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2000 J. Phys. A: Math. Gen. 33 1187

(http://iopscience.iop.org/0305-4470/33/6/307)

J. Phys. A: Math. Gen. **33** (2000) 1187–1197. Printed in the UK PII: S0305-4470(00)06247-8

The diamagnetic Coulomb problem at low field strength: I. Analysis of the spherical basis

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Received 22 July 1999

Abstract. Using Legendre polynomials (spherical basis) asymptotic expansions are given in the singularities $r = 0, \infty$ of the Schrödinger equation of the diamagnetic Coulomb problem with infinite nuclear mass. It is pointed out that the truncated expansion converges to an unbounded solution at $r = \infty$. The complete expansion has either a trivial or a divergent solution only.

1. Introduction

The quantum mechanics of a hydrogen atom of infinite nuclear mass in a strong homogeneous magnetic field $\boldsymbol{H}$ seems to be settled; the extensive results concerning eigenvalues, transition probabilities, and related problems are summarized by Ruder *et al* (1994) where it is indicated that basic new results are not expected concerning the low-lying levels. Current interest has shifted towards problems in which the established results constitute a basis to handle more involved problems like the search of quantum chaos, or to treat the effect of the finite nuclear mass, the motion of the whole hydrogen atom (Lai and Salpeter 1995, Kopidakis *et al* 1996, Potekhin 1998) or how to compute the opacity of the strongly magnetized hydrogen plasma (Potekhin and Pavlov 1993, Merani *et al* 1995). The results in these topics may play a crucial role in interpreting some laboratory experiments or the spectrum of stars with suspected strong magnetic fields (Jordan 1992, van Riper 1988, Ventura *et al* 1992).

Mathematical analysis of the diamagnetic Coulomb problem was more or less neglected by Ruder *et al* (1994) and Rösner *et al* (1984) because their main goal was seemingly to provide exhaustive numerical results including moderately excited levels which are not accessible by variational or upper–lower bound methods. Concerning the excited levels, their tables represent the sole published source of numerical results covering a wide range of field strengths. Their eigenvalues, wavefunctions and transition probabilities were based on the simplest eigenfunction expansions in terms of Legendre polynomials and harmonic oscillator wavefunctions—'spherical' and Landau basis, respectively. Using the basis of Liu and Starace (1987) (LaS) an analysis and numerical solution in the non-adiabatic approximation of the problem at high field strengths were given by Barcza (1996) and Balla and Benkő (1996). These studies confirmed the results from the Landau basis and indicated only that the LaS basis fits the problem better. Analysis and an efficient way of numerical solution of quasi-separable quantum mechanical eigenvalue problems by eigenfunction expansions were discussed in an earlier paper (Barcza 1994). This paper can be regarded as an actual example of its considerations.

At low and moderate field strength the mathematical and numerical analysis of the diamagnetic Coulomb problem is of great interest both in its own right and as a standard quasi-separable quantum mechanical eigenvalue problem which is of the simplest kind if the spherical basis is used. In this case the particularly simple structure of the coupled second-order ordinary differential equations arising from the use of the basis functions allows one to draw conclusions by almost purely analytical means, among them being the important conclusion that the truncated form of the wavefunction, which must be used to make the problem numerically tractable, converges to a wavefunction which is itself unbounded.

The paper is organized as follows. Section 2 describes the asymptotic analysis of the spherical basis and gives the complete set of solutions in the singular points of the eigenvalue problem. Section 3 discusses the truncated solutions which are all of finite norm but converge to an unbounded wavefunction. Section 4 gives the complete solution which differs fundamentally from the truncated solution: it is not convergent for even parity, i.e. its series representation does not have a limit and furthermore its norm is infinite, while for odd parity only the trivial solution exists. Sections 5 and 6 present a discussion and draw conclusions.

The atomic units ($\hbar = 1, m_e = 1, e = 1$) will be used throughout; here, and in a forthcoming paper, $\omega = e|\boldsymbol{H}|/2m_ec$ is the magnetic field parameter, and $\omega = 1$ if $|\boldsymbol{H}| = 4.70 \times 10^9$ G.

2. Expansions of the wavefunction in terms of Legendre polynomials

The Schrödinger equation for stationary states of the diamagnetic Coulomb problem with infinite nuclear mass is

$$\left[\left(\boldsymbol{p} - \frac{1}{2c}\boldsymbol{H} \times \boldsymbol{r}\right)^2 - \frac{2Z}{r} - 2E\right]\Psi(r, \eta, \varphi) = 0 \tag{1}$$

(Ruder *et al* 1994) where $\boldsymbol{r}(r, \theta, \varphi)$ are the spherical coordinates, $\eta = \cos\theta$, $\boldsymbol{p} = (\hbar/\mathrm{i})\nabla$, $Z = 1$, $c^{-1} = \frac{1}{137.037}$. By assuming

$$\Psi = (2\pi)^{-1/2} r^{-1} \psi(r, \eta) \exp(\mathrm{i}n_3\varphi) \tag{2}$$

φ is separated and (1) takes the form

$$\frac{\partial^2\psi}{\partial r^2} - \left(\omega^2 r^2 - 2E^* - \frac{2Z}{r}\right)\psi + \frac{1}{r^2}\left[\frac{\partial}{\partial\eta}(1-\eta^2)\frac{\partial\psi}{\partial\eta} - \left(\frac{n_3^2}{1-\eta^2} - \omega^2 r^4 \eta^2\right)\psi\right] = 0 \tag{3}$$

where $E^* = E - \omega n_3$ and n_3 is the magnetic quantum number.

