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The diamagnetic Coulomb problem: an eigenvalue problem with two singularities

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Abstract
By using the angular oblate spheroidal functions as basis functions a bounded wavefunction is constructed in the singularities of the Schrödinger equation of the diamagnetic Coulomb problem with infinite nuclear mass. The expansion in terms of these functions is a model to resolve singularities in an eigenvalue problem of non-separable partial differential equations of non-relativistic quantum mechanics. A comprehensive asymptotic analysis reveals the complete set of asymptotic solutions, makes possible a uniform numerical treatment of the bound, autoionizing continuum and continuum levels, and indicates how to find hitherto unknown low-lying stationary levels. An example, the splitting of the ground level, has been found numerically by an iterative shooting method.

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1. Introduction

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

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

(Ruder *et al* 1994) where $\mathbf{r}(r, \theta, \varphi)$ are the spherical coordinates, $-1 \leqslant \eta = \cos\theta \leqslant 1$, $\mathbf{p} = (\hbar/\mathrm{i})\nabla$, Z is the nuclear charge, E is the energy eigenvalue. Atomic units ($\hbar = 1, m_\mathrm{e} = 1, e = 1$) will be used throughout in the paper, $\omega = e|\mathbf{H}|/2m_\mathrm{e}c$ is the parameter of the problem, $\omega = 1$ if the homogeneous magnetic field $\mathbf{H}$ in z direction is equal to 4.70×10^9 G. The boundary conditions are the usual ones of non-relativistic quantum mechanics: boundedness in the whole domain of r, η, ϕ, quadratic integrability over space for bound levels and over momentum space for continuum levels. Astrophysical applications and the need to interpret laboratory measurements made this elementary problem of non-relativistic quantum mechanics a theoretical challenge some 20 years ago.

The potential $\omega^2 r^2(1-\eta^2) - 2Z/r$ has two singularities at $r = 0$ and ∞ if $\eta \neq \pm 1$ while on the axis z (i.e. $|\eta| = 1$): $\mathbf{r}$ and $\mathbf{H}$ are parallel and there is a Coulomb singularity only. The sum of spherically and cylindrically symmetric potentials allows the separation of φ only. Equation (1) is the simplest one among the numerous non-separable quantum-mechanical eigenvalue equations. The early studies of (1) were summarized by Ruder *et al* (1994). The solutions were numerically oriented: variational calculations with more and more sophisticated trial wavefunctions, expansions in different basis functions using $O(10^4)$ elements and diagonalization, or eigenfunction expansion in the spherical basis. Kravchenko, Liberman and Johansson (1996) gave another expansion in a basis built up directly from the partial differential equation. In these studies analytical behaviour of the wavefunction was scarcely apparent in the singularities, as well as an eventual relation of the found numerical solutions to the whole manifold of the solutions. The overwhelming majority of the numerical results of astrophysical interest was obtained in the spherical basis. However, an analysis revealed serious objections against the use of the spherical basis: it does not give the correct wavefunction in the singularity $r = \infty$ and it cannot account for the continuous spectrum (Barcza 2000).

The aim of the present paper is to construct the analytic asymptotic solutions in the singularities of diamagnetic Coulomb problem, to give insight into the complete set of solutions and in a robust numerical procedure for bridging over the finite domain between the singularities. Since the diamagnetic Coulomb problem is a prototype of non-relativistic non-separable eigenvalue problems in quantum mechanics the algebraic machinery to support a numerical solution will be interesting in itself.

We describe a solution using expansion of the wavefunction in terms of the angular oblate spheroidal functions; we elucidate the analytic properties of ψ at the singular points $r = 0$ and ∞, $\eta = \pm 1$ of the eigenvalue equation

$$
\begin{aligned}
-\frac{\partial}{\partial r} r^2 \frac{\partial \psi}{\partial r} + [\omega^2 r^4 - 2(E - \omega n_3) r^2 - 2Zr]\psi - \frac{\partial}{\partial \eta}(1-\eta^2)\frac{\partial \psi}{\partial \eta} \\
+ \left(\frac{n_3^2}{1-\eta^2} - \omega^2 r^4 \eta^2 \right) \psi = 0
\end{aligned}
\tag{2}
$$

which was obtained from (1) by separating φ: $\Psi = (2\pi)^{-1/2} \exp(\mathrm{i} n_3 \varphi) \psi(r, \eta)$, n_3 is the magnetic quantum number. An analytic solution to (2) is not known. Nevertheless, we shall find the complete set of the asymptotic solutions in analytic form and a limited number of numerical solutions will be given which demonstrate that the solutions from the spherical basis represent only a subset of all solutions. Further benefits of the use of angular oblate spheroidal functions are the rapid convergence (because products of these functions and appropriate functions depending on r are nearly congruent with the exact wavefunctions) and a fairly good representation of the wavefunction at small and large field strength as well. There is no need to use another expansion, e.g. the Landau basis (Ruder *et al* 1994) or LaS basis (Barcza 1996, Balla and Benkő 1996), to match two different expansions in the region of strong mixing because the sum of a few terms approximates well the wavefunction at any field strength. The use of the angular oblate spheroidal functions in the diamagnetic Coulomb problem was suggested and solved in the adiabatic approximation by Starace and Webster (1979). The coupling functions and a numerical solution of the non-adiabatic approximation were reported in Barcza (1994).

