PHILOSOPHICAL TRANSACTIONS OF THE ROYAL SOCIETY A MATHEMATICAL, PHYSICAL & ENGINEERING SCIENCES

Rotation of a Rigid Diatomic Dipole Molecule in a Homogeneous Electric Field III. New Phase-Integral Quantization Conditions, Expected to be Most Accurate When the Magnetic Quantum Number is Large or Equal to Zero, Expressed in Terms of Complete Elliptic Integrals: Survey of their Accuracy

Kilian Larsson

Phil. Trans. R. Soc. Lond. A 1994 **347**, 37-63
doi: 10.1098/rsta.1994.0038

Rotation of a rigid diatomic dipole molecule in a homogeneous electric field

III. New phase-integral quantization conditions, expected to be most accurate when the magnetic quantum number is large or equal to zero, expressed in terms of complete elliptic integrals: survey of their accuracy

By Kilian Larsson

Department of Theoretical Physics, University of Uppsala, Box 803, S-751 08 Uppsala, Sweden

Some new quantization conditions for the energy levels of a rigid diatomic dipole molecule in a homogeneous electric field of arbitrary strength, obtained by means of a phase-integral method involving phase-integral approximations of arbitrary order generated from two particular choices of the base function, are expressed in terms of complete elliptic integrals in the first, third and fifth order of the phase-integral approximation. One choice of the base function is especially useful for large absolute values of the magnetic quantum number m. The case $m = 0$ is considered with another choice of the base function, expected to be useful for small values of $|m|$. The great accuracy of the energy levels, yielded by the quantization conditions, is demonstrated for arbitrary electric fields in a number of diagrams pertaining to different values of the quantum numbers. For very weak and very strong electric fields explicit series expansions for the energy levels can be obtained from the quantization conditions, and these expansions are compared with previously obtained series expansions.

The investigation confirms that the phase-integral quantization conditions yield very accurate eigenvalues for all values of the electric field strength.

1. Introduction

This paper is the third in a series concerning the energy levels of a rigid diatomic dipole molecule rotating in a static homogeneous electric field. In the first of these papers (this Volume), which will hereafter be referred to as I, the historical background concerning the energy quantization problem according to quantum mechanics of a linear rigid polar rotator in a homogeneous electric field was outlined, and the Schrödinger equation for that system was recalled. Furthermore, new quantization conditions, valid for arbitrary strengths of the electric field, were obtained by means of a phase-integral method involving a phase-integral approximation of arbitrary order generated from an unspecified base function. In the second paper (this Volume), hereafter referred to as II, the case of field-free space as well as the limiting cases of very weak and very strong fields were considered, and for these cases the already known explicit expressions for the energy levels and their applicability were reviewed in a lucid way.

Phil. Trans. R. Soc. Lond. A (1994) **347**, 37–63

Printed in Great Britain

In this paper a quantization condition given in I, for a particular choice of the base function, which is particularly useful for large absolute values of the magnetic quantum number, $|m|$, is expressed in terms of complete elliptic integrals in the first, third and fifth order of the phase-integral approximation. Furthermore, quantization conditions for another choice of the base function, which is particularly useful for sufficiently small values of $|m|$, are also expressed in terms of complete elliptic integrals in the first, third and fifth order of the phase-integral approximation in the case that the magnetic quantum number equals zero. For very weak and very strong electric fields explicit series expansions for the energy levels can be obtained from the above-mentioned quantization conditions, and these series expansions are compared with the corresponding perturbation series. For arbitrary strengths of the electric field the great accuracy of the energy levels obtainable from the original quantization conditions is finally demonstrated in a number of diagrams; these diagrams also facilitate subsequent use of the quantization conditions.

Briefly reviewing the physical problem (cf. §2 in I), we consider a rigid diatomic molecule with a permanent electric dipole moment of the magnitude p. The moment of inertia of the rigid diatomic molecule about any axis through the centre of mass and perpendicular to the internuclear axis is denoted by I, and the polar angles of the internuclear axis are denoted by ϑ and φ. When the molecule is situated in an external static and homogeneous electric field of the strength F, which has the direction corresponding to $\vartheta = 0$, the potential energy is given by the expression

$$V(\cos\vartheta) = -pF\cos\vartheta. \tag{1.1}$$

If we introduce instead of the original wavefunction Ψ the new function ψ, defined by

$$\Psi = \psi(\vartheta)\,\mathrm{e}^{\mathrm{i}m\varphi} \tag{1.2}$$

for integral values of the magnetic quantum number m, and define the dimensionless quantities W and ω by the formulas

$$W = \frac{2I}{\hbar^2}E, \tag{1.3}$$

$$\omega = \frac{2I}{\hbar^2}pF, \tag{1.4}$$

where E is the energy, the Schrödinger equation for the stationary motion of the linear rigid polar rotator takes the form

$$\left[\frac{1}{\sin\vartheta}\frac{\mathrm{d}}{\mathrm{d}\vartheta}\left(\sin\vartheta\frac{\mathrm{d}}{\mathrm{d}\vartheta}\right) - \frac{m^2}{\sin^2\vartheta} + W + \omega\cos\vartheta\right]\psi = 0. \tag{1.5}$$

The energy eigenvalue problem is to be solved with the boundary conditions that ψ must vanish for $\vartheta = 0$ and for $\vartheta = \pi$.

It was demonstrated in I that the transformation

$$z = \cos\vartheta, \tag{1.6}$$

$$v = (1-z^2)^{\frac{1}{2}}\psi \tag{1.7}$$

reduces the differential equation (1.5) to the normal form

$$\frac{d^2v}{dz^2}+R(z)\,v=0, \tag{1.8}$$

where
$$R(z)=\frac{W+\omega z}{1-z^2}+\frac{1-m^2}{(1-z^2)^2}. \tag{1.9}$$

The eigenvalues of W are obtained by solving the differential equation (1.8) with the boundary conditions that v be equal to zero for $z=\pm 1$.

The differential equation (1.8) was the starting point for the phase-integral treatment of the energy eigenvalue problem in I. This equation has as approximate solutions the two linearly independent phase-integral functions (3.2) in I, i.e.

$$v=q^{-\frac{1}{2}}(z)\exp\left(\pm\mathrm{i}\int^{z}q(z)\,dz\right), \tag{1.10}$$

where, for the phase-integral approximation of the order $2N+1$,

$$q(z)=\sum_{s=0}^{N}Y_{2s}\,Q(z)\,dz, \tag{1.11}$$

$Q(z)$ being the unspecified base function, which is to be chosen conveniently. For the definition of the first few quantities Y_{2s}, see equations (3.4*a–c*) in I.

2. The base function

The square of the base function is conveniently chosen according to equation (3.8) in I, i.e.

$$Q^2(z)=\frac{W+\frac{1}{4}+\omega z}{1-z^2}-\frac{4\xi_0^2}{(1-z^2)^2}, \tag{2.1}$$

where ξ_0 is a constant which can be chosen conveniently. As was pointed out in I, there are two natural choices of ξ_0, namely $\xi_0=\frac{1}{2}|m|$ when $|m|$ is sufficiently large, and $\xi_0=0$ when $|m|$ is sufficiently small; for both these choices the phase-integral approximation yields the exact energy eigenvalues if $\omega=0$.

When $\xi_0=|m|/2>0$: the expression (2.1) takes the form

$$Q^2(z)=\frac{W+\frac{1}{4}+\omega z}{1-z^2}-\frac{m^2}{(1-z^2)^2}, \tag{2.2}$$

and with the aid of (1.9) we obtain

$$R(z)-Q^2(z)=-\frac{1}{4(1-z^2)}+\frac{1}{(1-z^2)^2}. \tag{2.3}$$

It is evident from (2.2) that $Q^2(z)$ has second-order poles at $z=\pm 1$. When $\omega>0$, the function $Q^2(z)$ has three simple, real zeros and we conveniently write (2.2) in the form

$$Q^2(z)=\omega\frac{(a-z)(z-b)(z-c)}{(1-z^2)^2}. \tag{2.4}$$

If W is an eigenvalue it turns out that a, b and c satisfy the inequalities

$$c < -1 < b < a < +1, \quad |b| < a. \tag{2.5}$$

This is proved in Appendix C, where further estimates of c are given as well.

When $\xi_0 = 0$ *and* $\omega > 0$: the expression (2.1) reduces to

$$Q^2(z) = \omega \frac{z-t}{1-z^2}, \tag{2.6}$$

where
$$t = -\frac{W+\frac{1}{4}}{\omega}. \tag{2.7}$$

Thus, in this case $Q^2(z)$ has a simple zero at $z = t$ and simple poles at $z = \pm 1$.

3. Phase-integral quantization conditions

In this paper we restrict the investigation to the case when $\xi_0 = \frac{1}{2}|m| > 0$ and to the case when $\xi_0 = 0$ and $m = 0$. In the $(2N+1)$th-order phase-integral approximation the energy eigenvalues of (1.8) are thus obtainable from the quantization conditions, cf. equations (3.17), (3.18), (4.10), (4.11*b*) and (4.12*a*) in I,

$$\sum_{s=0}^{N} \mathscr{L}^{(2s+1)} = (|m|+n+\tfrac{1}{2})\,\pi, \quad \xi_0 = \tfrac{1}{2}|m| > 0, \quad \text{the case in figure 1,} \tag{3.1}$$

$$\sum_{s=0}^{N} \mathscr{L}^{(2s+1)} = (n+\tfrac{3}{4})\,\pi - \varDelta, \quad \xi_0 = 0 \quad \text{and} \quad m = 0, \text{ the cases in figures 2 and 3,} \tag{3.2a}$$

where $n = 0, 1, 2, \ldots$, and

$$\mathscr{L}^{(2s+1)} = \frac{1}{2} \int_{\varLambda} Z_{2s}\, Q(z)\, \mathrm{d}z \tag{3.3}$$

with the first few Z_{2s} given by the expressions (3.6*a*–*c*) in I. The quantity $\varDelta$ in the right-hand member of (3.2*a*) is a phase obtained by means of comparison equation technique, and it is given by equation (4.3) in I. When t in figure 2 moves towards the left away from $z = -1$ or when t in figure 3 moves towards the right away from $z = -1$, the quantity $\varDelta$ tends to the constant value $\frac{1}{4}\pi$ (cf. formulas (4.8′) in I) and then we can replace (3.2*a*) by its limiting form (cf. equations (4.12*a*, *b*) in I)

$$\sum_{s=0}^{N} \mathscr{L}^{(2s+1)} = (n+\tfrac{1}{2})\,\pi, \quad \xi_0 = 0 \quad \text{and} \quad m = 0, \quad \text{the cases in figures 2 and 3,} \tag{3.2b}$$

where $n = 0, 1, 2, \ldots$.

(*a*) *The case when* $\xi_0 = \frac{1}{2}|m| > 0$

The square of the base function, $Q^2(z)$, pertaining to the case when $\xi_0 = \frac{1}{2}|m| > 0$ and $\omega > 0$, is given by (2.4) with the zeros a, b and c subject to the conditions (2.5). To define the base function $Q(z)$ completely, its phase must be specified. Thus, in order to make $Q(z)$ single-valued, a cut is introduced along the real axis from $z = -\infty$

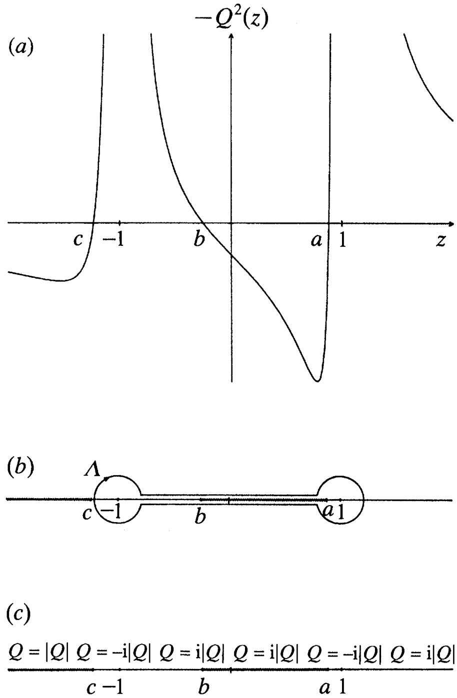


Figure 1. This figure refers to the case when $\xi_0 = |m|/2 > 0$ and $\omega > 0$. (a) Graphical representation of $-Q^2(z)$, i.e. the negative of the square of the base function, defined according to (2.2). The function $Q^2(z)$ has second-order poles at $z = \pm 1$ and three simple real zeros a, b and c which fulfil the inequalities (2.5), i.e. $c < -1 < b < a < +1$ and $|b| < a$. (b) The contour of integration Λ in the complex z-plane introduced in (3.3). (c) Phase chosen for the base function $Q(z)$. Cuts are denoted by wavy lines.

to $z = c$ and along the part $b < z < a$ of the real axis, where $Q^2(z) > 0$, and $Q(z)$ is defined to be positive on the upper lip of the last-mentioned cut (cf. figure 1). The contour of integration Λ in (3.3) encircles in the negative sense the poles at $z = \pm 1$, as well as the turning points b and a, but not the transition point c (cf. figure 1).