If

$$\psi = \sum_{l=|n_3|+p}^{\infty} u_l(r) P_l^{|n_3|}(\eta) \tag{4}$$

is assumed where $P_l^{|n_3|}$ is an associated Legendre polynomial, and some standard steps are performed (Ruder *et al* 1994), (3) can be transformed to the eigenvalue problem of the coupled system of second-order ordinary differential equations of the form

$$\begin{aligned}\frac{\mathrm{d}^2u_l}{\mathrm{d}r^2} - \left[L_0(l, |n_3|)\omega^2 r^2 - 2E^* - \frac{2Z}{r} + \frac{l(l+1)}{r^2}\right]u_l \\ +\omega^2 r^2[L_2(l, |n_3|)u_{l+2} + L_{-2}(l, |n_3|)u_{l-2}] = 0\end{aligned} \tag{5}$$

$l = |n_3| + p, |n_3| + p + 2, \ldots$

where $u_l(r)$ is called the channel coefficient,

$$L_{-2} = (l-1-|n_3|)(l-|n_3|)/(2l-3)(2l-1) \tag{6}$$

$$L_0 = [4l^3 + 6l^2 + 2l(2n_3^2 - 1) + 2n_3^2 - 2]/(4l^2 - 1)(2l+3) \tag{7}$$

$$L_2 = (l+2+|n_3|)(l+1+|n_3|)/(2l+5)(2l+3). \tag{8}$$

The definition of $P_l^{|n_3|}$ and the interrelations of the associated Legendre polynomials leading to (6)–(8) are given by Erdélyi (1953). Because of the invariance of (3) with respect to $\eta \leftrightarrow -\eta$, l runs in (4) and the following formulae over even or odd values, $p = 0, 1$ for even and odd solutions respectively. The boundary condition is that ψ must be bounded in the domain $-1 \leqslant \eta \leqslant 1$, $0 \leqslant r \leqslant \infty$. Equations (5) are, from a mathematical point of view, a finitely coupled infinite system of second-order ordinary differential equations. For reasons of practicality $1 \leqslant N < \infty$ terms can be taken into account in a numerical integration; these must be the first N terms; $E^{*(N)}$ will denote an eigenvalue of the truncated system. The norm is

$$(\Psi, \Psi) = \sum_{l=|n_3|+p}^{2N-2+|n_3|+p} \frac{2(l+|n_3|)!}{(2l+1)(l-|n_3|)!} \int_0^\infty \mathrm{d}r u_l^2(r) = \sum_l u_{\langle l \rangle}^2 \tag{9}$$

where the term l with the largest $u_{\langle l \rangle}^2$ can be regarded as the dominant term or channel.

The singular points of (5) are $r = 0$ and ∞, around them asymptotic expansions will now be given.

2.1. *The channel coefficients at* $0 \leqslant r < 1$

In the regular singularity $r = 0$, (5) is completely decoupled: in the interval $0 \leqslant r < 1$ its bounded solution begins in such a manner that the coupling does not enter in the terms $m = 0, 1$ of the series

$$u_l(r) = \sum_{m=0}^{\infty} c_m^{(l)} r^{m+l+1} \tag{10}$$

where

$$c_{m+1}^{(l)} = -\frac{2Zc_m^{(l)} + 2E^* c_{m-1}^{(l)} + \omega^2 [L_{-2} c_{m-1}^{(l-2)} - L_0 c_{m-3}^{(l)} + L_2 c_{m-5}^{(l+2)}]}{l[2l(m+1) + m^2 + 3m + 2]} \tag{11}$$

$$m = 0, 1, \ldots, c_{-1}^{(l-2)} = c_{-3}^{(l)} = c_{-2}^{(l)} = c_{-1}^{(l)} = c_{-5}^{(l+2)} = \cdots = c_{-1}^{(l+2)} = 0.$$

Because of the asymptotic decoupling the coefficients $c_0^{(l)}$ of number N are free parameters; one of them is the normalization factor. (By definition a parameter of an asymptotic solution is free if the boundary condition is automatically satisfied at its arbitrary value.) In the interval $1 \leqslant r < \infty$ the power series (10) is suitable for numerical purposes as well if its two deficiences are controlled: at $r \gg 1$ its convergence is slow and the loss of digits—$\max_m |c_m^{(l)} r^{m+l+1}/u_l(r)|$—is high when computing $u_l(r) \approx 0$.