Section 2 summarizes the use of angular oblate spheroidal functions: (2) will be transformed to a system of infinitely coupled second order ordinary differential equations of the form which is suitable for asymptotic analysis and unified treating bound, autoionizing stationary and the true continuum levels. In section 3 the complete set of asymptotic solutions will be given in the singularities $r = 0, \infty$. The sketch of the numerical procedure bridging over the asymptotic regions and selected numerical results for even parity, $n_3 = 0$ will be given in section 4. The results are discussed briefly in section 5. Section 6 draws the conclusions.

2. The expansion of the wavefunction and the coupled second order ordinary differential equations

The eigenfunctions of the η-dependent part in (2) are the angular oblate spheroidal functions (Abramowitz and Stegun 1968)

$$\left[\frac{\partial}{\partial\eta}(1-\eta^2)\frac{\partial}{\partial\eta} - \frac{n_3^2}{1-\eta^2} + \nu^2\eta^2 - \mu_n(\nu)\right]\Phi_n(\nu,\eta) = 0, \qquad \nu = \omega r^2 \tag{3}$$

with node number n and eigenvalue $\mu_n(\nu)$. At a fixed ν, n_3 and parity the functions Φ_n, $n = 0, 1, \ldots$ form a complete system of orthogonal functions with normalization $\int_{-1}^{1} \mathrm{d}\eta\,\Phi_n(\eta,\nu)\Phi_{n'}(\eta,\nu) = \delta_{nn'}$; therefore, we assume

$$\psi = \frac{1}{r}\sum_{n=0}^{\infty} y_n(r)\Phi_n(r,\eta). \tag{4}$$

The use of Φ_n provides for regular behaviour of ψ at $\eta = \pm 1$, i.e. the term $\nu^2\eta^2$ is automatically resolved in (2). Therefore, in the asymptotic analysis we have to deal with the singularities $r = 0, \infty$ only. The norm of Ψ can be expressed by the channel coefficients y_n:

$$\langle\Psi,\Psi\rangle = \int_0^{2\pi}\mathrm{d}\varphi\int_{-1}^{1}\mathrm{d}\eta\int_0^{\infty}\mathrm{d}r\,r^2\Psi^*\Psi = \sum_{n=0}^{\infty}\int_0^{\infty}\mathrm{d}r\,y_n^2(r) = \sum_{n=0}^{\infty}\langle y_n\rangle. \tag{5}$$

For bound levels $\langle\Psi,\Psi\rangle = 1$, for continuum levels norm (5) is infinite. The channels with infinite and finite $\langle y_n\rangle$ will be called free and bound channels respectively. Either for bound or continuum levels the boundary conditions are $y_n(0) = 0$, $\lim_{r\to\infty} r^{-1}y_n(r) = 0$, and $y_n(r)$ must be bounded for all channels.

Multiplication by $\Phi_{n'}$ and integration over η transforms (2) to the eigenvalue problem of the coupled inhomogeneous second order ordinary differential equations

$$\frac{\mathrm{d}^2 y_n}{\mathrm{d}r^2} + \left[2(E-\omega n_3) + \frac{2Z}{r} - \omega^2 r^2 + \frac{\mu_n(r)}{r^2} + A_{nn}\right]y_n + {\sum_{n'=0}^{\infty}}{}'\left[\left(A_{nn'} - \frac{B_{nn'}}{r}\right)y_{n'} + B_{nn'}\frac{\mathrm{d}y_{n'}}{\mathrm{d}r}\right] = 0, \qquad n = 0, 1, \ldots \tag{6}$$

where $\sum'$ indicates that the term $n' = n$ must be omitted in the summation. The coupling matrix elements are

$$B_{nn'}(r) = 2\int_{-1}^{1}\Phi_n\frac{\partial\Phi_{n'}}{\partial r}\mathrm{d}\eta, \tag{7}$$

$$A_{nn'}(r) = \int_{-1}^{1}\Phi_n\frac{\partial^2\Phi_{n'}}{\partial r^2}\mathrm{d}\eta + \frac{1}{r}B_{nn'}, \tag{8}$$

because of the normalization of Φ_n $B_{nn'} = -B_{n'n}$, $B_{nn} = 0$. For practical reasons the sum in (4) must be truncated to N elements in numerical computations, i.e. $n = 0, \ldots, N-1$ in (6). For bound states the truncation is warranted if the sum in (5) is convergent. The convergence can be investigated in the asymptotic domains $r \to 0$, $r \to \infty$ analytically or from a numerical solution directly or by introducing a solution $\{y_n\}_{n=0,\dots,N-1}$ in (6) and numerical integration to determine the errors $y_N, \dots$; this latter procedure can be applied for continuum levels as well.