If we introduce the quantities

$$A_\mu = \frac{1}{4Q^{\mu+2}(z)} \frac{\mathrm{d}^\mu Q^2(z)}{\mathrm{d}z^\mu}, \quad \mu = 0, 1, 2, \ldots, \tag{3.4}$$

$$B_\mu = \frac{1}{Q^{\mu+2}(z)} \frac{\mathrm{d}^\mu [R(z) - Q^2(z)]}{\mathrm{d}z^\mu}, \quad \mu = 0, 1, 2, \ldots, \tag{3.5}$$

we can conveniently write expressions (3.6*a–c*) in I as follows

$$Z_0 = 1, \tag{3.6a}$$

$$Z_2 = \tfrac{1}{12}(6B_0 - A_2) - \frac{\mathrm{d}}{\mathrm{d}\zeta}(\tfrac{5}{12}A_1), \tag{3.6b}$$

$$Z_4 = -\tfrac{1}{8}(B_0^2 - A_2 B_0 + \tfrac{1}{6}B_2 + \tfrac{7}{12}A_2^2 - \tfrac{5}{12}A_1 A_3) + \frac{1}{8}\frac{\mathrm{d}}{\mathrm{d}\zeta}(\tfrac{25}{18}A_1^3 + A_1 B_0 + \tfrac{1}{6}B_1 - \tfrac{5}{12}A_1 A_2), \tag{3.6c}$$

where
$$\zeta = \int^z Q(z)\,\mathrm{d}z. \tag{3.7}$$

The terms containing total derivatives with respect to ζ in (3.6a–c) give no contribution to the integral in the right-hand member of (3.3). Furthermore, the expressions are given in a form in which the powers of $Q(z)$, occurring in the denominators of the remaining terms in (3.6a–c), are as low as possible; cf. (3.4) and (3.5).

Since, according to (2.4), the base function $Q(z)$ is equal to the square root of a polynomial in z of the third degree without multiple zeros divided by $1-z^2$, the integral (3.3) can be expressed in terms of complete elliptic integrals. Adopting the notations of Byrd & Friedman (1971), we denote the complete elliptic integrals of the first, second and third kinds, defined by (A 1a,b), (A 2a,b) and (A 3a,b) in our Appendix A, by $K(k)$, $E(k)$ and $\Pi(\alpha^2, k)$, respectively. The number k is called the modulus, and α^2 is referred to as the parameter of the elliptic integral of the third kind.

By a convenient transformation of the independent variable z, which will simplify the calculation of $\mathscr{L}^{(2s+1)}$, we introduce the jacobian elliptic functions sn, cn and dn, defined according to (A 5), (A 6) and (A 7), respectively. Thus we put (cf. Byrd & Friedman 1971, §236)
$$z = a-(a-b)\,\mathrm{sn}^2\,u, \tag{3.8}$$
where we follow the convention of not indicating the dependence of the jacobian elliptic functions on the modulus k, which in the present case is defined by
$$k^2 = \frac{a-b}{a-c}. \tag{3.9}$$

Since according to (2.5) $c < b < a$, the inequality
$$0 < k^2 < 1 \tag{3.10}$$
holds. It easily follows from (3.8), (3.9), (A 8) and (A 9) that the numerator of $Q^2(z)$ in (2.4) transforms according to
$$(a-z)\,(z-b)\,(z-c) = (a-b)^2(a-c)\,\mathrm{sn}^2\,u\,\mathrm{cn}^2\,u\,\mathrm{dn}^2\,u, \tag{3.11}$$
and analogously the square root of the denominator of $Q^2(z)$ transforms according to
$$(1+z)\,(1-z) = \frac{(a-b)^2}{-\alpha_1^2\,\alpha_2^2}(1-\alpha_1^2\,\mathrm{sn}^2\,u)\,(1-\alpha_2^2\,\mathrm{sn}^2\,u), \tag{3.12}$$
with the parameters α_1^2 and α_2^2 defined by
$$\alpha_1^2 = \frac{a-b}{a+1} \quad (>0), \tag{3.13a}$$
$$\alpha_2^2 = \frac{a-b}{a-1} \quad (<0). \tag{3.13b}$$

With the aid of (3.9) and (3.13a,b) it is easy to show that
$$a-b = k^2(a-c) = \frac{2(-\alpha_1^2\,\alpha_2^2)}{\alpha_1^2-\alpha_2^2}. \tag{3.14}$$

By inserting (3.11), (3.12) and (3.14) into (2.4) we obtain

$$Q^2 = \frac{\omega(-\alpha_1^2\alpha_2^2)(\alpha_1^2-\alpha_2^2)}{2k^2}\frac{\mathrm{sn}^2 u\,\mathrm{cn}^2 u\,\mathrm{dn}^2 u}{(1-\alpha_1^2\,\mathrm{sn}^2 u)^2(1-\alpha_2^2\,\mathrm{sn}^2 u)^2}, \tag{3.15}$$

and by substituting (3.12) and (3.14) into (2.3), we obtain

$$R-Q^2 = \frac{(\alpha_1^2-\alpha_2^2)^2}{16(-\alpha_1^2\alpha_2^2)^2}\left(\frac{(\alpha_1^2-\alpha_2^2)^2}{(1-\alpha_1^2\,\mathrm{sn}^2 u)^2(1-\alpha_2^2\,\mathrm{sn}^2 u)^2}-\frac{-\alpha_1^2\alpha_2^2}{(1-\alpha_1^2\,\mathrm{sn}^2 u)(1-\alpha_2^2\,\mathrm{sn}^2 u)}\right). \tag{3.16}$$

Furthermore, by means of (3.8), (3.14) and (A 13) we obtain the operator identity

$$\frac{\mathrm{d}}{\mathrm{d}z} = -\frac{\alpha_1^2-\alpha_2^2}{4(-\alpha_1^2\alpha_2^2)}\frac{1}{\mathrm{sn}\,u\,\mathrm{cn}\,u\,\mathrm{dn}\,u}\frac{\mathrm{d}}{\mathrm{d}u}. \tag{3.17}$$

Although straight-forward, the calculation of $\mathscr{L}^{(2s+1)}$ by means of (3.3), (3.4)–(3.7) and (3.15)–(3.17) is lengthy, and the intermediate steps are far too bulky to be given here. Up to the fifth order of approximation, the integrand in the right-hand member of (3.3), when transformed to the variable u, turns out to be a sum of terms of the type

$$\frac{S(\mathrm{sn}^2 u, \mathrm{cn}^2 u, \mathrm{dn}^2 u)}{(1-\alpha_1^2\,\mathrm{sn}^2 u)^p(1-\alpha_2^2\,\mathrm{sn}^2 u)^p\,\mathrm{sn}^{2r} u\,\mathrm{cn}^{2r} u\,\mathrm{dn}^{2r} u}, \quad p=0,1;\, r=0,1,2,3, \tag{3.18}$$

where $S(\mathrm{sn}^2 u, \mathrm{cn}^2 u, \mathrm{dn}^2 u)$ denotes a polynomial in $\mathrm{sn}^2 u$, $\mathrm{cn}^2 u$, and $\mathrm{dn}^2 u$. The main problem is to decompose the integrand into partial fractions. To this end frequent use is made of (A 8)–(A 15). All the resulting partial fractions yield simple integrals which can be found in Byrd & Friedman (1971). It is convenient to define the quantities

$$\begin{aligned} g^{(1)}(k,\alpha_1^2,\alpha_2^2) = {} & \frac{2}{(-\alpha_1^2\alpha_2^2)^2}\left(\frac{2\omega(-\alpha_1^2\alpha_2^2)^3}{k^2(\alpha_1^2-\alpha_2^2)}\right)^{\frac{1}{2}}\Big\{\alpha_1^2\alpha_2^2[K(k)-E(k)] \\ & +[-(k^2+1)\alpha_1^2\alpha_2^2+k^2(\alpha_1^2+\alpha_2^2)]K(k) \\ & +\frac{\alpha_2^4(1-\alpha_1^2)(k^2-\alpha_1^2)}{\alpha_1^2-\alpha_2^2}\Pi(\alpha_1^2,k)+\frac{\alpha_1^4(1-\alpha_2^2)(k^2-\alpha_2^2)}{\alpha_2^2-\alpha_1^2}\Pi(\alpha_2^2,k)\Big\} \end{aligned} \tag{3.19a}$$

$$\begin{aligned} g^{(3)}(k,\alpha_1^2,\alpha_2^2) = {} & \frac{1}{12k'^4}\left(\frac{k^2(\alpha_1^2-\alpha_2^2)}{2\omega(-\alpha_1^2\alpha_2^2)^3}\right)^{\frac{1}{2}}\{(-(k^2+1)\alpha_1^2\alpha_2^2-(k^4-4k^2+1)(\alpha_1^2+\alpha_2^2) \\ & +(2k^6-3k^4-3k^2+2))[K(k)-E(k)] \\ & +(2\alpha_1^2\alpha_2^2-(k^2+1)(\alpha_1^2+\alpha_2^2)-(k^4-4k^2+1))k^2K(k)\} \end{aligned} \tag{3.19b}$$

$$\begin{aligned} g^{(5)}(k,\alpha_1^2,\alpha_2^2) = {} & \frac{1}{2880k'^{12}}\left(\frac{k^2(\alpha_1^2-\alpha_2^2)}{2\omega(-\alpha_1^2\alpha_2^2)^3}\right)^{\frac{3}{2}}\{((2k^8-298k^6-1200k^4-298k^2+2)\alpha_1^6\alpha_2^6 \\ & +(303k^8+2385k^6+2385k^4+303k^2)\alpha_1^4\alpha_2^4(\alpha_1^2+\alpha_2^2)-(168k^{12}-774k^{10}+3606k^8 \\ & -624k^6+3606k^4-774k^2+168)\alpha_1^4\alpha_2^4-(42k^{12}-186k^{10}+1716k^8+2232k^6+1716k^4 \\ & -186k^2+42)\alpha_1^2\alpha_2^2(\alpha_1^2+\alpha_2^2)^2+(1008k^{14}-4902k^{12}+9744k^{10}-474k^8-474k^6 \end{aligned}$$

