# Transfer of total angular momentum and quenching of fine-structure component of a Rydberg atom in collisions with neutral particles

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A theory of thermal collisions of neutral perturbing particles with Rydberg atoms is presented. The atoms are in selectively excited states nlJ with specified values of the principal and orbital quantum numbers n and l as well as of the total angular momentum J. General equations are obtained, within the framework of the impulse approximation of the quantum theory of the angular momentum, for the cross sections of inelastic transitions  $nlJ \rightarrow n'l'J'$ , inelastic scattering  $nlJ \rightarrow nlJ$ , and J-mixing of the fine structure components,  $nlJ \rightarrow nlJ'$  with  $J = |l - \frac{1}{2}|$  and  $J' = l + \frac{1}{2}$ . These equations describe the region of weak binding of the states and can be used for arbitrary form of the electron-atom scattering amplitude  $f_{eB}(k, \theta_{kk'})$ . Simple analytic expressions are derived by a classical approach, in the scattering-length approximation, for the cross sections and rate constants of the considered processes. These expressions are valid in both the weak and strong coupling regions. The results are used to analyze the role of the J-mixing process and of the inelastic n- and l-mixing processes in the quenching of the Rydberg levels  $n^2S_{1/2}n^2P_{1/2}$  and  $n^2D_{3/2}$  of Rb and Cs atoms undergoing thermal collisions with helium atoms. Specific calculations explain quantitatively the available experimental data for the processes in question.

#### **1. INTRODUCTION**

Many theoretical and experimental studies have been made recently of various processes involving collisions of Rydberg atoms A(nl) with neutral particles (see Refs. 1 and 2 and the citations therein). In the case of thermal collisions with atomic particles, the most actively studied were the broadening and shifts of highly excited *nl* levels and quenching an ionization of Rydberg atoms in their own gas or in a buffer gas. According to the current theory<sup>3-10</sup> the quenching of Rydberg *nl* states with very small quantum defect  $\delta_l \approx 0$  is due mainly to *l*-mixing, i.e., to quasielastic  $(\Delta \varepsilon_{nl,nl'} \approx 0)$   $nl \rightarrow nl'$  transitions with change of only the orbital momentum over a large group of hydrogenlike sublevels  $nl'(l' \neq l)$  of the same energy level n [see Ref. 1, Ch. 6, for details). The quenching of isolated *nl* levels with appreciable quantum defect  $\delta_l$  (i.e., *nS*, *nP*, and *nD* levels) is the result of inelastic transitions  $nl \rightarrow n'l' (\Delta \varepsilon_{nl,n'l'} \neq 0)$  with change of both the orbital momentum  $(2 \leq l' \leq n' - 1)$  and of the principal quantum number  $n' \neq n$  (see Refs. 11–19).

A theory of inelastic *n*- and *l*-mixing was developed in the scattering-length approximation in Ref. 13 in the framework of a quasiclassical model of a Fermi pseudopotential, and in Refs. 14 and 15 on the basis of the impulse approximation and the binary approximation for atomic form factors.<sup>16</sup> Simple analytic equations were obtained for the cross sections of the inelastic transitions  $nl \rightarrow n'$  (Refs. 13 and 15) and for inelastic transitions  $(n \rightarrow n')$  between hydrogenlike levels,<sup>13,15</sup> and also for the corresponding rate constants  $K_{nn'}(T)$  (Ref. 13) and Maxwell-averaged cross sections  $\langle \sigma_{n/n'} \rangle_T$  (Ref. 13) needed for comparison with the available experimental data. The existing theory of quasielastic<sup>3-12</sup> and inelastic<sup>13,15</sup>  $nl' \rightarrow n'$  transitions makes it possible on the whole to describe successfully the results of numerous experiments on the quenching of Rydberg atomic levels nS, nP, nD, and nF in thermal collisions with inert-gas atoms (for details see Refs. 1 and 2).

A general approach to the description of the inelastic transitions  $nl \rightarrow n'$  and  $n \rightarrow n'$ , valid for an arbitrary form of the scattering amplitude  $f_{eB}(k, \theta_{kk'})$  of an electron  $e^-$  by a perturbing particle B, was formulated in Refs. 17-19 in the context of the impulse approximation<sup>17,18</sup> and on the basis of the semiclassical model of a free electron.<sup>19</sup> In Refs. 17 and 18 the results were used for a quantitative explanation of the experimental data on quenching and to cast light on the role of the inelastic transitions  $nl \rightarrow n'$  in the broadening of the Rydberg nl levels of atoms in thermal collisions with alkalimetal atoms in the ground state. It was established that in this case it is necessary in principle to take into account, beside the usually considered potential electron-atom scattering, also the presence of a  ${}^{3}P$  resonance (with energy  $E_{r}$ and width  $\Gamma_r$  of order  $10^{-2}$ – $10^{-3}$  eV on the quasidiscrete level of the corresponding negative ion (see Refs. 17, 18, 20, and 21 for details).

It should be noted that the calculation results of Refs. 17 and 18 are valid in the region where the impulse approximation is valid, i.e., at  $n \ge 25-30$  for collisions with the heavy atoms K, Rb, and Cs. In this region the cross sections for quenching<sup>17</sup> and broadening<sup>18</sup> of the *nS* levels by the inelastic transitions  $nS \rightarrow n'$  decrease monotonically as *n* increases, and exceed substantially the cross sections for elastic scattering. For the region of lower n ( $15 \le n \le 25$ ), where oscillations of widths and shifts of the Rydberg levels (initially considered in Refs. 22 and 23 assuming a very narrow resonance  $\Gamma_r \ll E_r$ ,  $E_r \sim 10^{-3}$  eV within the framework of the asymptotic theory),<sup>24</sup> an adiabatic approach was recently proposed,<sup>21</sup> based on the model of quasi-intersection of terms of the Landau–Zener type.

We note also that the main contribution to the cross section of both quasielastic and inelastic quenching of highly excited nl levels in the experimentally investigated region of n is usually made by the scattering of the perturbing particle B from the quasifree electron  $e^-$  of the atom A(nl). In many situations, however (especially for inelastic  $nl \rightarrow n'$  transitions with large energy change  $\Delta \varepsilon_{nl,n'}$ ), the decisive factor is scattering by the atomic residue A<sup>+</sup> (see, e.g., Refs. 25-28).

Many experiments have also been performed by now on collisional quenching (see Refs. 1, 29–33, and the citations therein) and shock broadening and shift of highly excited Rydberg levels of heavy alkali (K, Rb, Cs) and alkalineearth (Sr, Ba) elements with specified values of both the principal (n) and orbital (l) quantum numbers, as well as of the total angular momentum J and the spin S of the atom. These processes have been very little studied theoretically even for Rydberg states of atoms with one valence electron. Thus, for example, an analysis of transitions between fine-structure components of alkali atoms at relatively low values of n was initially carried out<sup>29,34</sup> in the framework of a simple model of quasielastic *l*-mixing,<sup>7</sup> which leads as a rule for the *J*-mixing process to results that differ substantially from the experimental data (see Refs. 29 and 33 for details).

Only recently<sup>35</sup> was a numerical calculation made for the  $n^2D_{3/2} \rightarrow n^2D_{5/2}$  J-mixing process, with  $n \gtrsim 10-15$ , for cesium atoms in inert gases, using perturbation theory and the quasiclassical Fermi pseudopotential model (see Refs. 5 and 13). In Ref. 36 there were likewise obtained simple analytic expressions for the cross sections of the transitions  $n^2P_{1/2} \rightarrow n^2P_{3/2}$  and  $n^2D_{3/2} \rightarrow n^2D_{5/2}$  in the framework of the impulse approximation (for  $f_{eB} = -L = \text{const}$ , where L is the scattering length). The results of Refs. 35 and 36, however, are valid only in the weak-coupling region and cannot describe the region of the maximum cross section and its falloff with decrease of n at low values of the principal quantum number.

For collisions of selectively excited Rydberg atoms A(nlJ) and neutral particles there is thus at present no suitable theory capable of explaining and quantitatively describing jointly the behavior of the cross sections at high, low and intermediate values of n at different values of l and J and of spin-orbit splitting energy defects  $\Delta \varepsilon_{JJ'}$ . In particular, for arbitrary form of the scattering amplitude  $f_{eB}(k, \theta_{kk'})$ , neither inelastic transitions  $nlJ \rightarrow n'l'J'$ , nor even the simpler case of purely elastic scattering have been considered.

The aim of this paper is a detailed study of inelastic and elastic collisions of neutral particles B with Rydberg atoms A(nlJ) in states with specified quantum numbers n, l, and J. The investigations reported shed light on the role of J-mixing and inelastic n- and l-mixing processes in the quenching of selectively excited fine-structure components of highly excited atoms.

The analytic approach used in this paper is based on the impulse approximation and on the quantum theory of the angular momentum in the region of large n, and on the quasiclassical approximation in the region of small and intermediate n. The equations obtained are used for actual calculations of the cross sections for J-mixing as well as for n- and l-mixing, for thermal collisions of the Rydberg atoms Rb and Cs in the states  $n^2 S_{1/2}$ ,  $n^2 P_{1/2}$  and  $n^2 D_{3/2}$  with He atoms, and to explain the available experimental data for these processes. Substantial differences between quenching of selectively excited nlJ levels and of the previously investigated case of nl states. The main point is that is that quenching of Rydberg levels with specified values of quantum numbers n, l, and J in the region with relatively small  $n \leq 15$ -20 is predominantly the result of transfer of the total angular mo-

mentum  $nlJ \rightarrow nlJ'$  without change of the orbital momentum l and of the principal quantum number n. In the region of large n, however, the n- and l-mixing processes predominate, as before. Therefore the total cross section for quenching of a selectively excited nlJ level has an entirely different dependence on the principal quantum number n than for nl-states (cf. Figs. 2 and 3). In particular, two clearly pronounced maxima can occur here at low and high values of n (see Fig. 5).

