Creation, destruction, and transfer of atomic multipole moments by electron scattering: Quantum-mechanical treatment

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(Received 19 August 2008; revised manuscript received 18 November 2008; published 29 December 2008)

Using the wave-packet propagation method of Rodberg and Thaler and the density matrix method of Fano and Blum, we have defined by completely quantum-mechanical methods the cross sections for the creation, destruction, and transfer of atomic multipole moments by both elastic and inelastic scattering of electrons by atomic targets. All cross sections obtained quantum mechanically, except for the coherence transfer cross sections, agree in form with those obtained semiclassically by Fujimoto and co-workers. We also used the converged close-coupling (CCC) method to calculate numerically some of the above cross sections for selected transitions in electron scattering from hydrogen and barium atoms.

DOI: 10.1103/PhysRevA.78.062716 PACS number(s): 34.80.Pa, 34.80.Bm, 34.80.Dp, 52.20.Hv

I. INTRODUCTION

The rates for the creation, destruction, and transfer of atomic multipole moments by heavy-particle scattering have been studied for many years by Omont [1], D'yakonov and Perel [2], and Petrashen, Rebane, and Rebane [3–6] using semiclassical scattering theory along with the straight-line trajectory assumption for the scattering particle and by Dashevskaya, Nikitin, and Umanskii [7,8] using the multitrajectory semiclassical approximation. The main interest for these studies was the relaxation of atomic multipole moments in optical pumping or in laser- or electron-beam generated plasmas where it was reviewed extensively [9–13]. With the advent of plasma polarization spectroscopy (PPS) via the work of Fujimoto and collaborators [14–16] and Kazantsev and collaborators [17–19] the same rate coefficients became of interest for electronic collisions also in order to model these anisotropic plasmas. The semiclassical straight-line trajectory approach has been adopted for electron scattering by Fujimoto *et al.* [14] and Fujimoto and Kazantsev [15]. These latter authors have given definitions of alignment creation, destruction, and transfer cross sections for both elastic and inelastic electron scattering within the semiclassical straight-line trajectory approximation. In the case of inelastic scattering Kazantsev *et al.* [17,18] gave a quantum-mechanical definition of the alignment-creation cross section which was extended recently for elastic scattering by the present authors [20]. However, in this latter work the incident electron was treated as a distinguishable particle from the target electrons and spin-orbit-coupling and other semirelativistic effects were not taken into account for the incident electron and for elastic scattering only alignment creation was discussed. The purpose of this work is to use the methods of the present authors [20] to give general definitions for both elastic and inelastic scattering for the creation, destruction, and transfer cross sections of atomic multipole moments via the use of pure quantum-mechanical methods with due consideration for electron-exchange and for semirelativistic effects on the incident electron. In order to illustrate the order of magnitude, the sign, and the energy dependence of these cross sections in some cases, the various cross sections have been calculated using the convergent close-coupling (CCC) method for electron scattering from hydrogen and barium atoms [21,22].

II. GENERAL THEORY

Let us assume first that the incident electron is a distinguishable particle. Subsequently this assumption will be removed and the possibility of electron exchange with the target electrons introduced. In our previous work we also ignored the spin-orbit coupling effect and similar quasirelativistic effects for the incident electron. (They were considered for the target electrons.) However since those effects could be important for the interpretation of spin-polarization experiments [23–27] we will include them here into the Hamiltonian for all electrons. The relevant interactions are spin-orbit coupling, mass-velocity term, and the Darwin term (see, e.g., [28,29]). We shall include all those relativistic correction terms into our Hamiltonian for all electrons. Thus we arrive at a Hamiltonian that is identical to the one postulated by Cowan [30] and also used in some *R*-matrix theory electron scattering calculations by Bartschat and Burke. (In Ref. [31] Model Hamiltonian II.) In the terminology of Scott and Burke [32] our Hamiltonian will include the nonrelativistic Hamiltonian plus the one-body relativistic corrections. (It is an approximation to the Breit-Pauli Hamiltonian where all two-body relativistic corrections are ignored.)