3. Asymptotic analysis in the singular points $r = 0, \infty$

Analytic solutions to (6) are not known. In a numerical solution the integrator formulae become unstable at $r \to 0$ because of the singularity in the potential, and the infinite length $0 \leqslant r \leqslant \infty$ of the integration interval combined with a singularity of the potential poses serious problem as well. The goal of the following asymptotic analysis is to give the asymptotic series expansions in an analytic form by which the numerical integration can be reduced to a finite interval and the relation of numerical solutions to the complete set of solutions can be discussed.

3.1. Equation (3) at $r = 0, \infty$

By $\nu \to 0$ and $\nu \to \infty$ (3) is transformed to the differential equation of associated Legendre and Laguerre polynomials, respectively. Using this feature its asymptotic analysis provided asymptotic series expansions for $\Phi_n,\ A_{nn'},\ B_{nn'},\ \mu_n$ at $0 \leqslant \nu \ll 1$ and $\nu \gg 1$; the series in terms of increasing or decreasing powers of ν were summarized and formulae were given for computing them numerically at intermediate values of ν in Barcza (1994). It is an important feature of these expansions that $A_{nn'},\ B_{nn'}$ vanish at $r = 0, \infty$ leading to the asymptotic decoupling of equations (6): the asymptotic solutions are those of the adiabatic equations (i.e. $\sum' = 0$). For the eigenvalues

$$\mu(r) = -l(l+1) + O(r^4), \qquad l = 2n + |n_3| + p, \quad r \to 0, \tag{9}$$

$$\frac{\mu_n(r)}{r^2} - \omega^2 r^2 + A_{nn} = -2\omega(2n + |n_3| + 1) + O(r^{-4}), \qquad r \to \infty, \tag{10}$$

were found; $p = 0, 1$ for even and odd parities, respectively.

Owing to the use of the angular oblate spheroidal functions the singularity of the potential in (6) is resolved by (10). This is a decisive advantage in comparison with the spherical basis where asymptotic decoupling exists for $r \to 0$ only: in spherical basis finitely coupled equations of type (6) must be solved with $B_{nn'} \equiv 0$, but A_{nn}, $A_{nn'}$ and the potential are $\propto r^2$ for all channels leading to divergent or unbounded expansion of the wavefunction at $r \to \infty$ (Barcza 2000).

3.2. Equations (6) at $0 \leqslant r \ll 1$

At $r \to 0$ equations (6) have hydrogen-like asymptotic solutions; one of the two linearly independent solutions is bounded:

$$y_n = \sum_{m=0}^{\infty} c_m^{(l)} r^{l+1+m}, \tag{11}$$

E and $c_0^{(l)}$ are their asymptotically free parameters, i.e. the boundary conditions $\{y_n(0)\}_{n=0,\dots,N-1}$ are satisfied at their any finite value. One of $c_0^{(l)}$ is the normalization factor. N parameters of (11), i.e. $E(\omega)$ and $N-1$ coefficients $c_0^{(l)}(\omega)$ determine uniquely $\{y_n(r)\}_{n=0,\dots,N-1}$, $0 \leqslant r \leqslant \infty$.

The recursive formula for the first few coefficients $c_m^{(l)}$ shows that the coupling enters successively from the neighbouring channels (Barcza 1994), not earlier than in $c_2^{(l)}$, i.e. the asymptotic solutions of the adiabatic and non-adiabatic approximations ($\sum' = 0$ and $\neq 0$, respectively) are identical at least in $c_0^{(l)} r^{l+1}$, $c_1^{(l)} r^{l+2}$: equations (6) become finitely coupled in a given power of r. A corollary is that all elements with $0 \leqslant n \leqslant N-2$ must be included in a numerical computation with N elements.

Lemma [1]. The omission of a term $n \leqslant N-2$ leads to unbounded ψ at $r = 0$.