2.2. *The channel coefficients at* $r \to \infty$

In the irregular singularity $r = \infty$ by assuming

$$u_l(r) = C_l[1 + d_{-4}/r^4 + \mathrm{O}(r^{-5})] \exp(-\omega\Lambda r^2/2 + d_1 r + d_0 \ln r - d_{-1}/r) \tag{12}$$

equations (5) were transformed to the system of coupled equations

$$
\begin{aligned}
C_l\{\omega^2(\Lambda^2 - L_0)r^2 - 2\Lambda\omega d_1 r + d_1^2 - \Lambda\omega(2d_0+1) + 2E^* \\
+(2Z + 2d_1d_0 - 2\Lambda\omega d_{-1})/r + [d_0^2 - d_0 - 2d_1d_{-1} - l(l+1)]/r^2 \\
+\mathrm{O}(r^{-3})\}[1 + d_{-4}^{(l)}/r^4] + \omega^2 r^2\{C_{l+2}L_2[1 + d_{-4}^{(l+2)}/r^4] \\
+C_{l-2}L_{-2}[1 + d_{-4}^{(l-2)}/r^4]\} = 0 \qquad l = |n_3| + p, \ldots, |n_3| + p + 2N - 2.
\end{aligned}
\tag{13}
$$

The exponential factor of (12) regularized the singularity in the same sense as r^l of (10): it made it possible to find an asymptotic series in terms of r^{-1}, $0 \leqslant r^{-1} \ll 1$. This was done by transforming (5) into Ricatti equations. Since it is an identical factor for any l, it was omitted in (13). The first coefficient is d_{-4} which depends on l. By equating the coefficient of the different powers of r with zero in (13), Λ, d_1, d_0 etc can be determined.

If $N \geqslant 2$ the equations (13) remain coupled, i.e. the coefficient of r^2 gives a recurrence relation for C_l:

$$
\begin{aligned}
&L_{-2}(l, n_3)C_{l-2} + [\Lambda^2 - L_0(l, n_3)]C_l + L_2(l, n_3)C_{l+2} = 0 \\
&l = |n_3| + p, \ldots, |n_3| + p + 2N - 2.
\end{aligned}
\tag{14}
$$

(14) is a system of homogeneous linear equations of number N which has a non-trivial solution if its determinant vanishes as a function of Λ^2. In terms of a continued fraction this is expressed by

$$
F_N(\Lambda^2) = a_1 + \frac{b_1}{a_2+} \cdots \frac{b_{N-1}}{a_N} = 0 \tag{15}
$$

where $a_m = \Lambda^2 - L_0(l+2m-2, n_3)$, $b_m = -L_{-2}(l+2m, n_3)L_2(l+2m-2, n_3)$ with $l = |n_3| + p$. N' will denote the number of the roots $\Lambda_1^2, \ldots, \Lambda_{N'}^2$ of (15). In (13) the coefficients of r, r^0, r^{-1} give

$$
\begin{aligned}
&d_1 = 0 \qquad d_0 = E^*/\omega\Lambda - \tfrac{1}{2} \qquad d_{-1} = Z/\omega\Lambda \qquad \text{if} \quad \Lambda \neq 0 \\
&d_1 = \pm(-2E^*)^{1/2} \qquad d_0 = \mp Z/(-2E^*)^{1/2} \qquad \text{if} \quad \Lambda = 0
\end{aligned}
\tag{16}
$$

and the coefficients of the higher powers of r^{-1} can be elaborated successively, in principle, up to any order.

It is obvious that (5) has linearly independent bounded asymptotic solutions in number N': they are of the form (12) with $\Lambda_1, \ldots, \Lambda_{N'}$. These linearly independent solutions constitute a basis to expand the general asymptotic solution: the linear combination

$$
\begin{aligned}
u_l(r) = \sum_{m=1}^{N'} C_l^{(m)}[1 + d_{-4}^{(m,l)}r^{-4} + \mathrm{O}(r^{-5})]\exp[-\omega\Lambda_m r^2/2 + d_1^{(m)}r \\
+d_0^{(m)}\ln r - d_{-1}^{(m)}/r] \qquad l = |n_3| + p
\end{aligned}
\tag{17}
$$

will lead to the proper general asymptotic solution of (5) at $r \to \infty$ with the free parameters $C_{|n_3|+p}^{(m)}$ of number N'; one of them is the normalization factor. The other channel coefficients $u_l(r)$ with $l = |n_3| + p + 2, \ldots$ are likewise of the form (17); however, $C_{|n_3|+p+2}^{(m)}, \ldots$ are not free parameters but can be obtained by solving (14) with Λ_m, $m = 1, \ldots, N'$.

With the method used in this section a complete set of the allowed asymptotic channel coefficients was produced in the neighbourhood of both singular points of (5) and the number of free parameters of the bounded solutions was determined. The value of the free parameters $c_0^{(l)}$, $l = |n_3| + p, \ldots, |n_3| + p + 2N - 2$ and $C_{|n_3|+p}^{(m)}$, $m = 1, \ldots, N'$ can only be determined by numerical methods. By fixing their values an asymptotic particular solution is obtained. The omitted terms of the asymptotic channel coefficients—$\propto r^{-l}$ at $r = 0$, $\propto \exp(+\omega\Lambda r^2/2)$ at $r \to \infty$—had to be ruled out automatically because of unboundedness.

3. Truncated solutions

In the asymptotic range $r \to \infty$ the truncated solutions are formed by setting

$$C^{(m)}_{|n_3|+p+2\hat{N}} = 0 \qquad \text{for any } m \quad \hat{N} \geqslant N. \tag{18}$$

This is equivalent to approximation of ψ by a finite sum which involves an artificial termination of the infinite series (4). This step is warranted if (4) is convergent in any fixed point (r, η).

