Effect of fine structure on the line shape of hydrogenlike ions

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It is shown that allowance for the fine structure of a multiply charged ion (H ion) makes the line contours radically different from those in the relativistic treatment. The spectral function becomes asymmetric, and narrow components due in particular to the nonmonotonic variation of the terms appear. Detailed calculations were made for the $4 \rightarrow 3$ transitions of H ions with $Z = 22$ and 30 in a plasma with parameters $N_i \sim 10^{17} Z^2$ cm^{-3} and $T \sim Z^2$ eV.

1. INTRODUCTION

The mechanisms that broaden the lines of hydrogen and hydrogenlike ions (H ions) in a plasma have been investigated quite in detail.[1–3] The level splitting in the total angular momentum of the electron (i.e., of the fine structure), however, is usually neglected (see, e.g., Ref. 3, p. 32). It is nonetheless clear that this neglect is not justified in the analysis of multiply charged ion line shapes, since the role of the relativistic effects increases with the nuclear charge. At the same time, analysis of the influence of the fine structure on H-ion line contours is timely in view of the recent active research into highly ionized (and in particular, laser) plasma.[4–6]

We present here estimates (Sec. 2) that show the substantial role played by the fine splitting of $n \leqslant 4$ states for multiply charged H ions in a plasma having the frequently considered parameters[5–7] (ion density $N_i \sim 10^{17} Z^2$ cm^{-3}, ion temperature $T \sim Z^2$ eV, H-ion nuclear charge $Z > 10$).

We present also calculations (Sec. 3) that demonstrate the strong influence of the fine structure on the character of Stark splitting. For example, owing to the presence of quasi-crossing terms, certain adiabatic terms have a nonmonotonic dependence on the field strength.

We show, finally (Sec. 4), that the nonlinear character of the Stark effect leads to a radical change of the line contour compared with the results of the usual nonrelativistic treatment.[1–3,7] In particular, the line contour turns out to be asymmetric, there are several maxima near the frequencies corresponding to those microfield values at which the Stark shift reaches an extremum, and also near transitions between weakly displaceable components. Comparison with the results of the usual theory[1–3,7] shows that allowance for the fine struture decreases the effective line width.

2. SOME ESTIMATES

When considering the stark effect, the relativistic splitting of a level n can be neglected only if

$$\varepsilon_n^{\mathrm{rel}} \sim \alpha^2 Z^4/n^3 \text{ [a.u.]}$$

is much smaller than the splitting

$$\varepsilon_n(F) \sim D_z F \sim (n^2/Z) F \text{ [a.u.]},$$

due to the electric field F, i.e., if

$$F \gg \alpha^2 Z^5/n^5 \text{ [a.u.]}.$$

Here $\alpha = 1/137$ is the fine-splitting constant, Z the nuclear charge, and D_z the H-ion dipole moment. If we use for the estimate the average Holtsmark (static) microfield produced in the plasma by the ions (Ref. 3, p. 44), viz.,

$$\bar{F}_x = 8.8 \bar{Z} e N_i^{2/3}$$

(Z is the average charge of the plasma ions), it is clear that neglect of the fine structure is justified only at a sufficiently high ion density

$$N_i > 10^{17} Z^6/n^{15/2} \text{ [cm}^{-3}\text{]}. \qquad (1)$$

For simplicity we put here and elsewhere $\bar{Z} \approx Z$.

If condition (1) is not met, the stark effect becomes nonlinear in the field, and this should influence strongly the line shape.

Note that the condition that the field be quasistatic (i.e., that $|\dot{F}|/F$ be small compared with $D_z F$) sets also the lower bound of the ion density (Ref. 3, p. 27):

$$N_i > 4 \cdot 10^{16} T^{1/2} \text{ [eV]}/Z^{9/2}(n^2 - n'^2) \text{ [cm}^{-3}\text{]}. \qquad (2)$$

Here $\bar{Z} \approx Z$, $A = 2Z$ is the atomic weight of the ion, and n' is the principal quantum number of the lower level. It is clear, however, that for sufficiently large Z and moderate temperatures

$$T^{1/2}\text{[eV]}\, n^{1/2}/Z^{15/2} < 2$$

there exists a range of N_i at which the broadening by ions is static, but the fine structure must be taken into account in the calculation of the level shifts. This is the case, for example, for an H-ion plasma with parameters $N_i \sim 10^{17}$ cm^{-3}, $T \lesssim Z^2$, and $Z > 10$, which is of interest for the feasibility of amplification on the $4 \rightarrow 3$ transition of H ions.[5–7] We present therefore, below, calculations for the $4 \rightarrow 3$ transitions of multiply charged ions ($Z = 22$ and 30) at N_i and T such that the ion broadening can be regarded as static, but the fine structure is radically manifested in the line shape.

