp(1-(1-r)^2/4\alpha)[1]\}.\end{aligned} \tag{2.9}$$

III. THE SOLUTION AROUND $r=1$

On an interval containing the turning point $r=1$, Eq. (1.1) is of the form

$$(d^2F/dr^2)-\{\sigma^2\chi_0+\sigma\chi_1+\chi_2\}F=0, \tag{3.1}$$

with

$$\sigma=1/\alpha, \quad \chi_0=r-1/2, \quad \chi_1=-(\lambda+\tfrac{1}{2}), \quad \chi_2=l(l+1)/r^2. \tag{3.2}$$

This is again a type which has been considered by the author, and for which the forms of the solutions are known.[4] The equation is normal,

[3] R. E. Langer, "On the asymptotic solutions of ordinary differential equations, with reference to the Stokes' phenomenon about a singular point," Trans. Am. Math. Soc. 37, 397–416 (1935). We shall refer to this paper briefly by the notation (L. '35).

[4] R. E. Langer, "The asymptotic solutions of certain linear ordinary differential equations of the second order," Trans. Am. Math. Soc. 36, 90–106 (1934). We shall refer to this paper briefly by the notation (L. '34).

as that is defined in (L. '34), and for it

$$k=(\lambda/2)+\tfrac{1}{4},\quad \varphi=(r-1),\quad \xi=(r-1)^2/2\alpha,$$
$$\theta=l(l+1)/r^2.^5 \qquad (3.3)$$

It is supposed in (L. '34) that the interval in question is one upon which the function

$$\int |(\theta/\varphi)|dr$$

is bounded except near $r=1$. This is readily seen to exclude the point $r=0$ in the present case, but to impose no other condition. We may therefore take r in this section to have a range

$$a\leqq r<\infty,\ \text{with}\ 0<a<b. \qquad (3.4)$$

A solution of Eq. (1.1) which vanishes at $r=\infty$ is denoted in (L. '34) by $u_{0,2}$. For values of r such that $(r-1)$ is positive and sufficiently large, the form of this solution is given as

$$u_{0,2}=(1/\sigma^{\frac{1}{4}}\varphi^{\frac{1}{2}})\xi^k\exp(-\tfrac{1}{2}\xi)[1],$$

namely, in terms of the original variables as

$$u_{0,2}=(1/\sigma^{\frac{1}{4}}(2\alpha)^k)(r-1)^\lambda \times\exp(-(r-1)^2/4\alpha)[1]. \qquad (3.5)$$

For values of r near the turning point this solution is given to be of the form

$$u_{0,2}=(1/\sigma^{\frac{1}{4}}\varphi^{\frac{1}{2}})\{(\Gamma(-\tfrac{1}{2})/\Gamma(\tfrac{1}{4}-k))M_{k,1/4}(\xi) +(\Gamma(\tfrac{1}{2})/\Gamma(\tfrac{3}{4}-k))M_{k,-1/4}(\xi)\}+\log\sigma/\sigma O(1),$$

with $M_{k,\pm 1/4}$ designating the confluent hypergeometric function usually so denoted.[6] By use of the gamma-function relations

$$\begin{aligned}&\Gamma(\tfrac{1}{2})=(\pi)^{\frac{1}{2}},\quad \Gamma(-\tfrac{1}{2})=-2(\pi)^{\frac{1}{2}},\\ &\Gamma(x)\Gamma(1-x)=\pi/\sin\pi x,\\ &\Gamma(x)\Gamma(\tfrac{1}{2}+x)=(\pi)^{\frac{1}{2}}2^{1-2x}\Gamma(2x),^7\end{aligned} \qquad (3.6)$$

and, in terms of the original variables, it is thus found that near the turning point

$$u_{0,2}=(1/(\pi)^{\frac{1}{2}}\sigma^{\frac{1}{4}}(r-1)^{\frac{1}{2}}) \times\{2\sin(\lambda\pi/2)\Gamma(\lambda/2+1)M_{k,1/4}((r-1)^2/2\alpha) +\cos(\lambda\pi/2)\Gamma(\lambda+1/2)M_{k,-1/4}((r-1)^2/2\alpha)\} +\alpha\log\alpha O(1). \qquad (3.7)$$

