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The diamagnetic Coulomb problem at high field strength. Asymptotic analysis

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Abstract. The paper deals with asymptotic expansions in cylindrical coordinates for the Schrödinger equation of the diamagnetic Coulomb problem with infinite nuclear mass. The basis functions introduced by Liu and Starace are analysed: analytical asymptotic expansions are given for the basis functions and eigenvalues belonging to them. Using these, analytical asymptotic expansions are obtained for the coupling coefficients and solutions of the system of second-order ordinary differential equations which arise if the wavefunction is expanded in terms of the Liu–Starace basis functions. The role of the asymptotic expansions is elucidated for the numerical solution of the non-adiabatic approximation and for finding non-trivial auto-ionizing states.

1. Introduction

The Schrödinger equation of a hydrogen-like ion of nuclear charge Z and infinite nuclear mass in the homogeneous magnetic field $\boldsymbol{H}$ parallel to the axis z is the simplest problem of its kind in the enormous manifold of non-separable quantum-mechanical problems. At an arbitrary value of $\boldsymbol{H}$ the Hamiltonian cannot be split into small and large terms, consequently a conventional perturbative approach is not possible, thus the problem is often treated by variational calculations, as are other non-separable problems of small dimensions, or by diagonalization technique. These approaches are beyond the scope of the present paper, we turn to another method using special eigenfunction expansions which have been applied recently with success in several cases, for references of their simplest forms see Ruder *et al* (1994).

The problem takes the form in the cylindrical coordinates ϱ(= cylindrical radius) and z as follows.

$$\left[\frac{\partial^2}{\partial\varrho^2}+\frac{1}{\varrho}\frac{\partial}{\partial\varrho}+\frac{\partial^2}{\partial z^2}-\frac{n_3^2}{\varrho^2}+\frac{2Z}{(\varrho^2+z^2)^{1/2}}-\omega^2\varrho^2+2E^*\right]\psi=0$$
$$0\leqslant\varrho\leqslant\infty\qquad -\infty\leqslant z\leqslant\infty \tag{1}$$

where n_3 is the magnetic quantum number, φ is the azimuthal angle around z, the first factor of

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

was separated from (1), however, $\psi(z,\varrho)$ cannot be factorized in terms of functions of z and ϱ. $\omega=e|\boldsymbol{H}|/(2mc)$ and $E^*=E-\omega n_3$, E is measured in atomic units ($e=1$, $m=1$,

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$\hbar = 1$), $\omega = 1$ if $|\boldsymbol{H}| = 4.7 \times 10^5 T$. Equation (1) was derived by elementary operations, further analytical details are given by Liu and Starace (1987).

By transformation

$$\psi(z,\varrho) = \varrho^{n_3} \exp(-\omega\varrho^2/2) X(z,\varrho) \tag{3}$$

and introducing $\xi = \omega\varrho^2$ we obtain our standard form of (1):

$$\xi \frac{\partial^2 X}{\partial \xi^2} + [n_3 + 1 - \xi] \frac{\partial X}{\partial \xi} + \left[\frac{E^*}{2\omega} - \frac{1}{2}(n_3 + 1) \right] X + \frac{1}{4\omega} \left[\frac{\partial^2 X}{\partial z^2} + \frac{2Z}{(\xi/\omega + z^2)^{1/2}} X \right] = 0. \tag{4}$$

(Beginning from (3) n_3 denotes $|n_3|$, we omit the symbol of the absolute value.) The assumption

$$X = \sum_n f_n(z) g_n(z,\varrho) \tag{5}$$

(Liu and Starace 1987) and its analytical and numerical consequences will be the subject of this paper and paper II (Balla and Benkő 1996). From (4) it is evident that $1 \leqslant \omega \leqslant \infty$ is the field-strength domain where (5) will have favourable convergence.

The LaS basis functions are defined by

$$\frac{\partial^2 \Phi_n}{\partial \varrho^2} + \left[\frac{2Z}{(\varrho^2 + z^2)^{1/2}} - (n_3^2 - \tfrac{1}{4})\varrho^{-2} - \omega^2 \varrho^2 + \mu_n(z) \right] \Phi_n = 0 \tag{6}$$

where

$$\Phi_n(z,\varrho) = \varrho^{n_3 + 1/2} \mathrm{e}^{-\omega\varrho^2/2} g_n(z,\varrho) \tag{7}$$

(6) is suitable for numerical analysis while the equivalent form

$$\frac{\partial^2 g_n}{\partial \varrho^2} + \left[\frac{2n_3 + 1}{\varrho} - 2\omega\varrho \right] \frac{\partial g_n}{\partial \varrho} + \left[\frac{2Z}{(\varrho^2 + z^2)^{1/2}} - 2(n_3 + 1)\omega + \mu_n(z) \right] g_n = 0 \tag{8}$$

is convenient for an analytic asymptotic treatment. $\Phi_n(\infty,\varrho)\varrho^{-1/2}$ is obviously identical with the nth element of the Landau basis (Ruder *et al* 1994), therefore, the LaS basis can be regarded as a generalized Landau basis. By using the basis functions g_n the pole $\varrho = z = 0$ of (1) is eliminated because the composite wavefunction is chosen appropriately in the neighbourhood of the singularity.

If $\omega > 0$ equation (8) has discrete eigenvalues $\mu_n(z)$ only, its eigenfunctions are normalized as

$$(\Phi_n, \Phi_{n'}) = \int_0^\infty \varrho^{2n_3} \mathrm{e}^{-\omega\varrho^2} g_n(z,\varrho) g_{n'}(z,\varrho) \varrho \,\mathrm{d}\varrho = \delta_{nn'} \tag{9}$$

for any z in order to have

$$\left(\Phi_n, \frac{\partial \Phi_n}{\partial z} \right) = 0. \tag{10}$$

The regular behaviour of ψ and its quadratic integrability at the irregular singularity $\varrho = \infty$ of (1) is secured automatically by using $\Phi_n(z,\varrho)$ in the whole interval $-\infty \leqslant z \leqslant \infty$. The norm is

$$\langle \Psi, \Psi \rangle = \sum_n \int_{-\infty}^{\infty} f_n^*(z) f_n(z) \,\mathrm{d}z. \tag{11}$$

The coupled system of ordinary differential equations to be solved is obtained by introducing (5) in (4), using (8), a multiplication by $\varrho^{2n_3}\exp(-\omega\varrho^2)g_n$ from left and an integration over ϱ:

$$\frac{\mathrm{d}^2 f_n}{\mathrm{d}z^2} + [2E^* - \mu_n(z) + A_{nn}]f_n + \sum_{n'}{}' \left[A_{nn'}f_{n'} + B_{nn'}\frac{\mathrm{d}f_{n'}}{\mathrm{d}z}\right] = 0 \qquad n = 0, 1, \ldots \tag{12}$$

where

$$A_{nn'}(z) = \int_0^\infty \Phi_n \frac{\partial^2\Phi_{n'}}{\partial z^2}\,\mathrm{d}\varrho = \left(\Phi_n, \frac{\partial^2\Phi_{n'}}{\partial z^2}\right) \tag{13}$$

and

$$B_{nn'}(z) = 2\int_0^\infty \Phi_n \frac{\partial\Phi_{n'}}{\partial z}\,\mathrm{d}\varrho \tag{14}$$

are the elements of the coupling matrices, $\sum'$ indicates that the element $n' = n$ must be omitted.