The natural and the electron-impact broadening can be neglected at the plasma parameters of interest to us. Comparing thus the electronic width $\gamma_e \approx 30 N_e n^4 / Z^2 v_e$ (Ref. 2) (N_e is the electron density and $v_e \approx (2T_e/m_e)^{1/2}$ is their characteristic thermal velocity) with the static width $\sim n^2 N_i^{2/3}$, we find that the broadening by electrons is substantial only if

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$$N_i \gtrsim 10^{19} Z^6/n^6 \ [\mathrm{cm}^{-3}] \tag{3}$$

$T_e \sim Z^2$ eV and $N_e \sim ZN_i$). At these densities condition (1) is met and the fine structure of the levels is inessential.

We take into account below also the Doppler broadening due to the thermal motion of the radiating ions. The ion motion is here assumed free, which also limits their density. More accurately, the Doppler width should be less than the heavy-particle collision frequency (see, e.g., Ref. 8, p. 25).

For Coulomb collisions, this condition yields

$$N_i < 5\cdot 10^{18} Z^2 (T/Z^2)^2 (1/n^2 - 1/n'^2). \tag{4}$$

More substantial in an expanding plasma is frequently the Doppler effect due to the microscopic motion,[9,10] It can be easily taken into account in actual problems if the spatial distribution of the velocities is known.

It would be simplest to investigate the influence of relativistic effects on the contour of the L_α line ($2\to 1$ transition). This is, however, not of sufficient practical interest, since the main contribution to the broadening of this transition is made as a rule by the Doppler effect. On the other hand, when transition between excited states are considered, it is necessary to resort to numerical computations.

3. NONLINEAR STARK EFFECT DUE TO THE FINE STRUCTURE

H ion in the absence of a field

Disregarding the structure and the spin of the nucleus, a multiply charged H ion is described by the Dirac equation. The complete set of quantum numbers describing the electron state is n, l, j and m_j where l is the orbital quantum number, j the total angular momentum, and m_j the projection of the total momentum. The quantum number l is not a "good" one and determines only the parity of the state. The H-ion energy levels are given by the Sommerfeld equation[11-13]

$$E_{nj} = \left\{1 + \left[\frac{\alpha Z}{n-k+(k^2-\alpha^2 Z^2)^{1/2}}\right]^2\right\}^{-1/2}. \tag{5}$$

Here $k = j + 1/2 = 1,2,...,n$; $l = j \pm 1/2$ at $k \neq n$, $l = j - 1/2 = n - 1$ at $k = n$, and the relativistic units $m_e = c = \hbar = 1$ ($\alpha = e^2$) are used.

The wave eigenfunctions of the Dirac equation for an electron in a Coulomb field are of the form

$$|n,j,l,m_j\rangle = \begin{pmatrix} g_{nlj}(r)\Omega_{jlm_j}(\hat{r}) \\ i f_{nlj}(r)\Omega_{jl'm_j}(\hat{r}) \end{pmatrix}, \tag{6}$$

where Ω_{jlm_j} is a spherical spinor, $l = 0,1,...,n-1$, $l' = 2j - l$, r is the distance from the nucleus, and r are the angles characterizing the radius vector r; the radial wave functions g and f are normalized by the condition $\int (g^2 + f^2) r^2 dr = 1$.

The states described by (5) and (6) are degenerate both in the projections m_j of the total angular momentum and in the orbital momentum l. The radiative corrections to (5) lift the double degeneracy in l. The most significant here is the splitting of the states $ns_{1/2} - np_{1/2}$ (Lamb shift), but even this is $< 3\%$ of the total fine-structure interval (at $Z\sim 20$).[14] The radiative corrections to the levels $j \neq 1/2$ are negligibly small.

