An alternative method for computing dipole strengths

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Abstract. In this paper we complete the mathematical approach that aimed at computation of energy levels of bounded states for hydrogen atom in strong magnetic fields previously. By this accomplishment, we are allowed to compute any bound–bound dipole strengthfor hydrogen atom in strong magnetic field. In our method we obtain the values of these quadratic functionals directly. We derive initial value problems for some first order ordinary differential equations, their solutions provide to us the required values. Proceeding this way, we avoid both the computation of eigenfunctions and the cumbersome numerical integration of their compositions. The stability of our computations can be proven. In opposite to the traditional way, the accuracy of dipole strengths may be controlled directly.

1. Introduction

Atomic data like transition probabilities and oscillator strengths of hydrogen atom in strong magnetic field are necessary for modelling the spectra of magnetized white dwarf or neutron stars. When computing synthetic spectra we have to be aware of the strength of the lines. For allowed transitions the determination of the required oscillator strengths and transition probabilities is based on the evaluation of the dipole matrix elements. In the case of a one–electron system, $|\mathbf{p}_{nm}|^2$ is the squared Euclidean norm (the sum of the squared components) of vector

$$\mathbf{p}_{nm} := \int \Psi^*(E_n)\Psi(E_m)\mathbf{r}\mathrm{d}V \tag{1}$$

where Ψ–s are the eigenfunctions of the atomic system belonging to the eigenvalues E_m and E_n, respectively, $*$ denotes the complex conjugate. The volume integral is taken over the whole space. The eigenfunctions are assumed to be orthonormalized by

$$\int \Psi^*(E_n)\Psi(E_m)\mathrm{d}V = \delta_{nm}. \tag{2}$$

Expression (1) is used generally and it includes a number of considerations concerning the atom and its interactions with the electromagnetic field. For details see e.g. Schiff (1968). There are other formulae equivalent to (1) as it was described in the classical review by Bethe and Salpeter (1957).

Traditionally, when computing $|\mathbf{p}_{nm}|^2$ for a pair of indices (n, m), the first step is the numerical solution of the time-independent Schrödinger problem twice, providing in each turn an eigenvalue E and the corresponding eigenfunction $\Psi(E)$ simultaneously. Next, the value of the nonvanishing components of $\mathbf{p}_{nm}$ in (1) is obtained by numerical integration. Far from the center the eigenfunctions become inaccurate in a lot of methods. The weight function $\mathbf{r}$ in (1) amplifies the inaccuracy. An other source of errors is the numerical integration algorithm itself. As a result, there is no practical way to estimate the quality of numerical values for $\mathbf{p}_{nm}$.

For the diamagnetic Coulomb problem (hidrogen atom in strong, homogeneous magnetic field) we have elaborated an alternative method for determining the nonvanishing components of $\mathbf{p}_{nm}$. It seems to work in a wider class of non-separable cases (see Barcza 1994), as well.

2. The general description of the method

Provided the cylindrical coordinates ρ, z and the azimuthal angle φ around the axis z are introduced, one obtains the coordinates p_x, p_y, p_z of vector $\mathbf{p}_{nm}$ as follows (subscripts m, n are omitted):

$$\begin{aligned} p_x &= \int_{-\infty}^{\infty}\int_{0}^{\infty}\int_{0}^{2\pi} \Psi^*(E_n)\Psi(E_m)\rho^2\cos\varphi \mathrm{d}\varphi\mathrm{d}\rho\mathrm{d}z \\ p_y &= \int_{-\infty}^{\infty}\int_{0}^{\infty}\int_{0}^{2\pi} \Psi^*(E_n)\Psi(E_m)\rho^2\sin\varphi \mathrm{d}\varphi\mathrm{d}\rho\mathrm{d}z \\ p_z &= \int_{-\infty}^{\infty}\int_{0}^{\infty}\int_{0}^{2\pi} \Psi^*(E_n)\Psi(E_m)\rho z \mathrm{d}\varphi\mathrm{d}\rho\mathrm{d}z \end{aligned} \tag{3}$$

The orthonormalization condition (2) rewrites as

$$\int_{-\infty}^{\infty}\int_{0}^{\infty}\int_{0}^{2\pi} \Psi^*(E_n)\Psi(E_m)\rho \mathrm{d}\varphi\mathrm{d}\rho\mathrm{d}z = \delta_{nm}. \tag{4}$$