To our knowledge the form (12) was proposed by Liu and Starace (1987), and solved in adiabatic approximation, i.e. in (5) the sum was confined to one term. This restriction will be dropped and the differences originating from the non-adiabaticity will be indicated. Equation (8) is interesting in itself since it defines a system of orthogonal functions at a fixed value of z, because of the term $2Z/(\varrho^2 + z^2)^{1/2}$ its analytic treatment is possible in the regions $0 \leqslant |z| \ll 1$ and $|z| \gg 1$ only. In these domains of z analytical asymptotic expansions will be given to the basis functions g_n, the matrix elements $A_{nn'}$, $B_{nn'}$ (section 2) and the solution X as well by which a numerical integration of (12) will be easier and more transparent if the sum of (5) is extended to more than one element and important analytical results will be obtained for non-trivial auto-ionizing resonances (section 3). Concerning the equations which follow from the application of the LaS basis paper II is devoted to their numerical solution in the non-asymptotic range. The substantiation of (5) and its comparison with the numerous other possible forms of X are beyond the scope of the present paper, we mention here only that eigenvalues and eigenfunctions with a fixed accuracy will be obtained from (5) by the minimal number of necessary terms.

2. Asymptotic analysis of the basis equation and asymptotic expansions for the coupling matrix elements

By using the machinery of this section the time-consuming computation of $A_{nn'}$, $B_{nn'}$, will be reduced in the asymptotic domains to the evaluation of algebraic expressions or normalization factors or to the computation of some simple integrals. In addition to the computational simplifications the asymptotic formulae of the present section allows the construction of the analytical form of the complete ensemble of the solutions to (12) in its singular points $z = 0$ and $z = \infty$.

2.1. The range $0 \leqslant z \ll 1$

By introducing the variable

$$x = (z^2 + \rho^2)^{1/2} \qquad |z| \leqslant x \leqslant \infty \tag{15}$$

(8) takes the form

$$[H_0 + z^2 H' + \mu_n(z)]g_n(z, x) = 0 \tag{16}$$

where

$$H_0 = \frac{\partial^2}{\partial x^2} + \left[\frac{2n_3+1}{x} - 2\omega x\right]\frac{\partial}{\partial x} + \frac{2Z}{x} - 2\omega(n_3+1) \tag{17}$$

$$H' = -\frac{1}{x^2}\left[\frac{\partial^2}{\partial x^2} - \left(\frac{1}{x} + 2\omega x\right)\frac{\partial}{\partial x}\right]. \tag{18}$$

Equation (16) will be solved by a perturbation theory to obtain the coefficients of the series

$$\mu_n(z) = \mu_n^{(0)} + \mu_n^{(1)} z^2 + \cdots \tag{19}$$

and

$$g_n(z,x) = \chi_n^{(0)}(x) + \chi_n^{(1)}(x) z^2 + \chi_n^{(2)}(x) z^4 + \cdots \tag{20}$$

where

$$\chi_n^{(i)}(x) = \sum_m a_{nm}^{(i)} \chi_m^{(0)}(x) \qquad i = 1, 2 \tag{21}$$

and

$$[H_0 + \mu_m^{(0)}]\chi_m^{(0)}(x) = 0 \qquad m = 0, 1, \ldots \tag{22}$$

defines the basis to expand g_n. The perturbation theory is peculiar in the sense that the basis functions depend on z implicitly and for g_n the basis functions are exactly orthogonal at $z = 0$ only:

$$\int_{|x|}^{\infty} (x^2 - z^2)^{n_3} \mathrm{e}^{-\omega(x^2-z^2)} \chi_n^{(0)}(x)\chi_{n'}^{(0)}(x) x \, \mathrm{d}x = \begin{cases} 1 & \text{if } n = n' \\ \mathrm{O}(z^{2n_3+2}) & \text{if } n \neq n'. \end{cases} \tag{23}$$

By the steps of a conventional perturbation theory we find from the coefficient of z^2 that

$$\mu_n^{(1)} = -H'_{nn} + \mathrm{O}(z^{2n_3+2}) \tag{24}$$

and

$$a_{nn'}^{(1)} = \frac{H'_{n'n}}{\mu_{n'}^{(0)} - \mu_n^{(0)}} + \mathrm{O}(z^{2n_3+2}) \tag{25}$$

if $n' \neq n$ while $a_{nn}^{(1)}$ is arbitrary, formulae for efficient computation of $H'_{nn'}(z)$ are given in appendix A. By elaborating the coefficient of z^4 we obtain that

$$a_{nn'}^{(2)} = \frac{1}{\mu_{n'}^{(0)} - \mu_n^{(0)}}\left[\sum_m{}' a_{nn'}^{(1)} H'_{n'n} + \mu_n^{(1)} a_{nn'}^{(1)}\right] + \mathrm{O}(|z|^{2n_3+2}) \tag{26}$$

if $n \neq n'$ and $a_{nn}^{(2)}$ is arbitrary. The normalization (9) of g_n is satisfied if

$$a_{nn}^{(1)} = 0 \tag{27}$$

$$a_{nn}^{(2)} = -\tfrac{1}{2}\sum_{n'} a_{nn'}^{(1)^2}. \tag{28}$$

2.1.1. The solution of (22) If $\omega \to \infty$ (22) takes the form

$$\left[\hat{\xi}\frac{\mathrm{d}^2}{\mathrm{d}\hat{\xi}^2} + (n_3 + 1 - \hat{\xi})\frac{\mathrm{d}}{\mathrm{d}\hat{\xi}} + \frac{Z}{2(\omega\hat{\xi})^{1/2}} + \frac{\mu_n^{(0)}}{4\omega} - \frac{n_3+1}{2}\right]\chi_n^{(0)}(\hat{\xi}) = 0 \qquad (29)$$

where $\hat{\xi} = \omega x^2$ was introduced. The normalized regular solutions of (29) are

$$\chi_n^{(0)}(x) = \left[\frac{2\omega^{n_3+1}n!}{(n+n_3)!^3} + \mathrm{O}(z^{2n_3+2})\right]^{1/2} L_{n+n_3}^{n_3}(\hat{\xi}) + \mathrm{O}(\omega^{-1/2}) \qquad (30)$$

if

$$\mu_n^{(0)} = 2\omega(2n + n_3 + 1) + \mathrm{O}(\omega^{-1/2}) \qquad n = 0, 1, \ldots \qquad (31)$$

note that the factor $2\omega^{n_3+1}$ will harmonize (30) with (9).