PHILOSOPHICAL TRANSACTIONS OF THE ROYAL SOCIETY A MATHEMATICAL, PHYSICAL & ENGINEERING SCIENCES

$$+9744k^4-4902k^2+1008)\,\alpha_1^2\,\alpha_2^2(\alpha_1^2+\alpha_2^2)+(56k^{14}-271k^{12}+546k^{10}+565k^8+565k^6$$
$$+546k^4-271k^2+56)\,(\alpha_1^2+\alpha_2^2)^3-(1680k^{16}-8328k^{14}+16704k^{12}-16914k^{10}$$
$$+19092k^8$$
$$-16914k^6+16704k^4-8328k^2+1680)\,\alpha_1^2\,\alpha_2^2-(1008k^{16}-4968k^{14}+9858k^{12}$$
$$-9690k^{10}$$
$$+12960k^8-9690k^6+9858k^4-4968k^2+1008)\,(\alpha_1^2+\alpha_2^2)^2+(2688k^{18}-13368k^{16}$$
$$+26703k^{14}$$
$$-26670k^{12}+13335k^{10}+13335k^8-26670k^6+26703k^4-13368k^2+2688)\,(\alpha_1^2+\alpha_2^2)$$
$$-(1792k^{20}-8960k^{18}+18018k^{16}-18312k^{14}+9744k^{12}-2772k^{10}+9744k^8$$
$$-18312k^6$$
$$+18018k^4-8960k^2+1792))\,[K(k)-E(k)]+((89k^6+807k^4+807k^2+89)\,\alpha_1^6\,\alpha_2^6$$
$$-(90k^8+1254k^6+2688k^4+1254k^2+90)\,\alpha_1^4\,\alpha_2^4(\alpha_1^2+\alpha_2^2)+(84k^{10}+591k^8+2013k^6$$
$$+2013k^4+591k^2+84)\,\alpha_1^4\,\alpha_2^4+(21k^{10}+444k^8+2223k^6+2223k^4+444k^2$$
$$+21)\,\alpha_1^2\,\alpha_2^2(\alpha_1^2+\alpha_2^2)^2$$
$$-(504k^{12}-2388k^{10}+9204k^8-3888k^6+9204k^4-2388k^2+504)\,\alpha_1^2\,\alpha_2^2\,(\alpha_1^2+\alpha_2^2)$$
$$-(28k^{12}-132k^{10}$$
$$+750k^8+500k^6+750k^4-132k^2+28)\,(\alpha_1^2+\alpha_2^2)^3+(840k^{14}-4059k^{12}+7884k^{10}$$
$$-1977k^8$$
$$-1977k^6+7884k^4-4059k^2+840)\,\alpha_1^2\,\alpha_2^2+(504k^{14}-2421k^{12}+4650k^{10}-45k^8-45k^6$$
$$+4650k^4$$
$$-2421k^2+504)\,(\alpha_1^2+\alpha_2^2)^2-(1344k^{16}-6516k^{14}+12600k^{12}-12030k^{10}+14580k^8$$
$$-12030k^6$$
$$+12600k^4-6516k^2+1344)\,(\alpha_1^2+\alpha_2^2)+(896k^{18}-4368k^{16}+8505k^{14}-8274k^{12}$$
$$+4137k^{10}+4137k^8$$
$$-8274k^6+8505k^4-4368k^2+896))\,k^2K(k)\}, \tag{3.19c}$$

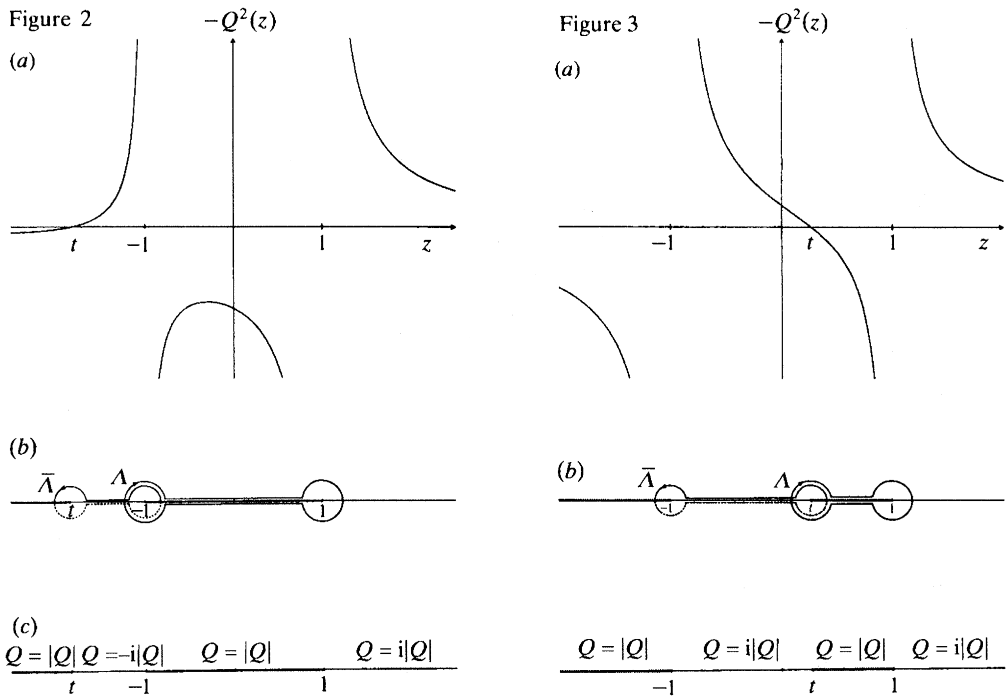
where k' is the complementary modulus related to k by (A 10), i.e.

$$k'^2 = 1-k^2. \tag{3.20}$$

We can then write the first-, third- and fifth-order contributions to the sum in the left-hand member of the quantization condition (3.1) as follows

$$\mathscr{L}^{(1)} = g^{(1)}(k,\alpha_1^2,\alpha_2^2)+|m|\,\pi, \tag{3.21a}$$
$$\mathscr{L}^{(3)} = g^{(3)}(k,\alpha_1^2,\alpha_2^2), \tag{3.21b}$$
$$\mathscr{L}^{(5)} = g^{(5)}(k,\alpha_1^2,\alpha_2^2), \tag{3.21c}$$

which is a result of simple residue calculus, the quantities $g^{(2s+1)}(k,\alpha_1^2,\alpha_2^2)$ originating from evaluation of the integrals $L^{(2s+1)}$ in I (cf. equations (3.14), (3.15) and (3.17)–(3.19) in I).



Figures 2 and 3. These figures refer to the two different cases $t < -1$ and $-1 < t < +1$, which can arise when $\xi_0 = 0$ and $\omega > 0$. In both cases the function $Q^2(z)$ reduces to (2.6), and has thus two first-order poles at $z = \pm 1$ and a single simple real zero $t = -(W + \frac{1}{4})/\omega$. 2 (*a*) Graphical representation of $-Q^2(z)$ when $t < -1$, which is the case when ω is sufficiently small. 3 (*a*) Graphical representation of $-Q^2(z)$ when $-1 < t < +1$, which is the case when ω is sufficiently large. 2 (*b*) and 3 (*b*). The contours of integration Λ and $\bar{\Lambda}$ in the complex z-plane introduced in connection with (3.3) and (3.28) respectively. The part of $\bar{\Lambda}$ which lies on a Riemann sheet adjacent to the complex z-plane under consideration is indicated by a dashed line. 2 (*c*) and 3 (*c*) Phase chosen for the base function $Q(z)$. Cuts are denoted by wavy lines.

In (3.19*a*–*c*) the terms are arranged so as to reveal certain symmetries, and such that the limiting cases when ω tends to zero and to infinity can be obtained easily. In both limits the modulus k tends to zero and then, according to (A 16), (A 17) and (A 18*a*, *b*), the quantities $K(k) - E(k)$ and $k^2K(k)$ are approximately proportional to k^2.

By analogy with the quantization condition (3.2*a*) for $\xi_0 = 0$ and $m = 0$, which is a special case of the quantization condition (4.11*b*) in I, there is also another quantization condition for $\xi_0 = \frac{1}{2}|m| > 0$, given by equation (4.11*a*) in I, which contains a phase Δ of importance when c is close to $z = -1$ (see figure 1). This quantity Δ can also be expressed in terms of the quantities $g^{(2s+1)}(k, \alpha_1^2, \alpha_2^2)$, given by (3.19*a*–*c*), with convenient choices of the moduli and the parameters. However, in this paper we restrict ourselves to considering the simple quantization condition (3.1) for $\xi_0 = \frac{1}{2}|m| > 0$, and we postpone the treatment of the quantization condition (4.11*a*) in I to the following paper (IV).

(*b*) *The case when* $\xi_0 = 0$ *and* $m = 0$

When $\xi_0 = 0$ and $\omega > 0$ the square of the base function, $Q^2(z)$, takes the simple form (2.6), where t is given by (2.7). Two separate cases arise, depending on whether $t < -1$ (figure 2) or $-1 < t < +1$ (figure 3). For both these cases we have, if $m = 0$, the quantization condition (3.2*a*) and its limiting form, the simple quantization condition (3.2b) with $\mathscr{L}^{(2s+1)}$ defined by (3.3), where Λ is now a contour of integration encircling in the negative sense the points delimiting the classically allowed part of the real axis, but leaving the third transition point (turning point or pole) outside the contour of integration (see figures 2 and 3).

(i) *The $\mathscr{L}$-integrals*

Although the base function for $\xi_0 = 0$ is quite different from the one for $\xi_0 = \frac{1}{2}|m| > 0$ and so simple that calculations similar to those presented in §3a for $\xi_0 = \frac{1}{2}|m| > 0$ could be performed with much less effort, it is nevertheless still simpler to obtain the quantities $\mathscr{L}^{(2s+1)}$ for $\xi_0 = 0$ and $m = 0$ as limiting cases of the ones pertaining to the case when $\xi_0 = \frac{1}{2}|m| > 0$, namely (3.21$a$–$c$). To this end it is possible to obtain an expression for the square of the base function, $Q^2(z)$, for $\xi_0 = 0$, which is analogous to (2.4) pertaining to $\xi_0 = \frac{1}{2}|m| > 0$, by multiplying both the numerator and the denominator of the right-hand member of (2.6) by $1 - z^2$. The zeros a, b and c of $Q^2(z)$, given by (2.4) for $\xi_0 = \frac{1}{2}|m| > 0$, then have their counterparts for the case $\xi_0 = 0$ and $m = 0$. Consequently, new moduli k and parameters α_1^2 and α_2^2 can be defined, and by substituting the appropriate values of k^2, α_1^2 and α_2^2 into (3.21a–c) and letting $m \to 0$, we obtain the quantities $\mathscr{L}^{(2s+1)}$ pertaining to the case $\xi_0 = 0$ and $m = 0$. Further details are given in Appendix B, where it is shown that the two expressions for $\mathscr{L}^{(2s+1)}$ pertaining to $t < -1$ and to $-1 < t < +1$, respectively, can be covered by a single expression (see (B 4a–c) with (B 3a, b)). In this section we shall, however, give the separate results obtained by substituting the values of α_1^2 given by (B 3a, b) into (B 4a–c).

When $t < -1$ the quantities $\mathscr{L}^{(2s+1)}$ thus take the form

$$\mathscr{L}^{(1)} = 2\left(\frac{2\omega}{k^2}\right)^{\frac{1}{2}} E(k), \tag{3.22a}$$

$$\mathscr{L}^{(3)} = \frac{1}{12k'^2}\left(\frac{k^2}{2\omega}\right)^{\frac{1}{2}} \{-(k^2-2)\,[K(k) - E(k)] - k^2 K(k)\}, \tag{3.22b}$$

$$\mathscr{L}^{(5)} = \frac{1}{2880k'^6}\left(\frac{k^2}{2\omega}\right)^{\frac{3}{2}} \{(56k^8 - 145k^6 + 129k^4 + 32k^2 - 16)\,[K(k) - E(k)]$$
$$- (28k^6 - 69k^4 + 105k^2 - 8)\,k^2 K(k)\}, \tag{3.22c}$$

where
$$k^2 = 2/(1-t). \tag{3.23}$$

When $-1 < t < +1$ the quantities $\mathscr{L}^{(2s+1)}$ analogously take the form

$$\mathscr{L}^{(1)} = 2(2\omega)^{\frac{1}{2}}\{-[K(k) - E(k)] + k^2 K(k)\}, \tag{3.24a}$$

$$\mathscr{L}^{(3)} = \frac{1}{12k^2k'^2}\frac{1}{(2\omega)^{\frac{1}{2}}}\{-(2k^2-1)\,[K(k) - E(k)] + k^2 K(k)\}, \tag{3.24b}$$

$$\mathscr{L}^{(5)} = \frac{1}{2880k^6k'^6}\frac{1}{(2\omega)^{\frac{3}{2}}}\{(16k^8 - 32k^6 - 129k^4 + 145k^2 - 56)\,[K(k) - E(k)]$$
$$- (8k^6 - 105k^4 + 69k^2 - 28)\,k^2 K(k)\}. \tag{3.24c}$$

where
$$k^2 = \tfrac{1}{2}(1-t). \tag{3.25}$$

PHILOSOPHICAL TRANSACTIONS OF THE ROYAL SOCIETY A MATHEMATICAL, PHYSICAL & ENGINEERING SCIENCES

(ii) *The η-integrals*

When the turning point t, given by (2.7), is located close to the pole at $z = -1$ (cf. figures 2 and 3) it is advantageous to use the quantization condition (3.2*a*) instead of the simple quantization condition (3.2*b*). These quantization conditions have the quantities $\mathscr{L}^{(2s+1)}$, given by (3.22*a*–*c*) when $t < -1$ and by (3.23*a*–*c*) when $-1 < t < +1$, in common. Furthermore, the quantity $\varDelta$ in (3.2*a*) is obtained by substituting $\xi_0 = 0$ and $m = 0$ into equation (4.3) in I. Using equations (4.3)–(4.5) in I, we thus have in the $(2N+1)$th-order of approximation,

$$\varDelta = \tfrac{1}{4}\pi + \arg\Gamma(\tfrac{1}{2}+\mathrm{i}\eta) - \eta\ln|\eta_0| + \sum_{s=0}^{N}\varDelta^{(2s+1)}, \tag{3.26}$$

where
$$\eta = \sum_{s=0}^{N}\eta_{2s}, \tag{3.27}$$

with
$$\eta_{2s} = \frac{\mathrm{i}}{2\pi}\int_{\bar{\varLambda}} Z_{2s}\,Q(z)\,\mathrm{d}z, \tag{3.28}$$