Description of the Stark effect

The only conserved quantum number in an external uniform electric field is the projection m_j of the angular momentum on the Z axis along which the field is directed. In a superweak field, when the level shift is much smaller than the Lamb shift, a quadratic Stark effect takes place. With increasing field, states with $l = j \pm 1/2$ are mixed in and the Stark effect becomes linear. The energy shifts are then determined in the Pauli approximation:

$$\varepsilon_{nj}(F) = \pm \frac{3}{4}[n^2 - (j+1/2)^2]^{1/2} \frac{nm_j}{j(j+1)} \frac{\alpha^{1/2} F}{\alpha Z}. \tag{7}$$

The $\pm$ sign pertains to sublevels with $j = l \mp 1/2$. The shift of the state with $j = n - 1/2$ is quadratic in the field.

Further increase of the field leads to mixing of states with different j. Analytic expressions for the shifts in such fields were obtained only in the case $n = 2$ (Ref. 15). For the cases $n = 3, 4$ of interest to us we must use numerical methods. In strong field, when $\varepsilon_{nj}(F) \gg E_{nn-1/2} - E_{n1/2}$, the fine structure is insignificant, the Stark effect is linear and is described by the known nonrelativistic parabolic-coordinate equations[11,12,16] (for the relativistic corrections see Ref. 15).

We shall be interested in the case of intermediate fields, when

$$\varepsilon_{nj}(F) \sim E_{nn-1/2} - E_{n1/2}. \tag{8}$$

The splitting $\varepsilon_{nj}(F)$ in the field is weak compared with the distance to the neighboring level with another quantum number $E_{nj} - E_{n'j'}$, $n \neq n'$, and the radiative corrections are neglected. In this case it is convenient for the unperturbed Hamiltonian H_0 to define in the Dirac Hamiltonian

$$H_D = \sum_{njm_j} E_{nj} P_{njm_j} = H_0 + V \tag{9}$$

in such a way that the perturbation is "reckoned" from the state $E_{n1/2}$

$$H_0 = \sum_n E_{n1/2} \sum_{jm_j} P_{njm_j}, \tag{10}$$

$$V = \alpha^{1/2} F z + \sum_{njm_j} (E_{nj} - E_{n1/2}) P_{njm_j}. \tag{11}$$

Here $P_{njm_j} = |n,j,m_j\rangle\langle n,j,m_j|$ is the operator of projection on the state $|n,j,m_j\rangle$.

Since the shifts are small, it suffices for our purpose to use first-order perturbation theory in the external field F.

Owing to the doublet degeneracy of the unperturbed states in l the zeroth-approximation wave functions must be chosen in the form of the symmetrized combinations:

$$|n,j,m_j\rangle^{(\pm)} = 2^{-1/2}(|n, j-1/2, j, m_j\rangle \pm |n, j+1/2, j, m_j\rangle)$$

$$\text{at} \quad j \neq n - 1/2 \tag{12}$$

and

$$|n, l, j, m_j\rangle \quad \text{at} \quad j=n-{}^1/_2.$$

The point is that the choice of any other basis leads, in first order perturbation theory, to a radical difference of the F-dependences of the physical quantities at $F = 0$. Incidentally, in our case the vicinity of the point $F = 0$ is inessential, since the microfield distribution function at this point is zero (see Sec. 4). We have therefore diagonalized the perturbation operator (11) in the basis of the functions $|n, l, j, m_j\rangle$.

Since m_j is a good quantum number, the matrix $\langle n, l, j, m_j | V | n, l', j', m_j'\rangle$ is block-diagonal and can be separately diagonalized for different values of m_j. For a fixed m_j, the diagonalized matrix V has a dimensionality $(2(n - |m_j|)$, its diagonal consists of the level shifts relative to the state $np_{1/2}$, and the off-diagonal quantities are

$$\alpha^{1/2} F\langle n, l, j, m_j|z|n, l', j', m_j\rangle.$$

The matrix element here is a particular case of the more general expression

$$t=\langle n, l, j, m_j|(4\pi/3)^{1/2} r \Upsilon_{1,-m}|n', l', j', m_j'\rangle$$

(Υ_{lm} are spherical harmonics), an expression necessary for the calculation of the radiative-transition probabilities. The explicit form of these expressions is given in the Appendix.