#### 2. FORMULATION OF PROBLEM

We start out from the general equation relating the cross section  $\sigma_{fi}$  of the inelastic transition  $|i\rangle \rightarrow |f\rangle$  between the initial  $|i\rangle$  and final  $|f\rangle$  states of an atom A\*\* with a scattering amplitude  $f_{fi}(\mathbf{q}',\mathbf{q})$  or with the corresponding matrix elements of the scattering amplitude  $T(\mathscr{C})$  on the energy surface<sup>11</sup>  $(\mathscr{C} = q^2/2\mu + \varepsilon_i = q'^2/2\mu + \varepsilon_f)$ :

$$\sigma_{fi} = \frac{q'}{q} \int |f_{fi}(\mathbf{q}', \mathbf{q})|^2 \, dO_{\mathbf{q}\mathbf{q}'}. \tag{1}$$

$$f_{fi}(\mathbf{q}',\mathbf{q}) = -\frac{\mu}{2\pi} \langle f | \langle \mathbf{q}' | T | \mathbf{q} \rangle | i \rangle, \quad T = V + V \mathscr{G} V. \quad (2)$$

Here  $\mathbf{q} = \mu \mathbf{v}$  and  $\mathbf{q}' = \mu v'$  are the moments of the relative motion of the particles A\*\* and B ( $\mu$  is the reduced mass),  $v = (2E/\mu)^{1/2}$  and E are respectively their initial velocity and kinetic energy;  $\mathscr{G}(\mathscr{C})$  is Green's operator, H and  $\mathscr{C}$  are the total Hamiltonian ( $H = H_0 + V$ ) and the energy of the system A\*\* + B, V is the interaction potential of the colliding particles,  $H_0 = H_A + K_{AB}$  is the zeroth-approximation Hamiltonian:

$$H_{\Lambda}|\alpha\rangle = \varepsilon_{\alpha}|\alpha\rangle, \quad |\alpha\rangle = |\psi_{\alpha}(\mathbf{r})\rangle, \quad H_{\Lambda} = -\frac{\Delta_{\mathbf{r}}}{2\mu_{e\Lambda^*}} + U(\mathbf{r}),$$
  
(3)

$$K_{AB} |\mathbf{q}\rangle = \frac{q^2}{2\mu} |\mathbf{q}\rangle, \quad |\mathbf{q}\rangle = |\exp(i\mathbf{q}\mathbf{R})\rangle, \quad K_{AB} = -\frac{\Delta_{\mathbf{R}}}{2\mu}.$$
(4)

Here  $H_A$  is the Hamiltonian of a Rydberg electron  $e^-$  with a radius vector **r** in the field U(r) of the atomic residue  $A^+$  $(U(r) \rightarrow -1/r \text{ as } r \rightarrow \infty)$ ;  $\alpha$  is the set of quantum numbers indicative of a highly excited state with energy  $\varepsilon_{\alpha}$  and wave function  $\psi_{\alpha}$  (**r**) ( $\langle \alpha | \alpha' \rangle = \delta_{\alpha \alpha'}$ ), is the kinetic-energy operator of the relative motion of the particles  $A^{**}$  and B,  $|\mathbf{q}\rangle$  is its wave eigenfunction ( $\langle \mathbf{q} | \mathbf{q}' \rangle = (2\pi)^3 \delta(\mathbf{q} - \mathbf{q}')$  and **R** is the radius vector joining the atom B with the mass center of the system  $A^+ + e^-$ .

In the case of selectively excited Rydberg levels with specified values of the quantum numbers n, l, and J (J = l + s,  $s = \frac{1}{2}$  is the electron spin), the wave functions of the initial and final states are

$$|i\rangle = |nlJM\rangle = R_{n,l}(r) Y_{JM}^{l/h}(\mathbf{n}_{r}),$$

$$|f\rangle = |n'l'J'M'\rangle = R_{n,l'}(r) Y_{J'M'}^{l'/h}(\mathbf{n}_{r}),$$
(5)

where  $R_{n_{\star},l}(r)$  is the radial part of the wave function of the highly excited atom A<sup>\*\*</sup> in the coordinate representation,  $n_{\star} = n - \delta_{lJ}$  is the effective principal quantum number.  $\delta_{lJ}$ is the quantum defect;  $Y_{JM}^{l\,1/2}(\mathbf{n}_r)$  is a spherical spinor (see Ref. 37, p. 176), and  $\mathbf{n}_r = \mathbf{r}/r$  is a unit vector defined by the angles  $\theta_r$  and  $\varphi_r$ . Thus, to calculate the cross section  $\sigma_{nlJ} n'^{I'J'}$  of a transition between fixed states nlJ and n'l'J' expression (1) must be averaged over the initial  $(M \equiv J_z)$  and summed over the final  $(M' \equiv J'_z)$  sublevels. To determine, however, the total cross section

 $\sigma_{nlj}^{el} = \sigma_{nlj}^{nlj}$ 

for the scattering of a perturbing particle B from a Rydberg atom A(*nlJ*) we separate, in accordance with the specific features of the processes investigated here and of the calculation method, the contributions  $\sigma_{nlJ}^{el} \equiv \sigma_{nlJ}^{nlJ}$  of the elastic scattering (transition  $nlJ \rightarrow nlJ$ ), of the J-mixing  $nlJ \rightarrow nlJ'$  of the structure components, and the total contribution (with  $J' \neq J$  and  $J = |l - \frac{1}{2}|$  or  $J = l + \frac{1}{2}$ ) and the main contribution  $\sigma_{nlJ}^{nl-ch}$  of all the inelastic transitions  $nlJ \rightarrow n'l'J'$  with change of the principal and orbital quantum numbers, i.e.,

$$\sigma_{nlJ}^{iol} = \sigma_{nlJ}^{el} + \sigma_{nlJ}^{inel}, \quad \sigma_{nlJ}^{inel} = \sigma_{nlJ}^{q} = \sigma_{nlJ}^{J-mix} + \sigma_{nlJ}^{n,l-ch}.$$
(6)

It is taken into account in (6) that the total contribution

$$\sigma_{nlJ}^{inel} = \sum_{n'l'J'} \sigma_{nlJ}^{n'l'J'}$$

of all the inelastic transitions  $nlJ \rightarrow n'l'J'$ , after subtraction (prime on the summation sign) the elastic-scattering cross section, determines the cross section  $\sigma_{nlJ}$  for collision quenching of the Rydberg nlJ level.

### 3. MATRIX ELEMENTS OF THE TRANSITIONS $nIJ \rightarrow n'I'J'$ AND $nIJ \rightarrow n'$ IN THE IMPULSE APPROXIMATION

The contribution of the scattering of the perturbing particle B by a quasi-free electron  $e^-$  and the residual atom A<sup>+</sup> can be calculated in the impulse approximation independently, i.e.,  $T_{imp} = T_{eB} + T_{A+B}$ . We consider here the matrix elements of the scattering operator  $T_{eB}$  $(T_{eB} = V_{eB} + V_{eB} \mathcal{T} V_{eB})$  which correspond to the potential  $V_{eB}$  of the interaction of particles  $e^-$  and B. According to the initial equation of the impulse approximation [38] we have for the quantity  $T_{fi}^{eB}(\mathbf{q}',\mathbf{q})$  [called also the scattering amplitude in the energy normalization, cf. Eq. (2)]

$$T_{fi^{eB}}(\mathbf{q}',\mathbf{q}) = \langle n'l'J'M' | \langle \mathbf{q}' | T_{eB} | \mathbf{q} \rangle | nlJM \rangle$$
  
$$= \langle G_{f}(\mathbf{p}') | t_{eB}(\mathbf{k}',\mathbf{k}) | G_{i}(\mathbf{p}) \rangle_{\mathbf{p}}$$
  
$$= \int G_{f} \cdot (\mathbf{p}') t_{eB}(\mathbf{k}',\mathbf{k}) G_{i}(\mathbf{p}) d\mathbf{p},$$
  
$$t_{eB}(\mathbf{k}',\mathbf{k}) = \langle \exp(i\mathbf{k}'\mathbf{r}_{eB}) | t_{eB} | \exp(i\mathbf{k}\mathbf{r}_{eB}) \rangle.$$
(7)

Here  $t_{eB}(\mathbf{k}',\mathbf{k})$  are the matrix elements of the two-particle operator  $t_{eB}$  for scattering of a free electron  $e^-$  by a particle B (the amplitude of the elastic electron-atom scattering in the energy normalization), while the relations between the momenta  $\mathbf{k}$ ,  $\mathbf{k}'$ ,  $\mathbf{p}$ ,  $\mathbf{p}'$  and the transferred momentum  $\mathbf{Q} = \mathbf{q} - \mathbf{q}'$  are

$$\mathbf{p}' - \mathbf{p} = \frac{M_{\Lambda^*}}{M_{\Lambda}} \mathbf{Q}, \quad \mathbf{k}' - \mathbf{k} = \frac{\mu_{eB}}{m_e} \left( \frac{M_{\Lambda^*}}{M_{\Lambda}} + \frac{m_e}{\mu} \right) \mathbf{Q},$$
$$\mathbf{k} = \frac{\mu_{eB}}{m_e} \mathbf{p} - \frac{\mu_{eB}}{\mu} \mathbf{q}.$$
(8)

If the collisions of the particles A\*\* and B are not too fast in

the entire region of interest for applications  $n \ll v^{-1}$  we can put (see Ref. 1, Ch. 8)

$$\mathbf{p} \approx \mathbf{k}, \ \mathbf{p}' \approx \mathbf{k}', \ \mathbf{k}' - \mathbf{k} \approx \mathbf{Q} = \mathbf{q} - \mathbf{q}'.$$
 (9)

The save functions of a Rydberg atom

$$G_{i}(\mathbf{p}) = g_{n_{*}i}(p) Y_{JM}^{i'_{h}}(\mathbf{n}_{p}), \quad G_{f}(\mathbf{p}') = g_{n_{*}i'}(p') Y_{J'M}^{i'_{h}}(\mathbf{n}_{p'})$$

can be written in the momentum representation in the form

$$G_{nlJM}(\mathbf{p}) = \frac{1}{(2\pi)^{\frac{1}{2}}} \int \psi_{nlJM}(\mathbf{r}) e^{-i\mathbf{p}\mathbf{r}} d\mathbf{r} = \sum_{m\sigma} C_{lm^{1}h\sigma}^{JM} G_{nlm}(p) \chi_{l\sigma}.$$
(10)

Here  $C_{lm1/2\sigma}^{M}$  are Clebsch-Gordan coefficients,  $\chi_{1/2\sigma}$  is the spin wave function  $G_{nlm}(\mathbf{p}) = g_{n \neq l}(p) Y_{lm}(\mathbf{n}_p)$ , and the radial functions  $g_{n \neq l}(p)$  and  $R_{n \neq l}(r)$  are connected by the relation

$$g_{n,l}(p) = (-i)^{l} \left(\frac{2}{\pi}\right)^{\prime h} \int_{0}^{\pi} R_{n,l}(r) j_{l}(pr) r^{2} dr, \qquad (11)$$

where  $j_l(z) = (\pi/2z)^{1/2} J_{l+1/2}(z)$  is a spherical Bessel function.