$\bar{\varLambda}$ being a closed contour of integration encircling both t and -1 in the positive sense (cf. figures 2 and 3). The quantities $\varDelta^{(2s+1)}$ in (3.26) are obtained by substituting $m = 0$ into equations (4.7*a*–*c*) in I with the result

$$\varDelta^{(1)} = \eta_0, \tag{3.29a}$$

$$\varDelta^{(3)} = -1/(24\eta_0), \tag{3.29b}$$

$$\varDelta^{(5)} = -\frac{\eta_2^2}{2\eta_0} + \frac{\eta_2}{24\eta_0^2} - \frac{7}{2880\eta_0^3}. \tag{3.29c}$$

Despite the fact that $\bar{\varLambda}$ differs from $\varLambda$ for the case $\xi_0 = 0$ and $m = 0$ as regards the transition points being encircled (cf. figures 2 and 3), we can, by analogy with the treatment in §3*b*(i), obtain also the quantities η_{2s} for $\xi_0 = 0$ and $m = 0$ (with due regard to the sign of η_{2s}) by substituting into (3.19*a*–*c*) the appropriate values of the moduli k and the parameters α_1^2 and α_2^2 and finally letting $m \to 0$. This is performed in the latter part of Appendix B, where we derive a single expression for η_{2s}, which covers the cases $t < -1$ and $-1 < t < +1$ (cf. (B 6*a*–*c*) with (B 7)). In this section we shall merely give the expression for η_{2s} obtained by substituting (B 7) into (B 6*a*–*c*).

When $t < -1$ we thus obtain

$$\eta_0 = -\frac{2}{\pi}\left(\frac{2\omega}{k'^2}\right)^{\frac{1}{2}}[K(k) - E(k)], \tag{3.30a}$$

$$\eta_2 = \frac{1}{12\pi}\frac{1}{k^2}\left(\frac{k'^2}{2\omega}\right)^{\frac{1}{2}}\{(k^2+1)[K(k)-E(k)] - 2k^2K(k)\}, \tag{3.30b}$$

$$\eta_4 = \frac{1}{2880\pi}\frac{1}{k^6}\left(\frac{k'^2}{2\omega}\right)^{\frac{3}{2}}\{(56k^8 - 79k^6 + 30k^4 - 79k^2 + 56)[K(k)-E(k)] - (28k^6 - 36k^4 - 36k^2 + 28)\,k^2K(k)\}, \tag{3.30c}$$

where
$$k^2 = (t+1)/(t-1). \tag{3.31}$$

PHILOSOPHICAL TRANSACTIONS OF THE ROYAL SOCIETY A MATHEMATICAL, PHYSICAL & ENGINEERING SCIENCES

When $-1 < t < +1$ we analogously obtain

$$\eta_0 = \frac{2}{\pi}(2\omega)^{\frac{1}{2}}\{-[K(k)-E(k)]+k^2K(k)\}, \tag{3.32a}$$

$$\eta_2 = \frac{1}{12\pi}\frac{1}{k^2k'^2}\frac{1}{(2\omega)^{\frac{1}{2}}}\{(2k^2-1)[K(k)-E(k)]-k^2K(k)\}, \tag{3.32b}$$

$$\eta_4 = \frac{1}{2880\pi}\frac{1}{k^6k'^6}\frac{1}{(2\omega)^{\frac{3}{2}}}\{(16k^8-32k^6-129k^4+145k^2-56)[K(k)-E(k)] -(8k^6-105k^4+69k^2-28)k^2K(k)\}, \tag{3.32c}$$

where

$$k^2 = \tfrac{1}{2}(t+1). \tag{3.33}$$

We have here treated the quantization condition (3.2*a*), which is the particular case corresponding to $m = 0$ of the quantization condition (4.11*b*) in I, where $|m|$ is assumed to be sufficiently small but not necessarily equal to zero. We postpone the treatment of the more general quantization condition (4.11*b*) in I to the following paper IV.

4. Energy levels obtained from the simple quantization condition pertaining to $\xi_0 = \frac{1}{2}|m| > 0$ expressed as series expansions for very weak and very strong electric fields, and their relation to previously obtained series expansions

In this section we derive series expansions for the energy levels for very weak and very strong electric fields from the simple quantization condition (3.1) pertaining to $\xi_0 = \frac{1}{2}|m| > 0$ with $\mathscr{L}^{(2s+1)}$ given by (3.21*a–c*). To see the possibility of obtaining such expansions, we note that the analytical series expansions for the complete elliptic integrals in powers of the square of the modulus, k^2, and the parameters α_1^2 and α_2^2 converge rapidly when k^2 is a small quantity, which is indeed found to be the case when W is an eigenvalue and the field is very weak or very strong. The quantities $\mathscr{L}^{(2s+1)}$ can thus be expressed as sums of powers of k^2, α_1^2 and α_2^2 in various combinations. The modulus and the parameters are defined in terms of the generalized classical turning points a, b and c, which according to (2.2) and (2.4) can be expressed in terms of m^2, ω and W. The quantization condition (3.1) can then be solved with respect to W, which will be obtained as a series expansion in powers of ω or $\omega^{-\frac{1}{2}}$ when the electric field is very weak or very strong respectively. The algebra involved is enormous, and the calculations were made possible by the use of the algebraic programming system REDUCE. It will be instructive to relate these expansions to the already available series expansions (see §§3 and 4 in II).

To carry out the calculations for obtaining the series expansions for W in the way described above, we must first express the generalized classical turning points in terms of m^2, ω and W. These expressions are obtained when we solve by iteration for the zeros of the right-hand member of (2.2), which is rearranged to single out small terms, proportional to ω for weak fields, and proportional to $1/\omega$ for strong fields.

(a) *Very weak electric fields*

When the electric field is very weak, the equation for the zeros of $Q^2(z)$, obtained from (2.2), is conveniently written

$$z^2 = A^2[1+\omega F(z)], \tag{4.1}$$

where
$$A^2 = \frac{W+\frac{1}{4}-m^2}{W+\frac{1}{4}} \tag{4.2}$$
and
$$F(z) = \frac{z(1-z^2)}{W+\frac{1}{4}}. \tag{4.3}$$
With $z = a$ $(0 < a < +1)$ we obtain from (4.1) the equation
$$a = +A[1+\omega F(a)]^{\frac{1}{2}}. \tag{4.4a}$$
Expanding the square root in (4.4*a*) in powers of $\omega F(a)$, which is supposed to be small, we can obtain the largest root a of equation (4.1) as a power series in ω by means of iteration. The intermediate root b, which for weak fields fulfils the inequality $-1 < b < 0$, is obtained analogously from the equation
$$b = -A[1+\omega F(b)]^{\frac{1}{2}} \tag{4.4b}$$
by iteration. Finally, the root c (< -1) is found by substituting the approximate series obtained for the roots a and b into the following relation between the zeros and the coefficients of $Q^2(z)$ (cf. (2.2) and (2.4))
$$c = -(a+b+(W+\tfrac{1}{4})/\omega). \tag{4.4c}$$
With the expressions for a, b and c obtained as described above, the quantities k^2, α_1^2 and α_2^2 can according to (3.9), (3.13*a*) and (3.13*b*), respectively, be expressed in terms of m^2, ω and W. Thus, we find that k^2 is approximately proportional to ω for very weak fields, and
$$0 < k^2 < \alpha_1^2 < 1, \tag{4.5a}$$
$$-\alpha_2^2 > 2. \tag{4.5b}$$
Consequently, $K(k)$ and $E(k)$ can be expanded in powers of k^2 according to (A 16) and (A 17), respectively, and the series expansion (A 19) is appropriate for both $\Pi(\alpha_1^2, k)$ and $\Pi(\alpha_2^2, k)$.

Substituting these series expansions into (3.3) with (3.21*a–c*) and (3.19*a–c*), and solving the resulting equation with respect to W, we get
$$W = j(j+1)+\left(\frac{1-3m^2/(j+\frac{1}{2})^2}{8(j+\frac{1}{2})^2}+\frac{1-15m^2/[4(j+\frac{1}{2})^2]}{8(j+\frac{1}{2})^4}+\frac{1-63m^2/[16(j+\frac{1}{2})^2]}{8(j+\frac{1}{2})^6}\right)\omega^2+\dots, \tag{4.6}$$
where
$$j = n+|m|. \tag{4.7}$$
The term which is independent of ω and the first contribution to the term proportional to ω^2 in the right-hand member of (4.6) originate from the first-order phase-integral approximation. The second and third contributions to the term proportional to ω^2 in (4.6) originate from the third- and fifth-order phase-integral approximations, respectively. Thus, the first-, third- and fifth-order approximations contribute to the coefficient of ω^2 in (4.6). It is seen from equation (3.2*b*) in II that this coefficient does not coincide with the corresponding one in the Rayleigh–Schrödinger perturbation series. If, which seems reasonable, phase-integral approximations of all orders contribute to this coefficient, i.e. if the contributions

proportional to ω^2 in (4.6) are regarded as the first three terms in a series, where the following terms are assumed to originate from successively higher orders of the phase-integral approximation, the question arises whether these terms, for infinite-order approximation, will sum up to a result, which is equal to the second term in the Rayleigh–Schrödinger perturbation series for weak fields. It seems plausible that this is the case, since the correction of second-order Rayleigh–Schrödinger perturbation theory, given by equation (3.2*b*) in II, can be written as follows

$$\begin{aligned}\frac{1-3m^2/[j(j+1)]}{2[4j(j+1)-3]} &= \frac{1-12m^2/\{[2(j+\frac{1}{2})]^2-1\}}{8[(j+\frac{1}{2})^2-1]}\\ &= \left(\frac{1}{8}\sum_{n=1}^{\infty}(j+\tfrac{1}{2})^{-2n}\right)\left(1-12m^2\sum_{n=1}^{\infty}[2(j+\tfrac{1}{2})]^{-2n}\right)\\ &= \frac{1}{8}\left(\frac{1}{(j+\frac{1}{2})^2}+\frac{1}{(j+\frac{1}{2})^4}+\frac{1}{(j+\frac{1}{2})^6}+\ldots\right)\\ &\quad -\frac{3m^2}{8}\left(\frac{1}{(j+\frac{1}{2})^4}+\frac{5}{4(j+\frac{1}{2})^6}+\frac{21}{16(j+\frac{1}{2})^8}+\ldots\right)\\ &= \frac{1-3m^2/(j+\frac{1}{2})^2}{8(j+\frac{1}{2})^2}+\frac{1-15m^2/[4(j+\frac{1}{2})^2]}{8(j+\frac{1}{2})^4}+\frac{1-63m^2/[16(j+\frac{1}{2})^2]}{8(j+\frac{1}{2})^6}+\ldots,\end{aligned} \tag{4.8}$$

and the first few terms in the expansion (4.8) are seen to reproduce the coefficient of ω^2 in (4.6).

