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The diamagnetic Coulomb problem at high field strength. Numerical analysis

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Abstract. With the help of the basis proposed by Liu and Starace, the solution of the Schrödinger equation with a strong magnetic field is investigated in this paper. Besides the analytical characterization, this basis allows an easy way for numerical treatment of the problem. We present an efficient numerical method for determining both the eigenvalues of the basis equation and those of the accompanying coupled equations without the computation of the eigenfunctions. The theoretically stable behaviour of the method is confirmed by numerical evaluations. For the parameter values which were involved into computations, the results are obtained with satisfactory accuracy.

1. Introduction

In this paper we deal with the numerical solution of the Schrödinger equation of a hydrogen-like ion of nuclear charge Z and infinite nuclear mass in the homogeneous magnetic field.

With the assumption that the magnetic field is parallel to axis z, the equation is written in cylindrical coordinates φ, ϱ, z. Then, the dependence on the azimuthal angle φ around axis z may be separated in the eigenfunction Ψ:

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

Thus, the eigenproblem in cylindrical coordinates takes the form of

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

where n_3 is the magnetic quantum number, $\omega = e|\boldsymbol{H}|/(2mc)$ and $E^* = E - \omega n_3$.

The representation

$$\psi(z, \varrho) = \sum_{n=0}^{\infty} f_n(z)\hat{\Phi}_n(z, \varrho) \tag{2}$$

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was proposed by Liu and Starace (1987) assuming that for any fixed z $\hat{\Phi}_n(z,\varrho)$ is a bounded function of variable ϱ and it is the nth eigenfunction belonging to the (nth) eigenvalue $\mu_n(z)$ of the problem

$$\left[\frac{\partial^2}{\partial\varrho^2}+\frac{1}{\varrho}\frac{\partial}{\partial\varrho}-\frac{{n_3}^2}{\varrho^2}+\frac{2Z}{(\varrho^2+z^2)^{1/2}}-\omega^2\varrho^2+\mu(z)\right]\hat{\Phi}(z,\varrho)=0 \qquad 0<\varrho<\infty. \tag{3}$$

The set of eigenfunctions of (3) corresponding to a fixed z will be called the Liu–Starace basis. They form an orthogonal system with respect to the scalar product

$$(\zeta,\eta)=\int_0^\infty \zeta(\varrho)\eta(\varrho)\varrho\,\mathrm{d}\varrho.$$

The eigenfunctions may be uniformly normalized to 1, i.e. the relations

$$(\hat{\Phi}_{n'},\hat{\Phi}_n)=\delta_{n'n} \tag{4}$$

become independent of z. In this case, equations (1) and (3) induce that the system of functions $\{f_n(z)\}_{n=0}^{\infty}$ must satisfy the infinite system of ordinary differential equations

$$\frac{\mathrm{d}^2 f_n}{\mathrm{d}z^2}+[2E^*-\mu_n(z)]f_n+\sum_{n'=0}^{\infty}\left[A_{nn'}f_{n'}+B_{nn'}\frac{\mathrm{d}f_{n'}}{\mathrm{d}z}\right]=0$$
$$-\infty<z<\infty \qquad n=0,1,\ldots \tag{5}$$

where

$$A_{nn'}(z)=\left(\hat{\Phi}_n,\frac{\partial^2\hat{\Phi}_{n'}}{\partial z^2}\right) \qquad B_{nn'}(z)=2\left(\hat{\Phi}_n,\frac{\partial\hat{\Phi}_{n'}}{\partial z}\right) \tag{6}$$

and due to orthonormalization (4), $B_{nn}=0$ and $B_{nn'}=-B_{n'n}$.

By our considerations, the solution of (1) is split into two subsequent steps. In the first step, the eigenvalues E^* of (1) are found. The present paper deals with this problem, only. Namely, the forthcoming material concerns eigenvalues and some functionals composed of eigenfunctions of (3) while the eigenfunctions of (3) themselves are not of interest at the moment. We will show that the evaluation of eigenvalues E^* of (1) in the following sections requires the computation of neither the eigenfunctions $\hat{\Phi}_n(z,\rho)$ nor those of the coupled system (5). On the other hand, it is shown that the methods below behave well numerically. These two features make the method distinguished among those for finding eigenvalues of Schrödinger equations.

Above the eigenvalues E^*, when explaining some phenomena and evaluating physical observations, the normalized wavefunctions ψ or rather their quadratic functionals like transition probabilities may be requested, too. We consider these evaluations as the second step in solving (1). Based on the results in this paper, methods that are compatible with those in the first step are developed for the first time. Since the eigenvalues are of interest on their own, another publication will be addressed to the second step.

In the next three sections, we will make intensive use of the results concerning singular boundary value problems and singular eigenvalue problems posed for ordinary differential equations. For the theoretical background and basic statements as well as for the error estimates in the case of regular singularity see Balla (1977, 1988), for irregular singularity we refer to Birger and Lyalikova (1965) and Abramov and Balla (1993). A survey of methods for singular eigenvalue problems is given in Abramov *et al* (1980). By a unified approach based on the above, specific problems (i.e. evaluation of eigenvalues and eigenfunctions and quadratic functionals involving eigenfunctions) for scalar ordinary Schrödinger equations regular and with singularities are highlighted in survey paper Kitoroage *et al* (1987). Additional material may be found in publications referred in the survey papers. Also, a lot

of physical problems solved by similar methods is cited or referred to there. No similar theory has been developed yet for the stable direct evaluation of normalized solutions and their quadratic functionals of solutions of (1) when basis is chosen in the manner as defined by (3). Together with the scheme of the second step and the numerical results we describe the underlying mathematical theory in a future publication.

The outline of the paper is as follows. In section 2 we will describe a method for finding the eigenvalues $\mu_n(z)$ that appear in equation (3). Section 3 will be devoted to the evaluation of matrix elements $A_{nn'}(z)$ and $B_{nn'}(z)$ given by (6). In section 4 we give a method for the computation of eigenvalues E_k^{*N}, $k = 0, 1, \ldots$ for arbitrary values of parameter n_3. These eigenvalues belong to finite, N-dimensional systems obtained by a proper truncation of (5), i.e. they approximate the values E_k^*, $k = 0, 1, \ldots$ (the dependence on n_3 is omitted in the notation E_k^*, E_k^{*N}). In section 5 we give figures and tables of μ_n, $A_{nn'}$ and $B_{nn'}$ for some values of parameters z, ω, n_3, n, n'. The results give a possibility both to evaluate the capacity of the proposed method and to compare them with previous results obtained either theoretically or numerically. The numerical experiments allow us to think that equations (3) and (5) and the approximation of the latter are sufficiently well chosen for the solution of problem (1). These conclusional remarks will be given in section 6. The paper is completed by an appendix on some technical details concerning the numerical algorithms and their implementation.

2. The eigenproblem for the Liu–Starace basis

By transformation $\Phi(\varrho, z) = \sqrt{\varrho}\hat{\Phi}(\varrho, z)$ equation (3) takes the form of

$$\Phi''(\varrho, z) + [q(\varrho, z) + \mu(z)]\Phi(\varrho, z) = 0 \tag{7}$$

where $'$ is the abbreviation for $\partial/\partial\varrho$,

$$q(\varrho, z) = \frac{\frac{1}{4} - {n_3}^2}{\varrho^2} + \frac{2Z}{(\varrho^2 + z^2)^{1/2}} - \omega^2\varrho^2. \tag{8}$$

First, we consider the case $z \neq 0$. For the potential $q(\varrho, z)$ the following representations are valid:

$$q(\varrho, z) = \frac{1}{\varrho^2}\sum_{i=0}^{\infty} q_i \varrho^{2i} \qquad \text{if } \frac{\varrho}{z} < 1$$

$$q(\varrho, z) = \varrho^2 \sum_{i=0}^{\infty} \tilde{q}_i \varrho^{-i} \qquad \text{if } \frac{\varrho}{z} > 1$$

where

$$q_0 = \tfrac{1}{4} - {n_3}^2 \qquad q_1 = \frac{2Z}{z} \qquad q_2 = -\frac{Z}{z^3} - \omega^2 \qquad q_i = \frac{Zc_{i-1}}{z^{2i-1}} \qquad \text{if } i \geqslant 3$$

and

$$\tilde{q}_0 = -\omega^2 \qquad \tilde{q}_1 = \tilde{q}_2 = 0 \qquad \tilde{q}_3 = 2Z \qquad \tilde{q}_4 = \tfrac{1}{4} - {n_3}^2$$
$$\tilde{q}_{2i+1} = 2Zc_{i-1}z^{2(i-1)} \qquad \text{if } i \geqslant 2.$$

Here $c_0 = 1, c_1 = -\frac{1}{2}$ and $c_i = -\frac{1}{2}[\sum_{l=1}^{i-1} c_l c_{i-l} + \sum_{l=0}^{i-1} c_l c_{i-l-1}]$ if $i \geqslant 2$. From now on, if no confusion arises, we omit argument z.

