Revising Data in Sholin's Tables for Calculating the Asymmetry of Hydrogenic Spectral lines in Plasmas

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ABSTRACT: Revisions to the data in Sholin's tables from his paper in *Optics and Spectroscopy* 26 (1969) 27, are presented. Since his data was used numerous times by various authors to calculate the asymmetry of hydrogenic spectral lines in plasmas, our corrections should motivate revisions of the previous calculations of the asymmetry and its comparison with the experimental asymmetry, and thus should have a practical importance.

Key words: asymmetry of spectral lines; corrections to input data; hydrogenic spectral lines in plasmas

Sholin's tables from paper [1] were used numerous times by various authors to calculate the asymmetry of hydrogenic spectral lines in plasmas. (The latest advances in the theory of the asymmetry can be looked up in papers [2, 3] and references therein). However, we found that there are incorrect entries tabulated in paper [1] for the the *Ly-γ*, *Ly-ϵ*, and *H-α* lines in both the intensity corrections and the quadrupole frequency corrections.

The dipole and quadrupole frequency corrections are given in paper [1] as

$$\Delta_k^{dipole} = nq - n'q', \tag{1}$$

and

$$\Delta_k^{quadrup} = \frac{1}{3}[n^4 - n^2 - 6n^2q^2 - n'^4 + n'^2 + 6n'^2q'^2], \tag{2}$$

where n and n' are the principal quantum numbers of the upper and lower energy levels, respectively; $q = n_1 - n_2$ and $q' = n_1' - n_2'$ are the combinations of the corresponding parabolic quantum numbers.

Frequency Corrections

For Ly-gamma ($n = 4$), Eq. (2) becomes:

$$\Delta_k^{quadrup}(q) = 80 - 32q^2. \tag{3}$$

It yields $\Delta_k^{quadrup}(0) = 80$, $\Delta_k^{quadrup}(\pm 1) = 48$, $\Delta_k^{quadrup}(\pm 2) = -48$, $\Delta_k^{quadrup}(\pm 3) = -208$. The comparison shows that in Sholin's table there are typographic errors in $\Delta_k^{quadrup}(0)$ entered as 60 (instead of 80) and in $\Delta_k^{quadrup}(\pm 3)$ entered as -206 (instead of -208).

For Ly-epsilon ($n = 4$), Eq. (2) becomes:

$$\Delta_k^{quadrup}(q) = 420 - 72q^2. \tag{4}$$

It yields $\Delta_k^{quadrup}(0) = 420, \Delta_k^{quadrup}(\pm1) = 348, \Delta_k^{quadrup}(\pm2) = 132, \Delta_k^{quadrup}(\pm3) = -228, \Delta_k^{quadrup}(\pm4) = -732,$ $\Delta_k^{quadrup}(\pm3) = -1380.$ The comparison shows that in Sholin's table there are typographic errors in $\Delta_k^{quadrup}(\pm2)$ entered as 108 (instead of 132).

Intensity Corrections

The intensity corrections are calculated from the corresponding corrections to the wave functions. The latter are given, e.g., in the Appendix of paper [4].

For H-alpha ($n = 3$ to $n = 2$ transition), the comparison shows that in Sholin's table there are typographic errors in $\epsilon_k^{(1)}$ corresponding to $\Delta_k^{dipole} = 2$ entered as -62 (instead of -62/9) and $\Delta_k^{dipole} = -2$ entered as 62 (instead of 62/9), as shown in detail below.