If $0 < \omega < \infty$ then (22) has no solutions in polynomial form except for a number of discrete $\mu_n^{(0)}$ and ω values (Taut 1995). For an arbitrary ω (22) was solved numerically by the following procedure (Barcza 1979). We assume

$$\chi_n^{(0)}(x) = \sum_m c_m^{(n)} x^{m+\gamma} \qquad (32)$$

after introducing it in (22) we obtain a recurrence relation for $c_m^{(n)}$:

$$(\gamma + m + 2)(\gamma + m + 2 + 2n_3)c_{m+2}^{(n)} + 2Zc_{m+1}^{(n)} - [2(\gamma + m + n_3 + 1)\omega - \mu_n^{(0)}]c_m^{(n)} = 0$$
$$m = -2, -1, \ldots, c_{-2}^{(n)} = c_{-1}^{(n)} = 0 \qquad (33)$$

from which it follows that $\gamma = 0$, $c_0^{(n)}$ is arbitrary and linearly present in any $c_m^{(n)}$, therefore, $c_0^{(n)}$ is just the normalization factor. By appropriate choice of $c_0^{(n)}$ the upper row of (23) must be satisfied, its z dependence will be of the form constant $+\,\mathrm{O}(z^{2n_3+2})$. Since

$$\lim_{m\to\infty}\frac{c_{m+2}^{(n)}}{c_m^{(n)}} = \frac{2\omega}{m} \qquad (34)$$

the expansion (32) is convergent for any finite x and this is fully sufficient for our purpose. (The asymptotic behaviour $\chi_n^{(0)} \propto \exp(2\omega x^2)$ of (32) would make it unacceptable only if it were extended for $x = \infty$.)

By using expansion (32) the equation

$$\chi_n^{(0)}(x_s, \mu_n^{(0)}(x_s)) = 0 \qquad (35)$$

was solved numerically for a particular x_s and $1.1x_s$, x_s was increased stepwise until satisfying the condition

$$|1 - \mu_n^{(0)}(1.1x_s)/\mu_n^{(0)}(x_s)| < 10^{-7}. \qquad (36)$$

Figures 1 and 2 are the plots of the computed values of the function $\mu_n^{(0)}(\omega)$ and of the value of x_s which was necessary to satisfy (36). Using double-precision arithmetic the levels up to some 15 nodes could be explored by solving (35). To check the quality of $\chi_n^{(0)}$ of the form (32) for the levels $n = 0$–5 (23) was computed, if $n \neq n'$ and $z = 0$ the absolute value of the integral was approximately 10^{-7} or less in the interval $0.1 < \omega < 1000$. An alternative method of solving (22) is given in appendix B.

Figure 1 shows a composite spectrum: at $\omega \to 0$ for the low-lying levels there is a Balmer-like behaviour without merging because at any value of ω with increasing node numbers the spacing of the eigenvalues converges to 4ω, i.e. to the Landau spacing. At $\omega \to \infty$ the Balmer-like behaviour disappears and the Landau spacing dominates.

Three remarks are appropriate.

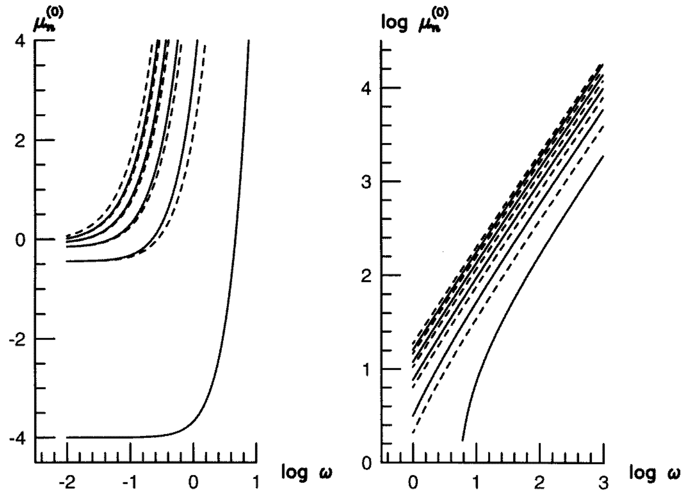

Figure 1. A plot of $\mu_n^{(0)}(\omega)$ for $Z = 1$, $n = 0, 1, 2, 3, 4$. Solid curves: $n_3 = 0$; broken curves: $n_3 = 1$.

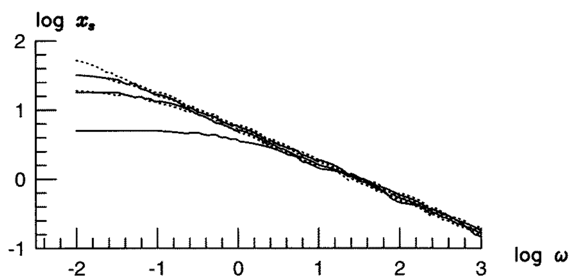

Figure 2. A plot of $x_s(\omega)$ for $n = 0, 1, 2$. Solid curves: $n_3 = 0$; dotted curves: $n_3 = 1$. The oscillation of the curves is a consequence of the stepwise increasing of x_s in (36) which was not smoothed out.

(a) The solutions $\chi_n^{(0)} \propto x^{-2n_3}$, which are valid solutions for $z > 0$ because of $x > 0$, must be excluded from continuity considerations in the point $z = 0$.

(b) If $\omega = 0$ (22) admits solutions of the form $p(x)\exp(\ldots x)$ where p is a polynomial which could be used to expand g_n in the domain $0 \leqslant \omega \ll 1$. (These are irrelevant for us and will not be discussed because (5) is an unsuitable assumption here.) The eigenvalues belonging to them are

$$\mu_n^{(0)} = \frac{-4Z^2}{(2n + 2n_3 + 1)^2} \tag{37}$$

the difference of the numerical values from (36) and (37) was about 10^{-5}–10^{-3} for $n = 0, 5$ at $\omega = 0.01$.

(c) The solutions of Taut (1995) are obtained from (33) by setting

$$\mu_n^{(0)} = 2\omega(m + n_3 + 1) \tag{38}$$

and

$$c_{m+1}^{(n)} = 0. \tag{39}$$

These conditions terminate (32) by $c^{(n)}_{m+2} = 0$, they are equivalent to an algebraic equation for the 'free' parameter ω of (33), its real roots degenerate (32) into a polynomial of degree m.

2.1.2.

The final form of the LaS basis functions is

$$\Phi_n(z,\varrho) = \varrho^{n_3+1/2}\mathrm{e}^{-\omega\varrho^2/2}\left\{\chi_n^{(0)}(x) + \left[\sum_m{}' \frac{H'_{mn}}{\mu_m^{(0)}-\mu_n^{(0)}}\chi_m^{(0)} + \sum_m \bar{a}^{(2)}_{nm}\chi_m^{(0)}\right]z^2 + \cdots\right\} \quad (40)$$

where $\bar{a}^{(2)}_{nm}$ is the coefficient of z^{-2} in (26) which is zero if $n_3 \geqslant 1$. On introducing it in (13) and (14)—remembering that $\partial/\partial z$ requires the inclusion $(z/x)\partial/\partial x$ etc—by comparing the two expansions we find for $n \neq n'$

$$B_{nn'} = B^{(0)}_{nn'} + B^{(*)}_{nn'} z \ln|z| + B^{(1)}_{nn'} z + \mathrm{O}(z^2 \ln|z|) \quad (41)$$

and

$$A_{nn'} = A^{(*)}_{nn'} \ln|z| + A^{(0)}_{nn'} + \mathrm{O}(z\ln|z|) = \tfrac{1}{2}[B^{(*)}_{nn'}\ln|z| + B^{(1)}_{nn'} + B^{(*)}_{nn'} + \mathrm{O}(z\ln|z|)]. \quad (42)$$