The boundedness of any solution Φ (with respect to ϱ) of equation (3) at the ends of the interval $(0, \infty)$ is equivalent to the following statements:

(i) For any sufficiently small ϱ ($\varrho \ll z$),

$$\varrho\Phi'(\varrho) = \gamma(\varrho)\Phi(\varrho) \tag{9}$$

where

$$\gamma = \sum_{i=0}^{\infty} \gamma_i \varrho^{2i} \tag{10}$$

$$\gamma_0 = \tfrac{1}{2} + |n_3| \qquad \gamma_1 = -\frac{q_1 + \mu}{2(1+|n_3|)} \qquad \gamma_i = -\frac{q_i + \sum_{l=1}^{i-1} \gamma_l \gamma_{i-l}}{2(i+|n_3|)} \qquad \text{if } i \geqslant 2 \tag{11}$$

(see Balla 1977).

(ii) For any sufficiently large ϱ ($\varrho \gg z$),

$$\Phi'(\varrho) = \varrho\beta(\varrho)\Phi(\varrho) \tag{12}$$

where

$$\beta \sim \sum_{i=0}^{\infty} \frac{\beta_i}{\varrho^i} \tag{13}$$

$$\beta_0 = -\omega \qquad \beta_1 = 0 \qquad \beta_2 = \frac{\mu}{2\omega} \qquad \beta_i = \frac{1}{2\omega}\left[\tilde{q}_i + \sum_{l=0}^{i-2} \beta_{l+1}\beta_{i-l-1} - (i-2)\beta_{i-2}\right] \qquad \text{if } i \geqslant 3 \tag{14}$$

due to Birger and Lyalikova (1965). Thus, if a small $\varrho = \varrho_0$ is fixed in (9) and a large $\varrho = \varrho_\infty$ is fixed in (12), then one arrives at an equivalent eigenvalue problem formed of equation (7) on the finite interval $[\varrho_0, \varrho_\infty]$ and boundary conditions (9) and (12) posed at the indicated points. This problem is free of singularities.

Now, we define functions $r(\varrho), \Theta(\varrho)$ implicitly by relations

$$\Phi(\varrho) = \frac{r(\varrho)}{\nu(\varrho)} \sin\Theta(\varrho) \qquad \Phi'(\varrho) = \nu(\varrho) r(\varrho) \cos\Theta(\varrho). \tag{15}$$

In fact, (15) is a modified Prüfer transformation where the function $\nu(\varrho)$ is an almost arbitrary function. We fix only that both limits $\lim_{\varrho\to 0} \nu(\varrho) = \nu_0$ and $\lim_{\varrho\to\infty} \nu(\varrho) = \nu_\infty$ exist. Modification by $\nu(\varrho)$ serves for scaling, i.e. for having smooth solutions of the equations in question. For lower modes the choice $\nu(\varrho) \equiv 1$ is satisfactory.

Having substituted relations (15) into equation (7), we arrive at the equation for phase Θ and amplitude r

$$\Theta' = \nu^2 \cos^2\Theta + \frac{1}{\nu^2}[q(\varrho, z) + \mu]\sin^2\Theta + \frac{(\nu^2)'}{\nu^2}\frac{\sin 2\Theta}{2} \tag{16}$$

$$r' = -v(\varrho, z) r \qquad v(\varrho, z) = \left[\frac{q(\varrho, z) + \mu(z)}{\nu^2(\varrho)} - \nu^2(\varrho)\right]\frac{\sin 2\Theta}{2} + \frac{[\nu^2(\varrho)]'}{\nu^2(\varrho)}\frac{\cos 2\Theta}{2}. \tag{17}$$

Conditions (9) taken at ϱ_0 and (12) taken at ϱ_∞ turn to

$$\Theta(\varrho_0) = \arctan\frac{\varrho_0 \nu^2(\varrho_0)}{\gamma(\varrho_0)} \tag{18}$$

and

$$\Theta(\varrho_\infty) = -\arctan\frac{\varrho_\infty \beta(\varrho_\infty)}{\nu^2(\varrho_\infty)} + \left(n + \frac{1}{2}\right)\pi. \tag{19}$$

As before, in the latter formula n denotes the index of the eigenfunction, which, in turn, coincides with the number of its zeros. Let us denote the solutions of the initial value

problems (16) with (18) and (16) with (19) by $\Theta_{\rm l}(\varrho)$ and $\Theta_{\rm r}(\varrho)$, respectively. When μ is an eigenvalue, then, for an arbitrarily fixed intermediate point $\varrho = \varrho_{\rm c} \in (\varrho_0, \varrho_\infty)$ the solutions of problems coincide, i.e. $\Theta_{\rm l}(\varrho_{\rm c}) = \Theta_{\rm r}(\varrho_{\rm c})$. Since the solutions of both initial value problems are monotone with respect to the parameter μ, each eigenvalue μ_n may be found by a bisection algorithm proceeding from a properly chosen interval that contains the eigenvalue.

Having the eigenvalues computed, in the next section we will intensively use the equation for amplitude $r(\varrho)$ defined by (17). It is a linear equation. In fact, we have two functions $r_{\rm l}(\varrho)$ and $r_{\rm r}(\varrho)$ with the coupling condition $r_{\rm l}(\varrho_{\rm c}) = r_{\rm r}(\varrho_{\rm c}) = r_{\rm c}$ that serves as an initial condition for equation (17) supplied with the corresponding indices l, r, respectively. The value of $r_{\rm c}$ is defined uniquely by the normalization of the eigenfunction in question. We notice here that solutions of equations (17) are needed neither for the computation of eigenvalues above in this section nor in the next sections where $A_{nn'}$ and $B_{nn'}$ and E^* are computed. We will need, however, the value $r_{\rm c}$. Namely, instead of computing the norm of an arbitrary, still not normalized eigenfunction by its numerical integration, we split the integral into two parts and decompose them following Kitoroage *et al* (1987). We introduce functions $h_{\rm l}(\varrho)$, $h_{\rm r}(\varrho)$ by

$$\int_0^{\varrho} \Phi^2(\xi, z)\,{\rm d}\xi = {r_{\rm l}}^2(\varrho, z)h_{\rm l}(\varrho, z) \qquad \text{and} \qquad \int_{\varrho}^{\infty} \Phi^2(\xi, z)\,{\rm d}\xi = -{r_{\rm r}}^2(\varrho, z)h_{\rm r}(\varrho, z). \tag{20}$$

Then, the differentiation of (20) yields equation

$$h_i'(\varrho) = \frac{1}{\nu^2(\varrho)} \sin^2 \Theta_i(\varrho) + 2v_i(\varrho)h_i(\varrho) \qquad i = {\rm l}, {\rm r} \tag{21}$$

if (17) is involved. Obviously, $\lim_{\varrho\to 0} {r_{\rm l}}^2 h_{\rm l} = 0$ which involves $\lim_{\varrho\to 0} h_{\rm l} = 0$. With the assumption of

$$h_{\rm l}(\varrho) = \sum_{j=1}^{\infty} h_{\rm l}^{(j)} \varrho^j$$

one gets $h_{\rm l}^{(1)} = h_{\rm l}^{(2)} = 0$, $h_{\rm l}^{(3)} = {\nu_0}^2/[{\gamma_0}^2(2\gamma_0 + 1)]$ where (10), (11) are taken into account. On the other hand, $h_{\rm r}(\varrho)$ remains bounded when $\varrho \to \infty$ and the assumption

$$h_{\rm r}(\varrho) \sim \sum_{j=0}^{\infty} \frac{h_{\rm r}^{(j)}}{\varrho^j}$$

with the help of (13), (14) results in $h_{\rm r}^{(0)} = {\nu_\infty}^2/[2\beta_0({\beta_0}^2 + {\nu_\infty}^4)]$. Thus, we get approximations for the values $h_{\rm l}(\varrho_0)$, $h_{\rm r}(\varrho_\infty)$. With these initial values, we form initial value problems for $h_{\rm l}, h_{\rm r}$ to be integrated in the stable directions. Namely, $h_{\rm l}$ is integrated from ϱ_0 and $h_{\rm r}$ is integrated from ϱ_∞ to an inner point $\varrho_{\rm c}$. Having integrated the equations, we use the orthonormalization condition (4) and get

$$r_{\rm c} = [h_{\rm l}(\varrho_{\rm c}) - h_{\rm r}(\varrho_{\rm c})]^{1/2}.$$

We remark again that the normalization is taken into account without the computation of the eigenfunction to be normalized. What we needed for that was the eigenvalue only. In the next section we will refer to the values above with an additional lower index indicating the index of the eigenvalue to which they belong.

