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Radiative Recombination for Parabolic and Spherical States in H-like Atoms

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Résumé. — Les éléments matriciels pour les transitions entre les états paraboliques de l'atome hydrogénoise sont exprimés par un ensemble de fonctions réelles satisfaisant des relations récursives très simples. La méthode de calcul suivant ces relations s'avère précise, rapide et efficace pour le calcul des sections différentielles et totales de la recombinaison radiative impliquant des états paraboliques. Nous étudions les distributions angulaires des photons ainsi que les populations des états Stark pour la recombinaison radiative.

Abstract. — The matrix elements for free-bound transitions between parabolic states of hydrogen-like atoms are expressed in terms of a set of real functions which satisfy quite simple recursion relations. The method of calculation based on them is shown to be precise, fast and efficient for the differential and total cross-sections for radiative recombination on parabolic states. We investigate the angular distributions of photons and branching rates for the subshells with the same principal quantum number $n$.

1. Introduction

The capture of a free electron by an ion and the emission of a photon — known as direct radiative recombination (DRR) — is one of the fundamental processes in the electromagnetic interactions of charged particles with atoms. In view of the time reversal relation between DRR and photoionization, the results for both processes are directly related by time reversal. Thus, the calculation of DRR cross-sections for hydrogenic system "... is a problem almost as old as quantum mechanics" [1].

Since in the case of a pure Coulomb field the initial and final wave functions are known analytically, the cross-sections for radiative recombination may be calculated exactly. Within the conventional nonrelativistic dipole approximation, i.e. neglecting retardation effects, the first extensive study of this problem was given by Stobbe [2], who derived the DRR cross-sections for arbitrary hydrogenic $(n,l)$ states in terms of hypergeometric functions of complex...
parameters, the only remaining problem being to find appropriate methods to perform the large volume of numerical calculations involved. In this respect notable results were obtained for the photoeffect by Karzas and Latter [3] who derived the corresponding transition probabilities as combinations of real hypergeometric polynomials with coefficients calculated recursively. Shafer and Bersohn [1] obtained similar results by different methods. Time reversal allows the translation of these results to the DRR process.

Extensive calculations in the nonrelativistic (conventional) dipole approximation are given in a recent paper by Aaron et al. [4], who represented the total cross-sections for arbitrary \((n, l)\) hydrogenic states in terms of simple and double sums of elementary functions of the incoming electron energy. They gave many numerical results for various atomic numbers \(Z\), pointing out the good agreement between the nonrelativistic results for the total atomic cross sections and the relativistic ones obtained by Kim and Pratt [5] for a rather large domain of incoming electron energies.

The studies of the dynamical group SO\((4, 2)\) for the hydrogen atom lead to the representation of the position and momentum operators in terms of generators and elements of this group. In this way, one obtains recursive methods for calculating electromagnetic transition probabilities within the nonrelativistic conventional dipole approximation [6].

In the same approximation Baratella et al. [7] reduced this problem to the exact calculation of four Gauss hypergeometric functions \(\,_{2}F_{1}\). After expressing the hypergeometric functions in terms of Jacobi polynomials, the numerical values were obtained recursively (for successive values of \(l\) at given \(n\)).

In this paper we will show that the DRR matrix elements and cross-sections for both parabolic and spherical states of completely ionized atoms may be expressed in terms of a set of real functions \(Y_j, j = 0, 1, 2, \ldots\) which are related to hypergeometric polynomials. The functions \(Y_j\) satisfy quite simple real three-term recursion relations. A brief announcement of this appeared in [8]. The use of the recursive method allows fast and accurate computations of the cross-sections. We will show that this method is faster and more efficient, using machine resources in an economic way, for both numeric and symbolic calculations. For illustrating the advantages of our method we studied the energy dependence of the branching ratios for the populations of the parabolic subshells with the same principal quantum number \(n\). We give the angular distributions of the photons emitted by recombination of electrons with various energies on parabolic and spherical states. Also given are expressions for the Gaunt factor and a comparison of the exact values obtained by our method and by the asymptotic expression derived in [9] establishing its precision and validity domain. As an additional test we calculated analytic expressions (using REDUCE) and numeric values for cross-sections obtaining excellent agreement with published ones.

2. Matrix Elements and Recursion Relations for Parabolic States

Within the electric dipole approximation the matrix element for the transition from the state \(|\kappa\rangle\) of the continuous spectrum to the parabolic bound state \(|\nu, m\rangle = |n, n_1, n_2, m\rangle\) with the emission of a photon of polarization \(s\) is given by

\[
M_{\nu, m, \kappa}(s) = s \cdot \mathbf{D}(\nu, m; \kappa).
\]

\[
\mathbf{D}(\nu, m; \kappa) = -i\hbar \int d^3x \Psi^*_{\nu, m}(r) \nabla \Psi_\kappa(r)
\]

where \(\hbar \kappa = p\) is the incoming electron's momentum and \(\nu\) is a shorthand for the parabolic quantum numbers \((n; n_1, n_2)\).
The continuous spectrum wave function is [11]

\[ \Psi_\kappa(r) = N_\kappa e^{i\kappa \cdot r} F(n', 1; i\kappa r - i\kappa \cdot r) \]  

where \( n' = 1/\kappa a, \) \( a = \hbar^2/Zm_e e^2 \) is the first Bohr radius of the H-like atom with nuclear charge \( Z \), \( F(\alpha, \gamma, z) \) is the confluent hypergeometric function \( \mathbb{1}_F(1) \) and

\[ N_\kappa = \sqrt{\frac{2\pi n'}{1 - e^{-2\pi n'}}} \]

is the normalization factor [12].