On the other hand, the assumption that the magnetic field $\mathbf{H}$ is parallel to axis z yields the separation of the azimuthal angle in the eigenfunction:

$$\Psi(E_n;\rho,z,\varphi) = (2\pi)^{-1/2}\exp(\mathrm{i}n_3^n\varphi)\psi(E_n;z,\rho) \tag{5}$$

where $n_3 = 0, \pm1, \pm2, \ldots$ is the magnetic quantum number, i is the imaginary unit. We used atomic units ($m_\mathrm{e} = e = \hbar = 1$) and inroduced the Larmor frequency $\omega = e|\mathbf{H}|/2m_\mathrm{e}c$. Substituting (5) into (3), one observes that depending on the value of

$$\Delta n_3 \stackrel{def}{=} n_3(\Psi(E_m)) - n_3(\Psi(E_n)) = n_3^m - n_3^n \tag{6}$$

the vectors $\mathbf{p_{nm}}$ differ qualitatively. Namely, when $\Delta n_3 = 0$ then $p_x = p_y = 0$ and

$$p_z = \int_{-\infty}^{\infty}\int_{0}^{\infty} \psi(E_n)\psi(E_m)\rho z \mathrm{d}\rho\mathrm{d}z. \tag{7}$$

(Arguments ρ, z in ψ are omitted.) When $\Delta n_3 = \pm 1$ then $p_z = 0$ and

$$p_x = \frac{1}{2}\int_{-\infty}^{\infty}\int_{0}^{\infty} \psi(E_n)\psi(E_m)\rho^2 \mathrm{d}\rho\mathrm{d}z \quad p_y = \pm\frac{\mathrm{i}}{2}\int_{-\infty}^{\infty}\int_{0}^{\infty} \psi(E_n)\psi(E_m)\rho^2 \mathrm{d}\rho\mathrm{d}z. \tag{8}$$

The latter value is not needed for $|\mathbf{p}_{nm}|^2$. When $|\Delta n_3| > 1$, then $p_z = p_x = p_y = 0$. Thus, in each case, the nonvanishing components lead to integrals of the form

$$I_s^{nm} = \int_{-\infty}^{\infty}\int_{0}^{\infty} \psi(E_n)\psi(E_m)s(\rho,z)\mathrm{d}\rho\mathrm{d}z \tag{9}$$

$$\text{where} \quad s(\rho,z) = \begin{cases} \rho z & \text{when} \quad \Delta n_3 = 0 \\ \rho^2 & \text{when} \quad \Delta n_3 = \pm 1. \end{cases} \tag{10}$$

Let us take parity into consideration. Since $\psi(E)$ is either odd or even with respect to z and so is s, one arrives at

$$I_s^{nm} = \begin{cases} 2\int_0^\infty\int_0^\infty \psi(E_n)\psi(E_m)\rho z \mathrm{d}\rho\mathrm{d}z, & \text{if} \quad \Delta n_3 = 0 \text{ and } \pi_{\mathrm{z}}^n \neq \pi_{\mathrm{z}}^m, \\ 2\int_0^\infty\int_0^\infty \psi(E_n)\psi(E_m)\rho^2 \mathrm{d}\rho\mathrm{d}z, & \text{if} \quad \Delta n_3 = \pm 1 \text{ and } \pi_{\mathrm{z}}^n = \pi_{\mathrm{z}}^m, \\ 0 & \text{otherwise,} \end{cases} \tag{11}$$

where π_{z}^n, π_{z}^m denote the z-parity of ψ_n, ψ_m, respectively. The normalization condition (4) yields also an integral of the form (9) with $n = m$, $s(\rho, z) = \rho$, since one has

$$\int_0^\infty\int_0^\infty \psi^2(E_n)\rho\mathrm{d}\rho\mathrm{d}z = \frac{1}{2}. \tag{12}$$

In order to simplify and unify the description of the method, above indicating the eigenvalues E_m or E_n in the notation of functions derived from the eigenfunctions ψ, we later indicate additionally their parities in superscripts when it seems necessary.

We adopt the framework of Balla and Benkő (1996) (hereafter BB96) and define $\psi(E_m)$ as

$$\psi(E_n) = \sum_{k=0}^{\infty} f_k^n(z)\hat{\Phi}_k^n(z,\rho) \tag{13}$$

where $\hat{\Phi}_0^n(z,\rho), \hat{\Phi}_1^n,(z,\rho),\ldots$ form the Liu-Starace basis belonging to eigenvalues $\mu_0^n(z), \mu_1^n(z),\ldots$ (see BB96, Barcza 1996, Liu and Starace 1987) and orthonormalized with respect to ρ by

$$\int_0^\infty \hat{\Phi}_k^n(z,\rho)\hat{\Phi}_l^n(z,\rho)\rho\mathrm{d}\rho \equiv \delta_{kl} \tag{14}$$

uniformly with respect to z, while E^{*n}, $f_0^n(z)$, $f_1^n(z),\ldots$ solve the eigenproblem

$$\frac{\mathrm{d}^2 f_k}{\mathrm{d}z^2} + [2E^* - \mu_k^n(z)]f_k + \sum_{k'=0}^{\infty}[A_{kk'}^n(z)f_{k'} + B_{kk'}^n(z)\frac{\mathrm{d}f_{k'}}{\mathrm{d}z}] = 0, \tag{15}$$
$$-\infty < z < \infty, \quad k = 0,1,2,\ldots,$$

with

$$A^n_{kk'}(z) = (\hat{\Phi}^n_k, \frac{\partial^2 \hat{\Phi}^n_{k'}}{\partial z^2}), \quad B^n_{kk'}(z) = 2(\hat{\Phi}^n_k, \frac{\partial \hat{\Phi}^n_{k'}}{\partial z}), \quad E^* = E - \omega n^n_3. \tag{16}$$