Calculation results

The matrix V defined by (11) was diagonalized by the Jacobi orthogonal rotations method.[17] This yielded a matrix S that diagonalizes the perturbation, $S^{-1}VS = E(F)$.

We note some of the results (see Fig. 1). At large values of m_j the Stark effect changes from quadratic to linear in weaker fields than in the case $m_j = 1/2$. This is due to the small splitting of the states with large angular momentum $n - 1/2 \geqslant j > m_j$. The terms of the interacting states do not cross in the adiabatic approximation, as is in fact the case for the dependences of ε_{nj} on F at various m_j. The repulsion of the terms in the quasicrossing terms leads to a nonmonotonic dependence of the shift of the symmetric state $|n, 1/2, 1/2\rangle^{(+)}$ on F. This circumstance is most important, since maxima of the spectral functions occur at frequencies corresponding to an extremum of the $\varepsilon_{nj}(F)$ dependence. When account is taken of the interaction of the fine-structure sublevels, the only terms that are not shifted are those with $|m_j| = j = n - 1/2$. Note that in the Pauli approximation (7) the states wth arbitrary m_j are not shifted at $j = n - 1/2$. This is due to neglect of the couplings of the states $j = n - 1/2$ to the other levels. Incidentally, the shifts of the levels that are immobile in the strong-field limit are small in intermediate fields. Near the corresponding frequencies there are also maxima of the spectral functions (see Sec. 4).

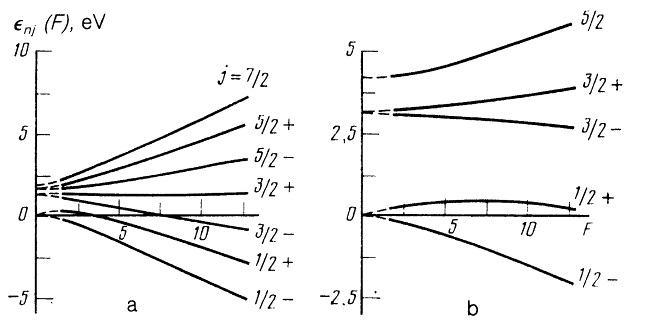

FIG. 1. Dependence of the Stark splitting of levels $n = 3$ (a) and $n = 4$ (b) at $m_j = 1/2$ of a multiply charged ion ($Z = 22$) on the field strength F. The field strength is in units of the characteristic Holtsmark field $F_0 = 2.2ZN_i^{2/3} \approx 10^8$ V/cm ($N_i = 10^{17}Z^2$ cm^{-3} = $4.84\cdot 10^{19}$ cm^{-3}). The + (−) sign indicates that the wave function corresponding to the given level becomes symmetric (antisymmetric) as $F \to 0$.

Probabilities of radiative transitions

Analysis of the relativistic effects on the probabilities of allowed, weak ($E2, M1$, etc.), and forbidden radiative transitions has shown that, accurate to 5%, the dipole approximation is adequate at $Z \lesssim 40$. The radiative-transition probabilities are then

$$A(n, \alpha, m \to n', \alpha', m') = {}^4/_3 \alpha \omega_{nn'}^3 \Big|\sum_{\beta,\beta'} S_{\alpha'\beta'}^{*} S_{\alpha\beta} t(n, \beta \to n'\beta')\Big|^2. \qquad (13)$$

Here $S_{\alpha\beta}(F)$ are elements of the matrix S, which determine the coefficients of expansion of the wave function of the state α of the "dressed" basis (which takes the field F into account) in terms of the wave functions β of the unperturbed basis, and $\omega_{nn'}$ are the frequencies of the $n \to n'$ transition.

The only selection rule for the radiative transitions (13) is the condition $|m - m'| \lesssim 1$. Other selection rules are substantially violated because of mixing of nj states of differing parity. The number of allowed transitions in the field is therefore quite large. For the $4 \to 3$ transition at a field intensity of the order of the splitting there are 298 transitions with probabilities ranging from 1% to 30% of the probabilities of the transitions allowed in the absence of the field.