The diagonal elements of the coupling matrix are obtained by derivation of (10) with respect to z: if $n_3 = 0$

$$A_{nn} = -\left(\frac{\partial\Phi_n}{\partial z}, \frac{\partial\Phi_n}{\partial z}\right) = A^{(0)}_{nn} + \cdots = -\sum_m{}' \left[\frac{H'^{(-1)}_{mn}}{\mu_m^{(0)}-\mu_n^{(0)}}\right]^2 + \mathrm{O}(z\ln|z|) \quad (43)$$

while $A_{nn} = A^{(2)}_{nn} z^2 + \cdots$ if $n_3 \geqslant 1$. The value of $A^{(0)}_{nn}$ is plotted in figure 3, the summation was extended from 10 to 15 elements in order to have relative accuracy 0.01. Formulae are given in appendix C for efficient computation of the coefficients of (41) and (42), and some characteristic values of $B^{(0)}_{nn'}$ and $B^{(1)}_{nn'}$ are plotted.

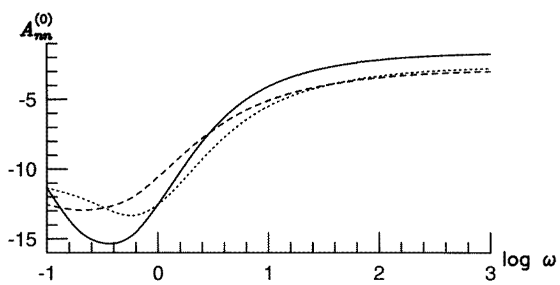

Figure 3. A plot of $A^{(0)}_{nn}(\omega)$ for $n = 0$: full curve; $n = 1$: dotted curve; $n = 2$: broken curve ($Z = 1$).

A numerical comparison of the asymptotic expansions (19) and (41)–(43) with the results of a numerical integration of (6) will be presented in paper II.

2.2. The asymptotics for $z \gg 1$

After expansions (8) takes the form

$$\xi\frac{\partial^2 g_n}{\partial\xi^2} + (n_3+1-\xi)\frac{\partial g_n}{\partial\xi} + \left\{\frac{Z}{2\omega|z|}\left[1 - \frac{\xi}{2\omega z^2} + \frac{3\xi^2}{8\omega^2 z^4} + \mathrm{O}(z^{-6})\right] + \frac{\mu_n(z)}{4\omega} - \frac{n_3+1}{2}\right\} g_n = 0 \quad (44)$$

where

$$\mu_n(z) = \sum_{m=0}^{\infty} \frac{b_m^{(\mu)}}{|z|^m} \tag{45}$$

and

$$g_n(z,\xi) = \sum_{k=0}^{\infty}\sum_{m=0}^{\infty} \frac{b_m^{(k)}}{|z|^k} L_{m+n_3}^{n_3}(\xi). \tag{46}$$

Equation (44) was solved by using (8) with $z = \infty$ (Laguerre differential equation), the relation

$$\xi L_{n+n_3}^{n_3} = -\frac{n+1}{n+n_3+1} L_{n+n_3+1}^{n_3} + (2n+n_3+1) L_{n+n_3}^{n_3} - (n+n_3)^2 L_{n+n_3-1}^{n_3} \tag{47}$$

among the associated Laguerre polynomials, and equating the coefficient of the different Laguerre polynomials with zero at every power of z^{-1}. The result is

$$g_n(z,\xi) = b_n^{(0)} L_{n+n_3}^{n_3}(\xi) + \sum_{k=1}^{\infty} \frac{1}{|z|^{2k+1}} \sum_{m=\max(-k,-n)}^{k} \left[b_{n+m}^{(2k+1)} + \frac{b_{n+m}^{(2k+2)}}{|z|} \right] L_{n+m+n_3}^{n_3}(\xi) \tag{48}$$

here the coefficients $b_m^{(k)}$ of (46) outside the domain indicated by the sum in (48) are zero, while the coefficients $b_n^{(k)}$ are arbitrary, and

$$\mu_n(z) = 2\omega(2n+n_3+1) - \frac{Z}{|z|}\left[2 - \frac{2n+n_3+1}{\omega z^2} + \frac{18n(n+n_3+1)+3n_3^2+9n_3+6}{16\omega^3 z^4} + \cdots\right]. \tag{49}$$

Those coefficients $b_{n\pm m}^{(2k+1)}$ of (48) which are necessary to calculate the first two non-vanishing terms of the asymptotic expansion of the coupling matrix elements $A_{nn'}$, $B_{nn'}$ can be given explicitly:

$$b_{n+k}^{(2k+1)} = \frac{Z b_n^{(0)}}{2\omega^{k+1} k k!} \prod_{m=0}^{k-1} (m+\tfrac{1}{2}) \prod_{m=1}^{k} \frac{n+m}{n+m+n_3} \tag{50}$$

$$b_{n-k}^{(2k+1)} = -\frac{Z b_n^{(0)}}{2\omega^{k+1} k k!} \prod_{m=0}^{k-1} (m+\tfrac{1}{2}) \prod_{m=0}^{k-1} (n-m+n_3)^2 \tag{51}$$

note that n is fixed in (50), (51), $k = 1, 2, \ldots$.

The normalization condition (9) must be satisfied by the appropriate choice of the arbitrary coefficients:

$$b_n^{(0)} = \left[\frac{2\omega^{n_3+1} n!}{(n+n_3)!^3}\right]^{1/2} \tag{52}$$

$$b_n^{(3)} = b_n^{(4)} = b_n^{(5)} = 0 \tag{53}$$

and

$$b_n^{(6)} = -\frac{Z^2[2n^2 + (n_3+1)(2n+1)]}{32\omega^4} b_n^{(0)} \tag{54}$$

$b_n^{(7)}, \ldots$ can similarly be obtained.

If $n \neq n'$ the first non-vanishing terms of the asymptotic expansions of the coupling matrix elements are given by

$$\left(\Phi_n, \frac{\partial^i \Phi_{n'}}{\partial z^i}\right) = \frac{(-1)^i (n! n'!)^{1/2} |z|^{-2|\Delta n|-i-1}}{[(n+n_3)!(n'+n_3)!]^{3/2}} \left[\frac{(n+n_3)!^3}{n!} \prod_{j=1}^{i} (2|\Delta n| + j) b_{n'-\Delta n}^{(2|\Delta n|+1)} + \frac{1}{|z|} \sum_{m=1}^{|\Delta n|-1} b_{n\pm m}^{(2m+1)} \prod_{j=1}^{i} (2|\Delta n| - 2m + j) b_{n'-(\Delta n \mp m)}^{(2|\Delta n|-2m+1)} \frac{(n \pm m + n_3)!^3}{(n \pm m)!} + \cdots \right] \tag{55}$$

where $\Delta n = n' - n$, the upper sign is valid if $\Delta n > 0$, $i = 1, 2$, finally $-\Delta n$ or $-(\Delta n \mp m)$ must be used in (50) and (51) instead of k for a fixed n or n'. If $n = n'$

$$A_{nn} = -\frac{9Z^2}{16\omega^4 z^8} [2n(n + n_3 + 1) + n_3 + 1] + \mathrm{O}(|z|^{-9}). \tag{56}$$

The values of the asymptotic expressions (55) and (56) will be compared with the computed coupling matrices in paper II. For the asymptotic analysis of (12) it is important to summarize from this section that all matrix elements $A_{nn'}$, $B_{nn'}$ vanish rapidly at $|z| \to \infty$. The only non-vanishing element is the first term of (49).