Due to normalizations (12) and (14),

$$\int_0^\infty \sum_{k=0}^{\infty} [f^n_k(z)]^2 \mathrm{d}z = \frac{1}{2} \tag{17}$$

holds. In BB96 we proposed a method for computation of $\{\mu^n_k(z)\}^\infty_{k=0}$, $\{A^n_{kk'}(z)\}^\infty_{k,k'=0}$ and $\{B^n_{kk'}(z)\}^\infty_{k,k'=0}$ which did not require the computation of the Liu-Starace basis $\{\hat{\Phi}^n_k(z)\}^\infty_{k=0}$ itself. Next, instead of (15) we considered the truncated eigenvalue problem

$$\frac{\mathrm{d}^2 F^N}{\mathrm{d}z^2} + \mathcal{B}_N(z)\frac{\mathrm{d}F^N}{\mathrm{d}z} + [\mathcal{A}_N(z) - \mathcal{M}_N(z)]F^N = -2E^{*N}F^N, \qquad 0 < z < \infty, \tag{18}$$

with respect to eigenvalue(s) E^{*N} and eigenfunction(s) $F^N(z) = (f^N_0(z), \ldots, f^N_{N-1}(z))^T$ where $f^N_k(z)$ are approximations to $f_k(z)$ of (15), T denotes the transposition. Here the entries of the skew-symmetrical matrix $\mathcal{B}_N(z)$ were approximations to $B^n_{kk'}(z)$, $k, k' = 0, \ldots, N-1$, while the entries of $\mathcal{A}_N(z)$ approximated $A^n_{kk'}(z)$, $k, k' = 0, \ldots, N-1$. The matrix $\mathcal{M}_N(z)$ was diagonal, $\mathcal{M}_N(z) = \mathrm{diag}[\mu^n_0(z), \ldots, \mu^n_{N-1}(z)]$, containing again numerical approximations. Note that in fact $\mathcal{A}_N(z), \mathcal{B}_N(z), \mathcal{M}_N(z)$ depended only on n^n_3 since so did $\{\hat{\Phi}^n_k(\rho, z)\}^\infty_{k=0}$.

In BB96 we also elaborated and described a method providing us with the approximate eigenvalues E^{*nN} without evaluating $F^{nN}(z)$. In order to proceed further and to get (9) with (12) when (13) is kept, we use the following splitting.

$$s(\rho, z) = \rho s_1(\rho) s_2(z) \tag{19}$$

$$s_1(\rho) = s^{(1)}_1(\rho) \equiv 1 \quad \text{or} \quad s_1(\rho) = s^{(2)}_1(\rho) = \rho \tag{20}$$

$$s_2(z) = s^{(1)}_2(z) \equiv 1 \quad \text{or} \quad s_2(z) = s^{(2)}_2(z) = z. \tag{21}$$

Next, let

$$K^{nmi}_{pq}(z) = \int_0^\infty \hat{\Phi}^n_p(\rho, z)\hat{\Phi}^m_q(\rho, z)\rho s^{(i)}_1(\rho)\mathrm{d}\rho \quad i = 1, 2. \tag{22}$$

Having $K^{nmi}_{pq}(z)$, (9) turns into

$$I^{nm}_s = 2\sum_{k=0}^{\infty}\sum_{l=0}^{\infty} \mathcal{F}^{nmij}_{kl} \tag{23}$$

where

$$\mathcal{F}^{nmij}_{kl} = \int_0^\infty f^n_k(z) f^m_l(z) s^{(j)}_2(z) K^{nmi}_{kl}(z)\mathrm{d}z \quad j = 1, 2. \tag{24}$$

With this notations, (12) rewrites as

$$2\sum_{k=0}^{\infty} \mathcal{F}^{nn11}_{kk} = 1. \tag{25}$$

(22) is an integral similar to the one we have computed in BB96. Moreover, due to the normalization of Liu-Starace basis, $K_{pq}^{nm1}(z) \equiv \delta_{pq}$ if $\Delta n_3 = 0$. In the Appendix we update the formula and the equations for obtaining $K_{pq}^{nmi}(z)$ for other values of the indices. For getting sufficiently accurate results, the number of channels may be different, this number is denoted by N when belongs to n and by M for m. When N and M have been fixed, formulae (17), (23) and (24) yield approximations

$$1 = 2\int_0^\infty F^{N\mathrm{T}}(z)F^N(z)\mathrm{d}z = 2\int_0^\infty F^{N\mathrm{T}}(z)\mathcal{K}^{nn11}(z)F^N(z)\mathrm{d}z \tag{26}$$

$$I_s^{nm} = 2\int_0^\infty F^{N\mathrm{T}}(z)\mathcal{K}^{nmij}(z)F^M(z)\mathrm{d}z \tag{27}$$