We substitute (11) in (10) and use the expansion of a spherical function of order l' + 1/2 (where  $\mathbf{k}' = \mathbf{k} + \mathbf{Q}$ ) in bipolar harmonics of rank (see Ref. 37, §5.17). We have then for the final-state wave function

$$G_{\mathbf{n}'l'\mathbf{m}'}(\mathbf{k}+\mathbf{Q}) = \exp(i\hat{\mathbf{Q}\mathbf{r}})G_{n'l'\mathbf{m}'}(\mathbf{k})$$
(12)

 $(\hat{\mathbf{r}} = i\partial/\partial \mathbf{k}$  is the momentum operator), we arrive at the expression

$$G_{n'l'm'}(\mathbf{k}+\mathbf{Q}) = (-1)^{l'} \left(\frac{2}{\pi}\right)^{\nu_{1}} \left(\frac{4\pi}{2l'+1}\right)^{\nu_{1}} \\ \times \sum_{\lambda_{1}\lambda_{2}} \sum_{\mathbf{x}_{1}\mathbf{x}_{2}} (-1)^{\lambda_{2}l\lambda_{1}-\lambda_{2}} [(2\lambda_{1}+1)(2\lambda_{2}+1)]^{\nu_{1}} \\ \times C_{\lambda_{1}0\lambda_{2}0}^{l'0} C_{\lambda_{1}\mathbf{w}_{1}\lambda_{2}\mathbf{x}_{2}} I'_{\lambda_{1}\mathbf{x}_{1}}(\mathbf{n}_{\mathbf{k}}) Y_{\lambda_{2}\mathbf{x}_{2}}(\mathbf{n}_{\mathbf{Q}}) \\ \times \int_{0}^{\infty} R_{n_{*}'l'}(r') j_{\lambda_{1}}(kr') j_{\lambda_{2}}(Qr')r'^{2} dr',$$
(13)

which is valid for k < Q. In the opposite case  $k \ge Q$  the substitution  $k \ne Q$  is necessary. With the aid of Eqs. (9)–(13) with allowance for the orthogonality relation for spherical functions,

$$\langle Y_{\lambda \varkappa}(\mathbf{n}_{\mathbf{k}}) | Y_{lm}(\mathbf{n}_{\mathbf{k}}) \rangle = \delta_{\lambda l} \delta_{\varkappa m},$$

the matrix element (7) of the scattering operator can be represented in the impulse approximation as

$$T_{fi}^{eB}(\mathbf{q}',\mathbf{q}) = (-1)^{i+l'+i} \left[ \frac{4\pi (2l+1)}{2l'+1} \right]^{\nu_{t}} \sum_{m\sigma,m'\sigma'} \sum_{\lambda x} (-1)^{\lambda} i^{\lambda}$$
$$\times (2\lambda+1)^{\nu_{t}} C_{lm\nu_{t}\sigma}^{JM} C_{l'm'\nu_{t}\sigma'}^{J'M'} C_{l0\lambda0}^{l'm'} C_{lm\lambdax}^{l'm'} Y_{\lambda x}^{*} (\mathbf{n}_{0}) \chi^{+}_{\nu_{t}\sigma'} \chi_{\nu_{t}\sigma} \Phi_{n,l,n,'l'}^{(\lambda)} (Q_{lm}) \chi_{\nu_{t}\sigma'}^{*} \chi_{\nu_{t}\sigma} \Phi_{n,l,n,'l'}^{*} (Q_{lm}) \chi_{\nu_{t}\sigma'}^{*} \chi_{\nu_{t}\sigma} \Phi_{n,l,n,'l'}^{*} (Q_{lm}) \chi_{\nu_{t}\sigma'}^{*} \chi_{\nu_{t}\sigma} \Phi_{n,l,n,'l'}^{*} (Q_{lm}) \chi_{\nu_{t}\sigma'}^{*} \chi_{\nu_{t}\sigma'}^{*} (Q_{lm}) \chi_{\nu_{t}\sigma'}^{*} \chi_{\nu_{t}\sigma'}^{*} (Q_{lm}) \chi_{\nu_{t}\sigma'}^{*} \chi_{\nu_{t}\sigma'}^{*} (Q_{lm}) \chi_{\nu_{t}\sigma'}^{*} (Q_{lm})$$

$$+1)^{\prime\prime\prime}C_{lm\prime\prime_{l\sigma}\sigma}C_{l^{\prime}m^{\prime\prime}_{l\sigma}\sigma'}C_{l0\lambda0}C_{lm\lambda\kappa}Y_{\lambda\kappa}^{*}(\mathbf{n}_{Q})\chi_{\prime\prime_{l\sigma}\sigma}^{\prime}\chi_{\prime\prime_{l\sigma}\sigma}\Phi_{n,l,n,\prime}^{(\prime\prime)}(Q).$$
(14)

The radial integral  $\Phi_{n_{\star}l,n_{\star}l'}^{(\lambda)}(Q)$  is given by

$$\Phi_{n,l,n,l'l'}^{(\lambda)}(Q) = i^{l-l'} \frac{2}{\pi} \int_{0}^{\infty} k^{2} dk \int_{0}^{\infty} k'^{2} dk' g_{n,l}(k) g_{n,l'l'}^{*}$$

$$\times (k') f_{eB}(k,k',Q) \int_{0}^{\infty} r'^{2} dr' j_{l}(kr') j_{\lambda}(Qr') j_{l'}(k'r'), \qquad (15a)$$

$$f_{eB}(k,k',Q) = -\frac{\mu_{eB}}{2\pi} t_{eB}(k,k',Q),$$

$$Q^{3} = k^{2} + k^{\prime 2} - 2kk^{\prime} \cos \theta_{kk^{\prime}}, \qquad (15b)$$

where  $\mu_{eB}$  is the reduced mass of the particles  $e^{-}$  and B (i.e.,  $\mu_{eB \approx m_e} = 1$  a.u.) and  $f_{eB}$  is the electron-atom scattering amplitude, which is generally expressed in the impulse approximation in terms of matrix elements  $t_{eB}(\mathbf{k}',\mathbf{k})$  of the twoparticle  $e^- \rightarrow B$  scattering operator both on  $(|\mathbf{k}'| \neq |\mathbf{k}|)$  and off  $(\mathbf{k} \text{ and } \mathbf{k}')$  the energy surface (see Ref. 38 for details). Just as any two function of two vectors, k, and k', the amplitude  $f_{eB}$  which is invariant to rotation of the coordinate frame depends generally speaking on the three variables  $k = |\mathbf{k}|, k' = |\mathbf{k}'|,$  and the cosine  $\cos \theta_{\mathbf{k}\mathbf{k}'}$  of the scattering angle [or the momentum transfer O, see (15b)]. We, however, shall use below (as in all calculations based on the impulse approximation), the usual amplitude of the electronatom scattering on the energy surface,  $f_{eB} = f_{eB}(k,Q)$  or k' = k $f_{eB}(k,\theta_{\mathbf{kk}'}),$ putting in (15b) and  $Q = 2k \sin(\theta_{\mathbf{k}\mathbf{k}'}/2).$ 

We express the Clebsch-Gordan coefficients in (14) in terms of 3*j* symbols and use their known properties (see, e.g., Ref. 37), and also the orthogonality relation  $\chi^+_{1/2\sigma'}\chi_{1/2\sigma} = \delta_{\sigma\sigma'}$  for spin functions. We have then for the quantity of interest

$$(2J+1)^{-1}\sum_{MM'}|T_{fi}(\mathbf{q}',\mathbf{q})|^2,$$

which determines the cross section of the  $nlJ \rightarrow n'l'J'$  transition, after summing in (14) over all the z-components of the angular momenta and after averaging over the directions of the momentum transfer,  $(1/4\pi) \int d\Omega_Q (\cdots)$ , we arrive at

$$\frac{1}{2J+1} \sum_{MM'} |T_{nlJM}^{n'l'J'M'}(\mathbf{q}',\mathbf{q}')|^{2} = (2\pi)^{2} \sum_{\lambda=|l'-l|}^{l'+l} A_{lJ,l'J'}^{(\lambda)} |\Phi_{n_{*}l,n_{*}'l'}^{(\lambda)}(Q)|^{2}.$$
(16a)

The angle coefficient  $A_{lJ,l'J'}^{(\lambda)}$  is expressed in terms of 3jand 6j symbols and has the same form as in the calculations [36] of the form factors of the transitions  $nlJ \rightarrow n'l'J'$ :

$$A_{lJ,l'J'}^{(\Lambda)} = (2l+1) (2l'+1) (2J'+1) (2\lambda+1) \\ \times \left(\frac{l' \ \bar{\lambda} \ l}{0 \ 0 \ 0}\right)^2 \left[\frac{l' \ J' \ 1/2}{J \ l \ \lambda}\right]^2.$$
(16b)

The radial integral (15a) can be written in the coordinate representation with the aid of (11) in the form

Expression (16c) acquires a particularly simple form if the amplitude  $f_{eB}$  depends only on the momentum transfer Q. In fact, taking  $f_{eB}(Q)$  outside the integral sign and using the orthogonality relation

$$\int_{0}^{\infty} j_{l}(kr) j_{l}(kr') k^{2} dk = \frac{\pi}{2} \frac{\delta(r-r')}{rr'}, \qquad (17)$$

we express  $\Phi_{n_{\bullet}l,n_{\bullet}'l'}^{(\lambda)}(Q)$  in terms of the radial matrix element  $P_{n_{\bullet}l,n_{\bullet}'l'}^{(\lambda)}(Q)$  of the spherical Bessel function for the  $nlJ \rightarrow n'l'J'$  transition

$$\Phi_{n_{*}l,n_{*}'l'}^{(\lambda)}(Q) = f_{eB}(Q) P_{n_{*}l,n_{*}'l'}^{(\lambda)}(Q), \qquad (18a)$$

$$P_{n_{*}l,n_{*}'l'}^{(\lambda)}(Q) = \langle n, l' | j_{\lambda}(Qr) | n \cdot l \rangle$$
  
=  $\int_{0}^{\infty} R_{n_{*}'l'}^{*}(r) R_{n_{*}l}(r) j_{\lambda}(Qr) r^{2} dr.$  (18b)

If the energy defect  $\Delta \varepsilon_{l'-1/2,l'+1/2}$  of the splitting of the fine-structure components of the final level n'l' with  $\mathbf{J}' = |l' \pm 1/2|$  is insignificant, one can sum over J' in (16) with the aid of the relation

$$\sum_{J'} (2J'+1) \left\{ \frac{l'}{J} \frac{J'}{l} \frac{\lambda}{\lambda} \right\}^2 - \frac{1}{2l+1}.$$
 (19)

As a result we have

$$\frac{1}{2J+1} \sum_{j',\underline{MM'}} |T_{nljM'}^{n'l'j'M'}(\mathbf{q},\mathbf{q}')|^2 = \frac{1}{2l+1} \sum_{mm'} |T_{nlm}^{n'l'}\overline{H}^{m'}(\mathbf{q},\mathbf{q}')|^2$$
$$= (2\pi)^2 \sum_{\lambda=(l'-l)}^{l'+l} B_{ll'}^{(\lambda)} |\Phi_{n_{\star}l,n_{\star}'l'}^{(\lambda)}(Q)|^2,$$
$$B_{ll'}^{(\lambda)} = (2l'+1) (2\lambda+1) \left(\frac{l'}{0} \frac{\lambda}{0} \frac{l}{0}\right)^2. \tag{20}$$

The calculation of the cross sections of the transitions  $nlJ \rightarrow n'l'$  (summed over J' = |l' + 1/2|) reduces thus in this case to a calculation of the cross sections of the transitions  $nl \rightarrow n'l'$ .