Proof. The omission is equivalent to $y_n(r) \equiv 0$ in (6) which takes the form for this channel

$$(A_{n,n+1} - B_{n,n+1}/r) y_{n+1} + B_{n,n+1} y'_{n+1} + O(r^{2n+|n_3|+p+4}) = 0. \tag{12}$$

From the asymptotic expansions of $A_{n,n+1}$, $B_{n,n+1}$ (Barcza 1994) it follows that

$$y'_{n+1} = \left(\frac{1}{r} - \frac{A_{n,n+1}}{B_{n,n+1}}\right) y_{n+1} + \cdots = -\frac{3}{2r} y_{n+1} + O(r) \tag{13}$$

for any n admitting the solution $y_{n+1} \propto r^{-3/2}$ and leading to $\psi \propto r^{-5/2}$. □

Without proof we mention that expansion (4) is obviously convergent with (11) if $0 \leqslant r < 1, -1 \leqslant \eta \leqslant 1$.

We denote by $\alpha_N^{(m)}(l_1, \ldots, l_m)$ the asymptotic solution with m zero asymptotically free parameters $c_0^{(l_1)} = 0, \ldots, c_0^{(l_m)} = 0$ and $N - m$ of non-zero $c_0^{(l)}$ in (11). The channel functions $y_{l_1}, \ldots, y_{l_m}$ vanish at $r \ll 1$ more rapidly than those with $c_0^{(l)} \neq 0$, and asymptotic behaviour of these channels is determined by the non-zero coefficients $c_0^{(l)}$ through $\sum'$, i.e. the number of the asymptotically free parameters for (6) is altogether $1 \leqslant N - m \leqslant N$.

3.3. Equations (6) at $r \to \infty$

In (6) the coefficient of any y_n is $-\lambda_n^2 + 2Z/r + O(r^{-4})$ (Barcza 1994) where

$$\lambda_n^2 = -2E + 2\omega(2n + |n_3| + 1 + n_3). \tag{14}$$

In adiabatic approximation equations (6) have hydrogen-like asymptotic behaviour with two differences: the term $-l(l+1)/r^2$ is missing because of the breakdown of spherical symmetry and the absorption threshold depends on n, it is at $\lambda_n = 0$. The adiabatic asymptotic solutions are

$$y_n^{\mathrm{ad}}(r) = \begin{cases} v_{nn}^{(+)}(r)\exp(\lambda_n r) r^{-Z/\lambda_n} + v_{nn}^{(-)}(r)\exp(-\lambda_n r) r^{Z/\lambda_n} & \text{if} \quad \lambda_n^2 > 0, \\ v_{nn}^{(\mathrm{c},0)}(r)\cos[(8Zr)^{1/2}] + v_{nn}^{(\mathrm{s},0)}(r)\sin[(8Zr)^{1/2}] & \text{if} \quad \lambda_n = 0, \\ v_{nn}^{(\mathrm{s})}(r)\sin\left(\bar{\lambda}_n r + \frac{Z}{\bar{\lambda}_n}\ln r\right) + v_{nn}^{(\mathrm{c})}(r)\cos\left(\bar{\lambda}_n r + \frac{Z}{\bar{\lambda}_n}\ln r\right) & \text{if} \quad \lambda_n^2 < 0, \end{cases} \tag{15}$$

$\bar{\lambda}_n^2 = -\lambda_n^2$. The exponential or trigonometric functions resolved the irregular singularity $r = \infty$ in the sense that for the functions $v_{nn}^{(\ldots)}$ with any superscript there exists an asymptotic expansion of the form

$$v_{nn}^{(\ldots)} = C_0^{(nn,\ldots)}\left[1 + C_1^{(nn,\ldots)} r^{-1} + \cdots\right]. \tag{16}$$

The asymptotically free parameters are E and the coefficients $C_0^{(\ldots)}$ except for $C_0^{(nn+)}$, one of $C_0^{(\ldots)}$ is the normalization factor. With expansions (16) (15) represents the two linearly independent solutions to each row in (6) forming a non-orthogonal basis to expand any asymptotic solution.

In (6) the coupling mixes $y_n^{\mathrm{ad}}(r)$ and its derivative multiplied by a power series of r^{-1} starting with $O(r^{-m})$, $m \geqslant 1$. If $E < \omega(2n^* + |n_3| + n_3 + 1)$, the general asymptotic solution is

$$y_n(r) = \sum_{m=0}^{n^*-1} \left[v_{nm}^{(\mathrm{s})}(r) \sin\left(\bar{\lambda}_m r + \frac{Z}{\bar{\lambda}_m} \ln r\right) + v_{nm}^{(\mathrm{c})}(r) \cos\left(\bar{\lambda}_m r + \frac{Z}{\bar{\lambda}_m} \ln r\right)\right]$$
$$+ \sum_{m=n^*}^{\infty} \left[v_{nm}^{(-)}(r) r^{Z/\lambda_m} \mathrm{e}^{-\lambda_m r} + v_{nm}^{(+)}(r) r^{-Z/\lambda_m} \mathrm{e}^{\lambda_m r}\right] \tag{17}$$

where $n^* = 0, 1, \ldots$ is the serial number of the continuum for which (17) applies. The asymptotically free parameters are those of (15). Bounded will be (17) if $C_0^{(nn+)}(E) = 0$ for all channels $n = n^*, \ldots, N-1$ involved in the expansion. We denote by $\beta_N^{(n^*)}(m_1, \ldots, m_{n^*-1})$ the asymptotic solutions (17) where $m_1, \ldots, m_{n^*-1}$ indicates the serial number m of the channel(s) with exponential vanishing, i.e. for which $C_0^{(mm\mathrm{c})} = C_0^{(mm\mathrm{s})} = 0$.