For $\Delta_k^{dipole} = 2$:

$$
\begin{aligned}
I_k = {} & <110''|z|010''>^2 \\
= {} & \Big(<110|z|010> -3\frac{a_o}{R}<200|z|010> +3\frac{a_o}{R}<020|z|010 \\
& > -\frac{a_o}{R}<110|z|100> +3\frac{a_o^2}{R^2}<200|z|100> -3\frac{a_o^2}{R^2}<020|z|100> \Big)^2 \\
\approx {} & <110|z|010>^2 -6\frac{a_o}{R}<200|z|010 \\
& > +6\frac{a_o}{R}<020|z|010> -2\frac{a_o}{R}<110|z|100> \\
= {} & I_k^{(0)}\Big(1-\frac{a_o}{R}\frac{62}{9}\Big).
\end{aligned}
\tag{5}
$$

For $\Delta_k^{dipole} = -2$:

$$
\begin{aligned}
= {} & \Big(<110|z|100> -3\frac{a_o}{R}<200|z|100> +3\frac{a_o}{R}<020|z|100 \\
& > +\frac{a_o}{R}<110|z|010> -3\frac{a_o^2}{R^2}<200|z|010> +3\frac{a_o^2}{R^2}<020|z|010> \Big)^2 \\
\approx {} & <110|z|100>^2 -6\frac{a_o}{R}<200|z|100 \\
& > +6\frac{a_o}{R}<020|z|100> +2\frac{a_o}{R}<110|z|010> \\
= {} & I_k^{(0)}\Big(1+\frac{a_o}{R}\frac{62}{9}\Big).
\end{aligned}
\tag{6}
$$

We note in passing that the robust perturbation theory developed by Oks and Uzer [5] allows calculating analytically corrections to the eigenfunctions due to the quadrupole interaction in a much simpler way than in Sholin paper [1]. Details are presented in Appendix.

For completeness we list below also previously known (for a long time) corrections to the tabulated entries from paper [1] for the H-beta line.

For the Stark components corresponding to the radiative transitions between the parabolic states 210 and 010 or between 120 and 100, the unperturbed intensity should be 81, instead of 16.

For the Stark component corresponding to the radiative transition between the parabolic states 210 and 001, the intensity correction $\epsilon_k^{(1)}$ should be -20 (instead of -16).

For the Stark component corresponding to the radiative transition between the parabolic states 120 and 001, the intensity correction $\epsilon_k^{(1)}$ should be 20 (instead of 16).

There are also two corrections (known for a long time) to the following typographic errors from paper [1].

In Table 2 for the H-alpha line, in the header of the last column, the scaling factor should be 10^6 instead of 10^5.

In Eq. (21), in its 2nd term in the right hand side, the coefficient should be (3/8) instead of (3/16). We note that after this correction, Eq. (21) from [1] coincides with the corresponding term (proportional to $1/R^4$) in Eq. (4.59) from book [5] after setting in the latter $Z_1 = 1$, $Z_2 = Z$. Equation (4.59) from book [5] was derived from the exact expression for the energy in elliptical coordinates for the two Coulomb center problem by expanding the latter in powers of $1/R$ up to (including) the term $\sim 1/R^6$. Therefore, Eq. (4.59) from book [5] can be considered, in particular, as the benchmark for testing Eq. (21) from [1]. Such a test confirms also that the 2nd term in the right hand side of Eq. (21) from [1] correctly contains the first power of Z (while there were incorrect suggestions that this term should contain Z^2).

In summary, since Sholin's tables from paper [1] were used numerous times by various authors to calculate the asymmetry of hydrogenic spectral lines in plasmas, our corrections should motivate revisions of the previous calculations of the asymmetry and its comparison with the experimental asymmetry, and thus should have a practical importance.

Appendix. Application of the robust perturbation theory [5] for calculating quadrupole corrections to the wave functions

In the present paper, the robust perturbation theory [6] was employed. The gist of it is as follows. If for the perturbed quantum system there is an operator A that commutes with the Hamiltonian H and the parts of these operators A_0 and H_0, characterizing the unperturbed quantum system, also commute, then the perturbation theory can be constructed in terms of the perturbation $(A - A_0)$ to the operator A_0, rather than in terms of the perturbation $(H - H_0)$ to the operator H_0. For calculating corrections to the wave functions (which are common for both A_0 and H_0), the advantage is that the eigenvalues of the operator A_0 are typically nondegenerate (in distinction to the eigenvalues of the operator H_0). Therefore, for calculating the first order corrections to the wave functions it is sufficient to use the first order of the nondegenerate perturbation theory with respect to the perturbation $(A - A_0)$ and it would not involve infinite summations. In distinction, for calculating the same corrections in terms of the perturbation $(H - H_0)$, one would have to proceed to the second order of the degenerate perturbation theory, involving infinite summations.