If $1 \leqslant N < \infty$, (15) is an Nth-degree polynomial in terms of Λ^2 with roots of number $N' = N$.

3.1. Adiabatic approximation

The adiabatic approximation for any l is defined by

$$\frac{\mathrm{d}^2 u_l}{\mathrm{d}r^2} - \left[L_0 \omega^2 r^2 - 2E^{*(1)} - \frac{2Z}{r} + \frac{l(l+1)}{r^2} \right] u_l = 0 \tag{19}$$

where $N = 1$, and its u_l approximates roughly the r dependence of the dominant channel. (19) has a composite spectrum (Barcza 1996) i.e. if $\omega \ll 1$ the low-lying levels follow Balmer spacing while the highly excited ones (where $2Z/r$ is negligible) follow the quasi-Landau spacing

$$E^{*(1)}_k \to \omega L_0^{1/2}(l, n_3)(l + 2k + \tfrac{3}{2}) \tag{20}$$

where $k \geqslant 0$ is a large integer, and a continuum does not exist for any $\omega > 0$. With increasing ω or $E^{*(1)}$ the Balmer spacing is replaced more and more by the quasi-Landau spacing. The norm (9) is finite for any u_l, the absorption threshold does not exist because at $r \to \infty$ the potential is proportional to r^2. The quasi-Landau spacing varies from $(\frac{8}{3})^{1/2}\omega \approx 1.63\omega$ $(l = 0)$ to $2^{1/2}\omega \approx 1.42\omega$ $(l \to \infty)$ if $n_3 = 0$, from $(\frac{16}{5})^{1/2}\omega \approx 1.78\omega$ to $2^{1/2}\omega$ if $n_3 = 1$ etc, which values allow even the experimentally found $\approx 1.5\omega$ at and somewhat above the absorption threshold (Veldt *et al* 1992). Compared with the case $1 < N < \infty$ the numerical solution of the adiabatic approximation (19) is much easier because of the possibility of continuing the expansion in the exponent of (12) and cutting short the interval in which a numerical integration is necessary to fit the solutions from (10) and (12).

In spite of the attractive physical and mathematical features the adiabatic approximation in the spherical basis is of scant value since $u_l(r)P_l^{|n_3|}(\eta)$ approximates ψ poorly.

3.2. Non-adiabatic approximations with finite N

If the non-adiabatic approximation of type $1 < N < \infty$ is considered the composite character of the spectrum is preserved: Balmer-like quantization if $0 < \omega \ll 1$ and $E^{*(N)} < 0$, with increasing $E^{*(N)}$ convergence to a quasi-Landau quantization of the levels of always-finite norm (9), and lack of continuum.

A rule is that at $\omega \approx 0$ the dominant channel has the value l belonging to the hydrogenic level from which the level evolves with increasing ω. This rule manifests itself in $|c_0^{(l)}| \gg |c_0^{(l\pm m)}|$, $m = 2, 4, \ldots, l - m \geqslant 0$.

Some eigenvalues are plotted in figure 1 from a numerical solution of (15) which indicates $\Lambda_m \to 0$ with increasing N, $m = 1, 2, \ldots, \ll N$. Since the exponentials with $\Lambda_2, \ldots, \Lambda_N$ vanish more rapidly at $r \to \infty$ the dominant term of (17) will be $m = 1$ if $C^{(1)}_{|n_3|+p} \neq 0$, $m = 2$ if $C^{(1)}_{|n_3|+p} = 0$ etc, this is the rule for $C^{(m)}_{|n_3|+p}$ at any ω. This asymptotic form anticipates the problem of convergence if N increases since from moderate to large values of r the terms $d_0^{(1)} \ln r - d_{-1}^{(1)}/r$ can exceed $\omega \Lambda_1 r^2/2$. However, it is obvious that by solving the truncated

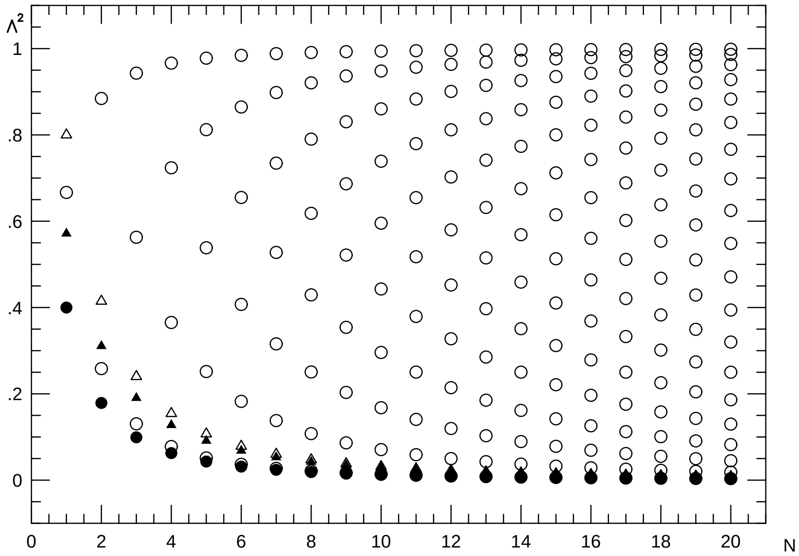

Figure 1. The eigenvalues of (15) as a function of N. Circles: $\Lambda_1^2, \ldots, \Lambda_N^2$ for $n_3 = p = 0$, filled circles: Λ_1^2 for $n_3 = 0$, $p = 1$, triangles and filled triangles: Λ_1^2 for $n_3 = 1$, $p = 0$ and 1, respectively.