Now, let us turn to the case $z = 0$. Then,

$$q(\varrho, 0) = \frac{\frac{1}{4} - {n_3}^2}{\varrho^2} + \frac{2Z}{\varrho} - \omega^2\varrho^2.$$

To show the similarity of the algorithm, it is worth having the representations of

$$q(\varrho,0)=\frac{1}{\varrho^2}\sum_{i=0}^{4}q_i\varrho^i \qquad q(\varrho,0)=\varrho^2\sum_{i=0}^{4}\tilde{q}_i\varrho^{-i} \tag{22}$$

where

$$q_0=\tfrac{1}{4}-{n_3}^2 \qquad q_1=2Z \qquad q_2=q_3=0 \qquad q_4=-\omega^2 \qquad (q_i=0,\ i>4)$$

and

$$\tilde{q}_0=-\omega^2 \qquad \tilde{q}_1=\tilde{q}_2=0 \qquad \tilde{q}_3=2Z \qquad \tilde{q}_4=\tfrac{1}{4}-{n_3}^2 \qquad (\tilde{q}_i=0,\ i>4).$$

Thus, for sufficiently small ϱ ($\varrho \ll 1$), relation (9) holds but (10), (11) are replaced by

$$\begin{gathered}\gamma=\sum_{i=0}^{\infty}\gamma_i\varrho^i \qquad \gamma_0=\tfrac{1}{2}+|n_3| \qquad \gamma_1=-\frac{2Z}{1+|n_3|} \qquad \gamma_2=-\frac{\gamma_1^2}{2+|n_3|}\\ \gamma_3=-\frac{2\gamma_1\gamma_2}{3+|n_3|} \qquad \gamma_4=\frac{\omega^2-\sum_{l=1}^{3}\gamma_l\gamma_{4-l}}{4+|n_3|} \qquad \gamma_i=-\frac{\sum_{l=1}^{i-1}\gamma_l\gamma_{i-l}}{i+|n_3|}.\end{gathered} \tag{23}$$

For sufficiently large ϱ ($\varrho \gg 1$), the relation (12) remains unchanged with the exception of some of the coefficients in (14) due to $\tilde{q}_i=0$, $i>4$. Otherwise, everything that was said in this section holds in the case $z=0$, as well. The basic ideas of this section rely upon the approach summarized in Abramov *et al* (1980).

3. Computation of the matrix elements

In this section we show that the direct computation of integrals in (6) involving the eigenfunctions and their derivatives may be avoided. Moreover, instead of numerically unstable processes due to numerical derivation, we propose a method free of instability. Also, analogously to the normalization process of the previous section, the computation of the integrands, i.e. the eigenfunctions is not needed.

Let us introduce the notations $\Omega_p=\partial\Phi_p/\partial z$ and $\Upsilon_p(\varrho,z)=\partial^2\Phi_p(\varrho,z)/\partial z^2$. Due to (7), $\Omega_p(\varrho,z)$ and $\Upsilon_p(\varrho,z)$ satisfy the equations

$${\Omega_p}''(\varrho,z)+[q(\varrho,z)+\mu_p(z)]\Omega_p(\varrho,z)=-\tau_p(z)\Phi_p(\varrho,z)-\frac{\partial q(\varrho,z)}{\partial z}\Phi_p(\varrho,z) \tag{24}$$

$$\begin{aligned}{\Upsilon_p}''(\varrho,z)+[q(\varrho,z)+\mu_p(z)]\Upsilon_p(\varrho,z)&=-2\tau_p(z)\Omega_p(\varrho,z)-2\frac{\partial q(\varrho,z)}{\partial z}\Omega_p(\varrho,z)\\ &\quad-\frac{\partial\tau_p(z)}{\partial z}\Phi_p(\varrho,z)-\frac{\partial^2 q(\varrho,z)}{\partial z^2}\Phi_p(\varrho,z)\end{aligned} \tag{25}$$

where $\tau_p(z)=\partial\mu_p(z)/\partial z$.

Let us multiply both sides of equation (24) by Φ_p and integrate over $(0,\infty)$. With partial integration and by taking the orthonormalization (4), equation (7) and the behaviour of the functions at the ends of the interval into account, we arrive at

$$\tau_p(z)=-\int_0^{\infty}{\Phi_p}^2(\varrho,z)\frac{\partial q(\varrho,z)}{\partial z}\,\mathrm{d}\varrho. \tag{26}$$

If (24) is multiplied by Φ_q, with $q\neq p$, then, the same process yields

$$\int_0^{\infty}\Omega_p(\varrho,z)\Phi_q(\varrho,z)\,\mathrm{d}\varrho=\frac{1}{\mu_q(z)-\mu_p(z)}\int_0^{\infty}\Phi_p(\varrho,z)\Phi_q(\varrho,z)\frac{\partial q(\varrho,z)}{\partial z}\,\mathrm{d}\varrho. \tag{27}$$

When $z \neq 0$, with the notations $l_1(\varrho, z) = 1/(\varrho^2 + z^2)^{3/2}$, $l_2(\varrho, z) = 1/(\varrho^2 + z^2)^{5/2}$,

$$I^i_{pq}(z) = \int_0^\infty \Phi_p(\varrho, z)\Phi_q(\varrho, z) l_i(\varrho, z)\,\mathrm{d}\varrho \qquad i = 1, 2 \tag{28}$$

$$J_{pq}(z) = \int_0^\infty \Omega_p(\varrho, z)\Phi_q(\varrho, z) l_1(\varrho, z)\,\mathrm{d}\varrho \tag{29}$$

expressions (26) and (27) simplify to

$$\tau_p(z) = 2Zz I^1_{pp}(z) \qquad \int_0^\infty \Omega_p(\varrho, z)\Phi_q(\varrho, z)\,\mathrm{d}\varrho = \frac{2Zz}{\mu_p(z) - \mu_q(z)} I^1_{pq}(z) \qquad p \neq q \tag{30}$$

while

$$\tau_p(0) = 0 \qquad \int_0^\infty \Phi_p(\varrho, z)\Phi_q(\varrho, z)\frac{\partial q(\varrho, z)}{\partial z}\,\mathrm{d}\varrho = 0 \tag{31}$$

hold trivially.

Applying the same arguments to equation (25) when $z \neq 0$ after some calculations we get

$$\int_0^\infty \Upsilon_p(\varrho, z)\Phi_q(\varrho, z)\,\mathrm{d}\varrho = \frac{2Z}{\mu_p(z) - \mu_q(z)} \times \left\{ I^1_{pq}(z) + 2z J_{pq}(z) - z^2 \left[3I^2_{pq}(z) + \frac{4Z}{\mu_p - \mu_q} I^1_{pp}(z) I^1_{pq}(z) \right] \right\} \qquad q \neq p. \tag{32}$$

The identity

$$\int_0^\infty \Upsilon_p(\varrho, z)\Phi_p(\varrho, z)\,\mathrm{d}\varrho = -\int_0^\infty \Omega^2_p(\varrho, z)\,\mathrm{d}\varrho \tag{33}$$

is due to orthonormalization.