where $\mathcal{K}^{nmij}(z)$ is a matrix with entries $(\mathcal{K}^{nmij}(z))_{kl} = s_2^{(j)}(z)K_{kl}^{nmi}(z)$, $k = 0, \ldots, N-1$, $l = 0, \ldots, M-1$. Thus, (27) is a quadratic functional and it may seem similar to (22). Application of ideas borrowed from Abramov *et al* (1980), Birger (1968) to the computation of $\mathcal{K}_{pq}^{nmi}(z)$, however, is worth for adjoint problems, only. In (24), however, $\{f_k^n(z)\}_{k=0}^\infty$ and $\{f_k^m(z)\}_{k=0}^\infty$ comes from the non-selfadjoint problem (15). Neither is its approximation (18) selfadjoint. Another version of differential factorization due to Bakhvalov (1973), however, admits extension to the evaluation of quadratic functionals of eigenfunctions of non-selfadjoint problems. Without going into the arguments leading to the differential factorization, we recall first the basic steps of Bakhvalov factorization in terms of the first order system

$$G^{N\prime} + \mathcal{P}_N(z, E^*)G^N = 0, \quad z_1 \le z \le z_\infty, \tag{28}$$

derived from (18) by introducing

$$G^N = \begin{pmatrix} F^N \\ F^{N\prime} \end{pmatrix}, \quad \mathcal{P}_N(z, E^*) = \begin{pmatrix} 0_N & -I_N \\ \mathcal{A}_N - \mathcal{M}_N + 2E^*I_N & \mathcal{B}_N \end{pmatrix}. \tag{29}$$

Here z_1 is small for $n_3 = 0$, otherwise $z_1 = 0$ and z_∞ is a large value. The left(=l) and right(=r) boundary conditions for $G(z)$ at z_1 and z_∞

$$U^{\mathrm{l}\pi_\mathrm{z}\mathrm{T}}G(z_1) = 0 \tag{30}$$

and

$$U^{\mathrm{r}\mathrm{T}}G(z_\infty) = 0, \tag{31}$$

where the z parity π_z is equal e(=even) or o(=odd),

$$U^{\mathrm{le}}(z_1) = \begin{pmatrix} 0_N \\ I_N \end{pmatrix}, \quad U^{\mathrm{lo}}(z_1) = \begin{pmatrix} I_N \\ 0_N \end{pmatrix}, \quad U^{\mathrm{r}}(z_\infty) = \begin{pmatrix} -\alpha_\infty^{\mathrm{T}} \\ I_N \end{pmatrix}, \tag{32}$$

0_N and I_N are quadratic zero and unit matrices and $\alpha_\infty = (\mathcal{M}_{\infty N} - 2E^*I_N)^{\frac{1}{2}}$. Now, we assume that the solutions of (28) satisfying (30) and (31), respectively, are represented as

$$G^{\mathrm{l}\pi_\mathrm{z}}(z) = Y^{\mathrm{l}\pi_\mathrm{z}}(z)\mathbf{c}^{\mathrm{l}\pi_\mathrm{z}}(z), \qquad G^{\mathrm{r}}(z) = Y^{\mathrm{r}}(z)\mathbf{c}^{\mathrm{r}}(z), \tag{33}$$

where

$$\frac{\mathrm{d}Y^{\mathrm{l}\pi_{\mathrm{z}}}}{\mathrm{d}z} + [I_{2N} - Y^{\mathrm{l}\pi_{\mathrm{z}}}(Y^{\mathrm{l}\pi_{\mathrm{z}}\mathrm{T}}Y^{\mathrm{l}\pi_{\mathrm{z}}})^{-1}Y^{\mathrm{l}\pi_{\mathrm{z}}\mathrm{T}}]\mathcal{P}Y^{\mathrm{l}\pi_{\mathrm{z}}} = 0 \tag{34}$$

with

$$Y^{\mathrm{lo}}(z_1) = \begin{pmatrix} 0_N \\ I_N \end{pmatrix}, \quad Y^{\mathrm{le}}(z_1) = \begin{pmatrix} I_N \\ 0_N \end{pmatrix}. \tag{35}$$

Equation for $Y^{\mathrm{r}}(z)$ is the same, but the initial value is

$$Y^{\mathrm{r}}(z_\infty) = \begin{pmatrix} (\alpha_\infty^{\mathrm{T}}\alpha_\infty + I_N)^{-1/2} \\ \alpha_\infty(\alpha_\infty^{\mathrm{T}}\alpha_\infty + I_N)^{-1/2} \end{pmatrix}, \tag{36}$$

while

$$\frac{\mathrm{d}\mathbf{c}}{\mathrm{d}z} - (Y^{\mathrm{T}}Y)^{-1}Y^{\mathrm{T}}\mathcal{P}Y\mathbf{c} = 0 \quad \text{for indices } \mathrm{l}\pi_{\mathrm{z}} \text{ and } \mathrm{r}. \tag{37}$$

In the latter formulae (28)–(37) we omitted the index $m(n)$.