equations (5) ψ is obtained with finite spatial norm (9) at any eigenvalue $E^{*(N)}$. An infinite spatial norm (9) is excluded: continuum wavefunctions cannot be obtained since for any l $u_l(r)$ is a sum of terms with $\propto \exp(-\omega\Lambda_m r^2)$, $\Lambda_m > 0$. Continuum solutions of (5) do not exist if $N < \infty$.

3.3. Numerical solution

By a shooting method using the Numerov integrator formula (Barcza 1994), (5) was solved. (This method may correspond to the 'direct numerical integration' to the 'exact solution' of Ruder *et al* (1994), as far as can be inferred from the sparse numerical detail given therein.) The outward and inward integrations were begun from (10) and (17), respectively, i.e. a number of initial value problems were solved on a finite interval $[0, r_s]$, $1 \ll r_s < \infty$ so that $E^{*(N)}$ and the asymptotically free parameters were varied in order to find the coincidence of $u_l(r_\mathrm{m})$ and $u_l(r_\mathrm{m} + h)$, $l = |n_3| + p, \ldots$ where h is the step size at the mesh point r_m. The number of coincidences to be achieved is $2N$, that of the free parameters is $2N + 1$; one of them, e.g. $c_0^{(|n_3|+p)}$, is the normalization factor. The balance is that the asymptotically free parameters are consumed completely by the fitting procedure and the uniqueness of a solution is provided by fixing $E^{*(N)}, c_0^{(|n_3|+p+2)}, \ldots, c_0^{(|n_3|+p+2N-2)}, C_{|n_3|+p}^{(1)}, \ldots, C_{|n_3|+p}^{(N')}$ since all $u_l(r)$, $\mathrm{d}u_l/\mathrm{d}r$ became continuous functions (up to $\mathrm{O}(h^5)$ of the Numerov integrator formula) in the whole interval $0 \leqslant r \leqslant \infty$.

The numerical solutions have shown that at $r \gg 1$ channel coefficients $u_l(r)$, $l = |n_3| + p, \ldots$ of the truncated equations (5) converge to the term $m = 1$ from (17): indication of $C_{|n_3|+p}^{(1)} = 0$ was not found in the interval $0 < \omega \ll 1$. Changes of sign in $c_0^{(l)}$ with a rapid reordering of the channel weights $u_{\langle l\rangle}^2$ were observed in narrow ranges of ω where the slope of curves $E^{*(N)}(\omega)$ changed strongly, e.g. at avoided crossings.

With increasing N the convergence of $E^{*(N)}$ slowed down or turned into a drift. Spurious abrupt changes of $E^{*(N)}$ were found if r_s was increased, instabilities appeared which indicated the loss of digits and could be mastered by increasing the accuracy of the computations. For example, in the interval $10^{-4} \leqslant \omega \leqslant 10^{-2}$, to achieve an accuracy 10^{-6} of E^* in integrations with $N = 2$ the double precision accuracy 10^{-15} was sufficient for the levels which originated from the main quantum number $n = 6$ at $\omega = 0$, while for $N = 4$ the extended precision accuracy 10^{-35} was necessary. For $N = 6$ some failures were found even with extended precision. The observed loss of digits in the integrations far exceeded the loss from the cumulative error of the integrator formula which was estimated according to Sloan (1968) and Johnson (1977). The most probable explanation for this computational finding seems to be that positive Lyapunov exponents exist if the evolution of $u_l(r)$, $0 \leqslant r \leqslant r_s$ is considered as a function of the free parameters $c_0^{(l)}$, $C^{(m)}_{|n_3|+p}$: the exponents $\ln|\Delta u_l(r_\mathrm{m})/\Delta c_0^{(l)}|$, $\ln|\Delta u_l(r_\mathrm{m})/\Delta C_l^{(1)}|$ (Contopoulos and Barbanis 1989) were found to be increasing positive numbers with increasing r_m and $r_s - r_\mathrm{m}$ where $\Delta u_l(r_\mathrm{m})$ is the relative error of $u_l(r_\mathrm{m})$ to which the relative error of $u_l(r)$ at $r \ll 1$ or $r \gg 1$ propagated; this latter relative error is given by $\Delta c_0^{(l)}$ and $\Delta C_l^{(1)}$, respectively. In other words: to obtain a fit of 10^{-6} accuracy in the mesh point the shooting—an initial value problem for the free parameters—had to be started by a much better accuracy, e.g. 10^{-20} or even 10^{-35}. With increasing ω, N or approaching an avoided crossing the digit loss became increasingly severe. Further discussion of this issue is beyond the scope of the present paper: e.g. whether these instabilities belong to an intrinsic feature of the diamagnetic Coulomb problem or to the non-optimal choice of the basis functions only.