3. Asymptotic analysis of the coupled equations

3.1. The domain $|z| \ll 1$

By assumption (5) the point $z = 0$ in (12) was converted to a regular point if $n_3 \geqslant 1$, while it is logarithmically singular in the non-adiabatic approximation if $n_3 = 0$. ψ will be regular in the interval $0 \leqslant z \ll 1$ and satisfy (12) if

$$f_n(z) = \sum_{m=0}^{\infty} d_m^{(n)} z^{\gamma_n + m} + D_n(z) \tag{57}$$

is assumed for all n together with $\gamma_n \geqslant 0$, where

$$D_n(z) = D_n^{(0)} z^2 (2 \ln |z| - 3)/4 + D_n^{(1)} z^3 (6 \ln |z| - 5)/36 + \cdots \tag{58}$$

will compensate the logarithmic singularity if $n_3 = 0$: $D_n^{(0)} = 0$ for the odd solutions, $D_n^{(1)} = 0$ for the even solutions, and of course $D_n^{(0)} = D_n^{(1)} = 0$ if $n_3 \geqslant 1$ or (5) is confined to a single term. Using (57) the complete ensemble of the bounded asymptotic solutions of (12) was constructed in the form of expansions which degenerate into Taylor series in the adiabatic approximation or if $n_3 \geqslant 1$.

After introducing (19), (41)–(43), and (57) in (12) we obtain from the coefficient of $z^{\gamma_n - 2}$ that $\gamma_n = \gamma = 0$ or $\gamma_n = \gamma = 1$ (corresponding to the even and odd solutions in z), the coefficients $d_0^{(n)}$ are arbitrary and at least one of them must be different from zero. From the coefficient of z^γ we obtain

$$d_2^{(n)} = \left[(\mu_n^{(0)} - 2E^* - A_{nn}^{(0)}) d_0^{(n)} - \sum_{n'}{}' A_{nn'}^{(0)} (1 + 2\gamma) d_0^{(n')}\right] / [(\gamma + 1)(\gamma + 2)]. \tag{59}$$

If $n_3 = 0$ and $\gamma = 0$ (59) gives $d_2^{(n)}$, $A_{nn}^{(0)}$ must be taken from (43). Checking for parity shows that $d_1^{(n)} = 0$. The coefficient of $\ln |z|$ is zero if

$$D_n^{(0)} = -\sum_{n'}{}' A_{nn'}^{(*)} d_0^{(n')}. \tag{60}$$

If $n_3 = 0$ and $\gamma = 1$ the elaboration of the powers z^0, $z \ln|z|$, z results in

$$d_1^{(n)} = -\tfrac{1}{2} \sum_{n'}{}' B_{nn'}^{(0)} d_0^{(n')} \tag{61}$$

$$D_n^{(1)} = -\sum_{n'}{}' (A_{nn'}^{(*)} + B_{nn'}^{(*)}) d_0^{(n')} \tag{62}$$

$$d_2^{(n)} = \tfrac{1}{6}\left[(\mu_n^{(0)} - 2E^* - A_{nn}^{(0)}) d_0^{(n)} - \sum_{n'}{}' (A_{nn'}^{(0)} + B_{nn'}^{(1)}) d_0^{(n')} + 2B_{nn'}^{(0)} d_1^{(n')}\right]. \tag{63}$$

Since sign (z) is a factor of $B_{nn'}^{(0)} d_1^{(n)} z^2$ will, while $B_{nn'}^{(0)} d_1^{(n')}$ will not change its sign at $z = 0$; consequently this term does not destroy the parity of f_n with respect to $z \to -z$.

The asymptotic solution (57) is useful to bridge over the critical region $0 \leqslant |z| \ll 1$ where a numerical integration of (12) is problematic because of the logarithmic singularity of $A_{nn'}$. Furthermore this analysis pointed out that at an outward (i.e. from $z = 0$ to $z = \infty$) numerical integration of (12) the appropriate vanishing of the vector–vector function $\boldsymbol{F}(\boldsymbol{E})$ must be found where $\boldsymbol{F}(z) = (f_0(z), f_1(z), \ldots)$ and each elements $f_n(z)$ depend on $\boldsymbol{E} = (E^*, d_0^{(1)}/d_0^{(0)}, \ldots)$ if $d_0^{(0)}$ is the non-zero element.

3.2. The domain $|z| \to \infty$

At $z = \pm\infty$ equations (12) have an irregular singularity: a series expansion of the type (57) e.g. in terms of the variable $t = |z|^{-1}$ does not exist. It is, however, possible through analytical reasoning to determine the 'tail' of the wavefunction (Bethe and Salpeter 1957) by finding the form of $f_n(z)$ for all indices n, to derive the thresholds in $E^*(\omega)$ which divide the bound and continuum states, and to show those solutions which correspond to auto-ionizing states.

If (49), (55) and (56) are introduced in (12) and the vanishing terms at $|z| \to \infty$ are neglected in adiabatic approximation the asymptotically good solutions are of the form

$$f_n = v_n(z) \exp\{-[2\omega(2n + n_3 + 1) - 2E^*]^{1/2}|z|\}. \tag{64}$$

The ionization thresholds are different for every channel n:

$$E_n^* = [\mu_n(\infty) - A_{nn}(\infty)]/2 = \omega(2n + n_3 + 1). \tag{65}$$

In non-adiabatic approximation $A_{nn'}$, $B_{nn'}$ mix solutions of type (64), therefore

$$f_n(z) = \sum_m v_{nm}(z) \exp\{-[2\omega(2m + n_3 + 1) - 2E^*]^{1/2}|z|\} \tag{66}$$

must be assumed. Using the variable t it can be pointed out that $v_n(z) \neq 0$ and $v_{nn}(z) \neq 0$ at $|z| \to \infty$, i.e. their behaviour does not change the unbounded character of (11) if the exponents of (64) and (66) are imaginary, the further properties of v are irrelevant for the asymptotic considerations. Consequently it is evident that in (12) the only threshold is at

$$E_0^* = \omega(n_3 + 1) \tag{67}$$

which is equivalent to two thresholds at $E = \omega$ and $E = (2n_3 + 1)\omega$ if $n_3 \neq 0$. The trivial auto-ionizing states are obtained if $n_3 > 0$ and $E(\omega) = E^*(\omega) + \omega n_3 > \omega$ occurs when increasing ω. If

$$(2n_0 + n_3 + 1)\omega < E^* < (2n_0 + n_3 + 3) \qquad n_0 = 0, 1, \ldots \tag{68}$$

$f_n(z)$ has oscillating components $n_0 + 1$ and the norm (11) will be unbounded. Furthermore, experience from numerical integration of (1) in spherical coordinates (Barcza 1994) has shown that with increasing ω the $n = 0$ term dominates the norm (11). Therefore, all levels are of continuum type with oscillating wavefunction if $E^* > E_0^*$.