Considerable interest attaches also to calculation of the matrix elements and cross sections  $\sigma_{nlJ,n'}$  of the transitions  $nlJ \rightarrow n'$  that determine the total contribution of all the inelastic transitions  $nlJ \rightarrow n'l'J'$  of the initial level nlJ to all the degenerate sublevels n'l'J' of the final hydrogenlike level n'. In this case the spin-orbit splitting  $\Delta \varepsilon_{l'-1/2,l'+1/2}$  of the sublevels n'l'J' with  $J' = |l' \pm 1/2|$  can certainly be neglected compared with the energy defect  $\Delta \varepsilon_{nl,n'} = |\delta_l + \Delta n|/n^3$  of the transition  $nl \rightarrow n' (\Delta n = n' - n)$ . We can therefore use directly for the transitions  $nlJ \rightarrow n'$  the already available calculation results<sup>17,39</sup> of the matrix elements of the  $nl \rightarrow n'$ 

transition, summed over l'm' and averaged over m in the impulse approximation:

$$\frac{1}{2J+1} \sum_{i'j'} \sum_{MM'} |T_{niJM}^{n'i'j'M'}(\mathbf{q},\mathbf{q}')|^{2}$$

$$= \frac{1}{2l+1} \sum_{m,m'l'} |\langle G_{n'l'm'}(\mathbf{k}+\mathbf{Q})|t_{eB}(\mathbf{k}+\mathbf{Q},\mathbf{k})|G_{nim}(\mathbf{k})\rangle_{\mathbf{k}}|^{2}$$

$$= \frac{(2\pi)^{2}}{2n'^{3}Q} \int_{k_{0}(\mathbf{Q})}^{\infty} |f_{eB}(k,Q)|^{2}|g_{n,l}(k)|^{2}k \, dk,$$

$$k_{0}(Q) = \frac{\Delta \varepsilon_{nl,n'} - Q^{2}/2}{Q}.$$
(21)

4. J-MIXING OF FINE-STRUCTURE COMPONENT AND

of electron scattering by a perturbing particle

Cross section of  $n|J \rightarrow n'|'J'$  transition for arbitrary amplitude

The general impulse-approximation formula for the cross section of the transition  $nlJ \rightarrow n'l'J'$  can be written, with the aid of the expression  $dO_{qq'} = d\varphi_{qq'}QdQ/qq'$  for the scattering solid angle in (1) and of the relation (16a), after inte-

**ELASTIC SCATTERING** 

4.1. Weak-coupling region

gration over  $d\varphi_{qq'}$  in the form

and the quantity  $\Phi_{n_{*}l,n_{*}l'}^{(\lambda)}(Q)$  is determined in the impulse representation by expression (15a) in which one must put  $n_{*} = n - \delta_{lJ}$  and  $t'_{*} = n' - \delta_{l'J'}$ . For the cross section of the transition  $nl \rightarrow n'l'$  we get similarly with the aid of

$$\sigma_{nl,n'l'}(v) = \frac{2\pi}{v^2} \sum_{\lambda=|l'-l|}^{l'+l} B_{ll'}^{(\lambda)} \int_{Q_{mln}}^{Q_{max}} |\Phi_{n_{\star}l,n_{\star}'l'}^{(\lambda)}(Q)|^2 Q \, dQ,$$
(22b)

where, however,  $Q_{\min} \approx |\Delta \varepsilon_{nl,n'l'}|v$ , while in the expression for the radial integral (15a) the effective quantum numbers of the initial and final states are equal respectively to  $n_{\star} = n - \delta_l$  and  $n'_{\star} = n' - \delta_{l'}$ .

For the transitions  $nlJ \rightarrow n'l'J'$  considered here, without change of the principal and orbital quantum numbers *n* and *l*, the angular coefficients  $A_{IJ,IJ'}^{(\lambda)}$  differ from zero only for even values  $\lambda = 2s$ , where s = 0, 1, 2, ... Calculation using (16b) leads then to the following result for the *J*-mixing process  $(J' \neq J, J = l - 1/2 \Rightarrow J' = l + 1/2)$ :

$$A_{ls,ls'}^{(2s)} = \frac{s(2s+1)(4s+1)(2l-2s)!}{l(2l+2s+1)!} \left(\frac{(2s)!(l+s)!}{(l-s)!(s!)^2}\right)^2,$$

$$A_{ls',ls'}^{(2*)} = \frac{2l}{2l+2} A_{ls,ls'}^{(2*)}.$$
 (23a)

(22a)

where

$$Q_{\min} = |q'-q| \simeq |\Delta \varepsilon_{n/J}^{n'/J'}|/v, \quad Q_{\max} = q' + q \approx 2\mu v,$$

 $\sigma_{ntr}^{n't'r'}(v) = \frac{2\pi}{v^3} \sum_{j=1,\dots,n}^{t'+t} A_{tr,t'r'}^{(b)} \int_{0}^{0} \sigma_{nr}^{(b)} |\Phi_{n,t,n,r't'}^{(b)}(Q)|^2 Q \, dQ,$ 

Here  $l \neq 0$ , since the s-state undergo no spin-orbit splitting. It is seen also that for arbitrary  $l \ge 1$  and  $J' \ne J$  the coefficient  $A_{IJ,IJ'}^{(2s)} = 0$  for s = 0. For the case of elastic scattering (J' = J) we obtain similarly

$$A_{lJ,lJ}^{(2s)} = \begin{cases} \frac{(4s+1)(2l+2s+1)(2l-2s)(2l-2s)!}{2l(2l+2s+1)!} \left(\frac{(2s)!(l+s)!}{(l-s)!(s!)^2}\right)^2, & J = l^{-1}/2, \ l \neq 0, \\ \frac{(4s+1)(2l+2s+2)(2l-2s+1)(2l-2s)!}{(2l+2)(2l+2s+1)!} \left(\frac{(2s)!(l+s)!}{(l-s)!(s!)^2}\right)^2, & J = l^{+1}/2. \end{cases}$$
(23b)

The values of the coefficients  $A_{U,U}^{(2s)}$  for the s, p, and d levels are listed in Table I.

For an arbitrary form of the scattering amplitude  $f_{eB}(k,Q)$ , the cross section  $\sigma_{nS_{1/2}}^{el} = \sigma_{n01/2}^{n01/2}$  for elastic scattering of a perturbing particles B by an atom A\*\* in the  $n^2S_{1/2}$  state has the simplest form. A contribution is made to (22a) by only one term with  $\lambda = 2s = 0$  (with  $A_{S_{1/2},S_{1/2}}^{(0)} = 1$ ), and the integral over dr' in (15a) can be calculated analytically. The result is

$$\sigma_{ns_{y_{i}}}^{*l}(v) = \frac{2\pi}{v^{2}} \int_{0}^{\infty} |\Phi_{n,0,n,0}^{(0)}(Q)|^{2} Q \, dQ, \qquad (24)$$

$$\Phi_{n,0,n,0}^{(0)}(Q) = \frac{1}{2Q} \int_{0}^{\infty} k \, dk f_{0B}(k,Q) g_{n,0}(k) \int_{|k-Q|}^{k+Q} k' \, dk' g_{n,0}^{*}(k').$$
(25)

Substituting in (25) the known expression for the radial wave function  $g_{n0}(k)$  of the hydrogenlike *ns* state:

$$g_{nn}(k) = \frac{4n^2}{(1+n^2k^2)^2} \frac{\sin[n\beta(k)]}{\sin[\beta(k)]},$$
  
$$\beta(k) = \arccos\left(\frac{n^2k^2 - 1}{n^2k^2 + 1}\right).$$
 (26)

TABLE I. Calculated angular coefficients  $A_{IJ,IJ}^{(\lambda)}$  [see (23) for  $\lambda = 2s, 0 \le s \le 1$ ] and of the quantities  $C_{IJ}^{(h)} = \xi_{IJ}^{(h)}$  ( $\nu = 0$ ) [see (30c)] determining the cross sections for J-mixing  $(nIJ \rightarrow nIJ', J' \ne J)$  and elastic scattering  $nIJ \rightarrow nIJ$  in s-, p-, and d-states. The values of  $C_{II}$  and  $B_{II}^{(\lambda)}$  [Eq. (31c)], calculated in Ref. 8 for  $nI \rightarrow nI$  transitions are shown for comparison.

ı	Transition	Elastic scattering $(J' = J)$	J-missing $(J' \neq J)$
8	$n^{\mathfrak{s}}S_{1_{\mathfrak{s}}} \rightarrow n^{\mathfrak{s}}S_{1_{\mathfrak{s}}}$	$A_{S_{1_4}, S_{1_4}}^{(0)} = 1, \ C_{1_4, 1_4}^{(a)} = 0,583$	
	$ns \rightarrow ns$	$B_{ss}^{(0)} = 1, \ C_{ss} = C_{y_2}^{(s)}, \ y_3} = 0,583$	
P	$n^{a}P_{J} \rightarrow n^{a}P_{J},$	$A_{P_{1_{4}}}^{(0)}, P_{1_{4}} = 1, \ A_{P_{1_{4}}}^{(2)}, P_{1_{4}} = 0$ $A_{P_{2_{1_{4}}}}^{(0)}, P_{3_{1_{4}}} = 1, \ A_{P_{4_{5}}}^{(2)}, P_{4_{5}} = 1$ $C_{1_{4_{4}}}^{(p)}, I_{2} = 0,583, \ C_{4_{1_{4}}}^{(p)}, I_{2} = 0,808$	$A_{P_{4_{4}}, P_{4_{1}}}^{(0)} = 0, \ A_{P_{4_{4}}, P_{4_{4}}}^{(2)} = 2$ $A_{P_{4_{4}}, P_{4_{4}}}^{(0)} = 0, \ A_{P_{4_{5}}, P_{4_{5}}}^{(2)} = 1$ $C_{4_{5}}^{(p)} = 0,451, \ C_{4_{5}, 4_{5}}^{(p)} = 0,226$
	np → np	$B_{pp}^{(0)} = 1, \ B_{pp}^{(2)} = 2, \ C_{pp} = \sum_{J'} C_{JJ'}^{(p)} = 1,034$	
d	$n^{\mathbf{a}}D_{J} \rightarrow n^{\mathbf{a}}D_{J},$	$A_{D_{b_{1_{s}}}, D_{s_{1_{s}}}}^{(0)} = A_{D_{s_{1_{s}}}, D_{b_{1_{s}}}}^{(2)} = 1, \ A_{D_{s_{1_{s}}}, D_{b_{1_{s}}}}^{(4)} = 0$ $A_{D_{b_{1_{s}}}, D_{b_{1_{s}}}}^{(0)} = 1, \ A_{D_{b_{1_{s}}}, D_{b_{1_{s}}}}^{(2)} = \frac{8}{7}, \ A_{D_{b_{1_{s}}}, D_{b_{1_{s}}}}^{(4)} = \frac{6}{7}$ $C_{s_{1_{s}}, s_{1_{s}}}^{(d)} = 0,808, \ C_{b_{1_{s}}, s_{1_{s}}}^{(d)} = 0,9866$	$A_{D_{b/_{s}}, D_{b/_{s}}}^{(0)} = 0, \ A_{D_{b/_{s}}, D_{b/_{s}}}^{(2)} = \frac{3}{7}, \ A_{D_{b/_{s}}, D_{b/_{s}}}^{(4)} = \frac{16}{7}$ $A_{D_{b/_{s}}, D_{b/_{s}}}^{(0)} = 0, \ A_{D_{b/_{s}}, D_{b/_{s}}}^{(2)} = \frac{3}{7}, \ A_{D_{b/_{s}}, D_{b/_{s}}}^{(4)} = \frac{12}{7}$ $C_{b/_{s}, b/_{s}}^{(d)} = 0,474, \ C_{b/_{s}, b/_{s}}^{(d)} = 0,316$
	$nd \rightarrow nd$	$B_{dd}^{(0)} = 1, \ B_{dd}^{(3)} = {}^{10}/_{7}, \ B_{dd}^{(4)} = {}^{18}/_{7}, \ C_{dd} = \sum_{J'} C_{JJ'}^{(d)} = 1,282$	

and calculating the integral over dk', we obtain

$$\Phi_{n0,n0}^{(0)}(Q) = \frac{1}{2Qn^2} \int_{0}^{\infty} f_{sB}(k,Q) \sin[n\beta(k)] \{\cos[n\gamma_1(k,Q)] -\cos[n\gamma_2(k,Q)]\} k \, dk,$$
  

$$\gamma_{1,2}(k,Q) = \arccos\left[\frac{n^2(k\pm Q)^2 - 1}{n^2(k\pm Q)^2 + 1}\right].$$
(27)