If e.g. $n^* = 0$ bound levels exist with $E < \omega(|n_3| + n_3 + 1)$ exclusively. The first absorption threshold $E = \omega$ is a multiple one since it belongs to all values $n_3 \leqslant 0$. If $n^* = 1$ 'monochromatic' continuum levels exist, this is the first continuum with $\omega(|n_3| + n_3 + 1) \leqslant E < \omega(|n_3| + n_3 + 3)$, etc. Nevertheless, $C_0^{(00\mathrm{s})} = C_0^{(00\mathrm{c})} = 0$ allows one to convert the free channel $n = 0$ to a bound one by $v_{00}^{(\mathrm{s})}(r) = v_{00}^{(\mathrm{c})}(r) = 0$ and $y_0 \to v_{01}^{(-)}(r) \exp(-\lambda_1 r) r^{(Z/\lambda_1)} \not\equiv 0$ where $v_{01}^{(-)} = -\lambda_1 C_0^{(11,-)} B_{01}^{(1)} r^{-1} + O(r^{-2})$, $B_{01}^{(1)}$ is the first non-vanishing coefficient in the expansion of $B_{nn'}$. Norm (5) of a level of this type will be finite. This is a non-trivial autoionizing stationary level in the first continuum. (An autoionizing level will be called trivial if $n_3 > 0$ and its energy eigenvalue lies above the first threshold: $E > \omega$.) The existence of non-trivial autoionizing levels is suggested by our asymptotic considerations; they can be found, if they exist, by numerical integration only.

The practical use of (17) is limited by the lack of a sufficient number of terms in expansion (16); however, it was possible to sort out the solutions with different vanishing at $r \to \infty$ and to determine the number of the asymptotically free parameters of the bounded solutions of (6).

At an eigenvalue E of a bound level the vanishing $\propto \exp(-\lambda_{n^*} r) r^{Z/\lambda_{n^*}}$ will dominate in all channel functions (17) at a sufficiently large r because $\lambda_{n^*} < \lambda_{n^*+1} < \lambda_{n^*+2} < \cdots$. In a channel m the asymptotic behaviour is $\propto \exp(-\lambda_{n^*} r) r^{(Z/\lambda_{n^*}) - |m-n^*|}$ ensuring the convergence of norm (5).

For free channels the exponential functions vanish at $r \to \infty$ and the trigonometric function(s) divided by a power $m \geqslant 0$ of r will dominate the asymptotic behaviour of $y_n(r)$ at any E.

4. Numerical solution of the truncated system (6)

Equations (6), $0 \leqslant n \leqslant N - 1$, were integrated simultaneously to a fixed value of the asymptotically free parameters by a modified Numerov procedure adapted to the presence of $B_{nn'} \mathrm{d}y_{n'}/\mathrm{d}r$ in $\sum'$ (Barcza 1994). To start the numerical integration from $0 < r_0 \ll 1$ outwards and from $r_\mathrm{s} \gg 1$ inwards the asymptotic series of the previous section were used. The step size h was varied in order to minimize the number of the necessary steps, 10^{-6} relative accuracy was prescribed for any step; this value was consistent with the accuracy 10^{-7} of $A_{nn'}$, $B_{nn'}$, μ_n. A shooting method was used to determine the asymptotically free parameters: at the mesh points r_m and at $r_\mathrm{m} - h$ $1 \leqslant n \leqslant 2N$ equations of type

$$\delta y_n(r_\mathrm{m}) = \left|1 - y_n^{(\mathrm{outward})}(r_\mathrm{m}) \big/ y_n^{(\mathrm{inward})}(r_\mathrm{m})\right| \leqslant 10^{-6}, \tag{18}$$

were satisfied. The computations were repeated without meshing, as a function of the asymptotically free parameters $\{y_n(r_s)\}_{n=0,\ldots,N-1} = 0$ was searched by a vectorized Newton procedure and r_s was increased until the convergence of E. The same results were obtained. The only noteworthy peculiarity is that approaching the first absorption threshold $E = \omega$ the loss of digits became more and more severe, and they were the same in the inward-outward or outward-only integration enabling the numerical determination $E(\omega)$ for the lowest six levels at a computational accuracy 10^{-17}. Increasing the accuracy to 10^{-34} shifted the limits to higher values of E and ω, but, principal improvement has not been found: the numerical instability does not originate from the noise of $A_{nn'}$, $B_{nn'}$, μ_n (being at level 10^{-7}) but the digit loss seems to be an inherent and not fully understood feature of equations (6) in non-adiabatic computations. In the adiabatic approximation the instability was found to be much much smaller; adiabatic eigenvalues could be computed for the lowest 50–60 levels without the failure of the shooting method with the Numerov integrator formula.