We extend the method to the computation of the functionals using the normalization as follows. (26) rewrites as

$$\int_0^\infty G^{N\mathrm{T}}(z)\tilde{\mathcal{K}}^{nn11}(z)G^N(z)\mathrm{d}z = \frac{1}{2}, \tag{38}$$

where

$$\tilde{\mathcal{K}}^{nn11} = \begin{pmatrix} \mathcal{K}^{nn11} & 0_N \\ 0_N & 0_N \end{pmatrix} = \begin{pmatrix} I_N & 0_N \\ 0_N & 0_N \end{pmatrix}. \tag{39}$$

Let the right-hand side be decomposed into a sum $\int_{z_1}^{z_\infty} = \int_{z_1}^{z} + \int_{z}^{z_\infty}$ and the matrices $H^{N\mathrm{l}\pi_{\mathrm{z}}}(z)$, $H^{N\mathrm{r}}(z)$ and the vectors $\mathbf{c}^{N\mathrm{l}\pi_{\mathrm{z}}}$, $\mathbf{c}^{N\mathrm{r}}$ be defined by

$$\begin{aligned} &\int_{z_1}^{z} G^{N\mathrm{T}}(\zeta)\tilde{\mathcal{K}}^{nn11}(\zeta)G^N(\zeta)\mathrm{d}\zeta = \mathbf{c}^{N\mathrm{l}\pi_{\mathrm{z}}\mathrm{T}}(z)H^{N\mathrm{l}\pi_{\mathrm{z}}}(z)\mathbf{c}^{N\mathrm{l}\pi_{\mathrm{z}}}(z), \\ &\int_{z}^{z_\infty} G^{N\mathrm{T}}(\zeta)\tilde{\mathcal{K}}^{nn11}(\zeta)G^N(\zeta)\mathrm{d}\zeta = -\mathbf{c}^{N\mathrm{r}\mathrm{T}}(z)H^{N\mathrm{r}}(z)\mathbf{c}^{N\mathrm{r}}(z). \end{aligned} \tag{40}$$

Then, discarding N,

$$\begin{aligned} &\frac{\mathrm{d}H^w}{\mathrm{d}z} - H^w(Y^{w\mathrm{T}}Y^w)^{-1}Y^{w\mathrm{T}}\mathcal{P}Y^w - Y^{w\mathrm{T}}\mathcal{P}^{\mathrm{T}}Y^w(Y^{w\mathrm{T}}Y^w)^{-1}H^w - Y^{w\mathrm{T}}\tilde{\mathcal{K}}^{nn11}Y^w = 0, \\ &H^{\mathrm{l}\pi_{\mathrm{z}}}(z_1) = 0_N \quad H^{\mathrm{r}}(z_\infty) = 0_N \qquad w = \mathrm{l}\pi_{\mathrm{z}}, \mathrm{r}. \end{aligned} \tag{41}$$

Due to normalization the identity

$$\mathbf{c}^{\mathrm{l}\mathrm{T}}(z_{\mathrm{c}})H^{\mathrm{l}}(z_{\mathrm{c}})\mathbf{c}^{\mathrm{l}}(z_{\mathrm{c}}) - \mathbf{c}^{\mathrm{r}\mathrm{T}}(z_{\mathrm{c}})H^{\mathrm{r}}(z_{\mathrm{c}})\mathbf{c}^{\mathrm{r}}(z_{\mathrm{c}}) = \frac{1}{2}, \tag{42}$$

holds for arbitrary but fixed point z_{c}, $z_1 \le z_{\mathrm{c}} < z_\infty$. For obtaining $\mathbf{c}^{\mathrm{l}\pi_{\mathrm{z}}}(z_{\mathrm{c}})$ and $\mathbf{c}^{\mathrm{r}}(z_{\mathrm{c}})$ we can use (42) and the continuity condition

$$Y^{\mathrm{l}\pi_{\mathrm{z}}}(z_{\mathrm{c}})\mathbf{c}^{\mathrm{l}\pi_{\mathrm{z}}}(z_{\mathrm{c}}) - Y^{\mathrm{r}}(z_{\mathrm{c}})\mathbf{c}^{\mathrm{r}}(z_{\mathrm{c}}) = 0 \tag{43}$$

noting that by equation (34), one has $Y^{\mathrm{T}}Y \equiv I_N$ (for all indicies not indicated here). Then, $\mathbf{c}^{\mathrm{l}\pi_z}(z_c) = a\mathbf{v}_1$, $\mathbf{c}^{\mathrm{r}}(z_c) = a\mathbf{v}_2$, where $\mathbf{v}_1$ is an arbitrary solution of

$$(Y^{\mathrm{l}\pi_z\mathrm{T}}(z_c)Y^{\mathrm{r}}(z_c)Y^{\mathrm{r}\mathrm{T}}(z_c)Y^{\mathrm{l}\pi_z}(z_c) - I_N)\mathbf{v}_1 = 0, \tag{44}$$

$$\mathbf{v}_2 = Y^{\mathrm{r}\mathrm{T}}(z_c)Y^{\mathrm{l}i}(z_c)\mathbf{v}_1, \quad a = (\mathbf{v}_1^{\mathrm{T}}H^{\mathrm{l}\pi_z}(z_c)\mathbf{v}_1 - \mathbf{v}_2^{\mathrm{T}}H^{\mathrm{r}}(z_c)\mathbf{v}_2)^{-\frac{1}{2}}. \tag{45}$$