In actual calculations of arbitrary values of the angular momenta l, J, and J' the cross section of the transition  $nlJ \rightarrow nlJ'$  has a particular convenient form when the scattering amplitude  $f_{eB}$  either depends only on the transferred momentum Q or is constant. We use in this case Eqs. (18a) and (22a) as well as the results of the classical calculations<sup>8,36</sup> of the radial matrix elements (18b) for  $l \leq n$  and  $\lambda = 2s$ :

$$P_{\mathbf{n}_{lj}^{(2*)}}^{(2*)}(Q) = j_{\bullet}(n.^{2}Q)J_{\bullet}(n.^{2}Q), \qquad (28)$$

which are valid both for elastic scattering at J' = J and  $\Delta \varepsilon_{JJ} = 0$  and for transitions between fine-structure components at  $J' \neq J$  and  $\Delta \varepsilon_{JJ'} \neq 0$  (details in Ref. 36). As a result we have

$$\sigma_{nlJ}^{nlJ'}(v) = \frac{2\pi}{v^2} \int_{|\Delta v_{JJ'}|/v}^{\infty} |f_{eB}(Q)|^2 \sum_{s=0}^{l} A_{lJ,lJ'}^{(2s)} j_{*}^{2}(n_{*}^{2}Q) \times J_{*}^{2}(n_{*}^{2}Q) Q \, dQ, \qquad (29)$$

where  $J_s(z)$  is a Bessel function of integer order, and  $j_s(z) = (\pi/2z)^{1/2} J_{s+1/2}(z)$ .

#### Scattering-length approximation

In the scattering-length approximation  $(f_{eB} = -L)$ Eq. (29) leads directly to an analytic expression for the cross section  $\sigma_{nlJ}^{el}$  of elastic scattering of a perturbing particle B by a Rydberg atom A(nlJ) and for the cross section  $\sigma_{nlJ}^{J-\text{mix}}$  for J-mixing of the fine-structure components,<sup>36</sup>

$$\mathbf{\sigma}_{nij}^{el} = \mathbf{\sigma}_{nij}^{nij} = \frac{2\pi C_{ij}^{(l)} L^3}{v^2 n^4}, \qquad (30a)$$

$$\mathbf{\sigma}_{n1J}^{J-mis} = \mathbf{\sigma}_{n1J}^{n1J'} = \frac{2\pi C_{JJ'}^{(i)}L^2}{v^2 n^4} \mathbf{\varphi}_{JJ'}^{(i)} (\mathbf{v}_{JJ'}),$$

$$v_{JJ'} = \frac{n_*^3 |\Delta \varepsilon_{JJ'}|}{v} = \frac{|\Delta \delta_{JJ'}|}{vn_*}.$$
 (30b)

Here  $C_{JJ'}^{(l)} = \xi_{JJ'}^{(l)}(0)$  are constant coefficients  $\varphi_{JJ'}^{(l)}(v_{JJ'}) = \xi_{JJ'}^{(l)}(v_{JJ'})/\xi_{JJ'}^{(l)}(0)$  is a function that determines the dependence of the J-mixing cross section on the inelasticity parameter  $v_{JJ'}$ , and  $\Delta \delta_{JJ'} = |\delta_{IJ} - \delta_{IJ'}|$  is the difference between the quantum defects. The quantity  $\xi_{JJ'}^{(l)}(v_{JJ'})$  can be represented in the form<sup>36</sup>

$$\xi_{JJ'}^{(1)}(\mathbf{v}_{JJ'}) = \sum_{s=0}^{l} A_{IJ,IJ'}^{(2s)} \int_{\mathbf{y}_{JJ'}}^{\infty} j_{s}^{2}(z) J_{s}^{2}(z) z \, dz,$$
(1) 2J+1 (1)

(30c)

 $\xi_{J'J}(v_{JJ'}) = \frac{1}{2J'+1}\xi_{JJ'}(v_{JJ'}),$ 

where we must put  $v_{JJ} = 0$  for elastic scattering (J' = J).

In the most interesting case of small  $l \ll n$  (for example, s-, p-, and d-states), a contribution is made to the sum over s in (30c) only by terms with  $s \leq l$ . The values of the corresponding coefficients  $C_{JJ'}^{(l)} \equiv \xi_{JJ'}^{(l)}(0)$  are listed in Table I, and the functions  $\varphi_{1/2,3/2}^{(p)}(\nu)$  and  $\varphi_{3/2,5/2}^{(d)}(\nu)$  as functions of the inelasticity parameter v are shown in Fig. 1 for the Jmixing processes  $n^2 P_{1/2} \leq n^2 P_{3/2}$  and  $n^2 D_{3/2} \leq n^2 D_{5/2}$ .

As seen from Fig. 1 and Eq. (30c), at  $v_{II'} \ll 1$ , (when  $\varphi_{JJ'}^{(l)}(v_{JJ'}) \approx 1$ ), the J-mixing process has a quasielastic character. The behavior of the cross section  $\sigma_{nlJ}^{J-\text{mix}}$  differs then from the elastic-scattering case (30a) only by the value of the constant coefficient. Thus, for small  $v_{II'} \ll 1$  we arrive with the aid of Eqs. (16b), (19), (20), and (30) at the following result for the total cross section of the J-mixing and elastic scattering:

$$\sigma_{nlj}^{el} + \sigma_{nlj}^{j-mix} = \sum_{j'} \sigma_{nlj'}^{nlj'} \xrightarrow{v_{jj'} \to 0} \sigma_{nl,nl} = \frac{2\pi C_{ll}L^2}{v^2 n^4}, \quad (31a)$$

$$C_{1l} = \sum_{J'=|l\pm J_{l}|} C_{JJ'}^{(l)} = \sum_{s=0}^{l} B_{ll}^{(2s)} \int_{j^{2}} (z) J_{s}^{2}(z) z \, dz,$$
  
$$B_{ll}^{(2s)} = (2l+1) (4s+1) \left( \frac{l}{0} \frac{2s}{0} \frac{l}{0} \right)^{2}.$$
 (31b)

The cross section  $\sigma_{nl}^{el} \equiv \sigma_{nl,nl}$  for elastic scattering of an atom B by a Rydberg atom A\*\* in the nl state was calculated in Ref. 8 (see also Table I for the values of  $B_{ll}^{2s}$  and  $C_{ll}$  at l = 0, 1, 2).

The inelastic character of the J-mixing process (when  $v_{II'} \ge 1$  and  $\varphi_{II'}^{(l)}(v) \ll 1$  becomes particularly important for thermal collisions of heavy atoms A(nlJ) and B, i.e., at low relative velocities v and for Rydberg atoms A\*\* with large atomic numbers Z (when the spin-orbit splitting of sublevels with  $J = l \pm 1/2$  is large).



FIG. 1. The functions  $\varphi_{1/2,3/2}^{(p)}(\nu)$  and  $\varphi_{3/2,5/2}^{(d)}(\nu)$  that determine the dependences of the transitions  $n^2 P_{1/2} = n^2 P_{3/2}$  (curve 1) and  $n^2 D_{3/2} = n^2 D_{5/2}$  (curve 2) on the value  $v_{JJ'} = n_*^2 |\Delta \varepsilon_{JJ'}| / v$  of the inelasticity parameter of the J-mixing process.

#### 4.2. Normalization of cross sections in the strong coupling region. General equation for high, low and intermediate n

Equations (22a), (29), (30), and (31) were obtained within the context of the quasi-free electron model and the impulse approximation.<sup>2)</sup> They are therefore valid for large enough  $n_* \gtrsim n_0(v)$  [see Eq. (35) below], i.e., in the region of weak coupling of states. In this region the cross sections for J-mixing and elastic scattering, calculated with the aid of these equations, turn out to be certainly smaller than the geometric cross section  $\sigma_{\text{geom}} = \pi \langle r^2 \rangle_{nl}$  of the Rydberg atom A\*\*.

We propose here a simple quasiclassical method of normalizing the cross sections (30) and (31). It makes it possible to obtain lucid analytic expressions (see (37) and (39) below) for J-mixing and elastic scattering. These expressions are valid for high  $(n_* \ge n_0)$ , sufficiently low  $(n_* \ll n_0)$ , and intermediate  $n_* \sim n_0$  values of  $n_*$ . We begin with the known equation for the cross section in the representation of the impact parameter  $\rho$ :

$$\sigma_{nlJ}^{nlJ'}(v) = 2\pi \int_{0}^{\infty} w_{nlJ}^{nlJ'}(\rho, v) \rho \, d\rho.$$
(32)

In view of the rapid exponential decrease of the wavefunctions  $R_{n_{\star}l}(r)$  in the classically forbidden regions past the turning points  $r < r_1$  and  $r < r_2$  (where  $r_1 \approx (l + 1/2)^2/2$ and  $r_2 \approx 2n_{\star}^2$  for  $l \ll n$ , the integration in (32) should in fact be carried out in the range  $0 \le \rho \le 2n^2$ . We define the transition probability  $\omega_{nlJ}^{nlJ'}$  as follows:

$$w_{nlJ}^{nlJ'}(\rho, v) = \begin{cases} w_1 = 5g_{J'}/8g = \text{const}, \\ \rho \leq \rho_0(v, n_1), \\ w_2(\rho, v) = \frac{C_{JJ'}L^2}{2v^2 n_*^6 \rho} \varphi_{JJ'}^{(l)}(v_{JJ'}), \\ \rho > \rho_0(v, n_2), \end{cases}$$
(33b)

where  $g_{J'} = 2J' + 1$  and  $g = \sum_{J} (2J + 1) = 2(2l + 1)$  are the statistical weights of the sublevel nlJ' and of the entire nllevel. The value of  $\rho_0$  is determined from the condition  $w_2(\rho_0, v) = w_1$ , i.e.,

$$\rho_0(v,n_*) = \frac{4gC_{JJ'}^{(1)}L^2}{5g_{J'}v^2n_*^6} \varphi_{JJ'}^{(1)}(v_{JJ'}). \tag{34}$$

We introduce next the principal quantum number  $n_0(v)$  in such a way that when  $n_* = n_0(v)$  the impact parameter (34) becomes equal to the radius  $r_2 \approx 2n_*^2$  of the Rydberg atom, i.e.,  $\rho_0(v, n_0) = 2n_0^2$ . As a result we obtain for the separation  $n_0(v)$  of the regions of weak  $n_* \ge n_0(v)$  and strong  $n_* \leq n_0(v)$  coupling of the states the following condition:

$$n_0^{\ 8}(v) = \frac{2}{5} \frac{g}{g_{J'}} \frac{C_{JJ'}^{(l)} L^2}{v^2} \varphi_{JJ'}^{(l)} [v_{JJ'}(n_0, v)]. \tag{35}$$

It assumes a particularly simple form when  $\varphi_{JJ'}^{(l)}(\nu) = 1$ , i.e., for elastic scattering and for J-mixing in the quasielastic limit ( $v_{II'} \ll 1$ ).