First, let us consider integrals $I^i_{pq}(z)$, $i = 1, 2$, $p, q = 0, 1, \ldots$, $z \neq 0$. For their evaluation we apply an idea similar to that used in (20) and described in Kitoroage *et al* (1987). Let

$$\begin{aligned} \int_0^\varrho \Phi_p(\xi, z)\Phi_q(\xi, z) l_i(\xi, z)\,\mathrm{d}\xi &= r_{p\mathrm{l}}(\varrho, z) r_{q\mathrm{l}}(\varrho, z) k^{\mathrm{l}i}_{pq}(\varrho, z) \\ \int_\varrho^\infty \Phi_p(\xi, z)\Phi_q(\xi, z) l_i(\xi, z)\,\mathrm{d}\xi &= -r_{p\mathrm{r}}(\varrho, z) r_{q\mathrm{r}}(\varrho, z) k^{\mathrm{r}i}_{pq}(\varrho, z) \end{aligned} \tag{34}$$

and for $j = \mathrm{l}, \mathrm{r}$ get

$$k^{ji\,\prime}_{pq}(\varrho) = [v^{ji}_p(\varrho) + v^{ji}_q(\varrho)] k^{ji}_{pq}(\varrho) + \frac{l_i \sin\Theta_p(\varrho) \sin\Theta_q(\varrho)}{\nu_p(\varrho)\nu_q(\varrho)}. \tag{35}$$

Approximating the initial values for these singular problems exactly as in section 2, in the case $z \neq 0$ we arrive at

$$k^{\mathrm{l}i}_{pq}(\varrho_0) = \frac{{\varrho_0}^3 \nu_{p0}\nu_{q0} l^i_0}{{\gamma_0}^2(2\gamma_0 + 1)} + \mathrm{O}({\varrho_0}^4) \qquad \text{where } l^1_0 = \frac{1}{z^3},\ l^2_0 = \frac{1}{z^5} \tag{36}$$

$$k^{\mathrm{r}1}_{pq}(\varrho_\infty) = \frac{\tilde{l}^1_0 \nu_{p\infty}\nu_{q\infty}}{2\beta_0[(\beta_0{}^2 + \nu_{p\infty}{}^4)(\beta_0{}^2 + \nu_{q\infty}{}^4)]^{1/2}} + \mathrm{O}\left(\frac{1}{\varrho_\infty}\right) \tag{37}$$

$$k^{\mathrm{r}2}_{pq}(\varrho_\infty) = \frac{\tilde{l}^2_0 \nu_{p\infty}\nu_{q\infty}{\varrho_\infty}^2}{2\beta_0[(\beta_0{}^2 + \nu_{p\infty}{}^4)(\beta_0{}^2 + \nu_{q\infty}{}^4)]^{1/2}} + \mathrm{O}(\varrho_\infty) \qquad \text{and} \qquad \tilde{l}^i_0 = 1,\ i = 1, 2.$$

One easily verifies that $I^2_{pq}(0)$ does not appear in the evaluation. In the computation of $I^1_{pq}(0)$, the only change is that $k^{l1}_{pq}(\varrho_0) = 1/[2{\gamma_0}^2(\gamma_0 - 1)] + \mathrm{O}(\varrho_0)$.

Finally,

$$I^i_{pq} z = \frac{k^{li}_{pq}(\varrho_c) - k^{ri}_{pq}(\varrho_c)}{r_{pc} r_{qc}} \tag{38}$$

for the relevant values of z and i.

$J_{pq}(z)$ and the expression on the right-hand side of (33) remain to be computed. For this purpose, we use the assumption that the expansion

$$\Omega_p(\varrho, z) = \sum_{t=0}^{\infty} \kappa_{pt}(z)\Phi_t(\varrho, z) \qquad \text{with } \kappa_{pt}(z) = \int_0^{\infty} \Omega_p(\varrho, z)\Phi_t(\varrho, z)\,\mathrm{d}\varrho \tag{39}$$

holds and, together with it

$$J_{pq}(z) = \sum_{t=0, t\neq p}^{\infty} \kappa_{pt}(z) I^1_{tq}(z) \tag{40}$$

is valid ($\kappa_{pp}(z) = 0$ by orthonormalization). It immediately yields that

$$\kappa_{pt}(z) = \frac{2Zz}{\mu_p - \mu_t} I^1_{pt} \qquad \text{when } p \neq t \tag{41}$$

$$\begin{aligned}\int_0^{\infty} \Omega^2_p(\varrho, z)\,\mathrm{d}\varrho &= \sum_{t=0}^{\infty} \kappa_{pt}(z) \int_0^{\infty} \Omega_p(\varrho, z)\Phi_t(\varrho, z)\,\mathrm{d}\varrho \\ &= 4Z^2 z^2 \sum_{t=0, t\neq p}^{\infty} \left[\frac{I^1_{pt}(z)}{\mu_p(z) - \mu_t(z)}\right]^2\end{aligned} \tag{42}$$

$$J_{pq}(z) = 2Zz \sum_{t=0, t\neq p}^{\infty} \frac{I^1_{pt}(z) I^1_{tq}(z)}{\mu_p(z) - \mu_t(z)}. \tag{43}$$

Before giving the final formulae for the matrix elements, notice that $I^i_{pq} = I^i_{qp}$. Now, the above considerations yield

$$B_{nn}(z) = 0 \qquad B_{nn'}(z) = \frac{4Zz}{\mu_{n'}(z) - \mu_n(z)} I^1_{nn'}(z) \qquad \text{when } n \neq n' \tag{44}$$

$$A_{nn}(z) = -4Z^2 z^2 \sum_{t=0, t\neq n}^{\infty} \left[\frac{I^1_{nt}(z)}{\mu_n(z) - \mu_t(z)}\right]^2 \tag{45}$$

$$\begin{aligned}A_{nn'}(z) = \frac{2Z}{\mu_{n'}(z) - \mu_n(z)} \Bigg\{ I^1_{nn'}(z) - z^2 \Bigg[3I^2_{nn'}(z) \\ + 4Z \left(\frac{I^1_{nn'}(z) I^1_{n'n'}(z)}{\mu_{n'}(z) - \mu_n(z)} - \sum_{t=0, t\neq n'}^{\infty} \frac{I^1_{n't}(z) I^1_{nt}(z)}{\mu_{n'}(z) - \mu_n(z)} \right) \Bigg] \Bigg\}.\end{aligned} \tag{46}$$

4. The coupled system

As it was said in section 1, instead of equation (5), we deal with a truncated one. Namely, for fixed N, $N = 1, 2, \ldots$, we investigate the eigenvalue problem

$$\frac{\mathrm{d}^2 F^N}{\mathrm{d}z^2} + \mathcal{B}(z)\frac{\mathrm{d}F^N}{\mathrm{d}z} + [\mathcal{A}(z) - \mathcal{M}(z)]F^N = -2E^{*N} F^N \qquad -\infty < z < \infty \tag{47}$$

where the vectorfunction F^N is assumed to be bounded. The vector $F^N(z)$ is formed as $F^N(z) = [f_0^N(z), f_1^N(z), \ldots, f_{N-1}^N(z)]^{\mathrm{T}}$ where f_i^N stands for f_i in the Nth truncated system, T denotes the transpose of the vector, later that of a matrix. The entries of the skew-symmetrical matrix $\mathcal{B}(z)$ are $B_{nn'}(z)$, $n, n' = 0, \ldots, N-1$, while the entries of $\mathcal{A}(z)$ are $A_{nn'}(z)$, $n, n' = 0, \ldots, N-1$. The matrix $\mathcal{M}(z)$ is diagonal, $\mathcal{M}(z) = \mathrm{diag}[\mu_0(z), \ldots, \mu_{N-1}(z)]$.

Due to (1) and (2), the eigenvectors F^N are either odd or even. Thus, when $n_3 \neq 0$ we may restrict the problem to the interval $[0, \infty)$ with imposing either the boundary condition $F^N(0) = 0$ for the odd solution or $F^{N\prime}(0) = 0$ for the even solution. (Within this section, $'$ denotes derivation with respect to z.) When $n_3 = 0$, the matrix $\mathcal{A}$ has a singularity at $z = 0$, while the solution in question is required to be regular. This case must be handled separately. The interval may be reduced again but to $[z_0, \infty)$ with a small $z_0 > 0$ and again, the proper boundary condition at z_0 must be imposed. The singularity of the system at $z = 0$, however, is a weak one, i.e. in contrast to cases studied in section 2, any linear condition at $z = 0$ remains admissible. Among them, those which produce odd and even solutions are admitted. At a point z_0 sufficiently close to $z = 0$, they may be approximated by $F^N(z_0) = 0$ or by $F^{N\prime}(z_0) = 0$.