To demonstrate the usefulness of our previous considerations some eigenvalues and the values of the asymptotically free parameters belonging to them will be reported for bound levels in subspace $n_3 = 0$, $p = 0$. This subspace is especially interesting because in (6) $\omega n_3 = 0$ (only quadratic Zeeman effect is present) and $l = 0$ are possible, meaning that $y_0 \neq 0$ on the z axis and, if it exists, only non-trivial autoionizing levels exist in this subspace.

Two methods were found for the numerical solutions.

4.1. Solution by simultaneous integration of N equations

A simultaneous integration of equations (6), $0 \leqslant n \leqslant N-1$ and solution of $2N$ relations of type (18) in outward-inward or N equations $\{y_n(r_s)\}_{n=0,\ldots,N-1} = 0$ in outward-only integration gave eigenvalues $E(\omega) < \omega$ in perfect agreement (accuracy 10^{-6}) with those obtained from the spherical basis (Ruder *et al* 1994). All solutions were found to be of type $\beta_N^{(0)}$ and $\alpha_N^{(0)}$ except for some discrete points on the $E(\omega)$ curves of type, e.g. $\alpha_2^{(1)}(0)$ was found at $E = 0.000\,2598$, $\omega = 0.042\,8052$, $\alpha_2^{(1)}(2)$ at $E = 0.130\,72$, $\omega = 0.167\,14$, etc, at these values of ω the sign of $c_0^{(0)}/c_0^{(2)}$ changed. In general, solutions $\alpha^{(m)}$, $m > 0$ were unbounded at $r \to \infty$.

For comparison the analogue equations to (6) from the spherical basis (i.e. those of Ruder *et al* (1994)) were integrated by the same method. To the same accuracy 10^{-6} in E the number of the necessary channels was larger by a factor ≈ 2 in comparison with using Φ_n. The numerical instability from the digit loss appeared more severely, already at lower E, and the convergence problems (Barcza 2000) manifested themselves when $E(\omega)$ approached the ionization limit ω.

4.2. Iterative solutions

Each row of (6) is a linear, inhomogeneous second order ordinary differential equation offering the possibility of an iterative solution. First a channel must be solved in the adiabatic approximation and in the next steps the channel functions of the previous step must be used in $\sum'$, i.e. inhomogeneous equations must be integrated. For the sake of simplicity all computations were outward-only. We have one free parameter for each channel enabling us to find $y_n(r_s) = 0$. The accuracy 10^{-6} of E was reached by 2–5 iterative steps.

Two different iterative solutions were found.

4.2.1. First we choose the dominant channel having the largest $\langle y_{n_d} \rangle$ in (5) (e.g. $n_d = 0$ for the ground state) and we solve $y_{n_d}(r_s, E) = 0$. We introduce $y_{n_d}(r, E)$ in the next

Table 1. The splitting of the ground state.

	From section 4.1			From section 4.2.2			
ω	$-E$	$\langle y_0 \rangle$	$10^6 \langle y_1 \rangle$	$-E$	$\langle y_0 \rangle$	$10^6 \langle y_1 \rangle$	$C^{(1,\infty)}$
0.01	0.509 899	0.999 999	0.085	0.509 896	0.999 999	1.2	1.000 01
0.02	0.519 600	0.999 999	0.73	0.519 541	0.999 992	7.9	1.0003
0.03	0.529 103	0.999 997	2.8	0.528 818	0.999 981	19	1.0006
0.05	0.547 526	0.999 983	17	0.545 794	0.999 959	41	1.0017

adjacent channel n_1 and solve $y_{n_1}\big(r_s, E, c_0^{(2n_1+|n_3|+p)}\big) = 0$ by varying $c_0^{(2n_1+|n_3|+p)}$. We introduce $y_{n_1}\big(r, E, c_0^{(2n_1+|n_3|+p)}\big)$ in $\sum'$ of channel n_d and solve now the inhomogeneous equation $y_{n_d}(r_s, E, y_{n_1}) = 0$, etc. The procedure can be extended, of course, to more adjacent channels.

This procedure confirmed the results reported in section 4.1.