Thus we will assume the following Hamiltonian for the electron plus atom system ($N+1$ electrons),

$$H = \sum_{i=1}^{N+1} h(\boldsymbol{r}_i) + \sum_{i=1}^{N+1} \xi(r_i)\boldsymbol{l}_i \cdot \boldsymbol{s}_i + \sum_{i<j=1}^{N+1} \frac{1}{r_{ij}}, \tag{1}$$

where $h(\boldsymbol{r})$ is assumed to have the form

$$h(\boldsymbol{r}) = \frac{\boldsymbol{p}^2}{2m} + \frac{eZ}{r} - \frac{\boldsymbol{p}^4}{8m^3c^2} - \frac{Ze^2\hbar^2}{8m^2c^2}\delta(\boldsymbol{r}). \tag{2}$$

In Eq. (1) $\boldsymbol{r}_i$ is the position coordinate of the ith electron, $\boldsymbol{l}_i$ and $\boldsymbol{s}_i$ are the orbital angular momentum and spin operators, respectively, of the ith electron. In Eq. (2) $\boldsymbol{p}$ is the momen-

tum operator of the electron, Z is the nuclear charge, r is the distance of the electron from the nucleus, and $\delta(\boldsymbol{r})$ is the Dirac δ function. In Eq. (1) $\xi(r)$ is defined by the formula

$$\xi(r) = -\frac{Z\hbar^2 e^2}{2r^3 m^2 c^2}. \tag{3}$$

Other, more accurate or semiempirical choices for $\xi(r)$ are also possible [33,34].

We note here that the Hamiltonian H, defined by Eq. (1), is totally symmetric in all electron coordinates.

The wave-packet treatment applied in our previous work [20] is applicable in the present case also, since the effect of the Darwin term is localized to the nucleus, and since,

$$\xi(r) \to 0 \quad \text{for } r \to \infty, \tag{4}$$

and therefore the incident electron can be described by the same wave packet used in our earlier work [20] except the energy of the incident electron will be given by the formula which incorporates the mass-velocity correction,

$$E_k = \frac{\hbar^2 k^2}{2m} - \frac{\hbar^4 k^4}{8m^2 c^2}. \tag{5}$$

We will assume that an incident electron is described by the wave packet [61],

$$|\Phi_{\boldsymbol{k}_{\text{in}},m_s}\rangle = (2\pi)^{-3} \int d\boldsymbol{k} A(\boldsymbol{k}) |\boldsymbol{k},m_s\rangle \exp\left(-\frac{i}{\hbar} E_k t\right), \tag{6}$$

where $\boldsymbol{k}$ refers to the wave vector (of magnitude k) and m_s to the spin of the incident electron, E_k is the energy of the incident electron and is given by Eq. (5) and $|\boldsymbol{k},m_s\rangle$ refers to a plane-wave state with wave vector $\boldsymbol{k}$ and spin m_s normalized as

$$\langle \boldsymbol{k},m_s|\boldsymbol{k}',m_s'\rangle = (2\pi)^3 \delta(\boldsymbol{k}-\boldsymbol{k}')\delta_{m_s,m_s'}.$$

We shall assume that the $A(\boldsymbol{k})$ function is strongly peaked around the value of the $\boldsymbol{k}_{\text{in}}$ wave vector with width $\delta k \ll k_{\text{in}}$ and is normalized according to the formula,

$$(2\pi)^{-3} \int d\boldsymbol{k} |A(\boldsymbol{k})|^2 = 1. \tag{7}$$

In order for the above assumption for the incident electron wave packet to be true we need for the electron-target interaction potential to be of short range implying that either we deal with an atomic target ($Z=N$) or with an ion immersed in a plasma where the plasma screens the Coulomb potential. The spatiotemporal representation of the wave packet can be given in the form

$$\Phi(\boldsymbol{r},\sigma,t) = (2\pi)^{-3} \int d\boldsymbol{k} A(\boldsymbol{k}) \exp(i\boldsymbol{k}\cdot\boldsymbol{r}) \chi_{m_s}(\sigma) \times \exp\left(-\frac{i}{\hbar} E_k t\right), \tag{8}$$

where $\boldsymbol{r}$ is the spatial variable, σ refers to the spin variable, and $\chi_{m_s}(\sigma)$ refers to the spinfunction of the electron with spin projection m_s.