Now, we turn to reducing the problem to a finite interval. When $z \to \infty$, $\mathcal{A}(z)$ and $\mathcal{B}(z)$ tend to 0 as a negative power of z, while $\mathcal{M}(z) = \mathcal{M}_\infty + \mathrm{O}(1/z)$. The true eigenvalues E_k^*, $k = 0, 1, 2, \ldots$ are known to be less than $\lim_{z\to\infty} \mu_n(z)/2$, $n = 0, 1, \ldots$ in non-autoionizing states. Due to monotonicity of $\mu_n(z)$ with respect to n for a fixed z and with respect to z for fixed n, one has $E_k^* < \lim_{z\to\infty} \mu_0(z)/2$ for all k. We assume that the same holds for the eigenvalues E_k^{*N} of the truncated system, i.e. the diagonal matrix $\mathcal{M}_\infty - 2E^* I_N$ is positive definite. (Here I is the identity matrix, the lower index refers to its order.) Then, the boundedness of a solution $F^N(z)$ when $z \to \infty$ involves that $F^{N\prime}(z) = \alpha(z) F^N(z)$ for sufficiently large z where $\lim_{z\to\infty} \alpha^2(z) = \mathcal{M}_\infty - 2E^* I$, $\alpha_\infty = \lim_{z\to\infty} \alpha(z)$ should be chosen negative definite (see Birger and Lyalikova 1965). For the approximation of this, we may use the boundary condition

$$F^{N\prime}(z_\infty) = \alpha_\infty F^N(z_\infty) \tag{48}$$

provided that z_∞ is chosen to be sufficiently large. A more accurate boundary condition $F^{N\prime}(z_\infty) = \hat{\alpha}_\infty F^N(z_\infty)$ may be obtained if a more accurate approximation $\hat{\alpha}_\infty$ is computed using

$$\alpha' + \alpha^2 + \mathcal{B}\alpha + \mathcal{A} - \mathcal{M} + 2E^* I_N = 0 \tag{49}$$

that defines function α. Exactly as in section 2, the more coefficients of the power series expansion of $\mathcal{A}$, $\mathcal{B}$ and $\mathcal{M}$ with respect to the non-positive powers of z are involved, the more coefficients in the power series expansion of $\alpha(z)$ may be computed.

Next, let us rewrite the odd and even problems in the form of

$$G' + \mathcal{P}(z, E^*) G = 0 \qquad z_1 \leqslant z \leqslant z_\infty \tag{50}$$

$$U_1^{\mathrm{liT}} G(z_1) = 0 \tag{51}$$

$$U_\infty^{\mathrm{rT}} G(z_\infty) = 0 \tag{52}$$

respectively, where

$$G = \begin{pmatrix} F^N \\ F^{N\prime} \end{pmatrix} \qquad \mathcal{P}(z, E^*) = \begin{pmatrix} 0_N & -I_N \\ \mathcal{A} - \mathcal{M} + 2E^* I_N & \mathcal{B} \end{pmatrix} \tag{53}$$

$z_1 = z_0$ when $n_3 = 0$, otherwise $z_1 = 0$, the Nth order zero matrix is denoted by 0_N and $i = \mathrm{e}, \mathrm{o}$. The index e belongs to even solution(s), the index o refers to the odd one(s) and

$$U_1^{\mathrm{le}} = \begin{pmatrix} 0_N \\ I_N \end{pmatrix} \qquad U_1^{\mathrm{lo}} = \begin{pmatrix} I_N \\ 0_N \end{pmatrix} \qquad U_\infty^{\mathrm{r}} = \begin{pmatrix} -\alpha_\infty^{\mathrm{T}} \\ I_N \end{pmatrix}. \tag{54}$$

It is reasonable to normalize the right boundary condition too, and thus $U_\infty^{\mathrm{rT}} = (-(\alpha_\infty^{\mathrm{T}}\alpha_\infty + I_N)^{-1/2}\alpha_\infty | (\alpha_\infty^{\mathrm{T}}\alpha_\infty + I_N)^{-1/2})$.

The classical theory of adjoint systems claims that if a vector function $G(z, E)$ is a solution of equation (50), then $U^{\mathrm{T}}(z, E)G(z, E) \equiv 0$ where $U(z, E) = V(z, E)W(z, E)$, $V(z, E)$ is a solution of problem $V' - P^{\mathrm{T}}(z, E)V = 0$, while $W(z, E)$ is arbitrary non-singular. In 1961, Abramov introduced a special choice of W providing the best U in the sense that the norm of U remained constant on the whole interval. There was no need either to compute the possibly unstable V or to find the proper W separately; the equation for U was derived directly.

The numerical problems of the type (50)–(52) are considered in a general setting in Abramov *et al* (1980). A consequence of (50)–(52) is that a vector function $G(z, E)$ is a solution if, for any $z \in [z_1, z_\infty]$, it satisfies the linear algebraic system

$$U^{li\mathrm{T}}(z)G(z, E) = 0 \qquad U^{\mathrm{rT}}(z)G(z, E) = 0 \tag{55}$$

where $(2N \times N)$ matrix functions $U^p(z)$, $p = \mathrm{l}i$, $i = \mathrm{o}, \mathrm{e}$ or $p = \mathrm{r}$ are the solutions of the initial value problems

$$U^{p\prime} - [I_{2N} - U^p(U^{p\mathrm{T}}U^p)^{-1}U^{p\mathrm{T}}]\mathcal{P}^{\mathrm{T}}U^p = 0 \tag{56}$$

with initial values

$$U^{\mathrm{l}i}(z_1) = U_1^{\mathrm{l}i} \qquad U^{\mathrm{r}}(z_\infty) = U_\infty^{\mathrm{r}} \tag{57}$$

respectively. In turn, $G(z, E)$ is a non-trivial solution, i.e. E is an eigenvalue if

$$\det \begin{pmatrix} U^{li\mathrm{T}}(z) \\ U^{\mathrm{rT}}(z) \end{pmatrix} = 0. \tag{58}$$

When $z = z_{\mathrm{c}}$ is fixed, then, the latter relationship is a non-linear algebraic equation with respect to the required eigenvalue. In order to find E_k^{*N} numerically, one has to solve a pair of problems (56), (57) for each guess E. The stability of the computations is ensured by the method of transfer (56) of the boundary condition, namely that

$$U^{p\mathrm{T}}(z)U^p(z) \equiv \text{constant} \tag{59}$$

holds. Due to normalization, the constant matrix on the right-hand side of (59) is I_N in each case.

When $N = 1$, the problem is a scalar, self-adjoint eigenvalue problem and one easily gets a rough estimate from below:

$$\mu_0(0)/2 < E_0^{*1} \tag{60}$$

and, obviously, $E_0^{*1} < E_1^{*1} < E_2^{*1} < \ldots$. In this case, equation (47) may undergo the Prüfer transformation and the sequence of eigenvalues may also be computed by the method described in section 2. Notice that the boundedness condition furnishing us with (48) provides an upper bound $\lim_{z\to\infty} \mu(z)/2$ for all E_k^{*N}. The method of section 2 reflects the number of zeros of the eigenfunctions when evaluating the eigenvalues, therefore the sequence $E_0^{*1} < E_1^{*1} < E_2^{*1} < \ldots$ with known lower and upper bounds may be computed without gaps.

5. Appraisal of numerical results

To obtain the energy eigenvalues E_k, the algorithm described in the previous sections was implemented by a FORTRAN program working on a SUN Sparc server 20. Some technical details about this program can be found in the appendix.

The numerical solution of (7) provided functions $\mu(z)$ at arbitrarily fixed values of the parameters ω, z and quantum numbers n and n_3. Some of them are shown in figure 1. All functions start at $z = 0$ from finite values and grow monotonically to $\mu_n^\infty = \lim_{z\to\infty} \mu_n(z)$. This behaviour follows from formula (26) where the right-hand side is, obviously, non-negative. When $n_3 = 0$ the functions $\mu_n(z)$ begin as a linear function of $|z|$ while for $n_3 \geqslant 1$ they behave as $\propto z^2$. Beyond this qualitative picture, the figure compares (in below panels) a few asymptotic analytical results (see Barcza 1996) to our results. The coincidence of the two types of treatments is demonstrated in both asymptotic ranges. Looking for polynomial radial eigenfunctions in a two-dimensional Schrödinger equation, Taut (1995) arrived at a problem that coincides with (7) at $z = 0$ and obtained values $\mu_n(0)$ analitically for certain pairs of ω and n. In these specific cases the results confirm each other. The eigenvalue μ as a function of ω at different and fixed values of z, $0 \leqslant z \ll 1$, $z \gg 1$ can be found in Barcza (1996). Our evaluations confirmed the behaviour stated there, and therefore we do not repeat these figures here.