4. The complete solution at the irregular singularity

Since the only parameter of the recurrence relation (14) is Λ^2 in its middle term the series of $C_{|n_3|+p+2N}$, $N \to \infty$ cannot be terminated by any value of Λ^2. Consequently, at $r \to \infty$ the presumed convergence of (4) must be examined in order to substantiate its approximation by a truncated sum. The infinite continued fraction in (15) represents a transcendental function and is principally different from $F_N(\Lambda^2)$ with finite N which is a polynomial.

A non-trivial asymptotic solution of type (12) can exist if $F_\infty(\Lambda^2)$ is convergent, i.e. if

$$\lim_{N\to\infty} \left| \frac{b_{N-1}}{a_{N-2}a_{N-1}} \right| \leqslant \frac{1}{4} \tag{21}$$

(Worpitzky theorem: Bulirsch and Stoer 1968). On expanding L_{-2}, L_0, L_2, assuming $\Lambda^2 = \lambda_0 + \lambda_1/l + \mathrm{O}(l^{-2})$, and introducing these expressions in (21), the criterion of convergence is that either

$$\Lambda^2 \leqslant \lim_{l\to\infty} (4n_3^2 - 1)/4l^2 = 0 \tag{22}$$

or

$$\Lambda^2 \geqslant \lim_{l\to\infty} 1 + \mathrm{O}(l^{-2}) = 1 \tag{23}$$

where $l = |n_3| + p + 2N$. A forbidden interval is $0 < \Lambda^2 < 1$ where the points are in figure 1: $F_\infty(\Lambda^2)$ is divergent here and (15) cannot be satisfied, which has the consequence that in the forbidden interval only the trivial solution exists: $C_l = 0$ for any l.

As a second step, outside the forbidden interval the roots Λ^2 must be determined which satisfy (15). $F_\infty(\Lambda^2)$ was expanded according to Bulirsch and Stoer (1968); figure 2 is a plot of its values for $n_3 = 0, 1, 2$ and $p = 0, 1$ which were obtained numerically. If $-\infty < \Lambda^2 < -0.5$ or $1.5 < \Lambda^2 < \infty$ the inclusion of a few (<10) fraction lines provides an accuracy 10^{-5} of $F_\infty(\Lambda^2)$, an expansion in terms of Λ^{-2} shows that there are no roots in these intervals. Approaching $\Lambda^2 = 0$ or 1 the number of necessary fraction lines to this accuracy

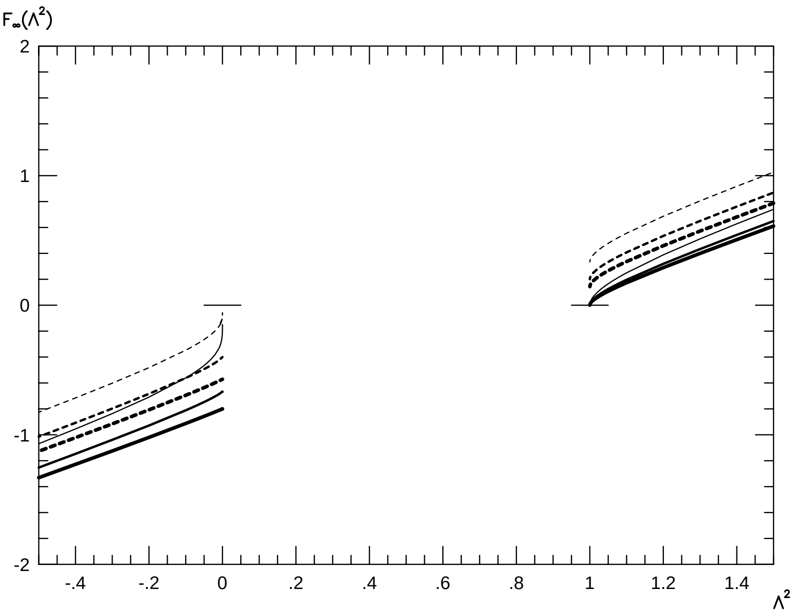

Figure 2. A plot of $F_\infty(\Lambda^2)$. Solid curves: $p = 0$; dashed curves: $p = 1$; the thin, moderately thick and thick curves correspond to $n_3 = 0, 1, 2$ respectively. $F_\infty(\Lambda^2)$ was found to be divergent in the empty region $0 < \Lambda^2 < 1$. The extrapolation of the solid curves touches the short horizontal line, $F_\infty(\Lambda^2) = 0$, asymptotically at $\Lambda^2 = 1$.

increases rapidly: at $\Lambda^2 = -10^{-5}$ or 1.000 01 some 100 fraction lines must be taken into account. This worsening of convergence is the consequence of approaching the limits (22), (23). Extrapolation of the numerical results indicates that the root of (15) is $\Lambda^2 = 1$ for $p = 0$, $n_3 = 0, 1, 2, \ldots$ while for the curves of $p = 1$ $F_\infty(\Lambda^2) \neq 0$ in the allowed domains $\Lambda^2 \leqslant 0$ or $\Lambda^2 \geqslant 1$. For computational convenience $N < 500$ was set, the nature of the divergence of $F_\infty(\Lambda^2)$ was examined numerically if $0 < \Lambda^2 < 1 : |F_\infty(\Lambda^2)| < \infty$ but $\lim_{N\to\infty} F_N(\Lambda^2)$ does not exist. Depending on the distance from $\Lambda^2 = \frac{1}{2}$, which is a critical value for (15) because of $a_N \to 0$, the values $F_N(\Lambda^2)$, $N = m_0, \ldots, m_c$ showed a quasi-periodicity where $m_c - m_0$ was a small integer at $\Lambda = \frac{1}{2}$, and a large integer at $\Lambda^2 \approx 0, 1$.