Neither the expression for W, obtained by retaining in the Rayleigh–Schrödinger perturbation series for very weak fields the first two terms, nor (4.6) give particularly accurate energy levels unless the field is extremely weak. However, by solving the quantization condition (3.1) with (3.21*a–c*) and (3.19*a–c*) numerically, we obtain already in the first order of approximation very accurate values of the energy levels, and, as soon as the field is not extremely weak, perturbation calculations of very high order are required to obtain this accuracy.

(*b*) *Very strong electric fields*

For very strong electric fields the equation for the zeros of $Q^2(z)$, obtained from (2.2), is rearranged as follows

$$z = -1+\frac{m^2/\omega}{(1-z)(z-1+\gamma)}, \tag{4.9}$$

where γ, defined by

$$(W+\tfrac{1}{4})/\omega = -1+\gamma, \tag{4.10a}$$

can be expanded as follows (cf. equation (4.28) in II)

$$\gamma = \gamma_1\omega^{-\frac{1}{2}}+\gamma_2\omega^{-1}+\gamma_3\omega^{-\frac{3}{2}}+\ldots, \tag{4.10b}$$

and γ_1, γ_2, γ_3, ... are coefficients that are independent of ω. The root c (<-1) is obtained from (4.9) by iteration. According to (2.2), (2.4) and (4.10*a*) the roots a, b and c of (4.9) are related to γ by the identity

$$-z^3+(1-\gamma)z^2+z-(1-\gamma+m^2/\omega) = (a-z)(z-b)(z-c), \tag{4.11}$$

from which the following relations between roots and coefficients are obtained

$$a+b+c = 1-\gamma, \tag{4.12a}$$

$$abc = -1+\gamma-m^2\omega^{-1}. \tag{4.12b}$$

By solving (4.12a,b) with respect to a and b we find that

$$a = -\tfrac{1}{2}(\gamma+c-1)+[(\tfrac{1}{2}(\gamma+c-1))^2-(\gamma-m^2/\omega-1)/c]^{\frac{1}{2}}, \tag{4.13a}$$

$$b = -\tfrac{1}{2}(\gamma+c-1)-[(\tfrac{1}{2}(\gamma+c-1))^2-(\gamma-m^2/\omega-1)/c]^{\frac{1}{2}}. \tag{4.13b}$$

By using (4.13a, b) with c obtained by iteration from (4.9) with $z = c$ we conclude that both k^2 and α_1^2 are approximately proportional to the small quantity $\omega^{-\frac{1}{2}}$. Then the complete elliptic integrals $K(k)$, $E(k)$ and $\Pi(\alpha_1^2, k)$ have the series expansions (A 16), (A 17) and (A 20) respectively. Analogously we find that, since $-\alpha_2^2 > 1$, (A 19) is the appropriate series expansion for $\Pi(\alpha_2^2, k)$.

By analogy with the treatment of very weak fields in §4a we substitute the series expansions obtained above into the quantization condition (3.1) with (3.21a–c) and (3.19a–c). By solving the resulting equation with respect to W, we obtain

$$W = -\omega+N\omega^{\frac{1}{2}}\sqrt{2}+\tfrac{1}{8}((3m^2-1)-N^2)+\frac{N}{64\sqrt{2}}(3(3m^2-1)-N^2)\,\omega^{-\frac{1}{2}}$$
$$+\frac{1}{2048}(-3(11m^4-14m^2+3)+34(3m^2-1)N^2-5N^4)\,\omega^{-1}$$
$$+\frac{N}{32768\sqrt{2}}(-3(271m^4-574m^2+135)+410(3m^2-1)N^2-33N^4)\,\omega^{-\frac{3}{2}}+O(\omega^{-2}), \tag{4.14}$$

where
$$N = 2n+|m|+1. \tag{4.15}$$

The terms proportional to ω^1, $\omega^{\frac{1}{2}}$ and ω^0 in the right-hand member of (4.14) originate from the first-order phase-integral approximation. The third-order approximation contributes to (4.14) with the term proportional to $\omega^{-\frac{1}{2}}$ and part of the term proportional to ω^{-1}, and the whole expression (4.14) is obtained in the fifth-order approximation. The expansion (4.14) is identical with the result obtained by means of fourth-order perturbation calculation as is seen from equations (4.28) and (4.29a–f) in II. However, by solving the quantization condition (3.1) with (3.21a–c) and (3.19a–c) numerically, we obtain eigenvalues with an accuracy, which is by no means achieved by using the fourth-order perturbation series, especially when the field is not very strong.

5. Survey of the accuracy: conclusions

The simple quantization condition (3.1) for $\xi_0 = \frac{1}{2}|m| > 0$, with $\mathscr{L}^{(2s+1)}$ given by (3.21a–c), as well as the quantization condition (3.2a) for $\xi_0 = 0$, $m = 0$ and its limiting form, the simple quantization condition (3.2b), with $\mathscr{L}^{(2s+1)}$ given by (3.22a–c) or (3.24a–c) and η_{2s} given by (3.30a–c) or (3.32a–c), were solved numerically in the first, third and fifth order of the phase-integral approximation by means of a standard iterative routine. For evaluating the complete elliptic integrals appearing in $\mathscr{L}^{(2s+1)}$ and η_{2s} very rapid standard library routines were used. The calculations were carried out on a VAX-11 computer in double precision, which gives an accuracy

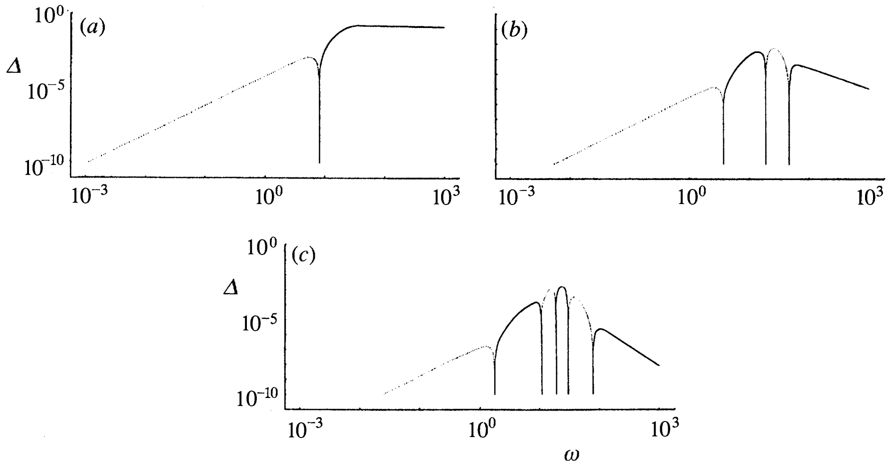


Figure 4. Detailed plots of the dependence on ω of the magnitude of the absolute error Δ in the approximate energy eigenvalue W obtained from (3.1), with the definition (5.1) for the quantum numbers $|m| = 2$ and $n = 2$ in the first, third and fifth order of the phase-integral approximation. Dotted/solid lines indicate that the exact eigenvalues are greater/less than the phase-integral values. (a) First order, (b) third order, (c) fifth order.

of at least 15 digits. The time of computation required for obtaining a single eigenvalue amounts to some 10 ms. To assure the correctness of the expressions for $\mathscr{L}^{(2s+1)}$ and η_{2s} in terms of complete elliptic integrals, given in §3, some eigenvalues were also calculated from the original quantization conditions with $\mathscr{L}^{(2s+1)}$ and η_{2s} given by (3.3) and (3.28), respectively, and thus not transformed to complete elliptic integrals. The eigenvalues thus obtained were found to agree within machine accuracy with those obtained with $\mathscr{L}^{(2s+1)}$ and η_{2s} expressed in terms of complete elliptic integrals, but the time of computation was about 100 to 1000 times longer.

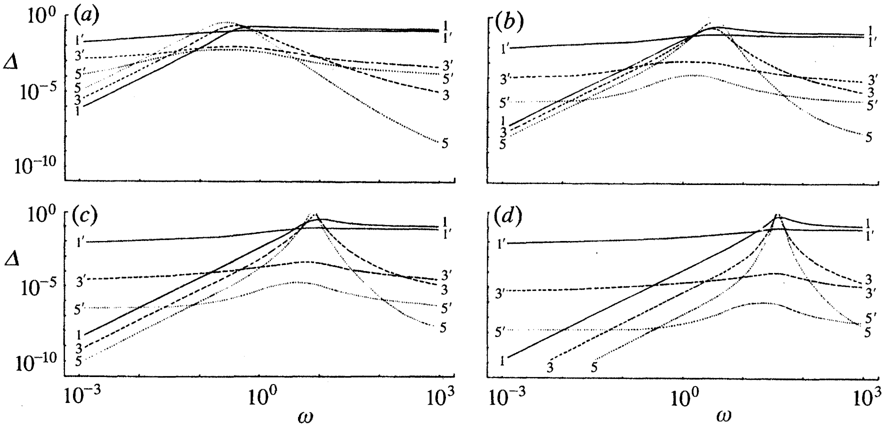
The eigenvalues obtained from the above-mentioned phase-integral quantization conditions were compared with sufficiently accurate numerical reference values obtained by means of the bisection method with the Sturmian chain and Richardson extrapolation when $|m| \geqslant 2$ and by means of a Prüfer transformation and a shooting method when $|m|$ is equal to 0 and 1.

The diagrams in figure 4 for the particular set of quantum numbers $|m| = n = 2$ have been picked out to demonstrate in detail the dependence on ω of the magnitude of the absolute error Δ [not to be confused with the phase (3.26)] in an eigenvalue W, i.e.

$$\Delta = |\text{accurate eigenvalue } W - \text{approximate eigenvalue } W|, \tag{5.1}$$

in the first, third and fifth order of the phase-integral approximation. The narrow minima in Δ, which are not very essential in practice, can be disregarded by constructing a smooth envelope, which connects with the original curve in such a way that the true values of Δ are always less than or equal to the values indicated by the envelope. By comparing figure 4a–c with figure 7c, the idea behind the construction of envelope curves can be fully understood. In figures 5–10 such envelopes demonstrating upper bounds for Δ against ω are plotted for some quantum numbers $|m|$ and n in the first, third and fifth order of the phase-integral approximation.

In all orders of approximation and for all combinations of $|m|$ and n that have been investigated it is obvious that, from being exact at $\omega = 0$ (due to our choice of base



Figures 5–10. Smooth envelopes representing the dependence on ω of Δ. Narrow minima, such as those in figure 4, are neglected, and the true values of Δ are always less than or equal to the values indicated by the envelopes.

In figure 5, where $m = 0$, the solid, dashed and dotted envelopes, which are indicated by 1, 3, 5, refer to the simple quantization condition (3.2*b*) in the first, third and fifth order of the approximation, respectively. Analogously, the envelopes indicated by 1′, 3′, 5′ refer to the quantization condition (3.2*a*).

In figures 6–10 for the quantum numbers $|m| = 1, 2, 3, 4$ and 5, respectively, the envelopes refer to the simple quantization condition (3.1) in the first, third and fifth order of the approximation. In all figures $n = 0\,(a)$, $1\,(b)$, $2\,(c)$ and $5\,(d)$.

function) and excellently accurate for very small values of ω, the eigenvalues become less accurate in the region of intermediate values of ω. In the first-order approximation Δ is almost constant when ω is greater than a certain value, which depends on the values of $|m|$ and n. In the third- and fifth-order approximations, however, Δ exhibits a pronounced peak in the centre of the intermediate region and decreases again for larger values of ω. For fixed quantum number $|m|$ and increasing quantum number n this peak is displaced towards larger values of ω. For fixed n the accuracy of W increases with increasing $|m|$ for small and intermediate values of ω.