When r is on the interval (3.4), but $r<1$, the relation $(r-1)=(1-r)\exp(\pi i)$ gives

$$\varphi=(1-r)\exp(\pi i)$$

and

$$\xi=(1-r)^2/2\alpha\exp(2\pi i). \qquad (3.8)$$

Accordingly, $\arg\xi=2\pi$, and for values of r not too near $r=1$ it is then given that

$$u_{0,2}=1/\sigma^{\frac{1}{4}}\varphi^{\frac{1}{2}}\{[A_{2,1}{}^{(0,1)}]\xi^{-k}\exp(\tfrac{1}{2}\xi) +[A_{2,2}{}^{(0,1)}]\xi^k\exp(-\tfrac{1}{2}\xi)\},$$

with

$$A_{2,1}{}^{(0,1)}=-\pi\{(-i\exp(2k\pi i)/\Gamma(\tfrac{1}{4}-k)\Gamma(\tfrac{3}{4}-k)) -(i\exp(2k\pi i)/\Gamma(\tfrac{3}{4}-k)\Gamma(\tfrac{1}{4}-k))\},$$

$$A_{2,2}{}^{(0,1)}=-\pi\{(i\exp(-(k-\tfrac{1}{4})\pi i)/\Gamma(\tfrac{1}{4}-k)\Gamma(\tfrac{3}{4}+k) -(i\exp(-(k+\tfrac{1}{4})\pi i)/\Gamma(\tfrac{3}{4}-k)\Gamma(\tfrac{1}{4}+k))\}.$$

These latter evaluations are easily reduced by means of the relations (3.6), and are thus found to be

$$A_{2,1}{}^{(0,1)}=\frac{\exp((2k-\frac{1}{2})\pi i)\sin(2k-\frac{1}{2})\pi\Gamma(2k+\frac{1}{2})}{(\pi)^{\frac{1}{2}}2^{2k-\frac{1}{2}}},$$

$$A_{2,2}{}^{(0,1)}=1.$$

In terms of the original variables, therefore,

$$u_{0,2}=\frac{\exp(-(1/4\alpha)+\lambda\pi i)}{\sigma^{\frac{1}{4}}(2\alpha)^k}\{-(2/\pi)^{\frac{1}{2}}\alpha^{\lambda+\frac{1}{2}} \times\exp((1/2\alpha)-\lambda\pi i)\Gamma(\lambda+1)[\sin\lambda\pi] \times(1-r)^{-\lambda-1}\exp(-1-(1-r)^2/4\alpha) +(1-r)^\lambda\exp(1-(1-r)^2/4\alpha)[1]\}. \qquad (3.9)$$

IV. THE CHARACTERISTIC VALUES AND FUNCTIONS

Formulas (2.9) and (3.9) are both valid between 0 and 1 on the interval $a\leqq r\leqq b$. They

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[5] It will be observed that certain symbols have here a meaning which is different from that which was assigned them in Section II. No confusion need arise from this, since the results are to be expressed promptly in terms of the original variables.

[6] Cf. E. T. Whittaker and G. N. Watson, *A Course in Modern Analysis* (Cambridge University Press, London, 1927), fourth edition, p. 337.

[7] Cf. N. Nielsen, *Handbuch der Theorie der Gammafunktion* (B. G. Teubner, Leipzig, 1906), pp. 14, 19.

describe, respectively, solutions which vanish at $r=0$ and at $r=\infty$. These solutions must be multiples of each other if the equation is to admit a characteristic solution (Eigenfunktion). This will evidently be so if and only if

$$(-1)^{l+1} = -(2/\pi)^{\frac{1}{2}}\alpha^{\lambda+\frac{1}{2}} \times \exp(1/2\alpha+\lambda\pi i)\Gamma(\lambda+1)[\sin\lambda\pi],$$

namely, if

$$[\sin\lambda\pi] = (\pi/2)^{\frac{1}{2}} \times ((-1)^l \exp(\lambda\pi i)/\Gamma(\lambda+1)\alpha^{\lambda+\frac{1}{2}} \exp(1/2\alpha)). \quad (4.1)$$

This is, therefore, the characteristic equation whose roots are the λ-Eigenwerte.