5. Discussion

The adiabatic approximation always has non-trivial and bounded solutions exclusively with a discrete spectrum which indicates the existence of a quasi-Landau quantization. The adiabatic wavefunctions $u_l(r)P_l^{|n_3|}(\eta)$ and (4) are, however, essentially different from a mathematical point of view.

The non-trivial asymptotic solutions of the truncated system (5) are bounded, and their norm is finite at any value of ω and $E^{*(N)}$. They report on discrete levels only; the continuum solution does not exist in the framework of this approximation. Their convergence is slow, and at fixed m and increasing N, $\Lambda_m^2 \to 0$ was found by the numerical solution of (15), i.e. at $r \to \infty$ the leading term of the asymptotic channel coefficients converges to

$$u_l(r) \to \hat{u}_l = C_l^{(1)}[1 + \mathrm{O}(r^{-2})] \exp[-(-2E^*)^{1/2}r + Z \ln r/(-2E^*)^{1/2}] \tag{24}$$

$$\lim_{l\to\infty} C_{l+2}^{(1)}/C_l^{(1)} = 1. \tag{25}$$

This solution has an absorption threshold at the wrong position $E^* = 0$; for any E^* its norm is infinite, and must be rejected on the ground that at $r \to \infty$ (24) and (25) lead to

$$\psi(r, \eta) \to \sum_l \hat{u}_l(r) P_l^{|n_3|}(\eta) \approx \hat{u}_{2N-2+|n_3|+p}(r) \sum_l P_l^{|n_3|}(\eta) \tag{26}$$

which becomes unbounded with $N \to \infty$ along the axis $\eta = \pm 1$, as can be seen from the generating function of $P_l^{|n_3|}(\eta)$ (Schiff 1968). All asymptotically free parameters of (17) now have a fixed value, and therefore, there are no parameters to avoid the behaviour (26) (e.g., by a combination of terms appearing on the right-hand side of (24)). The instabilities of the numerical solution reported in section 3.3 can probably have their origin in the unstable or wrong behaviour of (24) according to which the integrations started.

The wavefunctions from (17) with $m = 1$, and (24), have contradictory features; notwithstanding, saturation of $E^{*(N)}$ could be reported by Ruder *et al* (1994), even if increasing difficulties with the spherical basis were mentioned for the levels $n \geqslant 4$ (of $\omega = 0$): for the level $4s\sigma (n = 4, l = 0, n_3 = 0)$ $N = 2$–24, and for the level $5s\sigma$ $N = 23$–20 terms were necessary in the intervals $10^{-4} \leqslant \omega \leqslant 3 \times 10^{-2}$, $10^{-4} \leqslant \omega \leqslant 7 \times 10^{-4}$, respectively. If $E^{*(N)}$ is convergent with increasing N, it converges to pseudo-eigenvalues which belong to a wavefunction violating the boundary condition of boundedness at $r \to \infty$, $\eta = \pm 1$. Solving the truncated system (5) correctly does not guarantee $E^{*(N)} \to E^*$ in itself if N is increased. The relation of $E^{*(N)}$ to E^* depends upon whether by chance the truncated sum (4) does or does not approximate to ψ in the interval where the Hamiltonian gives large weight to it in the energy integral.

The complete system of equations (5) has either a trivial solution, i.e. $N' = 0$ for $p = 1$, or the solution belonging to the extrapolated $\Lambda^2 = 1$ if $p = 0, n_3 = 0, 1, \ldots$, i.e. $N' = 1$:

$$u_l(r) \to C_l^{(\infty)}[1 + O(r^{-4})] \exp[-\omega r^2/2 + (E^*/\omega - 1/2) \ln r - Z/\omega r] \tag{27}$$

$$\lim_{l\to\infty} C_{l+2}^{(\infty)}/C_l^{(\infty)} = -1. \tag{28}$$

Two objections can be raised against (27): it leads to the wavefunction of a discrete level but its norm is divergent according to (9) and the sum (4) is not convergent in the sense that its limit does not exist because of (28). For example, at $\eta = 1$, $r \gg 1$ the sum has two discrete values depending upon whether $l/2$ is even or odd for its last term:

$$\psi(r, 1) \to [1 + O(r^{-4})] \exp[-\omega r^2/2 + (E^*/\omega - 1/2) \ln r - Z/\omega r] \sum_l (-1)^{l/2}. \tag{29}$$

Numerical attempts failed to find this solution by setting $C_l^{(N)} \neq 0$, $C_l^{(m)} = 0$, $l = |n_3| + p, \ldots$, $m = 1, \ldots, N-1$ in (17). $2 \leqslant N \leqslant 6$ was used in the computations.