Since \( |\kappa\rangle \) and \( |\nu, m\rangle \) are orthogonal we obtain

\[ D(\nu, m; \kappa) = -i\hbar N_\kappa \int d^3x \, \Psi^*_\nu, m(r)e^{i\kappa \cdot r} \nabla F(n', 1; i\kappa r - i\kappa \cdot r) \]

and noting that

\[ \nabla F(n', 1; i\kappa r - i\kappa \cdot r) = i\kappa \left( \frac{\nabla}{\kappa} - \frac{\kappa}{\kappa} \right) F'(n', 1; i\kappa r - i\kappa \cdot r), \]

\[ F'(n', 1; i\kappa r - i\kappa \cdot r) = in' F(n' + 1, 2; i\kappa r - i\kappa \cdot r), \]

the matrix element may be expressed in the following form:

\[ D(\nu, m; \kappa) = \frac{i\hbar}{a} N_\kappa \int d^3x \, \Psi^*_\nu, m(r)e^{i\kappa \cdot r} \left( \frac{\nabla}{\kappa} - \frac{\kappa}{\kappa} \right) F(n' + 1, 2; i\kappa r - i\kappa \cdot r) \]

(5)

Using the parabolic coordinates \( \xi, \eta, \varphi \),

\[ \xi = r + z, \eta = r - z, \tan \varphi = y/x \]

(6)

\[ x = \sqrt{\xi \eta \cos \varphi}, y = \sqrt{\xi \eta \sin \varphi}, z = (\xi - \eta)/2. \]

(7)

and choosing the \( z \)-axis in the direction of the incoming electron’s momentum, one obtains

\[ D(\nu, m; \kappa) = \frac{i\hbar}{2a} N_\kappa \int_0^\infty d\xi \int_0^\infty d\eta \int_0^{2\pi} d\varphi \]

\[ \Psi^*_\nu, m(\xi, \eta, \varphi)e^{(i/2)\kappa(\xi-\eta)} F(n' + 1, 2; i\kappa \eta)(e_x\sqrt{\xi \eta \cos \varphi} + e_y\sqrt{\xi \eta \sin \varphi} - e_z \eta) \]

(8)

where the bound state function is given by [11]

\[ \Psi_{\nu, m}(\xi, \eta, \varphi) = N_{\nu, m}(\eta)^{\mu/2} \exp\left[-\varepsilon \frac{\xi + \eta}{2} + im\varphi\right] F(-n_1, \mu + 1; \varepsilon \xi) F(-n_2, \mu + 1, \varepsilon \eta), \]

(9)

where

\[ N_{\nu, m} = \frac{1}{\sqrt{\pi n^2(\mu)!^2}} \left( \frac{(n_1 + \mu)!(n_2 + \mu)!}{n_1!n_2!} \right)^{1/2} n^-\mu a^{-\mu-3/2}, \]

and

\[ \varepsilon = \frac{1}{na}, \mu = |m|, n_1 + n_2 + \mu + 1 = n = 1, 2, \ldots. \]

After performing the integration over \( \varphi \) in equation (8) we see that the only nonzero matrix elements are \( D_x(\nu, \pm 1; \kappa) \), \( D_y(\nu, \pm 1; \kappa) \), and \( D_z(\nu, 0; \kappa) \) and that

\[ D_x(\nu, 1; \kappa) = D_x(\nu, -1; \kappa) = iD_y(\nu, 1; \kappa) = -iD_y(\nu, -1; \kappa). \]

(10)
The matrix elements \( D_x(\nu, 1; \kappa) \) and \( D_x(\nu, 0; \kappa) \) may be written in the following form:

\[
D_x(\nu, 1; \kappa) = \frac{i\pi \hbar}{2a} N_\kappa N_{\nu, 1} I(n_1, 2); D_x(\nu, 0; \kappa) = -\frac{i\pi \hbar}{a} N_\kappa N_{\nu, 0} I(n_1, 1) J(n_2, 1) \tag{11}
\]

where

\[
I(n_1, \gamma) = \int_0^\infty d\xi \ e^{-\lambda_i \xi} \xi^{\gamma-1} F(-n_1, \gamma; \epsilon \xi), \tag{12}
\]

\[
J(n_2, \gamma) = \int_0^\infty d\eta \ e^{-\lambda_2 \eta} \eta F(in' + 1, 2; \kappa \eta) F(-n_2, \gamma; \epsilon \eta) \tag{13}
\]

for \( \gamma = 1, 2 \) and

\[
\lambda_1 = \frac{\epsilon - i\kappa}{2}, \quad \lambda_2 = \lambda_1^*, \quad \lambda_2 = \frac{\epsilon + i\kappa}{2} \tag{14}
\]

The integral \( I(n_1, \gamma) \) is given by equation (14) of [11]

\[
\int_0^\infty dz \ e^{-\lambda z} z^\nu F(-n, \gamma; kz) = \Gamma(\nu + 1)\lambda^{-\nu - 1} F(-n, \nu + 1, \gamma; k/\lambda) \tag{15}
\]

\[
= (-1)^n \Gamma(\nu + 1)(\lambda - k)^{n-\nu + 1} \frac{d^n}{d\gamma^n} \left[ \frac{\lambda^{-\nu - 1}(\lambda - k)^{\nu - 1 + 1}}{(\gamma + n - 1)} \right].
\]

Here \( \Re(\nu) > 1, \Re(\lambda) > 0, \) so that for \( \nu = \gamma - 1, \lambda = \lambda_1, n = n_1, k = \epsilon \) we obtain

\[
I(n_1, \gamma) = \frac{(-1)^n n_1 2\Gamma(\gamma)}{(\epsilon - i\kappa)^n} \rho^{n_1} \tag{16}
\]

where

\[
\rho = \frac{\epsilon + i\kappa}{\epsilon - i\kappa}. \tag{17}
\]