Nevertheless, from qualitative physical considerations it is expected, and in adiabatic approximation it was found (Ventura *et al* 1992, Ruder *et al* 1994), that by the z motion a Balmer-like merging is caused to any Landau level. These results apply strictly for $\omega = \infty$. For the domain $1 \leqslant \omega < \infty$ our asymptotic analysis revealed that these levels can be found in non-adiabatic approximation by eliminating the oscillating term $f_0(z)g_0(z, \varrho)$ from X if $n_0 = 0$, $f_0(z)g_0(z, \varrho)$ and $f_1(z)g_1(z, \varrho)$ if $n_0 = 1$ etc.

A simple omission of the element $n = 0$ from (5) is a first approximation to find these levels but it raises the question of the relation of this solution of (12) to that of (1). A mathematically appropriate way of eliminating f_0g_0 is to impose the condition

$$\sum_{n'=1}^{\infty} A_{0n'} f_{n'} + B_{0n'} \frac{\mathrm{d} f_{n'}}{\mathrm{d}z} = 0 \tag{69}$$

by which f_0 is completely decoupled from (12) and satisfies the homogeneous eigenvalue equation

$$\frac{\mathrm{d}^2 f_0}{\mathrm{d}z^2} + [2E^* - \mu_0(z) + A_{00}] f_0 = 0. \tag{70}$$

Its solution is of the form

$$f_0 = C_0 v_0(z) \exp\{-[2\omega(n_3 + 1) - 2E^*]^{1/2} |z|\} \tag{71}$$

C_0 is arbitrary. If $C_0 \neq 0$ in the bound domain $E^* < E_0^*$ the eigenvalues are already determined by (70) which is essentially an adiabatic approximation with discrete spectrum. However, these are not eigenvalues of the rest of the coupled equations ((12) with $n \geqslant 1$ and (69)), therefore the choice $C_0 = 0$ is necessary to convert (70) to identity at any E^*. In the continuum domain $E^* > E_0^*$ (70) has a continuous spectrum, the choice $C_0 \neq 0$ is possible by which a continuum-wavefunction is obtained if (12) with $n \geqslant 1$ and (69) are integrated numerically. From asymptotic analysis a criterion has not been found whether solutions of this type exist with discrete or continuous multitude of C_0. These solutions, if they exist for the whole axis z, constitute a subspace of the continuum of (1) which is rather a mathematical peculiarity and its eventual physical significance cannot be clarified merely from asymptotic analysis.

If $C_0 \to 0$ equations (12) with $n \geqslant 1$ and (69) degenerate into an eigenvalue problem for the non-trivial auto-ionizing resonance levels of $n_0 = 0$ with bounded norm (11) at the eigenvalues, the threshold is now at $E_1^* = \omega(n_3 + 3)$. This system of coupled differential equations can be solved by appropriate numerical methods; when looking for the best form of (69) to introduce it in (12) the asymptotic analysis of section 2 must be extensively used to avoid, e.g. an incorporation of unnecessary singularities which can be formed by a careless combination of singular or rapidly vanishing elements.

After having expressed $f_1(z)$ from (69) and introduced it in (12) we can find the non-trivial auto-ionizing resonance levels of $n_0 = 1$ if the auxiliary condition

$$\sum_{n'=2}^{\infty} \left\{ \left[A_{1n'} - (2E^* - \mu_1 + A_{11}) \frac{A_{0n'}}{A_{01}} \right] f_{n'} + \left[B_{1n'} - (2E^* - \mu_1 + A_{11}) \frac{B_{0n'}}{A_{01}} \right] f'_{n'} \right\} = 0 \tag{72}$$

is imposed on (12) with $n \geqslant 1$ and (69). In principle the imposition of auxiliary conditions can be continued to find the non-trivial auto-ionizing levels belonging to any higher Landau level. If eigenvalues satisfying $E^* > E_0^*$ are found from the numerical integration of (12) and auxiliary condition(s) as expected when $\omega \geqslant 1$ these are the non-trivial auto-ionizing states.

Because of (68) the thresholds follow each other by the Landau spacing. The position of the thresholds, the domains of the non-trivial auto-ionizing levels are an intrinsic feature of (1): if the expansions in terms of the Landau basis (Ruder *et al* 1994) or oblate angular spheroidal functions (Barcza 1994) are analysed the same results are obtained as in the present subsection. This feature is not apparent only if unsuitable basis functions are used to expand ψ.

4. Conclusions

The asymptotic analysis reported in this paper provides the basic first steps, a foundation for specifying efficient numerical integration methods for the solution of the system of coupled second-order ordinary differential equations (12) which arises from the choice of the LaS basis. The preliminary numerical tests indicate that the efficiency of the numerical methods is drastically improved by the incorporation of the established asymptotics especially at $z \gg 1$ where the time-consuming computation of $\mu_n(z)$ and coupling matrices can be avoided.

By the construction of asymptotic expansions for $f_n(z)$ at $0 \leqslant z \ll 1$ much computing time can be saved in a numerical integration of (12) if $n_3 = 0$ since the error of an integrator formula does not vanish when increasing its order. The values of $f_n(z \approx 0)$ became known by solving linear algebraic equations which makes a number of trial shootings unnecessary, and the asymptotically free parameters $d_0^{(n)}$ of the wavefunction were found. The asymptotic analysis of (12) at $z \to \infty$ revealed the asymptotic form of the wavefunction, the thresholds and gave hints on how to find the non-trivial auto-ionizing states by the numerical integration of (12).

As a result of the asymptotic analysis the $-\infty \leqslant z \leqslant \infty$ interval of a numerical integration could be confined to a finite interval $[0, z]$ but a more important result is that we have found analytical criteria which lead to non-trivial auto-ionizing resonance levels.