4. SPECTRAL FUNCTIONS OF THE TRANSITIONS 4→3

General formulas

The line contour of the H-ion $\alpha \to \beta$ transition in a plasma is determined by the convolution of the Doppler, impact, and Holtsmark contours:

$$S_{\alpha\beta}(E) = J_{\alpha\beta}(E)/N_{\alpha\beta}, \qquad (14)$$

$$N_{\alpha\beta} = \int_{-\infty}^{\infty} dE\, J_{\alpha\beta}(E) = \int_0^{\infty} E_{\alpha\beta}(F) A_{\alpha\beta}(F) H(F) \frac{dF}{F_0}, \qquad (15)$$

$$J_{\alpha\beta}(E) = \frac{\Gamma_{\alpha\beta}}{\pi^{-3/2}} \int_{-\infty}^{\infty} \frac{dv}{v_T} \exp\Big[-\Big(\frac{v}{v_T}\Big)^2\Big] \times \int_0^{\infty} \frac{E_{\alpha\beta}(F) A_{\alpha\beta}(F) H(F)\, dF/F_0}{\{E - E_{\alpha\beta}(F)(1+v/c)\}^2 + \Gamma_{\alpha\beta}^2}. \qquad (16)$$

Here

$$H(x) = \frac{2}{\pi x} \int_0^{\infty} y \sin y \exp\Big[-\Big(\frac{x}{y}\Big)^{3/2}\Big] dy$$

is the Holtsmark distribution function of the ionic micro-

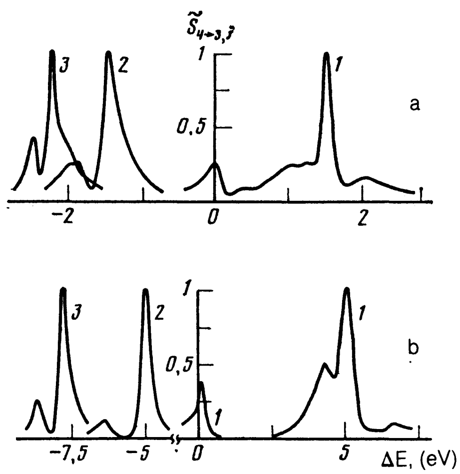

FIG. 2. Spectral functions $\tilde{S}_{4\to3,j}(E)$ for $Z = 22$ (a) and $Z = 30$ (b). Curves 1—$j = 1/2$, 2—3/2, 3—5/2. The energy origin is that of the $4_{p1/2} \to 3s_{1/2}$ transition [see Table I for the values of the maxima of the spectral functions $S^{\max}_{4\to3,j} = \max_E\{(S_{4\to3,j}(E)\}$ and of the rates of the spontaneous transitions $A(4\to3,j)$].

field, $F_0 = 2.6031ZeN_i^{2/3}$ is the characteristic value of the field,[1,3] $E_{\alpha\beta}(F)$ is the energy of the $\alpha\to\beta$ transition with allowance for the shifts of the levels α and β in the field F, v_T is the characteristic thermal velocity of the ions, and $\Gamma_{\alpha\beta}$ are the elements of the matrix that determines the relaxation due to radiative transitions and collisions with the electrons.

We shall neglect broadening due to spontaneous radiative transitions and to collisions with electrons. (Note that to take collision broadening into account it is necessary to diagonalize the operator $V + i\Gamma$). Calculating the limit (16) as $\Gamma_{\alpha\beta}\to 0$ we get

$$J_{\alpha\beta}(E) = \frac{1}{\pi^{1/2}}\frac{c}{v_T}\int_0^\infty A_{\alpha\beta}(F)H(F)\exp\left\{-\left[\frac{E-E_{\alpha\beta}(F)}{E_{\alpha\beta}(F)v_T/c}\right]^2\right\}\frac{dF}{F_0}. \quad (17)$$