If  $n_{\star} \leq n_0(v)$  the entire integration region  $(0 \leq \rho \leq 2n_{\star}^2)$ in (32) corresponds to close coupling, i.e.,  $w_{nlJ}^{nlJ'}(\rho, v) = w_1$ ,

for in this case  $\rho_0(v, n_*) \ge 2n_*^2$ . As a result we have with the aid of (33a)

$$\sigma_{nlJ}^{nlJ'}(v) = 2\pi \int_{0}^{2n_{\star}^{*}} w_{1}\rho \,d\rho = \frac{g_{J'}}{g} \sigma_{geom}(n_{\star}) = \frac{g_{J'}}{g} \pi \langle r^{2} \rangle_{nl},$$
(36a)

where  $\langle r^2 \rangle_{nl} \approx 5n_*^4/2$  if  $l \ll n$ .

In the opposite case  $n_* > n_0(v)$ , when  $\rho_0(v, n_*) < 2n_*^2$ , it is necessary to take into account in the impact-parameter region  $\rho_0 \le \rho \le 2n_*^2$  the decrease of the transition probability  $w_2(\rho, v)$  with increase of  $\rho$  [see (33b)], i.e., use the equation

$$\sigma_{nlJ}^{nlJ'}(v) = 2\pi \int_{0}^{\rho_0(v, n_*)} w_1 \rho \, d\rho + 2\pi \int_{\rho_0(v, n_*)}^{2n_*^*} w_2(\rho, v) \, \rho \, d\rho.$$
(36b)

In the weak coupling region (large  $n_* \ge n_0(v)$ ), when  $\rho_0(v,n_*) \le 2n_*^2$  and one can put  $\rho_0 = 0$ , Eq. (36b) leads directly to the result (30) given above for the *J*-mixing or elastic-scattering cross section. This, in particular, determines the specific form of  $w_2(\rho, v)$  in Eq. (33b).

In the general case of arbitrary values of  $\rho_0 \ll 2n_*^2$ , we ultimately have after substituting (33) and (34) in (33b), evaluating the corresponding integrals, and combining the result with (36a):

$$\sigma_{n'l'}^{n'l'}(v) = \begin{cases} \frac{2J'+1}{2(2l+1)} \frac{5\pi}{2} n.^4, & n. \leq n_0(v), \end{cases}$$
(37a)

$$\left(\frac{2\pi C_{JJ'}^{(1)}L^2}{v^2 n^4} \varphi_{JJ'}^{(1)}(v_{JJ'}) \left[1 - \frac{n_0^4(v)}{2n^8}\right], \ n \ge n_0(v).$$
(37b)

It is easily seen that at  $n_* = n_0(v)$  the quantities (37a) and (37b) become equal, as do their first derivatives. Given the relative velocity  $v = (2E/\mu)^{1/2}$  the maximum cross section of the  $nlJ \rightarrow nlJ'$  transition is reached at a value  $n_* = n_*^{\max}(v)$ determined from the condition

$$\left[\frac{n_{*}^{\max}(v)}{n_{0}(v)}\right]^{8} = \frac{3}{2} \frac{1 + \left[(v_{JJ'} d\varphi_{JJ'}^{(l)} / dv_{JJ'}) / 6\varphi_{JJ'}^{(l)} (v_{JJ'})\right]_{n_{*}=n_{*}^{\max}}}{1 + \left[(v_{JJ'} d\varphi_{JJ'}^{(l)} / dv_{JJ'}) / 4\varphi_{JJ'}^{(l)} (v_{JJ'})\right]_{n_{*}=n_{*}^{\max}}},$$
(38)

For elastic scattering  $(J' = J \text{ and } v_{JJ} = 0)$  and for J mixing in the quasielastic limit  $v_{JJ'} \leq 1$  we obtain  $\left[n_{*}^{\max}(v)/n_{0}(v)\right]^{8} = 3/2$  see also relation (35) for  $\varphi_{JJ'}^{(i)}(v_{JJ'}) = 1$ .

The value of  $n_0(v)$  for J-mixing of strongly split finestructure components with large values of  $\Delta \delta_{JJ'} = |\delta_{IJ} - \delta_{IJ'}|$  and for small enough relative velocities of the colliding particles A\*\* and B (when  $v_{JJ'} \ge 1$  and  $\varphi_{JJ'}^{(l)}(v_{JJ'}) \le 1$ ) remains extraordinarily small, i.e.,  $n_0(v) \le 1$ . There is then practically no region of close coupling of the channels (37a). The cross section of the inelastic transition  $nlJ \rightarrow nlJ'$  ( $J' \ne J$ ), is therefore described in the entire region where the theory presented here is valid  $(n_{**} \ge 1)$  by expression (37b) [or (30b) if  $n_* \ge n_0(v)$ ], and its value  $\sigma_{nlJ}^{nlJ'}$  is much less than the geometric cross section  $\sigma_{\text{geom}} \approx (5\pi/2) n_{\pm}^4$  of the Rydberg atom.

For comparison with the available experimental data, the cross section (37) must be averaged over a Maxwellian velocity distribution, i.e.,  $\langle \sigma_{nlJ}^{nlJ'} \rangle_T = \langle v \sigma_{nlJ}^{nlJ'}(v) \rangle_T / \langle v \rangle_T$ , where  $\langle v \rangle_T = (8T/\pi\mu)^{1/2} = 2v_T/\pi^{1/2}$  is the average thermal velocity and  $v_T = (2T/\mu)^{1/2}$ . The cross section  $\langle \sigma_{nlJ'}^{nlJ'} \rangle_T$ of an  $nlJ \rightarrow nlJ'$  transition with excitation of a Rydberg electron  $\varepsilon_{nlJ} < \varepsilon_{nlJ'}$  is then connected with the cross section of the inverse de-excitation process  $nlJ' \rightarrow nlJ$  by the detailed balancing relation:

$$\langle \sigma_{nlJ}^{nlJ'} \rangle_T = \frac{g_{J'}}{g_J} \langle \sigma_{nlJ'}^{nlJ} \rangle_T \exp\left(-\frac{|\Delta \varepsilon_{JJ'}|}{T}\right)$$

where  $g_J = 2J + 1$  and  $g_{J'} = 2J' + 1$  are statistical weights.

In the particular case when the energy defect  $\Delta \varepsilon_{JJ'}$  of the  $nlJ \rightarrow nlJ'$  transition is insignificant, the averaged cross section  $\langle \sigma_{nJJ'}^{nJ'} \rangle_T$  can be calculated analytically. In fact, putting  $\varphi_{JJ'}^{(l)}(v_{JJ'}) = 1$  in Eqs. (35) and (37) we obtain at  $v_{JJ'} \ll 1$  for pure elastic scattering  $J' = J(v_{JJ} = 0)$ , or for Jmixing of weakly split fine-structure components  $J' \neq J$ ,

$$\langle g_{nlJ}^{nlJ'} \rangle_{T} = \left[ \frac{5(2J'+1)C_{JJ'}^{(l)}}{2l+1} \right]^{l_{h}} \frac{\pi |L|}{2v_{T}} F(\zeta),$$
 (39a)

$$F(\zeta) = \zeta^{\frac{1}{2}} \left[ E_{2}(\zeta) + \frac{1 - e^{-\zeta}}{\zeta} \right],$$
  
$$\zeta = \frac{n_{0}^{s}(v_{T})}{n^{s}} = \frac{4(2l+1)}{5(2J'+1)} \cdot \frac{C_{JJ'}^{l}L^{2}}{v_{T}^{2}n^{s}}.$$
 (39b)

Here

$$\mathbf{E}_{2}(\zeta) = \int_{1}^{\infty} \frac{\exp\left(-\zeta t\right)}{t^{2}} dt$$

is an integral exponential function of second order, and  $\zeta$  is a parameter indicative of the collision "force." The cross section (39a) reaches a maximum at  $\zeta_{max} = 0.68$ , when  $F_{max} = F(\zeta_{max}) = 0.80$ . In the regions of weak ( $\zeta \ll 1$ ) and strong ( $\zeta \gg 1$ ) coupling of the channels, the transition cross section  $\sigma_{nlJ}^{nlJ}$  varies rapidly as a function of  $n_*$  (in proportion to  $n_*^{-4}$  and  $n_*^4$ , respectively, with  $F(\zeta) \to 0$  as  $\zeta \to 0$  and  $\zeta \to \infty$ . The function  $F(\zeta)$  is therefore similar to that obtained (see Ref. 40) for the averaged cross section of the *nl*level broadening by purely elastic scattering by using a quasiclassical approach based on calculation of the phase shifts. It should also be noted that the average cross section of the transition  $nlJ \to nlJ'$  in the region of small  $n_* \ll n_*^{max}(v_T)$  and large  $n_* \gg n_*^{max}(v_T)$  values of the principal quantum number can be written (for  $v_{JJ'} \ll 1$ ) in the form

$$\int_{1}^{n(J)} \frac{2J'+1}{2(2l+1)} \frac{5\pi}{2} n^{4}, \quad n \ll n^{max}, \quad (40a)$$

$$\langle \mathfrak{g}_{nlJ}^{nlJ} \rangle_{T} = \begin{cases} 2\pi C_{JJ}^{(l)} L^{2} \\ \frac{2\pi C_{JJ}^{(l)} L^{2}}{v_{T}^{2} n^{4}}, \qquad n \gg n.^{max}. \end{cases}$$
(40b)

The use of the approach proposed here to the calculation of the cross section  $\langle \sigma_{nl}^{el} \rangle_T$  of elastic scattering  $(nl \rightarrow nl)$  transition via collision of a perturbing particle B with a quasisi-free electron  $e^{-}$  leads to the expression

$$\langle \sigma_{nl}^{el}(\mathbf{B} \rightarrow e^{-}) \rangle_{T} = \left(\frac{5C_{ll}}{2}\right)^{\frac{1}{2}} \frac{\pi |L|}{v_{T}} F(\zeta),$$
  
$$\zeta = \frac{n_{0}^{s}(v_{T})}{n^{s}} = \frac{2C_{ll}L^{2}}{5v_{T}^{2}n^{s}}$$
(41a)

(see also Eq. (31b) and Table I for the values of  $C_{ll}$ ). To determine the total elastic-scattering cross section  $\sigma_{nl}^{el} = \sigma_{nl}^{el} (B \rightarrow e^{-}) + \sigma_{nl}^{el} (B \rightarrow A^{+})$  it is necessary to add to this expression the contribution

$$\langle \sigma_{nl}^{e_{l}}(\mathbf{B} \rightarrow \mathbf{A}^{+}) \rangle_{r} = 6,46 \left(\frac{\alpha}{v_{r}}\right)^{\frac{\omega}{2}},$$

$$\sigma_{nl}^{e_{l}}(\mathbf{B} \rightarrow \mathbf{A}^{+}) = \sigma_{e_{l}}^{\mathbf{B}\mathbf{A}^{+}}(v) = 7,16 \left(\frac{\alpha}{v}\right)^{\frac{\omega}{2}},$$

$$(41b)$$

due to the competing mechanism of scattering of the perturbing particle B by the atomic residue  $A^+$  of the Rydberg atom A(nl).