4.2.2. In addition to the hitherto known spectrum the following procedure resulted in new eigenvalues.

* By the shooting method with simultaneous integration we determine the eigenvalue $E^{(i)}$, the coefficients $c_0^{(l)}$, the channel functions $\big\{y_n^{(i)}(E^{(i)}, r)\big\}_{n=0,\dots,N-2}$, $i = 0$ is at the first step.
* We introduce the solution $\big\{y_n^{(i)}(E^{(i)}, r)\big\}_{n=0,\dots,N-2}$ in equation (6) for channel $n = N - 1$ and integrate it: at $r \to \infty$ the result will be unbounded: $y_{N-1}^{(i)}(r, E^{(i)}) \propto \exp(\lambda_{N-1} r) r^{-Z/\lambda_{N-1}}$ because the eigenvalue $E^{(i)}$ of the equations $n \leqslant N - 2$ is not an eigenvalue of the equation $n = N - 1$. We integrate the adiabatic equation $n = N - 1$ (i.e. $\sum' = 0$), because of the asymptotic decoupling its asymptotic behaviour is the same: $y_{N-1}^{\mathrm{ad},(i)}(r, E^{(i)}) \propto \exp(\lambda_{N-1} r) r^{-Z/\lambda_{N-1}}$, i.e. $C^{(N-1,N-1,+)}(E) \neq 0$ in (15). The ratio $y_{N-1}^{(i)}(r, E^{(i)}) \big/ y_{N-1}^{\mathrm{ad},(i)}(r, E^{(i)}) \to C^{(N-1,\infty)}$ was found in the computations, $C^{(N-1,\infty)}$ is a constant, differing slightly from unity. $C^{(N-1,\infty)} \neq 1$ means that these solutions are of type $\alpha_N^{(0)}$ at $r \to 0$ because $c_0^{(2N-2+|n_3|+p)} \neq 0$.
* By $y_{N-1}^{(i)}(r, E^{(i)}) - C^{(N-1,\infty)} y_{N-1}^{\mathrm{ad},(i)}(r, E^{(i)}) = y_{N-1}^{\mathrm{part},(i+1)}(r, E^{(i)})$ we find a bounded particular solution to channel $n = N - 1$ with vanishing $\propto \exp(-\lambda_{N-1} r) r^{Z/\lambda_{N-1}}$. We implement equations (6) by this channel function $y_{N-1}^{\mathrm{part},(i+1)}(r, E^{(i)})$ and repeat the procedure from [*] with $i = i + 1$.

If $\big|y_{N-1}^{\mathrm{part},(i+1)}(r, E^{(i)}) - y_{N-1}^{\mathrm{part},(i)}(r, E^{(i-1)})\big| \to 0$ for $0 \leqslant r \leqslant r_s$ and $E^{(0)}, E^{(1)}, \dots$ is a convergent series the limit of $E^{(i)}$ is an eigenvalue of equations (6) truncated to N elements, channel $n = N - 1$ vanishes with $r \to \infty$ in the same manner as $\big\{y_n^{(i)}(E^{(i)}, r)\big\}_{n=0,\dots,N-2}$. Solutions of this type have been found, at present the simplest ones, describing the splitting of the ground state. The results originate from $N = 2$ approximation, the inclusion channel $n = 2$ modifies the values in table 1 below 10^{-8}. Details are reported in table 1 and figure 1, for comparison the data of the ground state are given from simultaneous integration with $N = 2$.

In table 1 the limit $\omega = 0.05$ followed from losing the significant digits in $y_{N-1}^{\mathrm{part},(i+1)}(r, E^{(i)})$ since the difference $\propto \exp(-\lambda_{N-1} r) r^{Z/\lambda_{N-1}}$ could be computed from the unbounded non-adiabatic and adiabatic solutions $y_{N-1}^{(i)}(r, E^{(i)})$, $C^{(N-1,\infty)} y_{N-1}^{\mathrm{ad},(i)}(r, E^{(i)})$, both $\propto \exp(\lambda_{N-1} r) r^{-Z/\lambda_{N-1}}$ which were known to accuracy 10^{-6}.

Wavefunctions and eigenvalues of this type exist only in quasi-separable problems like (2) which can be converted to coupled inhomogeneous equations (6).