Calculation results

The line contours were calculated using Eq. (17) for a net with mesh 0.02 eV. The steps in F were variable, starting from the requirement that the line contours be described with accuracy not worse than 5%. To obtain the summary spectral function of the $4\to3$ transition, information is necessary on the relative populations of the level $n = 4$. Estimates show that at the considered plasma parameters ($N_e \approx 10^{17}Z^3$ [cm^{-3}], $T_e \approx Z^2$ [eV]) the states with $n = 4$ are distributed in proportion to the statistical weights. At the same time, the levels with $n = 3$ do not "have time" to be completely mixed. Only the populations of the degenerate states with like j are proportional here to the statistical weights. We therefore calculated in place of a single spectral function $W_{3\to4}(E)$ the three functions

$$S_{4\to3,j}(E) = \sum_{\alpha\beta} S_{\alpha\beta}(E)N_{\alpha\beta} \Big/ \sum_{\alpha\beta} N_{\alpha\beta} \quad (18)$$

for $j = 1/2$, 3/2, and 5/2 respectively. Here α "runs through" all the states with $n = 4$, and β all the states with $n = 3$ and with the given fixed j. Note that the normalization constants for $j = 1/2$, 3/2, 5/2 are related as 1:2.98:2.66 for $Z = 22$ and as 1:2.99:2.7 for $Z = 30$.

Figure 2 shows the spectral functions $\tilde{S}(E) = S(E)/S^{\max}$ normalized to their maximum values $S^{\max} = \max_E S(E)$. The values of $S^{\max}_{4\to3,j}$ and the probabilities of the spontaneous transitions are listed in Table I.

The most important feature is that the spectral functions are asymmetric (including also the summary spectral function $S_{4\to3}$). This is due to the asymmetric character of the fine splitting. Maxima exist near the extrema ($E\approx 0.03$ eV for $Z = 22$ and $E\approx 0.1$ eV for $Z = 30$) and at energies corresponding to weakly mixable components.

The line shapes for $Z = 22$ and 30 are different. The reason is that we have assumed $N_i \sim Z^2$ and accordingly $D_zF_0 \sim Z^{1/2}$. At the same time, the fine splitting is proportional to Z^4. Therefore the interaction of the sublevels with different j assumes a lesser role with increase of Z, and the shifts are described in the Pauli approximation (7). The largest deviation from (7) occurs at $Z\approx 15$.

5. CONCLUSION

We conclude by considering the extent to which the usual estimates of the quasistatic line width hold for multiply charged ions. It must be noted above all that in those cases when condition (1) is violated the concept "linewidth of the $n\to n'$ transition" becomes practically meaningless. One can speak of linewidth of the individual components $nj\to n'j'$, although their spectral functions can have several maxima. The effective widths obtained in the present paper for the transitions $4\to3$, $j = 1/2$, 3/2, 5/2 are respectively 0.16, 0.18, and 0.18 eV for $Z = 22$ and 0.56 and 0.4 eV for $Z = 20$. The customary estimate using the formula

$$\Delta E = 8{,}3\cdot10^{-15}(n^2-n'^2)(N_i\,[\mathrm{cm}^{-3}])^{2/3}\ [\mathrm{eV}],$$

proposed by Griem,[18] yields 0.8 eV for $Z = 22$ and 1.2 eV for $Z = 30$. These values are 2–5 times larger than the results of the numerical calculation. Estimates based on the approximate expression (7) for the term shifts come somewhat closer to the exact values of the effective widths, but they remain

TABLE I. Characteristics of $4\to3j$ transitions.

Z	T, eV	N_i, cm^{-3}	$A(4\to3,j)10^{13}$ s^{-1}			$S^{\max}_{4\to3,j}$, eV^{-1}			$E_{4p_{1/2}, 3s_{1/2}}$, eV
			$j=1/2$	$j=3/2$	$j=5/2$	$j=1/2$	$j=3/2$	$j=5/2$	
22	968	$4.84\cdot10^{19}$	0.967	2.88	2.57	1.42	1.9	2.44	322.7
30	1800	$9\cdot10^{19}$	3.32	9.92	9	0.667	1.67	1.59	604.3

incorrect for the terms with $n = n - 1/2$ (see Sec. 3). Thus, an adequate description of the Holtsmark broadening of multiply charged ions in a plasma calls for a complete analysis of the Stark splitting, similar to that carried out above

APPENDIX

We present an expression for t:

$$t(n_1l_1j_1m_1 \to n_2l_2j_2m_2) = (4\pi/3)^{1/2}$$
$$\times\langle n_2l_2j_2m_2|r\Upsilon_{1,-m}|n_1l_1j_1m_1\rangle = Q(l_1j_1m_1, l_2j_2m_2)\langle g_2rg_1\rangle + Q(l_1'j_1m_1, l_2'j_2m_2)\langle f_2rf_1\rangle. \quad \text{(A1)}$$