Below as the operator A we choose the projection A_z of the super-generalized Runge-Lenz vector, derived by Kryukov and Oks [7], on the axis connecting the nucleus of the hydrogenic atom/ion with the perturbing ion. The operator of the unperturbed projection $A_z^{(0)}$ has the well-known eigenvalues q/n - see. e.g., the textbook [8]. According to Eq. (12) from [6], the first non-vanishing term of the expansion of the operator $(A_z - A_z^{(0)})$ in terms of the small parameter n^2/R (here and below we use atomic units) is $-L^2/R$. Then the corrections to the wave functions are given by

$$-\frac{1}{R}\frac{(L^2)^{nq'm}_{nqm}}{A_{z,\alpha}^{(0)} - A_{z,\alpha'}^{(0)}} = \frac{n}{R}\frac{(L^2)^{nq'm}_{nqm}}{(q-q')}, \tag{A.1}$$

where the selection rules for non-zero matrix elements of the operator L^2 require $q - q' = \pm 2$.

The non-diagonal matrix elements of the operator L^2 in parabolic coordinates (as well as of the operators $L_\pm = L_x \pm iL_y$), have been calculated by Sholin, Demura, and Lisitsa in [9]:

$$<n_1+1, n_2 - 1, m|L^2 | n_1 n_2 m> = -[n_2 (n - n_2) (n_1 + 1) (n - n_1 - 1)]^{1/2},$$

$$< n_1 - 1, n_2 + 1, m|L^2 | n_1 n_2 m> = -[n_1 (n - n_1) (n_2 + 1) (n - n_2 - 1)]^{1/2}. \tag{A.2}$$

We note that matrix elements of the operator L_x in parabolic coordinates have been later reproduced by Gavrilenko in paper [10]. We also note that the non-diagoanal matrix elements of the operators $L_\pm$ can be also obtained using their proportionality (within the manifold of the fixed n) to the non-diagonal matrix elements of the operators $(x \pm iy)$:

$$<n, q \pm 2, m|L_\pm | nqm > = - (\pm 1) [2/(3n)] (x \pm iy). \tag{A.3}$$

(The underlying physical reason for the existence of relation (A.3) is, according to Demura [11], the O4 symmetry of hydrogenic atoms/ions.*/) Therefore, the non-diagonal matrix elements of the operator L^2 in parabolic coordinates can be obtained using their similar proportionality to the non-diagonal matrix elements of the operator $(x^2 + y^2)$. The latter matrix elements have been calculated by Clark [12].

Anyway, after substituting the non-diagonal matrix elements of the operator L^2 from Eq. (A.2) in Eq. (A.1), the latter equation yields the following result for the corrections to the wave functions (more rigorously, for the coefficients of the corresponding linear combinations of the unperturbed wave functions):

$$\frac{n[n_2(n - n_2)(n_1 + 1)(n - n_1 - 1)]^{1/2}}{2R}, \qquad q - q' = 2,$$

$$-\frac{n[n_1(n - n_1)(n_2 + 1)(n - n_2 - 1)]^{1/2}}{2R}, \qquad q' - q = 2. \tag{A.4}$$

This is the same result as in Sholin paper [1], but obtained in a simpler way: without the need to go to the second order of the perturbation theory.

Acknowledgements

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*/ Specifically, this is related to the following two facts within the manifold of the fixed n [11]. First, the mean value <**r**> of the radius vector of the bound electron is proportional to the unperturbed Runge-Lenz vector $\mathbf{A}^{(0)}$, as it is well-known. Second, the linear combinations $\mathbf{J}_\pm = (\mathbf{L} \pm \mathbf{A}^{(0)})/2$ obey the same commutation relations as the angular momentum.

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