Appendix A. The matrix elements for the perturbation series (20) and (21)

$$\begin{aligned} H'_{n'n}(z) &= \int_{|z|}^{\infty} (x^2 - z^2)^{n_3} \mathrm{e}^{-\omega(x^2-z^2)} \chi_{n'}^{(0)} H' \chi_n^{(0)} x \, \mathrm{d}x \\ &= \int_{|z|}^{\infty} (x^2 - z^2)^{n_3} \mathrm{e}^{-\omega(x^2-z^2)} \chi_{n'}^{(0)} \frac{1}{x} \left\{ \frac{2(n_3+1)}{x} \frac{\partial \chi_n^{(0)}}{\partial x} \right. \\ &\quad \left. + \left[\frac{2Z}{x} - 2\omega(n_3+1) + \mu_n^{(0)} \right] \chi_n^{(0)} \right\} \mathrm{d}x \\ &= H'^{(-1)}_{n'n} |z|^{-1} - H'^{(*)}_{n'n} \ln |z| + H'^{(0)}_{n'n} + \mathrm{O}(|z|). \end{aligned} \tag{A.1}$$

If $n_3 = 0$

$$H'^{(-1)}_{nn'} = -2Z c_0^{(n)} c_0^{(n')} \tag{A.2}$$

$$H'^{(*)}_{nn'} = 4Z^2 c_0^{(n)} c_0^{(n')} \tag{A.3}$$

$$\begin{aligned} H'^{(0)}_{nn'} &= 2Z c_0^{(n)} c_0^{(n')} [\omega^{1/2} \Gamma(\tfrac{1}{2}) - Z(C - \ln \omega)] \\ &\quad + \int_0^{\infty} \mathrm{e}^{-\omega x^2} [c_0^{(n)} \hat{S}_{n'}(3) + c_1^{(n)} \hat{S}_{n'}(2) + \bar{S}_n(2) \hat{S}_{n'}(1)] \, \mathrm{d}x \end{aligned} \tag{A.4}$$

where C is the Euler number,

$$\hat{S}_{n'}(m') = 2(n_3+1)\sum_{m=m'}^{\infty} m c_m^{(n')} x^{m-m'} + 2Z \sum_{m=m'-1}^{\infty} c_m^{(n')} x^{m-m'+1} + [\mu_{n'} - 2\omega(n_3+1)] \sum_{m=m'-2}^{\infty} c_m^{(n')} x^{m-m'+2} \tag{A.5}$$

$$\bar{S}_n(m') = \sum_{m=m'}^{\infty} c_m^{(n)} x^{m-m'}. \tag{A.6}$$

To obtain the value of (A.2) and (A.3) the relation

$$c_0^{(n)} = \lim_{\varrho\to 0} \Phi_n(0,\varrho)/\varrho^{-1/2} \tag{A.7}$$

is useful if Φ_n is determined by a numerical integration of (6).

If $n_3 \geqslant 1$

$$H'^{(-1)}_{nn'} = H'^{(*)}_{nn'} = 0 \tag{A.8}$$

$$H'^{(0)}_{nn'} = \int_0^{\infty} x^{2n_3-2} \mathrm{e}^{-\omega x^2} \bar{S}_n(0) \hat{S}_{n'}(1)\, \mathrm{d}x. \tag{A.9}$$

It is a remarkable feature of the asymptotic expansions (19)–(20) that if $n_3 = 0$ by (A.1) the vanishing of the first- and second-order terms in the perturbation series (19) and (20) are proportional to $|z|$ and z^2 respectively while the vanishing $\propto z^2$, z^4 is unchanged if $n_3 \geqslant 1$. This difference follows from the nature of the singularity of $2Z/\varrho - n_3^2/\varrho^2$ at $\varrho = 0$: the first term dominates if $n_3 = 0$ while the second one is dominating if $n_3 \geqslant 1$.

Appendix B. An alternative expansion to (22)

The numerical results of section 2.1.1 for $\mu_n^{(0)}$ will be confirmed here by an expansion which is interesting from an analytical point of view although it is computationally less efficient. We substitute

$$\Phi_n(0,\varrho) = \varrho^{n_3+1/2} \mathrm{e}^{\omega\varrho^2/2} \tilde{\chi}_n^{(0)}(\varrho) \tag{B.1}$$

for (7) in (6). The analogue of (22) reads in this case

$$\left\{ \frac{\mathrm{d}^2}{\mathrm{d}x^2} + \left[\frac{2n_3+1}{x} + 2\omega x \right] \frac{\mathrm{d}}{\mathrm{d}x} + \left[\frac{2Z}{x} + 2\omega(n_3+1) + \mu_n^{(0)} \right] \right\} \tilde{\chi}_n^{(0)} = 0 \tag{B.2}$$

its solution is assumed in the form

$$\tilde{\chi}_n^{(0)} = \sum_m \tilde{c}_m^{(n)} x^{m+\gamma}. \tag{B.3}$$

The recurrence relation for $\tilde{c}_m^{(n)}$ is

$$(\gamma+m+2)(\gamma+m+2+2n_3)\tilde{c}_{m+2}^{(n)} + 2Z\tilde{c}_{m+1}^{(n)} + [2(\gamma+m+n_3+1)\omega + \mu_n^{(0)}]\tilde{c}_m^{(n)} = 0$$
$$m = -2, -1, \ldots \qquad \tilde{c}_{-2}^{(n)} = \tilde{c}_{-1}^{(n)} = 0 \tag{B.4}$$

from which it follows that $\gamma = 0$, and

$$\lim_{m\to\infty} \frac{\tilde{c}_{m+2}^{(n)}}{\tilde{c}_{m+1}^{(n)}} = \pm\mathrm{i}\left(\frac{2\omega}{m}\right)^{1/2} \qquad \lim_{m\to\infty} \frac{\tilde{c}_{m+2}^{(n)}}{\tilde{c}_m^{(n)}} = -\frac{2\omega}{m} \tag{B.5}$$

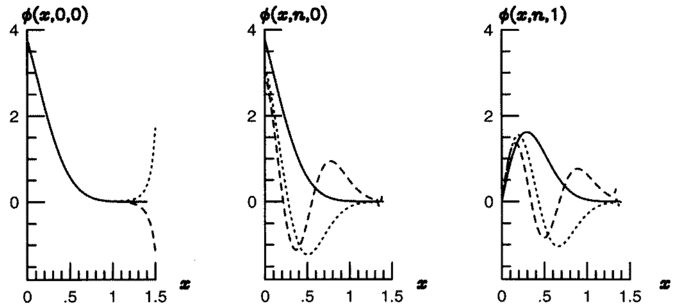

Figure B1. A plot of some $\phi(x,n,n_3) = x^{n_3}\exp(\omega x^2/2)\tilde{\chi}_n^{(0)}$ for $Z = 1$, $\omega = 10$. Full curves: $n = 0$, $\mu_0^{(0)} = 7.185\,762$ for $n_3 = 0$, $\mu_0^{(0)} = 34.25\,883$ for $n_3 = 1$. The dotted and broken curves in the left panel show the start of the divergent behaviour of $\phi(x,0,0)$ if $\mu_0^{(0)} = 7.183(< 7.185\,762)$ and $\mu_0^{(0)} = 7.188(> 7.185\,762)$ were used in (B.3). Dotted curves in the middle and right panel: $\mu_1^{(0)} = 51.28\,293$ for $n_3 = 0$, $\mu_1^{(0)} = 75.02\,968$ for $n_3 = 1$. Broken curves: $\mu_2^{(0)} = 92.68\,091$ for $n_3 = 0$, $\mu_2^{(0)} = 115.4932$ for $n_3 = 1$. These values of $\mu_n^{(0)}$ satisfy (B.7). The noisy end of $\phi(x,2,0)$, $\phi(x,2,1)$ indicates the value x where computational accuracy 10^{-15} becomes insufficient for computing $\tilde{\chi}_2^{(0)}(x)$ accurately enough. The noise at $x \approx 1.5$ is replaced by a vanishing behaviour corresponding to (B.7) if the computational accuracy is increased to some 10^{-18}, however, it reappears at larger values of x.