In the case \( \gamma = 2 \) the integral (13) of the product of two confluent hypergeometric functions is given by equation (10) of [11] :

\[
J(\lambda, \gamma; \alpha_1, \alpha_2; \epsilon_1, \epsilon_2) = \int_0^\infty dz \ e^{-\lambda z} z^\gamma F(\alpha_1, \gamma; \epsilon_1 z) F(\alpha_2, \gamma; \epsilon_2 z) \tag{18}
\]

\[
= \frac{\Gamma(\gamma)}{\lambda^{\gamma - \alpha_1 - \alpha_2}(\lambda - \epsilon_1)^{\alpha_1}(\lambda - \epsilon_2)^{\alpha_2}} \binom{\alpha_1, \alpha_2, \gamma; \epsilon_1 \epsilon_2}{\lambda - \epsilon_1, \lambda - \epsilon_2} \tag{18}
\]

where \( \lambda = \lambda_2, \gamma = 2, \alpha_1 = \epsilon_1 z, \alpha_2 = \epsilon_2 z, \epsilon_1 = i\kappa, \epsilon_2 = \epsilon \) yielding

\[
J(n_2, 2) = \frac{4(-1)^{n_2}}{\epsilon^2 + \kappa^2} \rho^{n_2} F_1(-n_2, in' + 1, 2; 1 - \rho^2). \tag{19}
\]

Using the functional relation

\[
\gamma F(\alpha, \gamma; z) = \alpha F(\alpha + 1, \gamma + 1; z) + (\gamma - \alpha) F(\alpha, \gamma + 1; z).
\]

(see e.g. [13], Eq (6.4/6)) for \( \alpha = -n_2, \gamma = 1 \) in the integral \( J(n_2, 1) \) we obtain

\[
J(n_2, 1) = (n_2 + 1)J(n_2, 2) - n_2 J(n_2 - 1, 2) \tag{19}
\]

\[
= \frac{4(-1)^{n_2} \rho^{n_2}}{\epsilon^2 + \kappa^2} \left[ (n_2 + 1)\rho^{-n_2} F_1(-n_2, in' + 1, 2, 1 - \rho^2) + n_2 \rho^{-n_2 + 1} F_1(-n_2 + 1, in' + 1, 2; 1 - \rho^2) \right].
\]
Following [8], we introduce the functions

\[ Y_j = (j + 1) \rho^{-j} {}_2F_1(-j, in' + 1, 2; 1 - \rho^2). \quad j = -1, 0, 1, \ldots \]  

such that the integrals (13) are now given by

\[ J(n_2, 2) = \frac{4(-1)^{n_2} \rho^{in'}}{(\varepsilon^2 + \kappa^2)(n_2 + 1)} Y_{n_2}; \quad J(n_2, 1) = \frac{4(-1)^{n_2} \rho^{in'}}{(\varepsilon^2 + \kappa^2)} (Y_{n_2} + Y_{n_2 - 1}). \]  

The functions \( Y_j \) defined by equation (20) satisfy simple recursion relations. Indeed, putting \( \alpha = -j, \beta = in' + 1, \gamma = 2, z = 1 - \rho^2 \) in the recursion relation

\[ (\gamma - \alpha) {}_2F_1(\alpha - 1, \beta, \gamma; z) + [2\alpha - \gamma + (\beta - \alpha)z] {}_2F_1(\alpha, \beta, \gamma, z) + \alpha(z - 1) {}_2F_1(\alpha + 1, \beta, \gamma, z) = 0 \]

([13], Eq. (2.8/28)) and by expressing the hypergeometric functions in terms of \( Y_j \) defined in equation (20) we obtain the recursion relation

\[ Y_{j+1} = \frac{1}{j + 1} \left[ (j + 1 - in')\rho^{-1} + (j + 1 + in')\rho \right] Y_j - Y_{j-1}. \]  

The coefficients in (22) are real and it is readily seen from (20) that the initial values for these three term recursion relation are

\[ Y_{-1} = 0, \quad Y_0 = 1 \]  

such that \( Y_j \) are real functions.

Let

\[ q = \frac{1}{n'} = \kappa a. \]  

\( q^2 \) is the energy of the incoming electron divided by \( Z^2 \text{Ry} \).

Now, the recursion relation (22) may be written in the following form:

\[ Y_{j+1} = -2 \left[ 1 + \frac{2(n - j - 1)}{(j + 1)(1 + n^2q^2)} \right] Y_j - Y_{j-1} \]  

The functions \( Y_j \) are particular cases, for \( k = 1, \) of the following functions:

\[ Y_{j}^{(k)} = (j + 1) \rho^{-j} {}_2F_1(-j, in' + k, 2k; 1 - \rho^2), \]  

\( j = -1, 0, 1, \ldots, k = 1, 2, \ldots \) which satisfy the recursion relation

\[ Y_{j+1}^{(k)} = \frac{j + 2}{j + 2k} \left[ (j + k + in')\rho + (j + k - in')\rho^{-1} \right] Y_j^{(k)} - Y_{j-1}^{(k)} \]  

and the same initial conditions (23). In a forthcoming paper [10] we will show that the retardation corrections to the cross-sections may be expressed in terms of \( Y_j^{(k)} \).