Caution is appropriate with an expansion of type (4): $\psi(r, \eta)$ was expanded in terms of the complete system of orthogonal functions $P_l^{|n_3|}(\eta)$; nevertheless, the truncated and the infinite expansions converge to physically unacceptable wavefunctions which are of a different type. Concerning the structure of the coupled equations for $u_l(r)$ the basic difference between $N < \infty$ and $N = \infty$ is that by the truncation singular terms of the complete system (5) are neglected. This radically modifies the character of the solutions in the singularity $r \to \infty$ since the coupling is proportional to r^2 in every equation.

6. Conclusions

It has been shown that in the diamagnetic Coulomb problem the spherical basis provides a doubtful expansion of the wavefunction. If the complete infinite expansion is used it allows only a trivial or a divergent solution. If the expansion is truncated arbitrarily with an increasing number of terms the solution converges to an unbounded wavefunction. From a mathematical point of view these possibilities are solutions to equations (5) but not to the diamagnetic Coulomb problem. In all respects, perfect expansion can be obtained to the diamagnetic Coulomb problem by using the angular oblate functions, since in this expansion the system of second-order ordinary differential equations is completely decoupled at $r \to \infty$ and here the asymptotic solution is the convergent sum of the solutions of adiabatic equations. Starace and Webster (1979) proposed the use of the angular oblate functions and solved the adiabatic approximation while the non-adiabatic approximation was solved by Barcza (1994) as an example for quasi-separable quantum mechanical eigenvalue problems; extensive tabular material from this expansion is not available yet. In a forthcoming paper the complete asymptotic analysis and numerical solution will be given using this basis. This will be the proper solution to the diamagnetic Coulomb problem at low and moderate field strength in the framework of eigenfunction expansions.

Acknowledgments

The author is grateful to Dr J Benkő and an anonymous referee for comments on the manuscript.

Appendix A. Equivalent forms to (4)

The general form of two conventional expansions is involved in (4). In a truncated form these expansions were used in the diagonalization technique (e.g., Holle *et al* 1986). These expansions are as follows.

(a) If the complete diamagnetic term $\omega^2 r^2(1-\eta^2)$ is taken as perturbation, the rest of (3) is separable. The assumption

$$\psi = \sum_{k,l} c_{kl}^{(\mathrm{a})} R_k^{(\mathrm{a})}(r) P_l^{|n_3|}(\eta) \tag{A.1}$$

will be appropriate where $R_k^{(\mathrm{a})}(r)$ is a hydrogenic radial wavefunction with $k = 1, 2, \ldots$ denoting the levels at a fixed l. By definition, the sum represents an appropriate integral over the continuum components. The first part of (3) without the term $\omega^2 r^2$ is the radial Schrödinger equation of hydrogen; in its hydrogenic energy spectrum $\epsilon^{(\mathrm{a})}$ there is one absorption threshold: $\epsilon^{(\mathrm{a})} = 0$.

(b) If the term $-\omega^2 r^2 \eta^2$ is taken as a perturbation, the rest of (3) is separable. The wavefunction must be assumed to be of the form

$$\psi = \sum_{k,l} c_{kl}^{(\mathrm{b})} R_k^{(\mathrm{b})}(r) P_l^{|n_3|}(\eta) \tag{A.2}$$

where $R_k^{(\mathrm{b})}$ satisfies (19) if $L_0 = 1$, $l = 0$, $E^{*(1)} = \epsilon^{(\mathrm{b})}$ are introduced. $\epsilon^{(\mathrm{b})}$ is of a composite-type spectrum without continuum: it follows Balmer spacing for the low-lying levels at $\omega \ll 1$, and Landau spacing 2ω for highly excited levels (Barcza 1996).

The spectrum $\epsilon^{(\mathrm{b})}$ consists of discrete elements only; the basis functions $R_k^{(\mathrm{b})}$ build up a complete orthogonal system. Consequently, any ψ of finite norm is represented by the form (A.2) (von Neumann 1980, Courant and Hilbert 1968). Since at $r \gg 1$ $R_k^{(\mathrm{b})}$ is proportional to $\exp(-\omega r^2/2)$, ψ is obtained by the truncated (A.2) which is of bound type at any energy eigenvalue.

The spectrum $\epsilon^{(\mathrm{a})}$ consists of discrete elements and a continuum as well. Depending on the values of $c_{kl}^{(\mathrm{a})}$, ψ can be of bound or continuum type. Above the hydrogenic absorption threshold, $E^* = 0$, a wavefunction of both types can be constructed by (A.1).

If (A.1) or (A.2) are used in practical computations for bound states a huge finite system of homogeneous linear equations must be solved for c_{kl} which has non-trivial solutions at discrete values of E^*—Holle *et al* (1986) gave an example for (A.1).

Using (4), ψ is expanded in terms of $P_l^{|n_3|}$ at each point r continuously; the assumptions (A.1) and (A.2) can be unified:

$$u_l(r) = \sum_k c_{kl}^{(j)} R_k^{(j)}(r) \qquad j = \text{a or b} \tag{A.3}$$

whose common form is (4). It can be guessed that these two expansions suffer from the same faults as (4).

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