In general, except for the case when $m = n = 0$, the accuracy of W improves with increasing order of approximation (at least up to the fifth order). When we use the simple quantization condition (3.2*b*) for $m = n = 0$, the contrary is the case to the left of the peak, i.e. in the region of small and intermediate values of ω. Furthermore, when $m = 0$ and $n \geqslant 2$ (3.2*b*) is useless in the region of the peak. This deficiency is removed by the use of the more general quantization condition (3.2*a*). The corresponding curves, plotted in figure 5 together with the ones pertaining to the simple quantization condition (3.2*b*), are seen to cross the latter ones well below the peak. It is, however, obvious that the quantization condition (3.2*a*) should be used only in the regions of the above-mentioned peaks. We recall that the simple quantization condition (3.2*b*) is obtained as a limiting form of the quantization condition (3.2*a*) when t recedes from the pole at $z = -1$ (cf. figures 2 and 3). The energy eigenvalues obtained from the simple quantization condition (3.2*b*) are thus expected to be least accurate when t is located close to -1, which according to (2.7) occurs when ω is close to $W+\frac{1}{4}$. This is the condition for the location of the peaks in figure 5 when $\xi_0 = 0$ and $m = 0$, and we find empirically that the same condition predicts the location of the peaks also for the simple quantization condition (3.1) pertaining to $\xi_0 = \frac{1}{2}|m| > 0$ (see figures 6–10). In figure 11 the quantity $W+\frac{1}{4}-\omega$ is

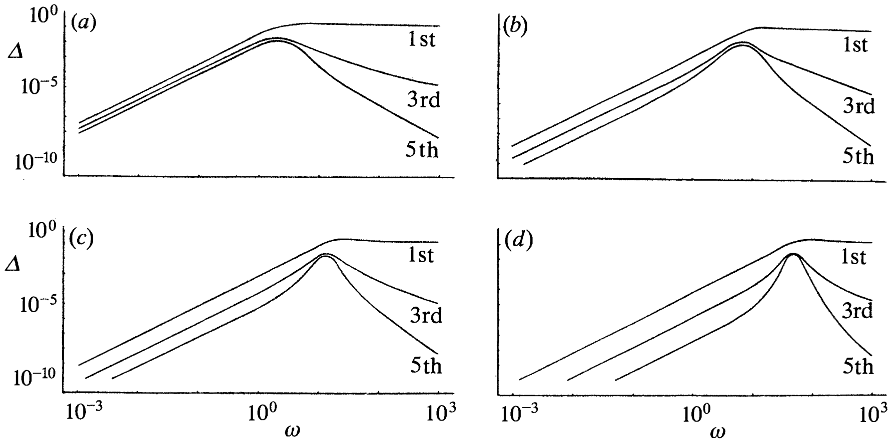


Figure 6. For details see figure 5 caption.

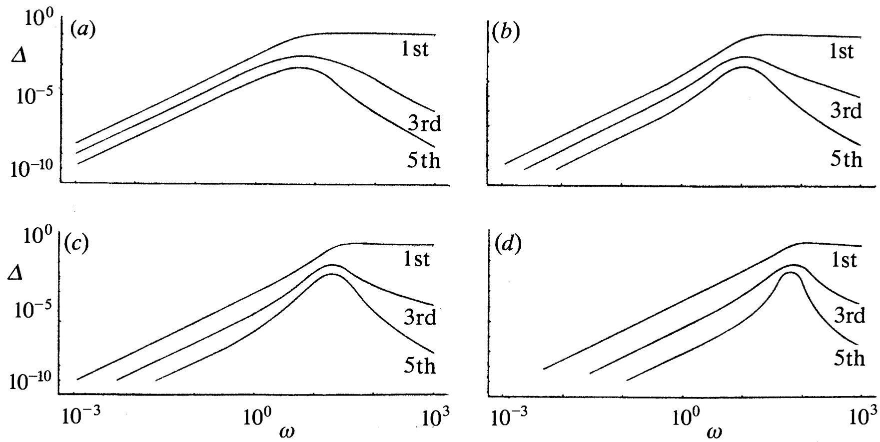


Figure 7. For details see figure 5 caption.

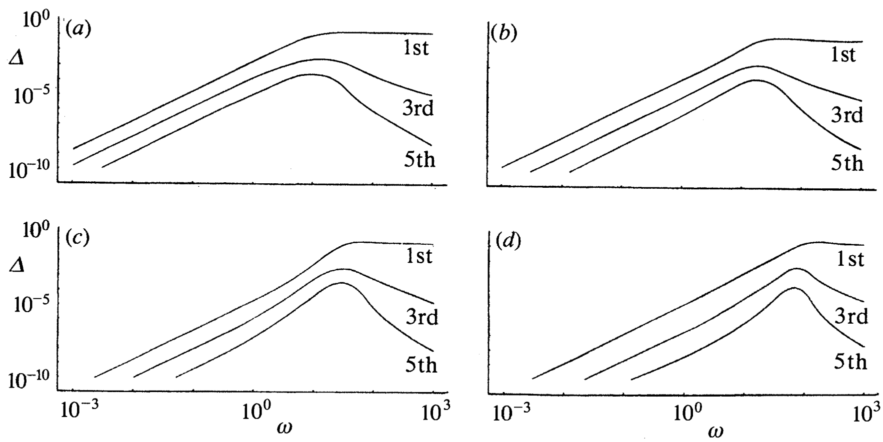


Figure 8. For details see figure 5 caption.

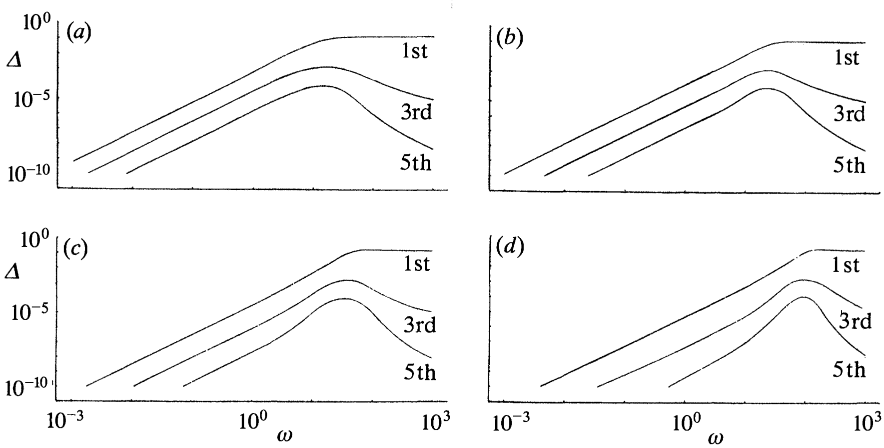


Figure 9. For details see figure 5 caption.

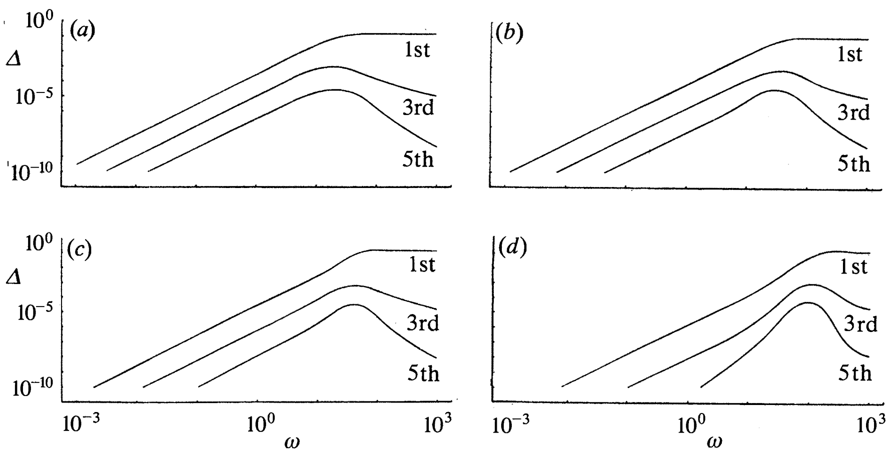


Figure 10. For details see figure 5 caption.

plotted against ω for the first 21 energy levels. Each curve is associated with an energy level indicated by the pair of quantum numbers $(j, |m|)$ and the intersection with the ω – axis thus defines a value of ω in the region around which the quantization condition (4.11 a) in I for $\xi_0 = \frac{1}{2}|m| > 0$ or the quantization condition (4.11 b) in I for $\xi_0 = 0$ should be used. If $m = 0$ this rule applies to the quantization condition (3.2 a), and the expressions (3.30 a–c) and (3.32 a–c) for η_{2s} are applicable for values of ω to the left and to the right of the point of intersection respectively.

The accuracy of the energy eigenvalues W obtained by means of the simple quantization conditions (3.1) and (3.2 b) is for very small values of ω found to be fully sufficient for probably all conceivable purposes already in the first-order phase-integral approximation. An analogous statement holds for very large values of ω in the third-order phase-integral approximation. The approximations are least good in the intermediate region of ω-values (cf. figures 5–10). When $m = 0$ it is advantageous, and if $m = 0$ and $n \geqslant 2$ even necessary, to make use of the quantization condition (3.2 a), and not its limiting form (3.2 b), to make the approximations useful in the whole intermediate region. The accuracy of W in the fifth-order phase-integral

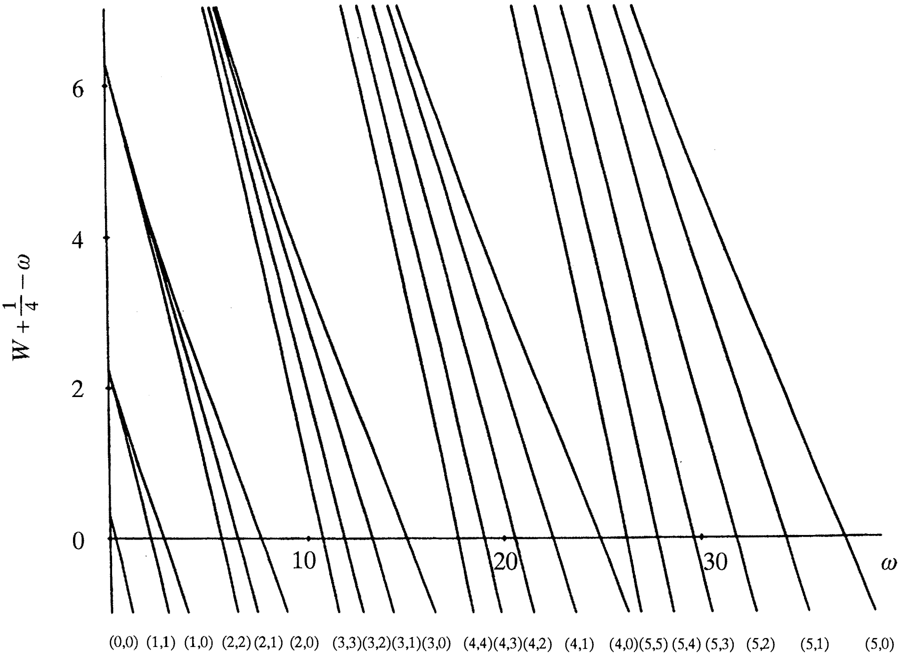


Figure 11. The quantity $W+\frac{1}{4}-\omega$ plotted against ω for the first 21 energy levels, indicated by the pair of quantum numbers $(j, |m|)$. For each energy level $(j, |m|)$ the intersection of the associated curve with the ω-axis defines a value of ω in the region around which it is favourable to use the quantization condition (4.11a) in I for $\xi_0 = \frac{1}{2}|m| > 0$ or the quantization condition (4.11b) in I for $\xi_0 = 0$. If $m = 0$ this rule thus applies to the quantization condition (3.2a), where the expressions (3.30a–c) or (3.32a–c) for η_{2s} are applicable for ω-values such that $W+\frac{1}{4}-\omega$ is greater than or less than zero respectively (see (2.7)).

approximation is then probably sufficient for most purposes when $m = 0$, possibly with the exception of the state $m = n = 0$. When we use the simple quantization condition (3.1) for $m \neq 0$ the intermediate regions are less troublesome. If, however, there is need for still better approximations in the intermediate region, which may be the case for small values of $|m|$, it is advantageous to use the quantization condition (4.11a) in I; this quantization condition will be investigated in IV. When extremely high accuracy is needed for intermediate values of ω a numerical method is preferable, but one must be aware of the fact that the use of a numerical integration routine may require a considerable time of computation. Moveover, by solving phase-integral quantization conditions in approximations of order larger than 5, one will probably increase the accuracy for all values of ω to a certain extent. Although the quantities $\mathscr{L}^{(2s+1)}$ seem to be too complicated to be expressed in terms of complete elliptic integrals for such orders of approximation, they can still be evaluated by numerical integration.