Obviously, the evaluation of the coupling matrix elements plays an important role in the solution of (47). For some parameter sets, the functions $A_{nn'}(z)$ and $B_{nn'}(z)$ are shown in figure 2. The matrix elements $A_{nn'}$ at $n_3 = 0$ and $n \neq n'$ have logarithmic singularity at $z = 0$. This feature is a consequence of the choice of the basis; no singularity arises in any other combination of parameter values. Another remarkable property of the matrix elements $A_{nn'}(z)$, the monotonicity on the whole z–interval $(0, \infty)$ seems to hold, independently of the other parameters. The monotonicity appears for $B_{nn'}(z)$ as well. When $n_3 = 1$, the monotonicity disappears. With increasing $|n - n'|$ the off-diagonal elements of $A_{nn'}$, $B_{nn'}$ vanish more and more rapidly when z is increasing. Together with the fast decrease of $A_{nn'}$, $B_{nn'}$ for small and intermediate values of z, this phenomenon demonstrates that the system of equations (47) is coupled mostly by elements close to diagonal. This is a good omen for the numerical solutions. We may expect a high accuracy in E_k using a few channels, only. Figure 3 shows the coupling matrix elements for some n, n' and at $n_3 = 0, 1$ near the asymptotic ranges. Panels of the figures display the validity of the asymptotic expressions by Barcza (1996) and the series expansion (39).

Some of the results are selected and demonstrated in tables 1 and 2, illustrating the relevance of the basis and efficiency of the applied numerical method. We did not face any difficulties in computations when increasing the magnetic number n_3. We also got values not having been provided anywhere else, even in Ruder *et al* (1994). While Ruder *et al* (1994) gives the results up to 6–8 digits at a very high number of channels (12, in general), the coincidence in the first 3–5 digits (4–6 digits in E^*) appears even when we use a very limited number of channels, 1, 2 or 3 and a very low accuracy at each step of the computation. (We stopped the iteration at the final step when the relative accuracy achieved 10^{-6}.) Thus, we verified this expectation of Liu and Starace (1987) for the first time both for low and higher values of n_3 and for non-adiabatic approximation and by a different numerical method. When the number of channels N increases and the accuracy is kept as before, our values E_0^N seem to change in the next digits only, and the agreement with results by Ruder *et al* (1994) is not getting worse. Since the bases are chosen differently and therefore no common intermediate values exist for comparison. No exact final values are available either, thus no general statement can be formulated in favour of any of the

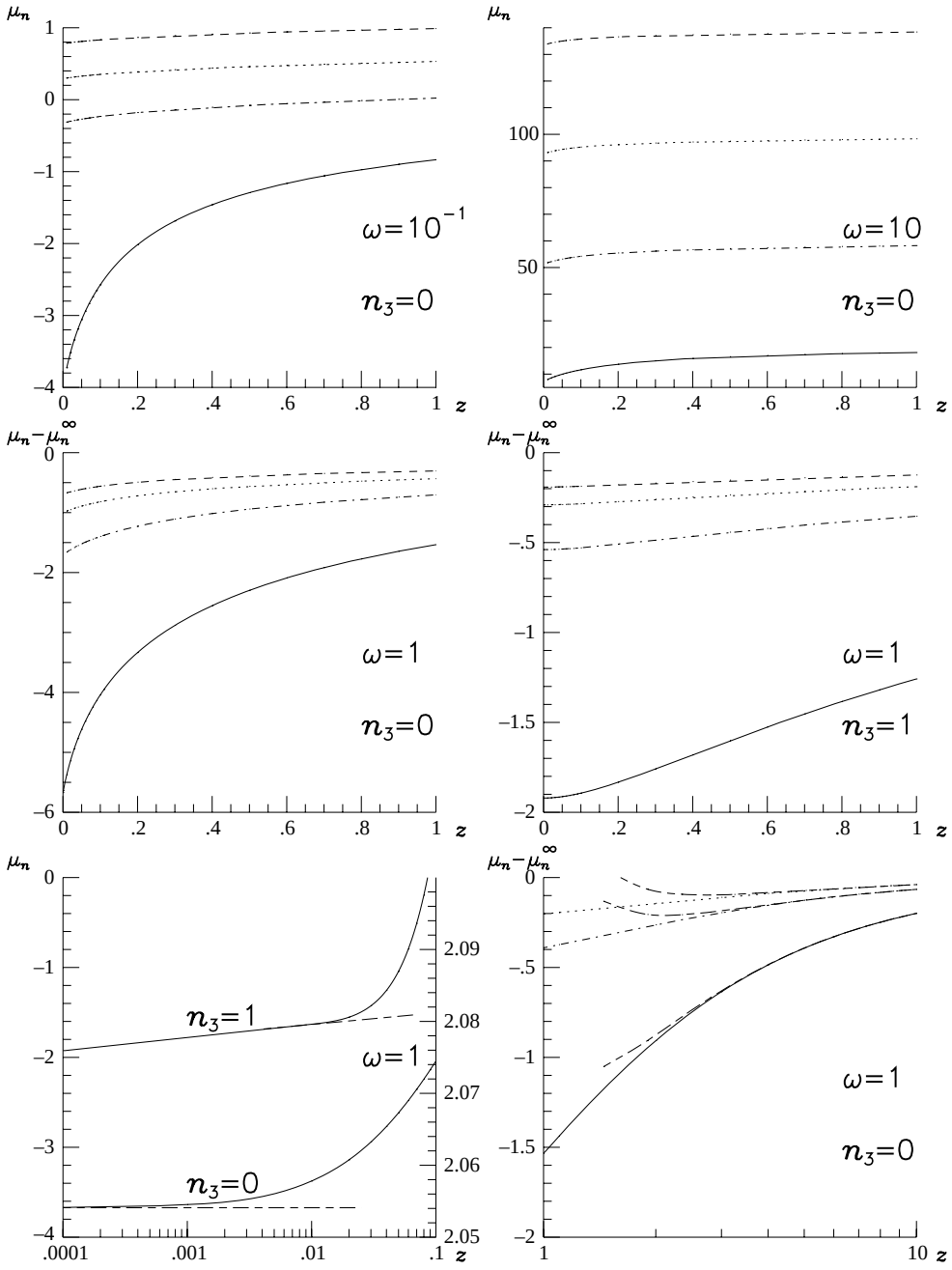

Figure 1. Eigenvalues μ_n of the basis equation (7) as a function of z for $\omega = 10^{-1}, 1, 10$, $n = 0, 1, 2, 3$. Full curves: $n = 0$, chain curves: $n = 1$, dotted curves: $n = 2$ and long-dash curves: $n = 3$. The short-dash–long-dash curves in the panels below are for showing the asymptotic behaviour of the computed eigenvalues in comparison with the asymptotic expansions in Barcza (1996). The right-hand side scale belongs to $n_3 = 1$. $\mu_n^\infty = 2\omega(2n + n_3 + 1)$.