If the atomic state of energy $E_{\alpha J}$ is described by the state vector $|\alpha JM\rangle$ where J refers to the total angular momentum of the atom, M to its projection along the z axis (the direction of the incidence of the electron), and α refers to all other quantum numbers, then the initial (noninteracting) electron plus atom system is described by the state vector,

$$|\Phi_{\alpha JM,\boldsymbol{k}_{\text{in}},m_s}\rangle = (2\pi)^{-3} \int d\boldsymbol{k} A(\boldsymbol{k}) |\boldsymbol{k},m_s\rangle |\alpha JM\rangle \times \exp\left(-\frac{i}{\hbar} E_k^{\alpha J} t\right), \tag{9}$$

where $E_k^{\alpha J} = E_k + E_{\alpha J}$ is the total energy of the electron plus atom system.

We shall now let the incident electron interact with the target (the atom), and we look at the sytem in the asymptotic future. First we shall introduce the notation for the noninteracting electron plus atom states,

$$|\boldsymbol{k}m_s;\alpha JM\rangle = |\boldsymbol{k}m_s\rangle |\alpha JM\rangle. \tag{10}$$

We can then use the completeness of the $|\boldsymbol{k}_1' m_s';\alpha JM\rangle$ basis set in the form

$$\mathcal{S}|\boldsymbol{k}_1 m_s;\alpha JM\rangle = (2\pi)^{-3} \sum_{\alpha' J' M'} \sum_{m_s'} \int d\boldsymbol{k}_1' |\boldsymbol{k}_1' m_s';\alpha' J' M'\rangle \times \langle \boldsymbol{k}_1' m_s';\alpha' J' M'|\mathcal{S}|\boldsymbol{k}_1 m_s;\alpha JM\rangle,$$

where $\mathcal{S}$ is the scattering operator, as defined, e.g., by Rodberg and Thaler [35], Chap. 7. We then obtain for the state vector of the electron-plus-atom system in the asymptotic future the form

$$|\Phi(t)\rangle_{\text{out}} = (2\pi)^{-6} \int d\boldsymbol{k}_1 A(\boldsymbol{k}_1) \exp\left(-\frac{i}{\hbar} E_{k_1}^{\alpha J} t\right) \times \int d\boldsymbol{k}_1' \sum_{\alpha' J' M'} \sum_{m_s'} \langle \boldsymbol{k}_1' m_s';\alpha' J' M'|\mathcal{S}|\boldsymbol{k}_1 m_s;\alpha JM\rangle \times |\boldsymbol{k}_1', m_s';\alpha' J' M'\rangle. \tag{11}$$

Let us assume that the initial atomic state is described by the density operator

$$\boldsymbol{\rho}^{\text{in}} = |\alpha JM'\rangle\langle \alpha JM|. \tag{12}$$

If we denote by $|\Phi(t)\rangle_{\text{out}}$ [$|\Phi'(t)\rangle_{\text{out}}$] the state vector at time t in the asymptotic future that evolved from the $|\boldsymbol{k}_1 m_s;\alpha JM\rangle$ ($|\mathbf{k}_1' m_s';\alpha' J' M'\rangle$) initial state of the atom-plus-electron system, then

$$\boldsymbol{\rho}_{\text{tot}}^{\text{out}} = |\Phi'(t)\rangle_{\text{out}\ \text{out}}\langle \Phi(t)|$$

describes that asymptotic state of the electron-plus-atom system in density operator form.