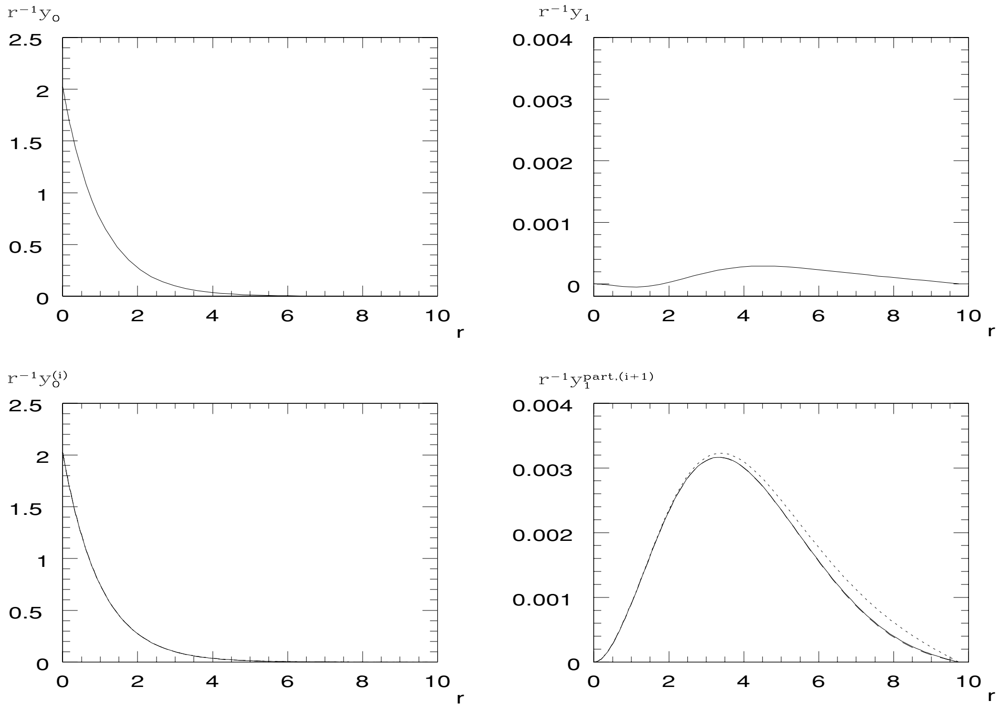

Figure 1. Channel coefficients at $\omega = 0.03$, $N = 2$. Upper panels: from simultaneous integration, section 4.1. Lower panels: from iterative solution, section 4.2.2. Lower right panel: dotted: $y_1^{\text{part},(1)}(r, E^{(0)})$, dashed: $y_1^{\text{part},(4)}(r, E^{(3)})$, line: $y_1^{\text{part},(5)}(r, E^{(4)})$. Lower left panel: because of the small difference in $y_0^{(i)}(r, E^{(i)})$, $i = 0, 3, 4$ the lines coincide within the line width.

5. Discussion

The results reported in sections 4.1 and 4.2.1 are modest from numerical point of view because the computed eigenvalues could only confirm those from the spherical basis while equations (6) are more complicated than those from the spherical basis where $B_{nn'} \equiv 0$, $A_{nn'} = L(n, n')r^2$. The confirmatory numerical results mean that in the spherical basis the wavefunction is well approximated in the domain of r and η which is influential for the energy eigenvalue.

The specific results from using the angular oblate spheroidal functions are the analytic asymptotic expansions, enabling us

- to resolve singularities
- to prove a lemma concerning the completeness of the expansion in terms of the basis functions
- to construct the complete set of asymptotic wavefunctions
- to determine their free parameters which have discrete values at an ω
- to find hitherto unknown low-lying stationary levels
- to handle the continuous spectrum as well
- to reduce the numerical integration to a finite interval.

This basis fits to the problem better than any other basis used in previous studies and promises a qualitative leap in treating the absorption thresholds, continuum which were treated in adiabatic approximation only (e.g. Ruder *et al* (1994), Potekhin and Pavlov (1994)).

In the adiabatic approximation we have an one threshold with one continuum; in the non-adiabatic approximation we have an infinite number of thresholds and continua separated by the Landau spacing 2ω. This is a principal difference.

The main new results are a corollary from the asymptotic decoupling at $r = 0$ and ∞; this is a feature of the expansion in terms of angular oblate functions.

6. Conclusions

The Schrödinger equation of the diamagnetic Coulomb problem has been analysed which is a prototype for the non-separable quantum mechanical eigenvalue problems. For expanding the eigenfunctions the angular oblate spheroidal functions were used as basis functions. By this expansion both singularities of the problem could be resolved and wavefunctions were found which are correct from an analytical point of view.

By algebra and analysis asymptotic series have been given in terms of $r, 0 \leqslant r \ll 1$ and $r^{-1}, r \gg 1$, respectively. The convergence radius of the series is small; however, both series could be used to start the numerical integration for $0 \leqslant r \leqslant \infty$ in the frame of a shooting method. For the complete set of solutions the number of the free parameters has been determined. The combination of analysis and algebraic machinery with numerical integration has provided much better insight into the structure of the bound and continuous spectrum; furthermore, in addition to the confirmation of the results from previous studies hitherto unknown low-lying levels have been discovered. This finding indicates that in the diamagnetic Coulomb problem a wealth of stationary levels is yet to be discovered, perhaps in the continuum as well, which have not been found by the simplest, common numerical procedures without comprehensive analysis.

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