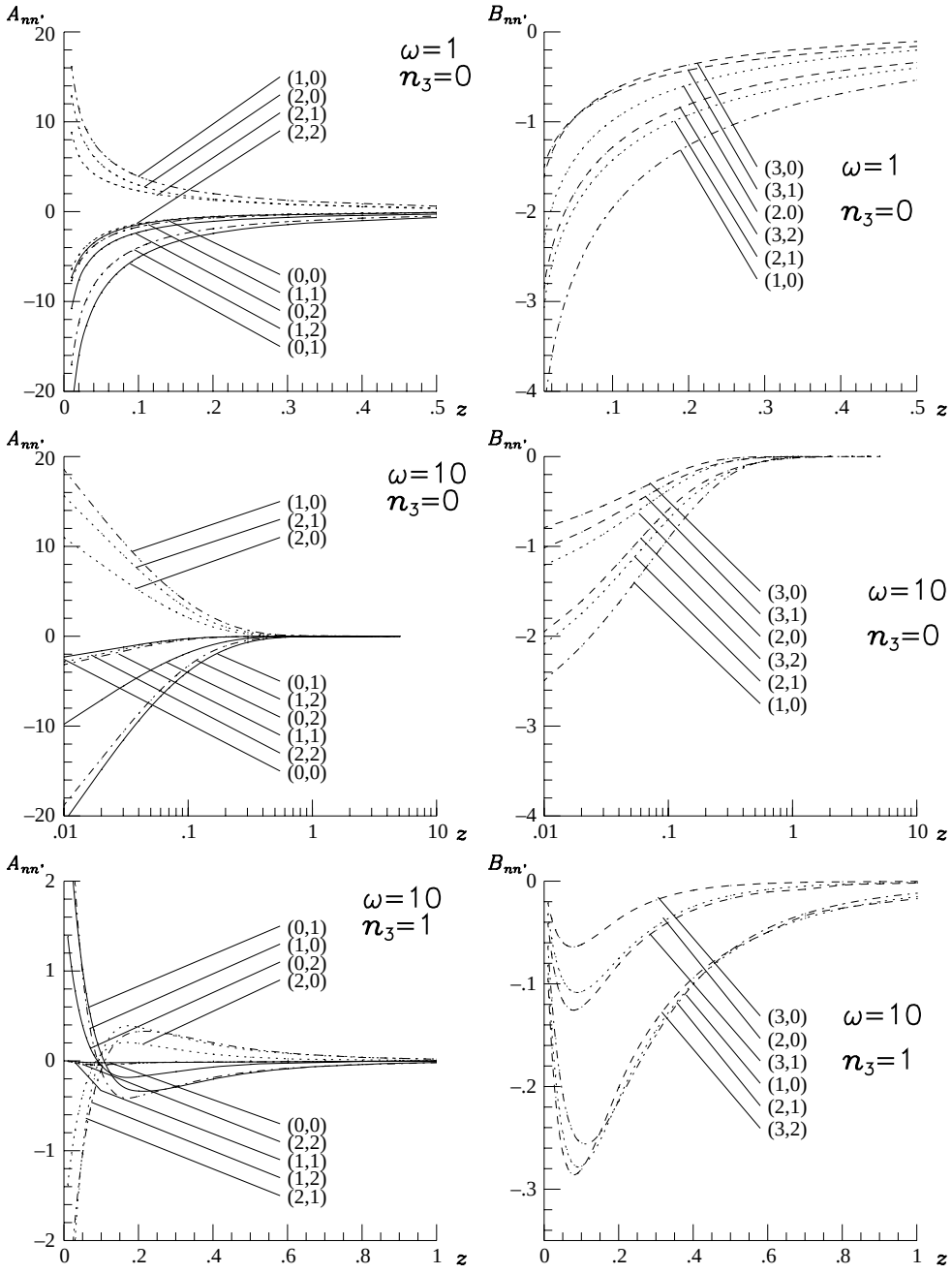

Figure 2. Coupling matrix elements $A_{nn'}$, $B_{nn'}$ as a function of z for $n_3 = 0, 1$. The line types indicate the first indices as in the figure 1. The assignments of labels are as (n, n'). The middle panels are scaled logarithmically in z.

compared final values. As far as we know, no computations have been carried out yet with the Liu–Starace basis using more than one channel, while we are able to do that. For the

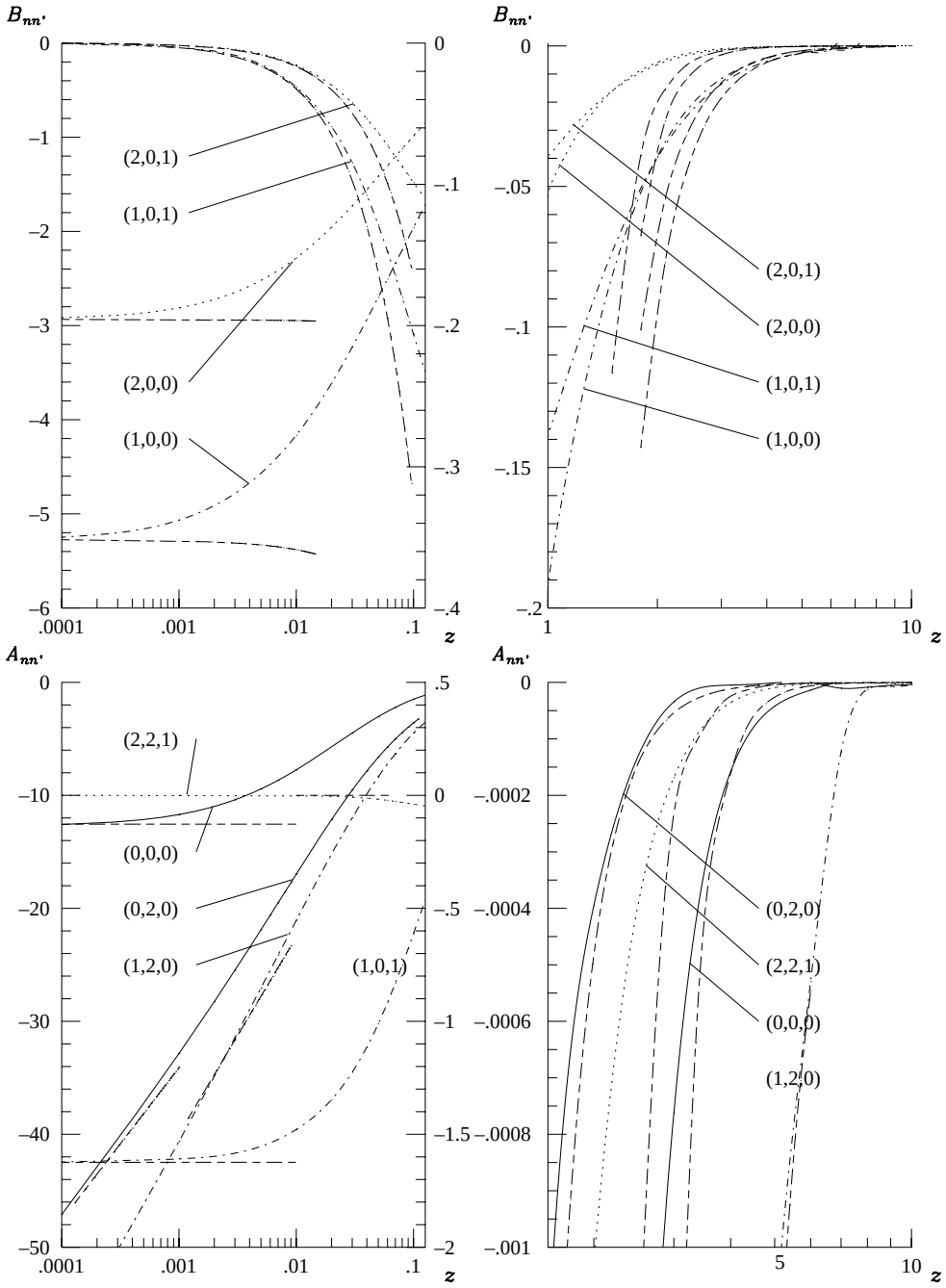

Figure 3. Asymptotic behaviour of the coupling matrix elements $A_{nn'}$, $B_{nn'}$ versus z. The labels refer to triple (n, n', n_3). The line types are the same as in figure 1, $\omega = 1$. The left and right axes belong to the parameter $n_3 = 0, 1$, respectively.

historical review of other approaches, their advantages and backdraws, we refer the reader to the latest survey by Ruder *et al* (1994).

Table 1. Energy eigenvalues E_k^N (in atomic units)[a] of the lowest state $k = 0$ of the H atom in a magnetic field with strength parameter ω when $\pi = +1$. The numbers in the brackets denote the number N of channels. The index R refers to the values taken from Ruder *et al* (1994). The uncertainty in the last digits are indicated by /.