Inserting (16) and (21) in equation (11), the matrix elements may be written as

\[ D_x(\nu, 1; \kappa) = \hbar \pi \sqrt{a f(n, q)} \rho^n \alpha_x(\nu). \quad D_x(\nu, 0; \kappa) = \hbar \pi \sqrt{a f(n, q)} \rho^n \alpha_z(\nu) \]  

(28)
where
\[ \alpha_x(\nu) = \frac{8\pi \nu \rho}{(1 + n^2 q^2)^2} \sqrt{\frac{n - n_2 - 1}{n_2 + 1}} Y_{n_2}. \quad a_z(\nu) = \frac{8\pi (1 + inq)}{(1 + n^2 q^2)^2} (Y_{n_2} + Y_{n_2-1}) \] (29)
and
\[ f(n, q) = \frac{(-1)^n \rho^{\text{inv}}}{\sqrt{q(1 - e^{-2\pi/q})}} \] (30)

Let us note that \( \rho^{\text{inv}} = \exp[-(2/q) \arctan(nq)] \) is a real quantity.

The results given by equation (28), derived here by a straightforward integration of (8), may be alternatively derived, as the limit for \( Q \to \kappa \), from a more general result of Đ. Belkić et al. [14, 15] who gave expressions for the matrix element
\[ D(\nu, m; \kappa, \mathbf{Q}) = -i h \int d^3 \mathbf{r} \, e^{i \mathbf{Q} \cdot \mathbf{r}} \Psi^{*}_{\nu, m} \nabla(\Psi_{\kappa} e^{-i \mathbf{K} \cdot \mathbf{r}}) \] (31)
for arbitrary values of \( \mathbf{Q} \) in terms of Lauricella hypergeometric functions of three variables.

Let us note that, although the matrix elements are complex, their phases are given by very simple expressions. The contributions from the \( \iota \) and \( 1 + inq \) factors depend only on the principal quantum number \( n \), while the factor \( \rho^{\text{inv}} \) has unit absolute value. Thus, for obtaining the cross sections for all the levels with principal quantum number \( n \) we need to compute recursively only the values of the \( n \) real functions \( Y_0, Y_1, \ldots, Y_{n-1} \).

Let us now consider the behaviour of the functions \( Y_j \) in the limiting cases of high and low energies. In the former, \( q \to \infty \), we note that the recursion relation (25) becomes
\[ Y_{j+1}|_{q=\infty} = -2Y_j|_{q=\infty} - Y_{j-1}|_{q=\infty} \] (32)
The solution of these equations, with initial conditions (23), is
\[ Y_j|_{q=\infty} = (-1)^{j+1}(j + 1) \] (33)
In the low energy limit, \( q \to 0 \), the recursion relation (25) becomes
\[ Y_{j+1}|_{q=0} = -2^{j-1} - \frac{1}{j+1} Y_j|_{q=0} - Y_{j-1}|_{q=0} \] (34)
with the solution
\[ Y_j|_{q=0} = (j + 1)F(-j; 2; 4n) \] (35)
The recursive numerical calculation of \( Y_j \) using (22) is very stable. Our method may be used for precise calculation of the cross sections for very high values of \( n \).

3. Cross Sections for Parabolic States

In non-relativistic dipole approximation the differential cross-section for DRR on the state with parabolic quantum numbers \( (\nu, m) \), for nonpolarized photons, is given by
\[ \frac{d\sigma_{\nu,m}(\kappa)}{d\Omega(k)} = \frac{1}{4\pi} \frac{r_0 \lambda_c}{\hbar^2 a} \frac{1 + n^2 q^2}{n^2 q} \sum_s |s \cdot D(\nu, m; \kappa)|^2. \] (36)
where \( \lambda_c \) is the reduced Compton wavelength and \( r_0 \) is the classical electron radius.
The sum over photon's polarizations is given by the well known formula
\[
\sum_s |s \cdot D|^2 = |D|^2 - \frac{1}{k^2} |k \cdot D|^2.
\] (37)

Introducing in equation (37) the vectorial matrix elements for \( m = 0 \) and \( 1 \),
\[
D(\nu, 0, \kappa) = e_x D_x(\nu, 0, \kappa), \quad D(\nu, \pm 1; \kappa) = (e_x \mp ie_y)D_x(\nu, \pm 1; \kappa)
\] (38)
and denoting by \( \theta \) the polar angle of the photon's momentum \( \hbar \mathbf{k} \), we obtain
\[
\sum_s |s \cdot D(\nu, 0; \kappa)|^2 = |D_x(\nu, 0; \kappa)|^2 \sin^2 \theta = \pi^2 \hbar^2 a f^2(n, q) |a_z(\nu)|^2 \sin^2 \theta,
\] (39)
\[
\sum_s |s \cdot D(\nu, \pm 1, \kappa)|^2 = |D_x(\nu, \pm 1; \kappa)|^2 (1 + \cos^2 \theta) = \pi^2 \hbar^2 a f^2(n, q) |a_z(\nu)|^2 (1 + \cos^2 \theta)
\]
where \( \alpha_x(\nu), a_z(\nu), f(n, q) \) are given by equations (29, 30).