i.e.

$$\tilde{\chi}_n^{(0)} \propto \mathrm{e}^{-2\omega x^2} \tag{B.6}$$

if $m \gg 1$. The asymptotic behaviour (B.6) implies a quadratically integrable vanishing of (B.1) which corresponds to a bound state, the only prescription is for (B.3) that the series must not be terminated. A few functions $\phi(x,n,n_3) = \Phi_n(0,x)x^{-1/2} = x^{n_3}\exp(\omega x^2/2)\tilde{\chi}_n^{(0)}$ are plotted in figure B1. The eigenvalue was obtained from the condition

$$\lim_{x\to\infty} \phi(x,n,n_3;\mu_n^{(0)}) = 0 \tag{B.7}$$

which is satisfied at discrete values of $\mu_n^{(0)}$ only. Full agreement was found with the numerical results originating from (35) and (36): our sophisticated method did not reveal new levels. The decreased efficiency of this procedure manifests itself in the loss of digits when computing (B.3) with increasing x where its convergence is similar to that of the Taylor expansion of $\exp(-2\omega x^2)$ at $x \gg 1$.

Solutions of type (B.1) were rejected in the early days of quantum mechanics (see e.g. Pauling and Wilson 1935 or any later textbook on the topic), from this remark it is obvious that this is not justified since the exponential divergence in (B.1) is compensated by the behaviour (B.6) of $\tilde{\chi}$.

Appendix C. The coefficients to the expansion of the matrix elements $A_{nn'}$, $B_{nn'}$ at $z \approx 0$

The coefficients for (41) and (42) were computed by expanding the relation

$$\frac{1}{2}B_{nn'} = \left(\Phi_n, \frac{\partial\Phi_{n'}}{\partial z}\right) = \frac{1}{\mu_{n'}(z) - \mu_n(z)}\int_{|z|}^{\infty} \Phi_n\Phi_{n'}\frac{2Zz}{x^3}\,\mathrm{d}x \tag{C.1}$$

(Barcza 1994). If $n_3 = 0$ the results are

$$B_{nn'}^{(0)} = \frac{B_{nn'}^{(*)}}{4Z} = \frac{4Zc_0^{(n)}c_0^{(n')}}{\mu_{n'}^{(0)} - \mu_n^{(0)}} \tag{C.2}$$

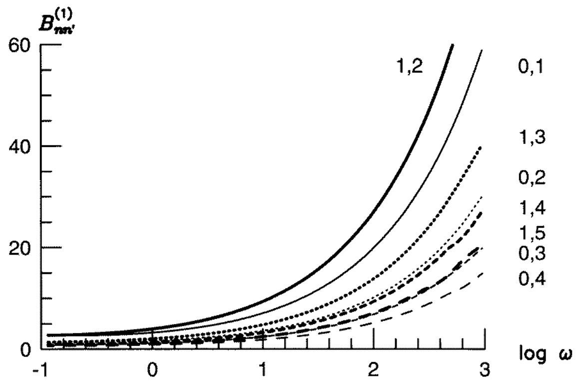

Figure C1. A plot of $B_{nn'}^{(1)}(\omega)$ for $Z = 1$, $n_3 = 1$, the curves are labelled by the value of nn'.

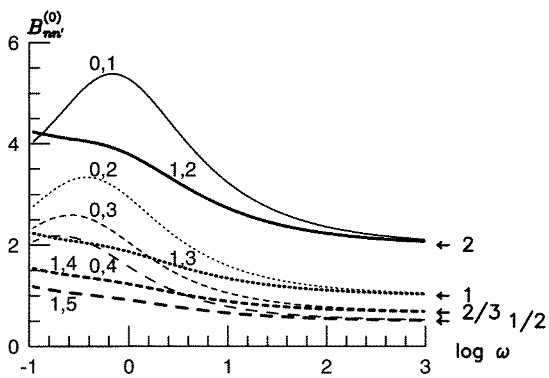

Figure C2. A plot of some values $B_{nn'}^{(0)}(\omega)$ for $Z = 1$, the curves are labelled by the value of nn'. The values of the asymptotic formula (C.8) are marked by arrows.

$$B_{nn'}^{(1)} = \frac{4Z}{\mu_{n'}^{(0)} - \mu_n^{(0)}} \left\{ c_0^{(n)} c_0^{(n')} \left[-\omega^{1/2}\Gamma\left(\frac{1}{2}\right) + 2Z(C + \ln\omega) + \frac{H'^{(-1)}_{n'n'} - H'^{(-1)}_{nn}}{\mu_{n'}^{(0)} - \mu_n^{(0)}} \right] \right.$$
$$+ c_0^{(n)} \sum_m{}' \frac{H'^{(-1)}_{mn'} c_0^{(m)}}{\mu_m^{(0)} - \mu_{n'}^{(0)}} + c_0^{(n')} \sum_m{}' \frac{H'^{(-1)}_{mn} c_0^{(m)}}{\mu_m^{(0)} - \mu_n^{(0)}}$$
$$\left. + \int_0^\infty \mathrm{e}^{-\omega x^2} [c_0^{(n)} \bar{S}_{n'}(2) + c_1^{(n)} \bar{S}_{n'}(1) + \bar{S}_n(2)\bar{S}_{n'}(0)]\,\mathrm{d}x \right\}. \tag{C.3}$$

If $n_3 \geqslant 1$ we obtain

$$B_{nn'}^{(0)} = B_{nn'}^{(*)} = 0, \tag{C.4}$$

$$B_{nn'}^{(1)} = \frac{4Z}{\mu_{n'}^{(0)} - \mu_n^{(0)}} \int_0^\infty x^{2n_3-2} \mathrm{e}^{-\omega x^2} \chi_n^{(0)} \chi_{n'}^{(0)}\,\mathrm{d}x. \tag{C.5}$$

A few values of $B_{nn'}^{(1)}$ are plotted in figure C1.

If $n_3 = 0$ and $\omega \to \infty$ on using (30) and

$$L_{n+n_3}^{n_3}(\hat{\xi}) = \sum_{m=0}^{n} \frac{(-1)^{m+1}(n+n_3)!^2 \hat{\xi}^m}{(n-m)!(m+n_3)!m!} \tag{C.6}$$

(Pauling and Wilson, 1935) we find that

$$\lim_{\omega\to\infty} c_0^{(n)} = (2\omega)^{1/2} \tag{C.7}$$

note that in (C.7) the minus sign was omitted from the constant term of (C.6). If $n \neq n'$ from (31), (C.2) and (C.7) we obtain that

$$\lim_{\omega\to\infty} B_{nn'}^{(0)} = \frac{2Z}{n' - n}. \tag{C.8}$$

The values of a few coupling constants $B_{nn'}^{(0)}$ as functions of ω are plotted in figure C2.

The accuracy 10^{-6} was reached easily in the components (C.2)–(C.5) except for the two sums in (C.3) which are different from zero only if $n_3 = 0$. This limitation is of secondary importance since $B_{nn'}^{(1)}$ is one of the constant terms of (42) and it is the third term of (41). These terms are preceded by non-zero elements which are much larger at $z \approx 0$.

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