In figure 12 the first 21 energy levels are plotted against ω. Similar figures have been produced before, usually by exact solution of the Schrödinger equation (cf. §1 in I) since in the region of intermediate values of ω the conventional perturbation calculations are more or less inadequate (see, for example, Peter & Strandberg 1956; von Meyenn 1970). Because of the great accuracy of the phase-integral approximation, which for small values of ω is a consequence of our judicious choice of base function, the entire energy spectrum can be obtained without the use of

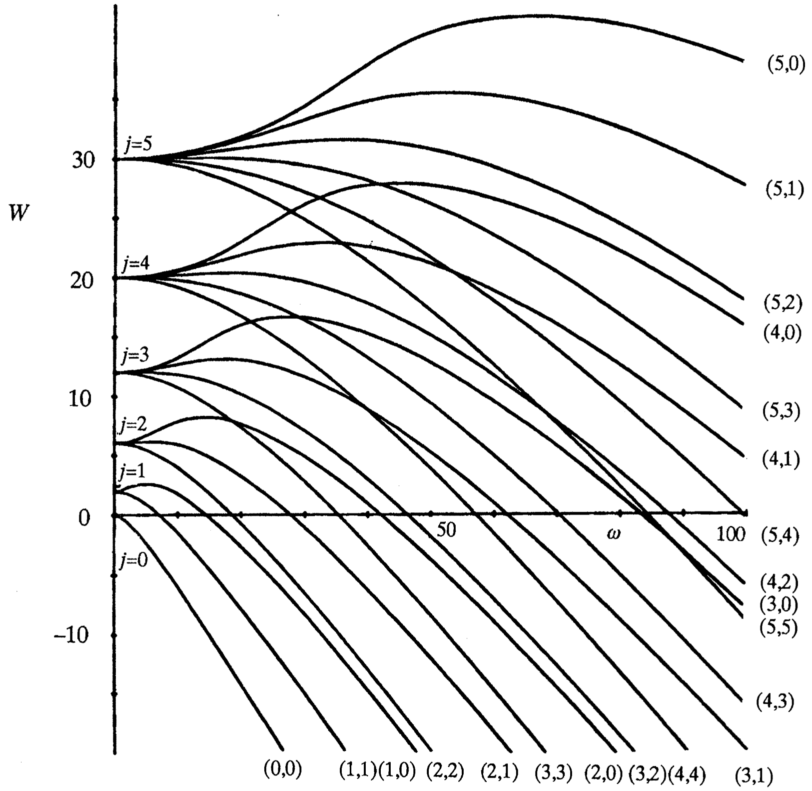


Figure 12. The first 21 energy levels, indicated by the pair of quantum numbers $(j, |m|)$, are plotted against ω.

complementary calculations, and figure 12 has thus been obtained wholly within the framework of this paper.

An alternative quantization condition, which was obtained by means of comparison equation technique, is given by equation (5.39) in I. With $\mathscr{L}^{(2s+1)}$ defined according to (3.3) and preferably expressed in terms of complete elliptic integrals, we can easily obtain the energy levels by the same iterative routines, which we use to solve the quantization conditions (3.1) and (3.2*b*). The quantization condition (5.39) in I has thus been tested numerically and was found to yield essentially the same accuracy of the eigenvalues W as the simple quantization conditions (3.1) and (3.2*b*).

Previous attempts to obtain the energy levels for a linear rigid polar rotator in a homogeneous electric field (cf. §1 in I and §5 in II) clearly indicate that there is need for a method yielding very accurate eigenvalues for all values of the electric field strength. This is accomplished as we have shown in this paper, by using the phase-integral quantization conditions derived in I.

I express my gratitude to Professor Nanny Fröman and Professor Per Olof Fröman for suggesting the problem and for stimulating discussions and constructive criticism of the manuscript. I am also indebted to Dr Finn Karlsson for fruitful discussions and to Anders Hökback for valuable advice concerning the numerical calculations.

Appendix A

In this appendix are collected, chiefly from Byrd & Friedman (1971), some formulas that are needed in this paper.

The normal elliptic integrals of the first, second and third kinds are defined by

$$F(\varphi, k) = \int_0^{\varphi} \frac{\mathrm{d}\vartheta}{(1-k^2\sin^2\vartheta)^{\frac{1}{2}}}, \tag{A 1a}$$

$$E(\varphi, k) = \int_0^{\varphi} (1-k^2\sin^2\vartheta)^{\frac{1}{2}}\,\mathrm{d}\vartheta, \tag{A 2a}$$

$$\Pi(\varphi, \alpha^2, k) = \int_0^{\varphi} \frac{\mathrm{d}\vartheta}{(1-\alpha^2\sin^2\vartheta)(1-k^2\sin^2\vartheta)^{\frac{1}{2}}}, \tag{A 3a}$$

where k is the modulus of the elliptic integrals and α^2 is the parameter of the elliptic integral of the third kind.

When $\varphi = \frac{1}{2}\pi$ the elliptic integrals are said to be complete, and the following notations are then used

$$K(k) \equiv F(\tfrac{1}{2}\pi, k), \tag{A 1b}$$

$$E(k) \equiv E(\tfrac{1}{2}\pi, k), \tag{A 2b}$$

$$\Pi(\alpha^2, k) \equiv \Pi(\tfrac{1}{2}\pi, \alpha^2, k). \tag{A 3b}$$

Introducing the variable

$$u = F(\varphi, k) \tag{A 4}$$

one defines the jacobian elliptic functions as follows

$$\mathrm{sn}\,u = \sin\varphi, \tag{A 5}$$

$$\mathrm{cn}\,u = \cos\varphi, \tag{A 6}$$

$$\mathrm{dn}\,u = (1-k^2\sin^2\varphi)^{\frac{1}{2}}. \tag{A 7}$$

They fulfil the relations

$$\mathrm{sn}^2 u + \mathrm{cn}^2 u = 1, \tag{A 8}$$

$$k^2\,\mathrm{sn}^2 u + \mathrm{dn}^2 u = 1. \tag{A 9}$$

Introducing the complementary modulus k', related to the modulus by

$$k'^2 = 1 - k^2, \tag{A 10}$$

one readily obtains the following alternative relations

$$\mathrm{dn}^2 u - k^2\,\mathrm{cn}^2 u = k'^2, \tag{A 11}$$

$$k'^2\,\mathrm{sn}^2 u + \mathrm{cn}^2 u = \mathrm{dn}^2 u. \tag{A 12}$$

Differentiation of the jacobian elliptic functions with respect to u yields

$$\mathrm{d}(\mathrm{sn}\,u)/\mathrm{d}u = \mathrm{cn}\,u\,\mathrm{dn}\,u, \tag{A 13}$$

$$\mathrm{d}(\mathrm{cn}\,u)/\mathrm{d}u = -\mathrm{sn}\,u\,\mathrm{dn}\,u, \tag{A 14}$$

$$\mathrm{d}(\mathrm{dn}\,u)/\mathrm{d}u = -k^2\,\mathrm{sn}\,u\,\mathrm{cn}\,u. \tag{A 15}$$

The complete elliptic integrals of the first and second kinds have the following series expansions

$$K(k) = \tfrac{1}{2}\pi \sum_{m=0}^{\infty} \left(\frac{(1/2)_m}{m!}\right)^2 k^{2m}, \quad k^2 < 1, \tag{A 16}$$

$$E(k) = \tfrac{1}{2}\pi \sum_{m=0}^{\infty} \frac{1}{1-2m}\left(\frac{(1/2-m)_m}{m!}\right)^2 k^{2m}, \quad k^2 < 1, \tag{A 17}$$

the Pochhammer symbol $(z)_m$ for arbitrary z being defined by

$$(z)_0 = 1, \tag{A 18a}$$

$$(z)_m = \prod_{j=0}^{m-1} (z+j), \quad m \geqslant 1. \tag{A 18b}$$

When $k^2 < 1$ and $-\alpha^2 > 1$ or when $k^2 < |-\alpha^2| < 1$, the complete elliptic integral of the third kind has the series expansion

$$\Pi(\alpha^2, k) = \sum_{m=0}^{\infty} c_m k^{2m}, \tag{A 19}$$

where

$$c_0 = \pi/[2(1-\alpha^2)^{\frac{1}{2}}], \tag{A 19a}$$

$$c_1 = \frac{\pi}{4\alpha^2}\left(\frac{1}{(1-\alpha^2)^{\frac{1}{2}}} - 1\right), \tag{A 19b}$$

$$2(m+1)\alpha^2 c_{m+1} = \frac{\pi}{2(2m-1)}\left(\frac{(1/2-m)_m}{m!}\right)^2 + (1-2m)c_{m-1} + (2m+1+2m\alpha^2)c_m, \quad m \geqslant 1. \tag{A 19c}$$

Alternatively, when $k^2 < 1$ and $|-\alpha^2| < 1$ the complete elliptic integral of the third kind has the series expansion

$$\Pi(\alpha^2, k) = \tfrac{1}{2}\pi \sum_{m=0}^{\infty}\sum_{j=0}^{m} \frac{(2m)!\,(2j)!}{4^m 4^j (m!)^2 (j!)^2} k^{2j} (\alpha^2)^{m-j}. \tag{A 20}$$

The complete elliptic integral $\Pi(\alpha^2, k)$ is singular when $\alpha^2 = 1$, but the singularity is so weak that

$$\lim_{\alpha^2 \to 1} (1-\alpha^2)\,\Pi(\alpha^2, k) = 0. \tag{A 21}$$

When $\alpha^2 = k^2$ the complete elliptic integral of the third kind reduces to

$$\Pi(k^2, k) = E(k)/k'^2. \tag{A 22}$$

Appendix B

In this appendix we shall first obtain the quantities $\mathscr{L}^{(2s+1)}$ for $\xi_0 = 0$ and $m = 0$ from the expressions (3.21 a–c) for $\mathscr{L}^{(2s+1)}$ pertaining to $\xi_0 = \frac{1}{2}|m| > 0$ by letting $m \to 0$, and then we shall show that also the quantities η_{2s} for $\xi_0 = 0$ and $m = 0$ can be obtained analogously. To this end it is for $\xi_0 = 0$ convenient to write the square of the base function, given by (2.6), in the form

$$Q^2(z) = \omega(1-z)(z+1)(z-t)/(1-z^2)^2. \tag{B 1}$$

By comparing (B 1) with (2.4) it is obvious that the zeros a, b and c pertaining to $\xi_0 = \frac{1}{2}|m| > 0$ correspond, in the limit when $m \to 0$, to

$$a = 1, \quad b = -1, \quad c = t, \quad \text{if} \quad t < -1 \tag{B 2a}$$

$$a = 1, \quad b = t, \quad c = -1, \quad \text{if} \quad -1 < t < +1. \tag{B 2b}$$

We now turn to the problem of obtaining the quantities $\mathscr{L}^{(2s+1)}$ for $\xi_0 = 0$ and $m = 0$. According to (3.9) and (3.13a, b) the limiting values (B 2a, b) yield

$$k^2 = 2/(1-t), \quad \alpha_1^2 = 1, \quad \alpha_2^2 = -\infty, \quad \text{if} \quad t < -1 \tag{B 3a}$$

$$k^2 = \tfrac{1}{2}(1-t), \quad \alpha_1^2 = k^2, \quad \alpha_2^2 = -\infty, \quad \text{if} \quad -1 < t < +1. \tag{B 3b}$$

All terms in the expressions (3.19a–c) for $g^{(2s+1)}(k, \alpha_1^2, \alpha_2^2)$ are found to be finite in the limit when $m \to 0$, and in particular it is obvious from the definition (A 3a, b) in Appendix A that $\Pi(\alpha_2^2, k)$ then vanishes. Furthermore, the term containing $\Pi(\alpha_1^2, k)$ tends to zero when $m \to 0$ in both cases $t < -1$ and $-1 < t < +1$ (cf. (A 21) and (A 22)).