The angular dependence of the differential cross sections may be usefully evidenced by their expansion in a series of Legendre polynomials. Defining the coefficients \( K_j(\nu, m) \) by the relation
\[
\sum_s |s \cdot D(\nu, m, \kappa)|^2 = \frac{\pi^2 \hbar^2 a}{2} \frac{n^2}{1 + n^2 q^2} f^2(n, q) \sum_j K_j(\nu, m) P_j(\cos \theta)
\] (40)
we may write
\[
\sum_s |s \cdot D(\nu, 0; \kappa)|^2 = \frac{2}{3} \pi^2 \hbar^2 a f^2(n, q) |a_z(\nu)|^2 [1 - P_2(\cos \theta)],
\] (41)
\[
\sum_s |s \cdot D(\nu, \pm 1, \kappa)|^2 = \frac{2}{3} \pi^2 \hbar^2 a f^2(n, q) |a_z(\nu)|^2 [2 + P_2(\cos \theta)].
\]
The only nonzero coefficients \( K_j(\nu, m) \) are the following
\[
K_0(\nu, 0) = \frac{4}{3} \frac{1 + n^2 q^2}{n^2} |a_z(\nu)|^2 = \frac{2^8}{3(1 + n^2 q^2)^2} (Y_{n_2} + Y_{n_2-1})^2,
\]
\[
K_2(\nu, 0) = -K_0(\nu, 0).
\] (42)
and
\[
K_0(\nu, 1) = K_0(\nu, -1) = \frac{8}{3} \frac{1 + n^2 q^2}{n^2} |a_z(\nu)|^2 = \frac{2^9}{3(1 + n^2 q^2)^3} \frac{n - n_2 - 1}{n_2 + 1} Y_{n_2},
\]
\[
K_2(\nu, 1) = K_2(\nu, -1) = \frac{1}{2} K_0(\nu, 1)
\] (43)
In terms of the coefficients \( K_j \) the differential cross-section is given by
\[
\frac{d\sigma_{\nu, m}(\kappa)}{d\Omega(k)} = \frac{\pi r_0 \lambda_c h(n, q)}{4q^2} \left[ K_0(\nu, m) + K_2(\nu, m) P_2(\cos \theta) \right]
\] (44)
where
\[
h(n, q) = \frac{e^{-(4/q)} \arctan nq}{1 - e^{-2\pi/q}}.
\] (45)
Table I. — The $K_0(\nu,m)$ coefficients, defined by equations (42, 43), written as $K_0(\nu,m) = \frac{A_0}{(1 + x^2)^{m+1}} \left[ \sum_{k \geq 1} A_k(\nu,m) \frac{1}{(1 + x^2)^k} \right]^2$. $x = nq$.

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The numerical stability of the recursive algorithm for the computation of \( Y_j \) leads to rather efficient codes for computing the cross-sections on Stark levels. Symbolic calculations (using REDUCE) are also reasonably fast for obtaining analytic results.

As a first example, we summarize in the Table I the analytic expressions of \( K_0(n, n_1, n_2, m) \) for the final states with \( n \leq 8 \) obtained by a REDUCE program [17] as functions of the variable \( x = nq \).

Finally, the cross-section \( \sigma_{\nu, m}(\kappa) \) is given by the equation

\[
\sigma_{\nu, m}(\kappa) = \frac{\pi^2 r_0 \lambda_c h(n, q)}{q^2} K_0(\nu, m). \tag{46}
\]

The differential and integrated cross-sections for the transition to the \( n \)-th shell will be given by the relations

\[
\frac{d\sigma_n(\kappa)}{d\Omega(k)} = \frac{\pi r_0 \lambda_c h(n, q)}{4q^2} [K_{0n} + K_{2n} P_2(\cos \theta)], \tag{47}
\]

and

\[
\sigma_n(\kappa) = \frac{\pi^2 r_0 \lambda_c h(n, q)}{q^2} K_{0n} \tag{48}
\]

where

\[
K_{jn} = \sum_{n_1=0}^{n-1} K_j(n, n_1, n - n_1 - 1, 0) + 2 \sum_{n_1=0}^{n-2} K_j(n; n_1, n - n_1 - 2, 1), \quad j = 1, 2. \tag{49}
\]
Fig. 1. — The reduced cross-sections $s_d$ for DRR on the Stark states $(n, n_1, n_2, m)$, equation (50), versus photon-emission angle $\theta$ for $n = 3$ and for the incident electron energy parameter $q = \sqrt{E/\text{Ry}Z^2} = 1$. The curves are labelled by the parabolic quantum numbers $n, n_1, n_2, m$.

We have chosen to give the $q$ dependence for the cross-sections divided by $r_0 \lambda_c$ and multiplied by $q^2$ because this dependence is universal (in the dipolar non-relativistic approximation). The $q^2$ factor cancels the low-energy $q^{-2}$ singularity of the cross-sections. Thus, our data may be immediately rescaled to other systems of interest, such as positronium, proton-antiproton etc.

In Figure 1 we show the data obtained by our computer program for

$$s_d(\nu, m) = \frac{q^2}{r_0 \lambda_c} \frac{d\sigma_{\nu, m}(\kappa)}{d\Omega(k)}$$

for $n = 3$. We point the reader's attention to the differences in the behaviour for $m = 0$ and $m = 1$.

As a further illustration of the efficiency of the recursive algorithm we reproduced the results of [4] for the summed cross-section on the first 100 shells, $\sigma^{(100)} = \sum_{n=1}^{100} \sigma_n$. Our code takes about 2 seconds per energy value on a 80386DX/40 MHz PC with 387 coprocessor. We also checked the numerical stability of the computation based on the equations (22, 29, 42-46) for many Stark levels. For $n \leq 100$ we compared the results of exact calculations (using 50 digits) with single- and double-precision calculations of the differential and total cross-sections. We obtain an accuracy between 5 and 6 digits in single-precision and between 12 and 14 digits in double-precision.

Based on these results, we believe that the use of parabolic states is of practical interest for fast and accurate computations of differential and integrated cross-sections on one or several $n$-shells.