It is easy to show, using the excited-electron shake-off method (see Refs. 18 and 26), that the very same expression (41b) is valid also for the contribution of the  $B \rightarrow A^+$  scattering to the cross section of the  $nlJ \rightarrow nlJ'$  transition and should be added to Eq. (39a) obtained above (at J' = J) for the contribution of  $B \rightarrow e^-$  scattering. Yet the contribution of the  $B \rightarrow A^+$  scattering to the cross section of the J-mixing process (the transition  $nlJ \rightarrow nlJ'$  at  $J' \neq J$ ) turns out to be exceedingly small at not too high values  $n_* \leq (\mu v/M_{A^+})^{-1/2}$  and can be neglected.

#### **5. RESULTS AND DISCUSSION**

The theory developed here can be used to explain and to describe quantitatively the experimental results on collision quenching of Rydberg nlJ levels with specified values of the quantum numbers n, l, and J, for atoms with one electron in excess of a filled shell. We investigate here by way of example the case of thermal collisions of heavy atoms of the alkali metals Rb\*\* with Cs\*\* with He atoms in the ground state. Reliable experimental data at high, low, and intermediate values of n are available for this purpose. The actual calculations reported here for the J-mixing as well as n- and l-mixing cross sections for  $n^2 S_{1/2} - n^2 P_{1/2}$  and  $n^2 D_{3/2}$  states identify the basic laws and the relative roles of these processes in the quenching of selectively excited components of the fine structure of "single-electron" Rydberg atoms. It should be noted that for collisions between highly excited atoms and helium atoms one can use in practically the entire range of nthe scattering-length approximation:  $f_{e,He} = -L_{He}$  $\times (L_{\rm He} = 1.19 \text{ a.u.})$  for the amplitude of the elastic electron-atom  $e^- \rightarrow$  He scattering amplitude. This makes it possible, in particular, to use clear analytic equations (37) and (39) for the J-mixing cross sections. Calculations of the Maxwell-averaged cross sections  $\langle \sigma_{nlJ,n'} \rangle_T$  of the  $nl \rightarrow n'$ transitions were made above with the aid of Eq. (38) of Ref. 13, which was derived for inelastic  $nlJ \rightarrow n'$  transitions within the framework of the quasiclassical model of the Fermi pseudopotential. It was taken into account here that by virtue of relation (21) the cross section

$$\sigma_{nlJ,n'} = \sum_{l'J'} \sigma_{nlJ}^{n'l'J'},$$

of the  $nl \rightarrow n'$  transition, summed over all the quantum numbers l' and J', is equal to the cross section of the transition  $nl \rightarrow n'$ , i.e.,  $\sigma_{nlJ,n'} = \sigma_{nl,n'}$ .

#### Thermal atomic collisions $Rb(n^2S_{1/2})$ , $Rb(n^2D_{3/2}) + He$

We consider first the thermal collisions (T = 520 K,  $v_T = (2T/\mu)^{1/2} = 6.8 \cdot 10^{-4}$  a.u.) of Rb ( $n^2 D_{3/2}$ ) atoms with helium atoms. The calculated Maxwell-averaged Jmixing cross sections  $\langle \sigma_{nD_{3/2}}^{J-\text{mix}} \rangle_T$  and of the total contribution

$$\langle \sigma_{nD_{q_1}}^{n,l-ch} \rangle_T = \sum_{n'} \langle \sigma_{nD_{q_1},n'} \rangle_T$$

of all the inelastic transitions  $n^2 D_{3/2} \rightarrow n'$  $(2 < l' \le n' - 1, J' = 3/2, 5/2)$  are shown in Fig. 2. The values  $\delta_D^{\text{Rb}} = 1.34$  and  $\delta_{D_{5/2}}^{\text{Rb}} = 0.002$  were used for the quantum defects. It follows directly from (37) that the inelasticity parameter  $v_{3/2,5/2}^{(d)} = |\Delta \delta_{3/2,5/2}^{(d)}|/v_T n_{\bullet}$  for the transition  $n^2 D_{3/2} \rightarrow n^2 D_{5/2}$  is small  $(v_{3/2,5/2}^{(d)} \le 1)$  in the entire considered range of *n* and, correspondingly,  $\varphi_{3/2,5/2}^{(d)}(v) \approx 1$  (see Fig. 1). The averaged cross section  $\langle \sigma_{nD_{3/2}}^{J-\text{mix}} \rangle_T$  (dashed curve in Fig. 2) was therefore calculated in this case using the simple analytic equation (39) corresponding to the



FIG. 2. Cross sections of thermal collisions (T = 520 K) of the atoms  $Rb(n^2D_{3/2}) + He$ . Dashed curve—calculation using Eq. (39) of the cross section  $\langle \sigma_{nD_{3/2}}^{\prime - \text{mix}} \rangle_T$  of J-mixing  $(n^2D_{3/2} \rightarrow n^2D_{3/2})$ ; dotted—total cross section  $\langle \sigma_{nD_{3/2}}^{\prime - 1} \rangle_T = \Sigma_n \langle \sigma_{nD_{3/2}} \rangle_T$  of all inelastic  $n^2D_{3/2} \rightarrow n'$  transitions, which determines the  $nD_{3/2}$ -level quenching cross section  $\langle \sigma_{nD_{3/2}}^{\prime - 1} \rangle_T \equiv \zeta \sigma_{nD_{3/2}}^{\prime - 1} \rangle_T \oplus (T = 520 \text{ K})$  and O(T = 296 K)—corresponding experimental data of Ref. 29 and of Refs. 41, 42. The dash-dot curves correspond to the contribution  $\langle \sigma_{nD_{3/2}} \rangle_T = \langle \sigma_{nD_{3/2}}^{\prime - 1} \rangle_T$  of individual inelastic  $n^2D_{3/2} \rightarrow n'$  transitions [calculated using Eq. (38) of Ref. 13]. Solid curve—total cross section  $\langle \sigma_{nD_{3/2}}^{\prime} \rangle_T = \langle \sigma_{nD_{3/2}}^{\prime - 1} \rangle_T$  for quenching a selectively excited  $n^2D_{3/2}$  level;  $\triangle(T = 520 \text{ K})$  and 30.

quasielastic limit  $v_{JJ'} \rightarrow 0$ ) of the J-mixing process (we must put here l = 2, J' = 5/2, and  $C_{3/2,5/2}^{(d)} = 0.474$ , see Table I). This equation leads to results that agree very well with the available experimental data<sup>29,30</sup> for the considered J-mixing process at low, high, and intermediate values of *n*. It follows from (39), in particular, that the maximum of the cross section  $\langle \sigma_{nD_{3/2}}^{J-\text{mix}} \rangle_T^{\text{max}} \approx 1 \cdot 10^{-13} \text{ cm}^2$  is reached at  $n_{\text{max}}^{J-\text{mix}} = 8$ . With increase of  $n > n_{\text{max}}^{J-\text{mix}}$  the cross section of the transition  $n^2 D_{3/2} \rightarrow n^2 D_{5/2}$  tends very rapidly to the asymptotic limit of weak coupling of the states:  $\langle \sigma_{nD_{3/2}}^{J-\text{mix}} \rangle_T \propto n_*^{-4}$  [more details in (30b)], recently considered in Ref. 36.

The calculated averaged cross sections  $\langle \sigma_{nD_{3/2},n'} \rangle_T$  of inelastic transitions  $n^2 D_{3/2} \to n'$  with change of the principal and orbital quantum numbers and their total contribution  $\langle \sigma_{nD_{3/2}}^{n,l-ch} \rangle_T$  for the possible values of n' are shown in Fig. 2 by dash-dot and dotted curves. It can be seen that the maximum  $\langle \sigma_{nD_{3/2}}^{n,l-ch} \rangle_T^{\max} \approx 8.8 \cdot 10^{-15} \text{ cm}^2$  of the cross section of n- and lmixing is reached at  $n_{\max}^{n,l-ch} = 22$ . The largest contribution to the cross section  $\langle \sigma_{nD_{3/2}}^{n,l-ch} \rangle_T$  is made by the transitions  $n^2 D_{3/2} \to n - 1$  and  $n^2 D_{3/2} \to n - 2$ , which have the smallest energy defects  $\Delta \varepsilon_{nD,n-1} = 0.34/n^3$  and  $\Delta \varepsilon_{nD,n-2} = 0.66/n^3$ . At large  $n \gtrsim 40-50$ , inelastic transitions  $n^2 D_{3/2} \to n'$  to other degenerate hydrogenlike sublevels n'l'J' (l' > 2) with  $n' \neq n - 1, n - 2$  become substantial.

The total quenching cross section

$$\langle \sigma_{nD_{y_1}}^{\mathfrak{c}} \rangle_T = \langle \sigma_{nD_{y_1}}^{\overline{\mathfrak{g}}-mis} \rangle_T + \langle \sigma_{nD_{y_1}}^{\mathfrak{n},t-st} \rangle_T,$$

which is determined by the total contribution of the J-mixing and n- and l-mixing, is shown by the solid curve of Fig. 2. Thus, for large  $n \gtrsim 20$  the quenching of a selectively excited  $n^2 D_{3/2}$  level is due mainly to inelastic  $n^2 D_{3/2} \rightarrow n'$  transitions with change of the principal and orbital quantum numbers, while at low  $n \le 15$  mainly to the transition  $n^2 D_{3/2} \rightarrow n^2 D_{5/2}$  with change of only the angular momentum. These processes make comparable contributions in the region  $n \sim 15-20$ .