Finally, let $I_s^{nm} = \int_{z_1}^{z} + \int_{z}^{z_\infty}$ and let

$$\begin{aligned}
&\int_{z_1}^{z} G^{N\mathrm{T}}(\zeta)\tilde{\mathcal{K}}^{nmij}(\zeta)G^{M}(\zeta)\mathrm{d}\zeta = \mathbf{c}^{M\mathrm{l}\pi_z\mathrm{T}}(z)Q^{nm\mathrm{l}\pi_z}(z)\mathbf{c}^{N\mathrm{l}\pi_z}(z),\\
&\int_{z}^{z_\infty} G^{N\mathrm{T}}(\zeta)\tilde{\mathcal{K}}^{nmij}(\zeta)G^{M}(\zeta)\mathrm{d}\zeta = -\mathbf{c}^{M\mathrm{r}\mathrm{T}}(z)Q^{nm\mathrm{r}}(z)\mathbf{c}^{N\mathrm{r}}(z),
\end{aligned} \tag{46}$$

where

$$\tilde{\mathcal{K}}^{nmij} = \begin{pmatrix} \mathcal{K}^{nmij} & 0_{N\times M} \\ 0_{N\times M} & 0_{N\times M} \end{pmatrix}. \tag{47}$$

Then, for Q^{nmw} one has

$$\begin{aligned}
&\frac{\mathrm{d}Q^{nmw}}{\mathrm{d}z} - Q^{nmw}(Y^{mw\mathrm{T}}Y^{mw})^{-1}Y^{mw\mathrm{T}}\mathcal{P}^{m}Y^{mw}\\
&-Y^{nw\mathrm{T}}\mathcal{P}^{nw\mathrm{T}}Y^{nw}(Y^{nw\mathrm{T}}Y^{nw})^{-1}Q^{nmw} - Y^{mw\mathrm{T}}\tilde{\mathcal{K}}^{nmij}Y^{nw} = 0\\
&Q^{nm\mathrm{l}\pi_z}(z_1) = 0_{N\times M} \qquad Q^{nm\mathrm{r}}(z_\infty) = 0_{N\times M}.
\end{aligned} \tag{48}$$

Now, the functionals can be obtained as

$$I_s^{nm} = \mathbf{c}^{m\mathrm{l}\mathrm{T}}(z_c)Q^{nm\mathrm{l}}(z_c)\mathbf{c}^{n\mathrm{l}}(z_c) - \mathbf{c}^{m\mathrm{r}\mathrm{T}}(z_c)Q^{nm\mathrm{r}}(z_c)\mathbf{c}^{n\mathrm{r}}(z_c). \tag{49}$$

3. Numerical results and conclusions

In order to verify our method we have chosen transitions which cover a wide range of phyisically relevant parameters. In table 1 we have listed the dipole strengths compared with those published by Ruder *et al* (1994). The initial and final states are always labelled by both their asymptotic quantum numbers: n_p, l, n_3 if $\omega = 0$ and n, n_3, ν if $\omega \to \infty$. In figure 1 a Grotrian-type diagram demonstrates the transitions computed by us at a fixed field strength ($\omega = 1$). Altogether, Table 1 and figure 1 show that no problems arose when computing transitions of different type (neither when $\Delta n_3 = 0$ nor when $\Delta n_3 \neq 0$). Difficulties appear neither at higher value of n_3 nor for all three magnitudes of the strength of the field.

In the cases when former results exist, they and our ones confirm each other, although we used approximations of significantly lower order. We also have computed dipole strengths for transitions, where – as far as we know – no values has been published yet.

We want to summarize the main conceptual and practical results of the paper.

The theoretical point:

Table 1. Dipole strengths $|\mathbf{p}|^2$ for diamagnetic Coulomb problem compared with the results of Ruder *et al* (1994) $|\mathbf{p}_{\mathrm{R}}|^2$. The strength of magnetic field is parametrized by Larmor frequency ω in atomic units. ($\omega = 1$ if $|\mathbf{H}| = 4.7 \times 10^5$ T.) The transitions are labelled by their asymptotic quantum numbers. The number of channnels used in computation are given in brackets.