Let us define the branching ratio for the population of the Stark subshells of the shell with principal quantum number $n$ as

$$p(\nu, m) = \frac{\sigma_{\nu, m}}{\sigma_n}.$$ 

In Figure 2 we give the energy dependence of the branching ratios for the $n = 4$ shell. At high energies, $q \to \infty$, the branching ratios for the states with $m = 0$ go to the same value, $p(\nu, m) \to 1/n$, while the ones for $|m| = 1$ tend to zero as $q^{-2}$. This is easily understood from the expressions for $p(\nu, m)$ in terms of $Y_j$: 
Fig. 2. — The branching ratios $p$ for the population of the Stark subshells $(n; n_1, n_2, m)$, equation (51), versus incident electron energy parameter $q = \sqrt{E/\text{RyZ}^2}$ for $n = 4$. The curves corresponding to the various subshells are labelled by the parabolic quantum numbers $n, n_1, n_2, m$.

$$p(\nu, m) = \left[\frac{2(n - n_2 - 1)}{n_2 + 1}\right]^{\left|m\right|} \left(1 + n^2 q^2\right)^{1-\left|m\right|} \frac{[Y_{n_2} + (1 - \left|m\right|)Y_{n_2-1}]^{2}}{\sum_{j=0}^{n-1} \left(1 + n^2 q^2\right)(Y_j + Y_{j-1})^2 + 4 \left(\frac{n - j - 1}{j + 1}\right) Y_j^2},$$

(52)

and by considering the limiting cases given in equations (33) and (35). At high energies the recombination takes place predominantly on the spherical $l = 0$ state, [18], and all the parabolic $m = 0$ states have the same weight in it. In the low energy limit, $q \rightarrow 0$, the branching ratios decrease with $n_1$ and increase with $n_2$. Thus the maximal value of the branching ratio is attained for the $(n, 0, n - 1, 0)$ state.

At low energies Kramers’ quasiclassical formula [19]

$$\sigma_n^{(\text{Kr})}(E) = \frac{2^5 \pi r_0 \lambda_c}{3\sqrt{3nq^2(1 + n^2 q^2)}}$$

(53)

is often used. The error of Kramers’ formula is given by the Gaunt factor $g_n(q)$:

$$\sigma_n(q) = g_n(q) \sigma_n^{(\text{Kr})}(q)$$

(54)

which, by using (48), is obtained as

$$g_n(q) = \frac{8\sqrt{3}\pi n h(n, q)}{(1 + n^2 q^2)^2} \sum_{n_2=0}^{n-1} \left[(1 + n^2 q^2)(Y_{n_2} + Y_{n_2-1})^2 + 4 \left(\frac{n - n_2 - 1}{n_2 + 1}\right) Y_{n_2}^2\right].$$

(55)

Using the generalized steepest descent approach [20, 21] of Vrejoiu et al. (1), an asymptotic expression for the Gaunt factor was obtained in [9]

$$g_n^{(a)}(q) = 1 - A_n(q) - B_n(q) + 2A_n(q)B_n(q),$$

(56)

(1) This also was done by Campbell et al. [22].
Fig. 3. — The relative errors $\varepsilon_n(n;q)$, equation (60), of the asymptotic Gaunt factor $g_n^{(a)}(q)$, (Eqs. 56-59), versus incident electron energy parameter $q = \sqrt{E/\text{Ry}Z^2}$ for various values of the principal quantum number $n = 1, n = 2, n \geq 3$.

where

$$\omega = \frac{1 + n^2 q^2}{n^2}, \quad E = q^2 \quad (57)$$

$$A_n(E) = 0.172825 \omega^{-2/3} (n^{-2} - E), \quad (58)$$

$$B_n(E) = 0.033060 \omega^{-4/3} (E^2 - \omega E + 1.5 \omega^2). \quad (59)$$

In Figure 3 the relative error

$$\varepsilon_n(n;q) = 100 \times \frac{g_n^{(a)}(q) - g_n(q)}{g_n(q)} \quad (60)$$

of the asymptotic Gaunt factor (56-59) is plotted against the energy-parameter $q$ for $n = 1, 2, 3$ and $\infty$. Although the theoretical domain of applicability of (56-59) is low energies and high $n$, we may see that even for $n = 1$ the relative error does not exceed 1% for $q \leq 1.5$.

4. Matrix Elements and Cross Sections for Spherical States

The matrix elements for the transitions to the spherical states are obtained by using the expansions of the spherical hydrogen-like wave functions $\Psi_{n_1,n_2}(r, \theta, \varphi)$ in terms of the corresponding parabolic hydrogen-like wave functions.

$$\Psi_{n_1,n_2}(r, \theta, \varphi) = \sum_{n_1,n_2} A_{n_1,n_2}^{n_1,n_2} \Psi_{n_1,n_2,m}(\xi, \eta, \varphi). \quad (61)$$

Tarter [23] has expressed the coefficients $A_{n_1,n_2}^{n_1,n_2}$ in terms of the generalized hypergeometric function

$$\binom{\alpha_1, \ldots, \alpha_m}{\beta_1, \ldots, \beta_q} x^n = \sum_{n=0}^{\infty} \frac{(\alpha_1) \ldots (\alpha_p) x^n}{(\beta_1) \ldots (\beta_q) n!} \quad (62)$$
and for $m \geq 0$

$$A_{n_{1}, n_{2}, m}^{n_{1}, n_{2}} = (-1)^{l-m} \frac{(n-m-1)!}{m!} \sqrt{\frac{(2l+1)(l+m)!}{(n+n_1+n_2)!}} \frac{(l-m)!(n_1+m)!}{(l-m)!} \frac{(n_2+m)!}{(n_1+n_2+m)!} \times \sum_{m=0}^{m-2} \frac{1}{n(n+m-1)} \rho_{n_{1}} a_{x}(n_{1}, n - n_{1} - 1) \rho_{n_{2}} a_{x}(n_{2}, n - n_{2} - 1) \rho_{n_{1}} a_{x}(n_{1}, n - n_{1} - 2) \rho_{n_{2}} a_{x}(n_{2}, n - n_{2} - 2)$$

(63)

The nonpositivity of the integer arguments $-l + m$ and $-n_2$ of $3F_2$ implies that it reduces to a polynomial of degree $N = \min(l - m, n_2) \leq n - 1$.