$-n_3$	ω	$E_{0,\mathrm{R}}^N$	E_0^N
1	0.7	0.178 993 (13)	0.178 57 (3)
			0.178 69 (5)
	1	0.400 387 (15)	0.400 59 (2)
			0.400 55 (5)
			0.400 587 (7)
	10	8.5344/5 (12)	8.5329 (1)
			8.534 40 (3)
	15	13.2945/6 (12)	13.2930 (1)
			13.2944 (2)
	100	96.652 83/8 (12)	96.65278 (1)
2	1	0.528 828 (19)	0.528 67 (1)
			0.528 76 (3)
	10	8.806 36/7 (12)	8.806 17 (1)
			8.806 30 (2)
	100	97.197/8 (12)	97.19785 (1)
3	1	0.596 759 (21)	0.596 50 (1)
			0.596 71 (2)
	10	8.959 320/1 (12)	8.959 63 (1)
			8.959 30 (2)
	100	97.516 28/9 (12)	97.5164 (1)
4	1	0.640 649 (12)	0.640 51 (1)
			0.640 63 (2)
	10	9.061 413 (12)	9.061 39 (1)
			9.061 44 (2)
	100	97.733 63 (12)	97.7338 (1)
5	1	—	0.672 02 (1)
			0.672 10 (2)
	10	—	9.136 12 (1)
			9.136 20 (2)
	100	—	97.8958 (1)

[a] We recall that $\omega = 1$ if $|\boldsymbol{H}| = 4.7 \times 10^5$ T.

It is worth putting an accent again on the gain in the computational efficiency. It is achieved first because we do not evaluate the eigenfunctions of (3), instead of that, we directly obtain the coefficients of (5), i.e. the functions $\mu(z)$, $A_{nn'}(z)$ and $B_{nn'}(z)$. Neither are the vector-functions $F^N(z)$ belonging to the iteration steps computed when the eigenvalues E_k^N are defined by iteration as described in the previous sections. Secondly, all intermediate evaluations in the definition of the eigenvalues E_k^N consist of the solution of initial value problems which are stable and have smooth solutions. This allows us to use both simple methods for the numerical integration of these equations and large integration steps.

6. Conclusions

The numerical investigations of the Liu–Starace basis were presented in this work. We determined the eigenvalues $\mu_n(z)$ of the basis equation (7) on the whole z-interval $[0, \infty)$ without computing eigenfunctions by solving a first order differential equation only. This is a profound simplification compared to the generally accepted view when treating equations

Table 2. Energy eigenvalues E_k^N (in atomic units) of the lowest state $k = 0$ of H atom in magnetic field with strength parameter ω when $\pi = -1$. Designations are the same as in table 1.

$-n_3$	ω	$E_{0,\mathrm{R}}^N$	E_0^N
1	1	0.754 75 (12)	0.754 759 (1)
	10	9.623 880 (12)	9.623 80 (1)
	100	99.538 178 (12)	99.5388 (1)
2	1	0.782 545 (12)	0.782 545 7 (1)
	10	9.647 807 (12)	9.647 81 (1)
	100	99.549 420 (11)	99.5495 (1)
3	1	0.800 862 (12)	0.801 86 (1)
	10	9.665 419 (12)	9.665 42 (1)
	100	99.558 673 (9)	99.5589 (1)
4	1	—	0.814 45 (1)
	10	—	9.679 39 (1)
	100	—	99.5669 (1)

similar to (7). The usual procedure is to solve a second order differential equation which leads simultaneously to the eigenvalue and eigenfunction. In this manner we saved much computing time. We showed that the numerical treatment is in keeping with the asymptotic one in both relevant domains. We reduced the computation of coupling matrix elements $A_{nn'}(z)$, $B_{nn'}(z)$ to determining the values of some quadratic functionals. Each functional was computed in an efficient and stable way by solving ordinary differential equations. The results of the numerical computations and the asymptotic expansions fit well where the latter is valid. It is not true only in the case of $A_{nn'}(z)$ if $n_3 = 0$, $n \neq n'$ and $z \to 0$. Here the series expansion (39) converges slowly. Lastly, we completed our report by showing a method for obtaining the eigenvalues of coupling equations (47) analogous to that used for the basis equation (7). Both methods are based upon the same factorization where the functions satisfy relations $U^{\mathrm{T}}U' = 0$, $U^{\mathrm{T}}U = I$ at each point. It corresponds to a continuous orthogonalization. We note that, based on the theoretical results in Konyukhova and Pak (1987), the above method may also be modified for being suitable for computations at large values of ω. The problem is, however, beyond the scope of this paper.

The Liu–Starace basis that was chosen naturally allows us to compute the energy levels of a hydrogen-like ion in a strong magnetic field more efficiently than it was done by bases of other types. Accordingly, we can evaluate higher excited states than were available before. Moreover, we might get a chance to map some resonances in the continuum.

Our main purpose with the present work was the exact mathematical establishment of the numerical solution of the problem as it was posed in the introduction. We remark that, for small ω, the oblate spheroidal system of coordinates with a similar expansion of the eigenfunction is more relevant (see Barcza 1994), while for larger values of ω, this setting fits well. For evaluating the energy levels of hydrogen atom in strong magnetic fields, we gave an almost complete set of mathematical tools and with its help, we carried out a number of computations.

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Appendix

To solve equations (56) a hierarchically organized FORTRAN program was developed. At the lowest level of the program, the fourth order Runge–Kutta (R–K) algorithm with an adaptive stepsize control due to Press *et al* (1992) is plugged in. It integrates (16) twice in each step with initial conditions (18) and (19), respectively. The value ϱ_0 was chosen equal to $z \times 10^{-4}$. For approximation of $\gamma(\varrho_0)$, a truncated sum of (10) was taken. Due to the fast convergence the accuracy became suitable when the consequent sums differed less than by 10^{-3}. The value ϱ_∞ cannot be fixed similarly since (13) is an asymptotic expression only. A numerical procedure was used for simultaneous choise of ϱ_∞ and truncation. For both cases, exact error estimates are available, see Abramov and Balla (1993) and Balla (1977). The intermediate point ϱ_c was set equal to z except in the case $z = 0$ where $\varrho_c = 1$ was taken. The routine on the next level determined μ_n by a simple bisection method as indicated in section 2. It was stopped when either the relative accuracy reached that of the machine one in μ_n i.e. $|(\mu_n^{(i-2)} - \mu_n^{(i-1)})/\mu_n^{(i)}| \leqslant 10^{-15}$ or the relative error $|[\Theta_l(\varrho_c) - \Theta_r(\varrho_c)]/\Theta_l(\varrho_c)|$ became less than 10^{-12}. The upper indices in the previous formula denote the number of iterations. The coupling matrix elements were computed as has been described in section 3 by simultaneous integration of equations (16), (21) and (35). Again, the above R–K algorithm was used for numerical integration.

When computing E_k^N for a fixed k and N, both the value of the determinant and the relative deviation of E_k^N in the consequent iterations were checked. For evaluation of the components building up the determinant we integrated equation (56). The basic integration routine was as above. To approximate the identity (59), we checked its defect at M equidistant points $z_i = z_0 + (z_\infty - z_0)i/M$ where $M = 8$ was chosen. Aiming at a global error ε, on each subinterval $[z_i, z_{i+1}]$ the local error $\varepsilon_{loc} = \varepsilon/M$ was allowed and inequality

$$\sum_{i,j}(U^T U - I)_{i,j}^2 < \varepsilon_{loc} \tag{A1}$$

was controlled. On the subintervals the starting stepsize was chosen to be $s = (z_{i+1} - z_i)/M_0$. $M_0 = 8$ was set on the first subinterval. If the condition did not hold, then the algorithm returned to the left end of the subinterval and M_0 was doubled. Otherwise, either the stepsize was kept for the next subinterval or it was doubled, provided it had been accepted at least once before. This stepper method allowed us to compute all necessary quantities $(\mu_n, A_{nn'}, B_{nn'})$ at a fixed z no more than once and to store them in a linked list structure.

During the integration of coupled equations (56), the inverse of the matrices $U^T U$ was needed at each z. Since these matrices are symmetrical and close to the identity matrix, the most efficient method, that is, the Cholesky decomposition (see e.g. Press *et al* 1992) was used. For finding the determinant in (58), an LU decomposition was used. As we said before the relative accuracy of the eigenvalue was one of the checkpoints. If $|(E_k^{(i-1)} - E_k^{(i)})/E_k^{(i)}| \leqslant 10^{-6}$, the process was stopped and $E_k^{(i)}$ was accepted as a starting value for the computation at a larger number N of channels or for a more excited level in the spectrum. It is remarkable that these two types of iterations are practically independent, so the processes could have been parallelized. When $n_3 \neq 0$, we always choose $z_0 = 0$, otherwise $z_0 = 10^{-3}$. The largest right end was $z_\infty = 10$ while the intermediate point z_c was always close to z_0 and depended on the length of the z-interval.

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