transition	ω	$\lvert\mathbf{p}_{\mathrm{R}}\rvert^2$	$\lvert\mathbf{p}\rvert^2$
$2p_{-1}/0-10 \longleftrightarrow 3d_{-1}/0-11$	1	1.189	1.187[2]
			1.1892[6]
	10	$3.188 \cdot 10^{-1}$	$3.19 \cdot 10^{-1}$[2]
			$3.188 \cdot 10^{-1}$[4]
	100	$8.018 \cdot 10^{-2}$	$8.235 \cdot 10^{-2}$[1]
$2p_{-1}/0-10 \longleftrightarrow 3d_{-2}/0-20$	1	$8.741 \cdot 10^{-1}$	$8.743 \cdot 10^{-1}$[6]
	10	$9.665 \cdot 10^{-2}$	$9.665 \cdot 10^{-2}$[4]
	100	$9.901 \cdot 10^{-3}$	$9.905 \cdot 10^{-3}$[1]
$3p_{-1}/0-12 \longleftrightarrow 3d_{-1}/0-11$	1	8.241	8.2408[6]
	10	4.369	4.3688[2]
	100	3.303	3.308[1]
$3p_{-1}/0-12 \longleftrightarrow 3d_{-2}/0-20$	1	$9.146 \cdot 10^{-3}$	$9.147 \cdot 10^{-3}$[6]
	10	$2.465 \cdot 10^{-4}$	$2.464 \cdot 10^{-4}$[4]
	100	$7.391 \cdot 10^{-6}$	$7.398 \cdot 10^{-6}$[1]
$2p_{-1}/0-10 \longleftrightarrow 4d_{-1}/0-13$	1	—	$4.4502 \cdot 10^{-4}$[6]
	10	—	$9.699 \cdot 10^{-3}$[4]
	100	—	$1.7276 \cdot 10^{-2}$[1]
$3p_{-1}/0-12 \longleftrightarrow 4d_{-1}/0-13$	1	—	$4.3792 \cdot 10^{-2}$[6]
	10	—	$1.2318 \cdot 10^{-3}$[4]
	100	—	7.2918[1]
$3d_{-2}/0-20 \longleftrightarrow 4f_{-2}/0-21$	1	—	1.7866[6]
	10	—	$4.3063 \cdot 10^{-1}$[4]
	100	—	$1.2401 \cdot 10^{-1}$[1]
$4f_{-2}/0-21 \longleftrightarrow 4d_{-2}/0-22$	1	—	9.6021[6]
	10	—	5.1284[4]
	100	—	2.9267[1]
$2p_{-1}/0-10 \longleftrightarrow 4d_{-2}/0-22$	1	—	$1.649 \cdot 10^{-4}$[6]
	10	—	$1.359 \cdot 10^{-5}$[4]
	100	—	$7.496 \cdot 10^{-6}$[1]

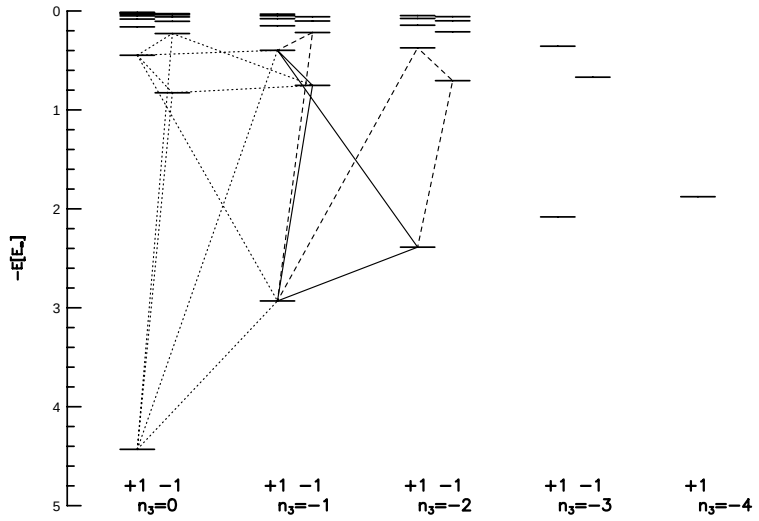

Figure 1. A Grotrian type diagram demostrating the calculated transitions ($\omega = 1$). Dipole strength were computed by either Ruder *et al* (1994) (dotted lines) or us (dashed lines) or by both (continuous lines).

(i) It is known, that the computation of a quadratic functional where the matrix functions are solutions of selfadjoint problem is straightforward, see Kitoroage *et al* (1989). We showed now that a similar idea applies to quadratic functionals for a set of non-selfadjoint cases in the frame of Bakhvalov factorization. The factorization method in general has numerous advantages compared to the other treatments. Among others, for getting the eigenvalues it does not require computation of the eigenfunctions.

(ii) The theoretical observation (i) allowed us to develop a mathematically consistent method for computing both the eigenvalues – that is the energy levels – and the quadratic functionals – transition probabilities – for a non-separable quantum mechanical problem, namely, the diamagnetic Coulomb problem by the use of a non-trivial basis. This paper completed the mathematical studies of our previous work BB96. From an other point of view, these two papers may be considered as an analysis of the problem in Liu–Starace basis in non-adiabatic approximation.