The matrix element for the transition to the state with the spherical quantum numbers $(n, l, m)$, $m = 0, \pm 1$, is

$$M_{n, l, m, \kappa}(s) = s \cdot \mathbf{D}(n, l, m; \kappa),$$

(64)

where the vector matrix element is

$$\mathbf{D}(n, l, m; \kappa) = -i \hbar \int d^3x \Psi^{*}_{n, l, m}(r) \nabla \Psi_{\kappa}(r).$$

(65)

Let us express it through the parabolic matrix elements computed by introducing the wave function expansions (61) in (65)

$$\mathbf{D}(n, l, m; \kappa) = -i \hbar \sum_{n_1, n_2} A_{n_{1}, n_{2}, m}^{n_{1}, n_{2}} \int d^3x \Psi^{*}_{n, l, n_{1}, n_{2}, m}(r) \nabla \Psi_{\kappa}(r)$$

(66)

$$= \sum_{n_1, n_2} A_{n_{1}, n_{2}, m}^{n_{1}, n_{2}} \mathbf{D}(n_{1}, n_{2}, m; \kappa).$$

Now, it is easy to see that the cross-sections for the transitions to the $(n, l, m)$-states are given by the relations (44, 46, 47) with the substitutions

$$a_{x}(n_{1}, n_{2}) \rightarrow \tilde{a}_{x}(n, l) = \sum_{n_1=0}^{n-1} A_{n_{1}, l, 0}^{n_{1}, n_{2}, n_{2}} \rho_{n_{1}} a_{x}(n_{1}, n - n_{1} - 1)$$

(67)

$$= \sum_{n_1=0}^{n-1} A_{n_{1}, l, 0}^{n_{1}, n_{2}, n_{2}} \rho_{n_{1}} a_{x}(n_{1}, n - n_{1} - 1) \rho_{n_{2}} a_{x}(n_{2}, n - n_{2} - 1) \rho_{n_{1}} a_{x}(n_{1}, n - n_{1} - 2) \rho_{n_{2}} a_{x}(n_{2}, n - n_{2} - 2)$$

(68)

and for $m \geq 0$

$$A_{n_{1}, n_{2}, m}^{n_{1}, n_{2}} = (-1)^{l-m} \frac{(n-m-1)!}{m!} \sqrt{\frac{(2l+1)(l+m)!}{(n+n_1+n_2)!}} \frac{(l-m)!(n_1+m)!}{(l-m)!} \frac{(n_2+m)!}{(n_1+n_2+m)!} \times \sum_{m=0}^{n-2} \frac{1}{n(n+m-1)} \rho_{n_{1}} a_{x}(n_{1}, n - n_{1} - 1) \rho_{n_{2}} a_{x}(n_{2}, n - n_{2} - 1) \rho_{n_{1}} a_{x}(n_{1}, n - n_{1} - 2) \rho_{n_{2}} a_{x}(n_{2}, n - n_{2} - 2)$$

(69)

$$K_0(n; n_1, n_2, 0) \rightarrow \tilde{K}_0(n, l, 0) = \frac{4}{3} \frac{1 + n^2 q^2}{n^2} \tilde{a}_x(n_1, l)^2 \tilde{K}_2(n, l, 0) = -\tilde{K}_0(n, l, 0),$$

(70)

The differential and total cross-sections for the transitions to the $(n, l)$-states will be given by the following formulas:

$$\frac{d\sigma_{nl}}{d\Omega} = \frac{\pi r_0 \lambda \hbar(n, q)}{4q^2} \left[ \tilde{K}_0(n, l, 0) + 2 \tilde{K}_0(n, l, 1) - \left( \tilde{K}_0(n, l, 0) - \tilde{K}_0(n, l, 1) \right) P_2(\cos \theta) \right].$$

(71)
Therefore, after defining
\[ a(n, l) = \frac{1}{4} \left[ \tilde{K}_0(n, l, 0) + 2\tilde{K}_0(n, l, 1) \right], \quad b(n, l) = \frac{1}{4} \left[ \tilde{K}_0(n, l, 0) - \tilde{K}_0(n, l, 1) \right] \]  

we obtain
\[ \frac{d\sigma_{nl}}{d\Omega} = \frac{\pi r_0 \lambda_c h(n, q)}{q^2} \left[ a(n, l) - b(n, l)P_2(\cos \theta) \right] \]  

and finally,
\[ \sigma_{nl} = \frac{\pi^2 r_0 \lambda_c h(n, q)}{q^2} \left[ \tilde{K}_0(n, l, 0) + 2\tilde{K}_0(n, l, 1) \right] = \frac{4\pi^2 r_0 \lambda_c h(n, q)}{q^2} a(n, l) \]

As an illustration, we give the analytic expressions for \( a(n, l) \) and \( b(n, l) \) for \( n \leq 5 \). These expressions were obtained as functions of the variable \( x = nq \) by a symbolic program in REDUCE.