Despite the fact that the explicit presence of α_1^2 in $g^{(2s+1)}(k, \alpha_1^2, \alpha_2^2)$ for $\xi_0 = 0$ and $m = 0$ is wholly dependent upon the use of (B 1) instead of (2.6), it may be advantageous not to substitute the values of α_1^2 given by (B 3a, b) into (3.19a–c), since the two separate cases $t < -1$ and $-1 < t < +1$ are then covered by one expression for $\mathscr{L}^{(2s+1)}$, namely

$$\mathscr{L}^{(1)} = \lim_{\alpha_2^2 \to -\infty} g^{(1)}(k, \alpha_1^2, \alpha_2^2)$$
$$= \frac{2}{\alpha_1^4}\left(\frac{2\omega\alpha_1^6}{k^2}\right)^{\frac{1}{2}} \{-\alpha_1^2[K(k)-E(k)] + [(k^2+1)\,\alpha_1^2 - k^2]K(k)\}, \tag{B 4a}$$

$$\mathscr{L}^{(3)} = \lim_{\alpha_2^2 \to -\infty} g^{(3)}(k, \alpha_1^2, \alpha_2^2)$$
$$= \frac{1}{12k'^4}\left(\frac{k^2}{2\omega\alpha_1^6}\right)^{\frac{1}{2}} \{((k^2+1)\,\alpha_1^2 + (k^4 - 4k^2 + 1))\,[K(k)-E(k)]$$
$$-(2\alpha_1^2 - (k^2+1))\,k^2 K\}, \tag{B 4b}$$

$$\mathscr{L}^{(5)} = \lim_{\alpha_2^2 \to -\infty} g^{(5)}(k, \alpha_1^2, \alpha_2^2)$$
$$= \frac{1}{2880k'^{12}}\left(\frac{k^2}{2\omega\alpha_1^6}\right)^{\frac{3}{2}} \{(-(2k^8 - 298k^6 - 1200k^4 - 298k^2 + 2)\,\alpha_1^6$$
$$-(303k^8 + 2385k^6 + 2385k^4 + 303k^2)\,\alpha_1^4$$
$$+(42k^{12} - 186k^{10} + 1716k^8 + 2232k^6 + 1716k^4 - 186k^2 + 42)\,\alpha_1^2$$
$$-(56k^{14} - 271k^{12} + 546k^{10} + 565k^8 + 565k^6 + 546k^4 - 271k^2$$
$$+56))\,[K(k)-E(k)] + (-(89k^6 + 807k^4 + 807k^2 + 89)\,\alpha_1^6$$
$$+(90k^8 + 1254k^6 + 2688k^4 + 1254k^2 + 90)\,\alpha_1^4$$
$$-(21k^{10} + 444k^8 + 2223k^6 + 2223k^4 + 444k^2 + 21)\,\alpha_1^2$$
$$+(28k^{12} - 132k^{10} + 750k^8 + 500k^6 + 750k^4 - 132k^2 + 28))\,k^2K(k)\}, \tag{B 4c}$$

where either $\alpha_1^2 = 1$ or $\alpha_1^2 = k^2$ in accordance with (B 3a, b).

We shall now obtain expressions for the quantities η_{2s} pertaining to $\xi_0 = 0$ and $m = 0$ analogously. As is seen from the definition (3.28), η_{2s} resembles $\mathscr{L}^{(2s+1)}$ except for the contour of integration and a constant factor. We conclude from (B 1) and (B 2*a*, *b*) that the contour $\bar{A}$ of η_{2s}, depicted in figures 2 and 3, encircles the counterparts to c and b. We now assume that $Q^2(z)$ is given by (2.4). By calculations analogous to those in §3*a* for obtaining the quantities $\mathscr{L}^{(2s+1)}$ pertaining to $\xi_0 = \frac{1}{2}|m| > 0$, we find that also the quantities η_{2s} for $\xi_0 = 0$ and $m = 0$ can be expressed in terms of the functions $g^{(2s+1)}(k, \alpha_1^2, \alpha_2^2)$, given by (3.19*a*–*c*), the values of the moduli k and the parameters α_1^2 and α_2^2 being defined with regard to the zeros encircled by $\bar{A}$. It is thus possible to obtain η_{2s} for $\xi_0 = 0$ and $m = 0$ by substituting the appropriate values of k, α_1^2 and α_2^2 into the function $g^{(2s+1)}(k, \alpha_1^2, \alpha_2^2)$ multiplied by the convenient constant factor, and finally letting $m \to 0$. We now find from (B 2*a*, *b*) and §233 in Byrd & Friedman (1971) that

$$k^2 = (t+1)/(t-1), \quad \alpha_1^2 = k^2, \quad \alpha_2^2 = 1, \quad \text{if} \quad t < -1 \tag{B 5a}$$

$$k^2 = \tfrac{1}{2}(t+1), \quad \alpha_1^2 = k^2, \quad \alpha_2^2 = \infty, \quad \text{if} \quad -1 < t < +1. \tag{B 5b}$$

We note that because of (B 5*a*, *b*), (A 3*a*, *b*), (A 21) and (A 22) the terms in the right-hand member of (3.19*a*), which contain complete elliptic integrals of the third kind, vanish in both cases $t < -1$ and $-1 < t < +1$. We also recall that according to (B 5*a*, *b*) $1/\alpha_2^2$ is equal to 1 for $t < -1$ but equal to zero for $-1 < t < +1$, while α_1^2 is equal to k^2 in both cases. The quantities η_{2s} can then for both cases be written

$$\eta_0 = -\frac{1}{\pi}\lim g^{(1)}(k, k^2, \alpha_2^2)$$

$$= \frac{2}{\pi}\left(\frac{2\omega}{1-\beta k^2}\right)^{\frac{1}{2}}\{-[K(k)-E(k)]+(1-\beta)\,k^2K(k)\}, \tag{B 6a}$$

$$\eta_2 = +\frac{1}{\pi}\lim g^{(3)}(k, k^2, \alpha_2^2)$$

$$= \frac{1}{12\pi}\frac{1}{k^2k'^2}\left(\frac{1-\beta k^2}{2\omega}\right)^{\frac{1}{2}}\{((2k^2-1)-(k^4+2k^2-2)\,\beta)$$
$$\times[K(k)-E(k)]-(1-(2k^2-1)\,\beta)\,k^2K(k)\}, \tag{B 6b}$$

$$\eta_4 = -\frac{1}{\pi}\lim g^{(5)}(k, k^2, \alpha_2^2)$$

$$= \frac{1}{2880\pi}\frac{1}{k^6k'^6}\left(\frac{1-\beta k^2}{2\omega}\right)^{\frac{3}{2}}\{((16k^8-32k^6-129k^4+145k^2-56)$$
$$-(56k^{14}-247k^{12}+435k^{10}-446k^8-430k^6-564^4+392k^2-112)\,\beta)$$
$$\times[K(k)-E(k)]+(-(8k^6-105k^4+69k^2-28)+(28k^{12}-120k^{10}$$
$$+156k^8+8k^6-261k^4+189k^2-56)\,\beta)\,k^2K(k)\}, \tag{B 6c}$$

where the symbol 'lim' indicates that $\alpha_2^2 \to 1$ if $t < -1$ and $\alpha_2^2 \to \infty$ if $-1 < t < +1$, and where

$$\beta = \begin{cases} 1 & \text{if} \quad t < -1, \\ 0 & \text{if} \quad -1 < t < +1. \end{cases} \tag{B 7}$$

MATHEMATICAL, PHYSICAL & ENGINEERING SCIENCES
THE ROYAL SOCIETY A
PHILOSOPHICAL TRANSACTIONS OF

Appendix C

To obtain estimates of the zeros of the square of the base function when $\xi_0 = \frac{1}{2}|m| > 0$ and $\omega > 0$ we conveniently write (2.2) as follows (cf. (2.4))

$$Q^2(z) = \omega P(z)/(1-z^2)^2, \tag{C 1}$$

where
$$P(z) = -z^3 - \frac{W+\frac{1}{4}}{\omega}z^2 + z + \frac{W+\frac{1}{4}-m^2}{\omega} = (a-z)(z-b)(z-c), \tag{C 2}$$

the zeros of $Q^2(z)$ being denoted by a, b and c (see figure 1). The zeros are obtained as the roots of the equation.

$$\omega z + W + \tfrac{1}{4} - m^2 = m^2 z^2/(1-z^2). \tag{C 3}$$

From graphical representations of the functions in the two members of (C 3) a number of conclusions can be drawn. For fixed $\omega > 0$ there is always one real root in the interval $-\infty < z < -1$, and there are two real roots in the interval $-1 < z < +1$ when W is larger than a certain critical value, W_c, which depends on m^2 only. For this critical value $P(z)$ has a double root in the interval $0 < z < +1$, and consequently $P(z)$ and its derivative with respect to z have a common zero in the interval $0 < z < +1$, which is given by

$$z = -(W_c+\tfrac{1}{4})/(3\omega) + [((W_c+\tfrac{1}{4})/(3\omega))^2 + \tfrac{1}{3}]^{\frac{1}{2}}. \tag{C 4}$$

This quantity must fulfil the inequality $z < +1$, from which it follows that

$$(W_c+\tfrac{1}{4})/\omega > -1. \tag{C 5}$$

Substitution of (C 4) into the second member of (C 2) yields the equation

$$[((W_c+\tfrac{1}{4})/(3\omega))^2+\tfrac{1}{3}]^{\frac{3}{2}} - ((W_c+\tfrac{1}{4})/(3\omega))^3 + (W_c+\tfrac{1}{4})/(3\omega) - m^2/(2\omega) = 0. \tag{C 6}$$

As $(W_c+\frac{1}{4})/\omega$ increases from -1 to $+\infty$, the expression on the left-hand side of (C 6) increases monotonically from $-m^2/(2\omega)$ to $+\infty$. When $m \neq 0$ it is thus precisely one value of $(W_c+\frac{1}{4})/\omega$ which satisfies (C 6) and also fulfils the inequality (C 5). The equation (C 3) is thus seen to have two real roots in the interval $-1 < z < +1$ when $(W+\frac{1}{4})/\omega$ satisfies both of the conditions

$$(W+\tfrac{1}{4})/\omega > -1 \tag{C 7}$$

and
$$[((W+\tfrac{1}{4})/\omega)^2+3]^{\frac{3}{2}} - ((W+\tfrac{1}{4})/\omega)^3 + 9(W+\tfrac{1}{4})/\omega > \frac{27}{2}\frac{m^2}{\omega}. \tag{C 8}$$

Then the two roots $z = b$ and $z = a$ of equation (C 3) fulfil the inequality

$$-1 < b < a < +1. \tag{C 9}$$

From the graphical representations of the functions in the two members of (C 3) it is then obvious that a is positive, whereas b may be positive or negative but must satisfy the condition

$$|b| < a. \tag{C 10}$$

According to the conclusions below (C 3) it is obvious that

$$-\infty < c < -1. \tag{C 11}$$

PHILOSOPHICAL TRANSACTIONS OF THE ROYAL SOCIETY A MATHEMATICAL, PHYSICAL & ENGINEERING SCIENCES

To obtain further estimates of c we use the relation

$$a+b+c=-(W+\tfrac{1}{4})/\omega. \tag{C 12}$$

From (C 12) and the inequalities (C 9) and (C 10) we conclude that

$$-2-(W+\tfrac{1}{4})/\omega < c < -(W+\tfrac{1}{4})/\omega. \tag{C 13}$$

Furthermore, by substituting $z=-1$ into (C 2), we obtain the following equation

$$(1+a)(1+b)(1+c)=-m^2/\omega. \tag{C 14}$$

By solving (C 14) with respect to c, we get

$$c=-1-(m^2/\omega)/[(1+a)(1+b)]. \tag{C 15}$$

By means of (C 15) and the inequalities (C 9) and (C 10) we find that

$$c<-(1+m^2/4\omega). \tag{C 16}$$

References

Byrd, B. F. & Friedman, M. D. 1971 *Handbook of elliptic integrals for engineers and scientists*, 2nd edn. Berlin, Heidelberg, New York: Springer-Verlag.

von Meyenn, K. 1970 *Z. Physik* **231**, 154–60.

Peter, M. & Strandberg, M. W. P. 1957 *J. chem. Phys.* **26**, 1657–9.

Received 6 January 1992; accepted 5 February 1993

PHILOSOPHICAL TRANSACTIONS OF THE ROYAL SOCIETY A MATHEMATICAL, PHYSICAL & ENGINEERING SCIENCES