The angle integrals Q can be expressed in terms of Clebsch-Gordan coefficients and $6j$ symbols[9] ($l' = 2j - l$):

$$Q(l_1j_1m_1, l_2j_2m_2) = (-1)^{j_1+1/2+l_2-1}[j_1l_1]C^{j_2m_2}_{j_1m_1,1,m_2-m_1}C^{l_20}_{l_1010}\begin{Bmatrix} l_1 & 1/2 & j_1 \\ j_2 & 1 & l_2 \end{Bmatrix}, \quad \text{(A2)}$$
$$[a \ldots b] \equiv [(2a+1) \ldots (2b+1)]^{1/2}.$$

The radial integrals $\langle g_2rg_1\rangle$ and $\langle f_2rf_1\rangle$ are given by

$$\begin{Bmatrix} \langle g_2rg_1\rangle \\ \langle f_2rf_1\rangle \end{Bmatrix} = \begin{Bmatrix} A_{12} \\ B_{12} \end{Bmatrix} \{n_{r_1}n_{r_2}R(-n_{r_1}+1, -n_{r_2}+1)$$
$$\mp n_{r_1}(N_2-\varkappa_2)R(-n_{r_1}+1, -n_{r_2}) \mp (N_1-\varkappa_1)n_{r_2}R(-n_{r_1}, -n_{r_2}+1) + (N_1-\varkappa_1)(N_2-\varkappa_2)R(-n_{r_1}, -n_{r_2})\}. \quad \text{(A3)}$$

$$\begin{Bmatrix} A_{12} \\ B_{12} \end{Bmatrix} = \left(\frac{4}{N_1N_2}\right)^{3/2}\frac{1}{\alpha Z}\left[\frac{\Gamma(2\gamma_1+n_{r_1}+1)\Gamma(2\gamma_2+n_{r_2}+1)}{n_{r_1}!n_{r_2}!16N_1N_2} \times\frac{(1\pm\varepsilon_1)(1\pm\varepsilon_2)}{(N_1-\varkappa_1)(N_2-\varkappa_2)}\right]^{1/2}\frac{2^{\gamma_1+\gamma_2-2}}{\Gamma(2\gamma_1+1)\Gamma(2\gamma_2+1)N_1^{\gamma_1-1}N_2^{\gamma_2-1}}. \quad \text{(A4)}$$

Here Γ is the Euler gamma function, ε_i are the Dirac energies of the level $n_i\, j_i$, and the remaining quantities are defined as follows:

$$\varkappa_i = -(j_i+1/2), \quad j_i = l_i+1/2,$$
$$\varkappa_i = +(j_i+1/2), \quad j_i = l_i-1/2,$$
$$n_{r_i} = n_i - |\varkappa_i|, \quad N_i = [n_i^2 - 2n_{r_i}(|\varkappa_i| - \gamma_i)]^{1/2}, \quad \text{(A5)}$$
$$\gamma_i = [(j_i+1/2)^2 - (\alpha Z)^2]^{1/2}.$$

The integrals R, from which we have left out some of the invariant parameters, are expressed in terms of integrals of confluent hypergeometric functions Φ:

$$R(n_1, n_2) \equiv R(\gamma_1, \gamma_2, 2/N_1, 2/N_2, n_1, n_2),$$

$$R(a, b, \alpha, \beta, n_1, n_2) = \int_0^\infty x^{a+b+1}e^{-(\alpha+\beta)x/2}\Phi(-n_1, 2a+1; \alpha x)$$
$$\times\Phi(-n_2, 2b+1; \beta x)\,dx = \left(\frac{2}{\alpha+\beta}\right)^{a+b+2}\sum_{i=0}^{n_1}\frac{(-n_1)_i}{(2a+1)_i}\left(\frac{2\alpha}{\alpha+\beta}\right)^i \times\frac{\Gamma(a+b+2+i)}{i!}\,{}_2F_1\left(-n_2, a+b+2+i; 2b+1; \frac{2\beta}{\alpha+\beta}\right), \quad \text{(A6)}$$

where ${}_2F_1$ is the Gauss hypergeometric function and $(a)_i$ is the Pochhammer symbol.

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