It should be noted that this constitutes the main difference between the quenchings of the levels  $n^2 D_{3/2}$  (Fig. 2) and  $n^2 S_{1/2}$  (Fig. 3) off alkali metal atoms. In fact, since there is no spin-orbit splittings at l=0, the  $n^2S_{1/2}$  state is quenched only as a result of inelastic  $n^2 S_{1/2} \rightarrow n'$  transitions with changes of the principal and orbital quantum numbers. In view of the substantial difference between the quantum defects  $\delta_S^{\text{Rb}} = 3.15$  and  $\delta_D^{\text{Rb}} = 1.34$ , the cross sections  $\langle \sigma_{nS_{1/2}}^{n,l-ch} \rangle_T$  and  $\langle \sigma_{nD_{3/2}}^{n,l-ch} \rangle_T$  themselves and the relative roles of the individual transitions  $nlJ \rightarrow n'$  in the *n*- and *l*-mixing of the  $n^2 S_{1/2}$  and  $n^2 D_{3/2}$  levels turn out too differ significantly. In particular, the maximum value of the cross section  $\langle \sigma_{nS_{1/2}}^{n,l-ch} \rangle_T^{max} = 2 \cdot 10^{-14} \text{ cm}^2 \text{ at } n_{max}^{n,l-ch} = 18 \text{ is much higher}$ than the corresponding value  $\langle \sigma_{nD_{3/2}}^{n,l-ch} \rangle_T^{max}$  for the  $n^2 D_{3/2}$  level (cf. Figs. 2 and 3). In addition, by virtue of the small energy defect ( $\Delta \varepsilon_{nS,n-1} = 0.15/n^3$ ) of the  $n^2 S_{1/2} \rightarrow n'$  transition, its role in the quenching of  $n^2 S_{1/2}$  is particularly important (see Ref. 13 for details). However, the allowance made in the present paper for the contributions of other transitions  $n^2 S_{1/2} \rightarrow n'$  with  $n' \neq n - 3$  leads to a less sloping decrease of the cross section  $\langle \sigma_{nS_{1/2}}^q \rangle_T$  with increase of *n* in the region  $n > n_{max}$  compared with the contribution of the cross section  $\langle \sigma_{nS_{1/2},n-3} \rangle_T$ of the separate transition



FIG. 3. Cross sections  $\langle \sigma_{nS_{1/2}}^{\prime} \rangle_T = \sum_{n'} \langle \sigma_{nS_{1/2},n'} \rangle_T$  for quenching  $n^2 S_{1/2}$  levels for thermal collisions (T = 520 K) of R $(n^2 S_{1/2}) +$  He atoms (solid curves)  $\bigoplus (T = 520$  K) and  $\bigcirc (T = 296$  K) are the corresponding experimental data of Ref. 29 and of Refs. 41 and 42, respectively. The dash-dot curves correspond to the contribution of individual inelastic transitions  $n^2 S_{1/2} \rightarrow n'$  (calculated using Eq. (38) of Ref. 13).

 $n^2 S_{1/2} \rightarrow n - 3$ . This leads to a good description of the available experimental data<sup>41,42</sup> in the entire investigated range of n.

## Thermal collisions of the atoms $Cs(n^2P_{1/2})$ and $Cs(n^2D_{3/2})$ + He

We investigate now the total angular momentum transfer  $nlJ \rightarrow nlJ'$  and the *n*- and *l*-mixing for  $n^2P_{1/2}$  and  $n^2D_{3/2}$ states of Cs<sup>\*\*</sup> atoms in thermal collisions (T = 353 K,  $v_T = (2T/\mu)^{1/2} = 5.58 \cdot 10^{-4}$  a.u.) with He atoms. The quantum defects used in the calculations are  $\delta_P^{Cs} = 3.58$ ,  $\delta_{P_{1/2}}^{Cs} - \delta_{P_{3/2}}^{Cs} = 0.033 \text{ and } \delta_D^{Cs} = 2.47, \ \delta_{D_{3/2}}^{Cs} - \delta_{D_{5/2}}^{Cs} = 0.009.$ The corresponding cross sections  $\langle \sigma_{nP_{1/2}}^{J-\text{mix}} \rangle_T$  $\langle \sigma_{nD_{3/2}}^{J-\text{mix}} \rangle_T$  of the transitions  $n^2 P_{1/2} \rightarrow n^2 P_{3/2}$ and  $n^2 D_{3/2} \rightarrow n^2 D_{5/2}$ , obtained by averaging the common expression (37) over the Maxwellian distribution of the velocities, is shown by the dashed curves of Figs. 4 and 5. It is evident from Fig. 4 that in the case of J-mixing of the levels  $n^2 D_{3/2} \rightarrow n^2 D_{5/2}$  our theoretical results are in good agreement with the available experimental data, and they describe well the observed behavior of the cross sections  $\langle \sigma_{nD_{3/2}}^{J-\text{mix}} \rangle_T$ not only in the weak-coupling region at  $n \gtrsim 11-12$  (as was done in Refs. 35 and 36), but simultaneously also in the strong coupling region at  $n \sim 8-11$ , i.e., in the immediate vicinity of the maximum  $\langle \sigma_{nD_{3/2}}^{J-\text{mix}}(n=9) \rangle_T^{\text{max}} = 1.03 \cdot 10^{-13}$ cm<sup>2</sup>. There are no experimental data at present for the  $n^2 P_{1/2} \rightarrow n^2 P_{3/2}$  J-mixing of the levels of the atoms Cs<sup>\*\*</sup> in helium, so that particular interest attaches to the corresponding calculations and their comparative analysis with the case of the  $n^2 D_{3/2} \rightarrow n^2 D_{5/2}$ , transition.

The substantial differences in the behavior and values of the cross sections  $\langle \sigma_{nD_{3/2}}^{J-\text{mix}} \rangle_T$  and  $\langle \sigma_{nP_{1/2}}^{J-\text{mix}} \rangle_T$  are due primarily to the qualitatively different influence of the inelas-



FIG. 4. Total cross sections  $\langle \sigma_{nD_{3/2}}^q \rangle_T = \langle \sigma_{nD_{3/2}}^{J-\text{mix}} \rangle_T + \langle \sigma_{nD_{3/2}}^{n,l-ch} \rangle_T$  for quenching of  $n^2 D_{3/2}$  levels for thermal collisions (T = 353 K) of  $\operatorname{Cs}(n^2 D_{3/2})$  + He atoms (solid curve). Dashed curves—J-mixing cross sections for the direct  $n^2 D_{3/2} \rightarrow n^2 D_{5/2}$  (1) and inverse  $n^2 D_{5/2} \rightarrow n^2 D_{3/2}$  (2) transitions, calculated by Maxwell-averaging over the velocities in Eq. (37);  $\bigcirc (T = 353 \text{ K})$ —corresponding experimental data;<sup>33</sup> dotted—combined cross sections  $\langle \sigma_{nD_{3/2}}^{n,l} \rangle_T = \sum_{n'} \langle \sigma_{nD_{3/2}n'} \rangle_T$  of all inelastic  $n^2 D_{3/2} \rightarrow n'$  transitions, calculated from Eq. (38) of Ref. 13.

ticity parameters  $v_{3/2,5/2}^{(d)} = |\Delta \delta_{3/2,5/2}^{(d)}|/v_T n_*$  and  $v_{1/2,3/2}^{(p)} = |\Delta \delta_{1/2,3/2}^{(p)}|/v_T n_*$  in these two cases. Thus, for the collisions  $\operatorname{Cs}(n^2 D_{3/2})$  + He the value of  $v_{3/2,5/2}^{(d)}$  is small enough already at  $n \gtrsim 12$  (when  $v_{3/2,5/2}^{(d)} \lesssim 1.7$  we can put  $\varphi_{3/2,5/2}^{(d)}(v) \approx 1$ ) and leads only at  $n \sim 8-11$  to small devia-



FIG. 5. Total cross sections  $\langle \sigma_{nP_{1/2}}^q \rangle_T = \langle \sigma_{nP_{1/2}}^{J-\min} \rangle_T + \langle \sigma_{nP_{1/2}}^{n,l-ch} \rangle_T$  of  $n^{2}P_{1/2}$ -level quenching for thermal collisions (T = 353 K) of  $Cs(n^2P_{1/2})$  + He atoms (solid curve). Dashed curve—cross sections of  $(n^2P_{1/2} \rightarrow n^2P_{3/2})$ , *J*-mixing obtained by Maxwell-averaging of the velocities. Dotted—total cross sections  $\langle \sigma_{nP_{1/2}}^{n,l-ch} \rangle_T = \Sigma_n \langle \sigma_{nP_{1/2}n} \rangle_T$  of all inelastic  $n^2P_{1/2} \rightarrow n'$  transitions, calculated using Eq. (38) of Ref. 13.

tions in the behavior of the J-mixing processes from the purely quasielastic case v = 0. In fact, at n = 8, 9, 10, and 11, when  $v_{3/2,5/2}^{(d)} = 2.92, 2.47, 2.14, \text{ and } 1.89$ , we have from (30c) and from Fig. 1 respectively  $\varphi_{3/2,5/2}^{(d)}(\nu) = 0.65; 0.84;$ 0.9 and 0.94. By virtue of the appreciable increase of the energy splitting  $\Delta \varepsilon_{1/2,3/2}^{(p)}$  of the fine-structure components of the Rydberg  $n^2P$  levels compared with the corresponding value  $\Delta \varepsilon_{3/2,5/2}^{(d)}$  for  $n^2 D$  levels  $(\Delta \delta_{1/2,3/2}^{(p)} / \Delta \delta_{3/2,5/2}^{(d)} \approx 3.67)$ , the inelasticity parameter turns out to be large,  $v_{1/2,3/2}^{(p)} \ge 1$ , in practically the entire considered region of n. For example at n = 40 and n = 8 we have respectively  $v_{1/2,3/2}^{(p)}(40) = 1.62$ ,  $\varphi_{1/2,3/2}^{(p)}(\nu) = 0.85$  and  $\nu_{1/2,3/2}^{(p)}(8) = 13.4$ ,  $\varphi_{1/2,3/2}^{(p)}(\nu)$ = 0.046. This lowers substantially the cross sections for J mixing of the levels  $n^2 P_{1/2} \rightarrow n^2 P_{3/2}$  compared with the cross sections of the  $n^2 D_{3/2} \rightarrow n^2 D_{5/2}$  transition, not-withstanding the insignificant difference between the coefficients  $C_{1/2,3/2}^{(p)} = 0.451$  and  $C_{3/2,5/2}^{(d)} = 0.474$  and between the statistical weights.

The calculated cross sections  $\langle \sigma_{nlJ}^{n,l-ch} \rangle_T$  of the *n*- and *l*mixing processes for collisions of the atoms  $Cs(n^2D_{3/2})$ ,  $Cs(n^2P_{1/2}) + He$  (obtained, just as for Rb\*\* + He collisions, with allowance for the contribution of many inelastic  $nlJ \rightarrow n'$  transitions) are shown (dotted) in Figs. 4 and 5. It should be noted that by virtue of the close values of the energy defects ( $\Delta \varepsilon_{nD,n-2} = 0.47/n^3$ ,  $\Delta \varepsilon_{nD,n-3} = 0.53/n^3$  and  $\Delta \varepsilon_{nP,n-4} = 0.42/n^3$ , and  $\Delta \varepsilon_{nP,n-3} = 0.58/n^3$ ) of the most substantial transitions, the cross sections  $\langle \sigma_{nD_{3/2}}^{n,l-ch} \rangle_T$  and  $\langle \sigma_{nP_{1/2}}^{n,l-ch} \rangle_T$  turn out to be exceptionally close. The total quenching cross sections  $\langle \sigma_{nlJ}^q \rangle_T$  of the selectively excited levels  $n^2D_{3/2}$  and  $n^2P_{1/2}$  of the Cs\*\* atoms differ considerably in the region of the low values  $n \leq 20$ , where the decisive role is played by angular-momentum transfer without a change of the principal and orbital quantum numbers.

- <sup>1)</sup> We use here the atomic units  $e = m_e = \hbar = 1$ .
- <sup>2)</sup> The criteria for the applicability of the quasifree electron model and of the impulse approximation were considered in many papers for both quasielastic *l*-mixing and elastic scattering (see Ref. 1, Ch. 6-8), as well as for inelastic transitions  $nl \rightarrow n'$  and  $n \rightarrow n'$  (Refs. 13, 17, 18) and ionization<sup>39</sup> of a Rydberg atom.
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