The left-hand member of Eq. (4.1) stands for a quantity which differs from $\sin\lambda\pi$ by a term of at most the order of $\alpha \log\alpha$. Since (at least for moderate values of λ) the right-hand member is small relative to $\alpha \log\alpha$, Eq. (4.1) can be assured to give only the result

$$\sin\lambda\pi = O(\alpha \log\alpha).$$

The characteristic values thus differ from integers by terms of at most the order of $\alpha \log\alpha$, namely,

$$\lambda = v + O(\alpha \log\alpha), \quad (4.2)$$

with v an integer.

Let us designate the characteristic solution by F. It is a multiple of the function $z^{\frac{1}{2}}u_1$, of Section II, and likewise of $u_{0,2}$ of Section III. If, for convenience, we determine it by the relation

$$F = \rho^{-(\beta+\frac{1}{2})}z^{\frac{1}{2}}u_1, \quad (4.3)$$

formula (2.6) shows it to have, for values of r near $r=0$, the form

$$F = (\{1-(1-r)^2\}^{l+1}/(1-r)^{\frac{1}{2}})\{\xi^{-(l+\frac{1}{2})}J_{l+\frac{1}{2}}(\xi) + \{1-(1-r)^2\}O(1)\}, \quad (4.4)$$

with ξ as given in Section II. Although this value of ξ is purely imaginary, the term $\xi^{-(l+\frac{1}{2})}J_{l+\frac{1}{2}}(\xi)$ is real. It may be written alternatively as $|\xi|^{-(l+\frac{1}{2})}I_{l+\frac{1}{2}}(|\xi|)$. For values of r between 0 and 1, but not too near either 0 or 1, the form as obtained from (2.9) is

$$F = ((4\alpha)^{l+1}/(2\pi)^{\frac{1}{2}})\{(-1)^{l+1}(1-r)^{-\lambda-1} \times \exp(-1-(1-r)^2/4\alpha)[1] + (1-r)^{\lambda}\exp(1-(1-r)^2/4\alpha)[1]\}. \quad (4.5)$$

The relation between F and $u_{0,2}$ is easily determined from (4.3) and a comparison of formulas (2.9) and (3.9). It is thus found that

$$F = ((4\alpha)^{l+1}(2\alpha)^k \exp(1/4\alpha - \lambda\pi i)/(2\pi)^{\frac{1}{2}})u_{0,2}.$$

In accordance with (4.2) we may use in this the evaluation

$$\exp(-\lambda\pi i) = (-1)^v[1].$$

The formula (3.7) thus shows that for values of r near $r=1$

$$F = ((-1)^v(4\alpha)^{l+1}(2\alpha)^k e^{1/4\alpha}/\pi\sqrt{2}) \times \{2\sin(\lambda\pi/2)\Gamma(\lambda/2+1)M_{k,1/4}((r-1)^2/2\alpha) + \cos(\lambda\pi/2)\Gamma(\lambda+1/2) \times M_{k,-1/4}((r-1)^2/2\alpha) + O(\alpha^{\frac{1}{4}}\log\alpha)\}, \quad (4.6)$$

with $k=\lambda/2+\frac{1}{4}$. Finally, for values of r that are larger than 1 and not too near 1, the formula (3.5) shows that

$$F = ((-1)^v(4\alpha)^{l+1}e^{1/4\alpha}/(2\pi)^{\frac{1}{2}})(r-1)^{\lambda} \times \exp(-(r-1)^2/4\alpha)[1]. \quad (4.7)$$