The practical point:

(iii) We have shown that for arbitrary transitions our calculations and the former ones are consistent while we have used only a few channels to reach the same accuracy.

(iv) We have determined dipole strengths for some transitions for the first time.

Appendix

Computation of $K_{pq}^{nmi}(z)$.

In analogy with the procedure described in BB96 for getting functionals I_{pq}^{i}, let

$$K_{pq}^{nmi}(z) = r_p^n(\rho_c, z) r_q^m(\rho_c, z)[k_{pq}^{nmil}(\rho_c, z) - k_{pq}^{nmir}(\rho_c, z)]$$

where, as in BB96, $r_s^t(\rho_c, z) = [h_s^{tl}(\rho_c, z) - h_s^{tr}(\rho_c, z)]^{-1/2}$ and $(t, s) = (m, q)$ or (n, p), while

$$\frac{\mathrm{d}k_{pq}^{nmiw}(\rho, z)}{\mathrm{d}\rho} = [v_p^n(\rho, z) + v_q^m(\rho, z)]k_{pq}^{nmiw}(\rho, z) + \frac{\sin\theta_p^n(\rho, z)\cos\theta_q^m(\rho, z)}{\nu_p(\rho)\nu_q(\rho)} s_1^{(i)}(\rho)$$

$$k_{pq}^{nmil}(\rho_0, z) = \frac{\nu_{p0}^n \nu_{q0}^m}{(\frac{1}{2} + |n_3^n|)(\frac{1}{2} + |n_3^m|)(1 + i + |n_3^n| + |n_3^m|)} \rho_0^{2+i} + O(\rho_0^{3+i})$$

$$k_{pq}^{nmir}(\rho_\infty, z) = -\frac{\nu_{p\infty}^n \nu_{q\infty}^m}{2\omega^3} \rho_\infty^{-4+i} + O(\rho_\infty^{-5+i}).$$

Equation for K_{pq}^{nmiw} coincides with (35) in BB96 if the proper change of weight function is taken into account. The difference is in v_p^n, v_q^m where different n_3^n, n_3^m may appear. Above these values, the behaviour of the new weight functions have an impact on the initial values. All other quantities were defined and/or computed in BB96.

Implementation.

The computations of the components of dipole matrix elements (7) and (8) were carried out by a FORTRAN program running on a Sun workstation. Some subroutines of standard numerical methods were taken from Press *et al* (1992). The input parameters E^m, E^n, $\mathcal{P}^m(z)$, $\mathcal{P}^n(z)$ and $K_{pq}^{nmi}(z)$ were provided by a slightly modified version of the program described in BB96.

We evaluated the functionals in two subsequent steps. First, we solved the matrix differential equations (34) and (41) for pairs $Y^{nN}(z)$, $H^{nN}(z)$ and $Y^{mM}(z)$, $H^{mM}(z)$, simultaneously. The fourth order Runge–Kutta process was modified to solve matrix equations with an adaptive stepsize control. We integrated the equations from both z_1 and z_∞ to z_c. Determination of $\mathbf{c}$ is equivalent to finding an arbitrary eigenvector belonging to the eigenvalue 1 of the algebraic problem (44). We have found $\mathbf{c}$ by the help of a Jacobi algorithm which provides approximation to the complete set of eigenvalues. The eigenvalue closest to 1 was chosen and its eigenvector was normalized by (45). The difference of the best eigenvalue from the value 1 indicated the accuracy of our $\mathbf{c}$, as well.

For the second main step, we solved the matrix differential equation (48) for $Q^{nmw}(z)$ from the z_0^{Q}, z_∞^{Q} to z_c, where z_0^{Q} and z_∞^{Q} were chosen so that $Q^{nmw}(z)$ be defined in the

common part of the interval of definition of $H^{nN}(z)$ and $H^{mM}(z)$. In all necessary cases linear interpolation was applied. When inverses appeared, the matrices were inverted by a Cholesky-type decomposition.

Errata to BB96.

Here would like to indicate the error occuring in (37) in BB96. The correct expressions there should be

$$k_{pq}^{\mathrm{r}1}(\rho_\infty) = \frac{\tilde{l}_0^1 \nu_{p\infty}\nu_{q\infty}\rho_\infty^{-6}}{2\beta_0^3} + O(\rho^{-7})$$

$$k_{pq}^{\mathrm{r}2}(\rho_\infty) = \frac{\tilde{l}_0^2 \nu_{p\infty}\nu_{q\infty}\rho_\infty^{-8}}{2\beta_0^3} + O(\rho^{-9})$$

A correction also should be made on p. 6751. $h_{\mathrm{r}}(\rho) \sim \rho^{-6}\sum_{j=0}^{\infty} h_{\mathrm{r}}^{(j)}\rho^{-j}$, $h_{\mathrm{r}}^{(0)} = \nu_\infty^2/(2\beta_0^3)$. This correction improves the behaviour of our method for smaller ω.

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