\[
\begin{align*}
    a(1, 0) &= \frac{64}{3(x^2 + 1)^2} \\
    a(2, 0) &= \frac{128(x^2 + 4)}{3(x^2 + 1)^3} \\
    a(2, 1) &= \frac{128(x^2 + 11)}{3(x^2 + 1)^4} \\
    a(3, 0) &= \frac{64(3x^2 + 7)^2(x^2 + 9)}{9(x^2 + 1)^5} \\
    a(3, 1) &= \frac{512(3x^2 + 11)^2(x^2 + 9)}{9(x^2 + 1)^6} \\
    a(4, 0) &= \frac{256(3x^2 + 18x^2 + 23)^2(x^2 + 16)}{27(x^2 + 1)^7} \\
    b(1, 0) &= a(1, 0) \\
    b(2, 0) &= a(2, 0) \\
    b(2, 1) &= \frac{1024}{3(x^2 + 1)^4} \\
    b(3, 0) &= a(3, 0) \\
    b(3, 1) &= \frac{512(7x^2 + 45)}{3(x^2 + 1)^5} \\
    b(3, 2) &= \frac{512(7x^2 + 45)}{9(x^2 + 1)^6} \\
    b(4, 0) &= a(4, 0) \\
    a(4, 1) &= \frac{256(75x^8 + 1700x^6 + 9954x^4 + 21124x^2 + 14907)}{15(x^2 + 1)^7} \\
    b(4, 2) &= \frac{2048(9x^2 + 210x^2 + 135)}{27(x^2 + 1)^7} \\
    b(4, 3) &= \frac{16384(21x^2 + 37)(x^2 + 16)(x^2 + 4)}{135(x^2 + 1)^8} \\
    b(4, 3) &= \frac{16384(3x^2 + 19)(x^2 + 16)(x^2 + 4)}{135(x^2 + 1)^8} \\
    a(5, 0) &= \frac{64(15x^6 + 165x^4 + 509x^2 + 455)^2(x^2 + 25)}{135(x^2 + 1)^9} \\
    b(5, 0) &= a(5, 0)
\end{align*}
\]
\[
\begin{align*}
\alpha(5,1) &= \frac{512(675x^{12} + 26100x^{10} + 297459x^8 + 1489344x^6 + 3689289x^4 + 4429100x^2 + 2055425)}{135(x^2 + 1)^9} \\
\beta(5,1) &= \frac{512(687x^6 + 8421x^4 + 27965x^2 + 26375)(15x^4 + 66x^2 + 67)}{135(x^2 + 1)^9} \\
\alpha(5,2) &= \frac{1024(2205x^8 + 26754x^6 + 106010x^4 + 169534x^2 + 94955)(x^2 + 25)}{189(x^2 + 1)^9} \\
\beta(5,2) &= \frac{512(441x^8 + 16968x^6 + 100498x^4 + 201008x^2 + 130861)(x^2 + 25)}{189(x^2 + 1)^9} \\
\alpha(5,3) &= \frac{229376(3x^4 + 13x^2 + 13)(4x^2 + 25)(x^2 + 25)}{135(x^2 + 1)^9} \\
\beta(5,3) &= \frac{16384(6x^4 + 65x^2 + 101)(4x^2 + 25)(x^2 + 25)}{135(x^2 + 1)^9} \\
\alpha(5,4) &= \frac{32768(9x^2 + 25)(9x^2 + 14)(4x^2 + 25)(x^2 + 25)}{945(x^2 + 1)^{10}} \\
\beta(5,4) &= \frac{16384(9x^2 + 25)(4x^2 + 25)(3x^2 + 13)(x^2 + 25)}{945(x^2 + 1)^{10}}
\end{align*}
\]

We point out that the anisotropy parameter \(\beta_{nl}\) defined by

\[
\frac{1}{\sigma_{nl}} \frac{d\sigma_{nl}}{d\Omega} = \frac{1}{4\pi} \left[ 1 - \frac{1}{2} \beta_{nl} P_2(\cos \theta) \right]
\]

may be expressed in terms of \(a(n,l)\) and \(b(n,l)\) as

\[
\beta_{nl} = 2 \frac{b(n,l)}{a(n,l)}.
\]

The sums (67, 68) giving the transition amplitudes for spherical states in terms of the parabolic ones become rather ill conditioned for large values of \((n, l)\), especially at higher energies. The results for small \((\leq 5)\) values of \(l\) quoted in [4] may be readily reproduced. For higher Rydberg states the accuracy of even double precision calculations decreases (for a given \(n\)) when the quantum number \(l\) increases. Thus, for \(q = 0.1\) we obtain 9 digit accuracy for the \(s\) states, 7 digit accuracy for \((n, l) = (15, 14)\), 3 digits for \((n, l) = (20, 19)\); for \(n = 25, 30\) the double precision calculations have only 1 digit accuracy at \(l = 20\), respectively \(l = 25\) and worse thereafter. The precision losses increase with the incident electron energy, such that for \(q = 1\) the double precision calculations have only 1 digit accuracy at \((n, l) = (15, 13)\) and \((20, 12)\), 2 digits for \((n, l) = (25, 11)\), \((30, 11)\) and worse thereafter. This accuracy loss for Rydberg states was noted in [16] for bound-free atomic charge exchange calculations.

The effect of the numerical instability of the sums (67, 68) may be observed in the final results if we represent, for example, \(|\tilde{a}_{l}|^2\) as

\[
|\tilde{a}_{l}|^2 \sim \sum_{n_1=0}^{n-1} A_{n_1}^{n_2} (Y_{n_2} + Y_{n_2-1})^2 + 2 \sum_{n_1=0}^{n-2} \sum_{n_1'=n_1+1}^{n-1} \cos[2(n_1 - n_1')\chi] A_{n_1}^{n_1'} A_{n_1}^{n_2} (Y_{n_2} + Y_{n_2-1})(Y_{n_2} + Y_{n_2'-1}),
\]

and \(|\tilde{a}_{l}|^2\) in a similar form, where \(\chi = \arctan(nq)\). For higher \((n, l)\) levels the two terms generated by the double and single sums in (77) become of opposite signs with very close
magnitudes. The number of the first identical digits in the two terms increases quickly when \( l \rightarrow n \), yielding small results for the cross sections, and the precision degree of calculations necessary for obtaining a correct result increases too. Such, for example, for \((n,l) = (30,29)\) the two sums in (77) have opposite signs and 41 identical digits(2).

Nevertheless, as remarked in section 3 above, computing the total DRR cross-section and the angular distribution on a \( n \)-shell using the parabolic amplitudes is simpler, faster and more precise than the one using the spherical amplitudes.

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References

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(2) We thank an anonymous referee for bringing this to our attention.