If the initial free-electron state is described by the free-electron density operator

$$\boldsymbol{\rho}^{\text{free}} = |\boldsymbol{k}_1 m_s\rangle\langle \boldsymbol{k}_2 m_s|,$$

then the initial state of the electron-plus-atom system can be described by the density operator

$$\boldsymbol{\rho}_{\mathrm{tot}}^{\mathrm{in}} = |\boldsymbol{k}_1 m_s; \alpha J M'\rangle\langle \boldsymbol{k}_2 m_s; \alpha J M| \equiv \boldsymbol{\rho}^{\mathrm{in}} \times \boldsymbol{\rho}^{\mathrm{free}}. \quad (13)$$

The reduced density operator of the final state of the atomic system is obtained by taking the trace over the electron states $|\boldsymbol{k}_0 m_{s_0}\rangle$ in the form (see, e.g., Blum [36], p. 66)

$$\boldsymbol{\rho}^{\mathrm{out}} = \frac{1}{2}(2\pi)^{-3} \sum_{m_s, m_{s_0}} \int d\boldsymbol{k}_0 \langle \boldsymbol{k}_0 m_{s_0} | \boldsymbol{\rho}_{\mathrm{tot}}^{\mathrm{out}} | \boldsymbol{k}_0 m_{s_0}\rangle,$$

where we have also introduced an averaging over the spin of the incident electron assuming an unpolarized incident electron beam [62]. Using Eq. (11) in the above equation we obtain

$$\begin{aligned}\boldsymbol{\rho}^{\mathrm{out}} = {} & \frac{1}{2}(2\pi)^{-9} \sum_{m_s, m_{s_0}} \int d\boldsymbol{k}_0 \int d\boldsymbol{k}_1 A(\boldsymbol{k}_1) \exp\left(-\frac{i}{\hbar} E_{k_1}^{\alpha J} t\right) \\ & \times \int d\boldsymbol{k}_2 A^*(\boldsymbol{k}_2) \exp\left(\frac{i}{\hbar} E_{k_2}^{\alpha J} t\right) \sum_{\alpha_1', \alpha_2', J_1', J_2', M_1', M_2'} |\alpha_1' J_1' M_1'\rangle \\ & \times \langle \alpha_2' J_2' M_2' | \langle \boldsymbol{k}_0 m_{s_0}; \alpha_1' J_1' M_1' | \mathcal{S} | \boldsymbol{k}_1 m_s; \alpha J M'\rangle \\ & \times \langle \boldsymbol{k}_2 m_s; \alpha J M | \mathcal{S}^\dagger | \boldsymbol{k}_0 m_{s_0}; \alpha_2' J_2' M_2'\rangle. \end{aligned} \quad (14)$$

For the matrix element (within the $\alpha' J'$ manifold) of this reduced density operator we obtain

$$\begin{aligned}&\langle \alpha' J' M_1' | \boldsymbol{\rho}^{\mathrm{out}} | \alpha' J' M_2'\rangle \\ &\quad \equiv \rho_{M_1' M_2'}^{\mathrm{out}} = \frac{1}{2}(2\pi)^{-9} \sum_{m_s, m_{s_0}} \int d\boldsymbol{k}_0 \int d\boldsymbol{k}_1 A(\boldsymbol{k}_1) \\ &\qquad \times \exp\left(-\frac{i}{\hbar} E_{k_1}^{\alpha J} t\right) \int d\boldsymbol{k}_2 A^*(\boldsymbol{k}_2) \exp\left(\frac{i}{\hbar} E_{k_2}^{\alpha J} t\right) \\ &\qquad \times \langle \boldsymbol{k}_0 m_{s_0}; \alpha' J' M_1' | \mathcal{S} | \boldsymbol{k}_1 m_s; \alpha J M'\rangle \\ &\qquad \times \langle \boldsymbol{k}_2 m_s; \alpha J M | \mathcal{S}^\dagger | \boldsymbol{k}_0 m_{s_0}; \alpha' J' M_2'\rangle. \end{aligned} \quad (15)$$

If we denote by $a, b, \ldots$ all the quantum numbers of states $|a\rangle, |b\rangle, \ldots$ of the noninteracting electron-plus-atom system [defined by Eq. (10)] and by $E_a, E_b, \ldots$ the corresponding energies, then we can define the transition operator, $\mathcal{T}$, by its matrix elements, $\mathcal{T}_{ab}$, via the equation, (see, e.g., Bransden [37], p. 141)

$$\mathcal{S}_{ab} = \langle a|b\rangle - 2\pi i \delta(E_a - E_b) \mathcal{T}_{ab}. \quad (16)$$

The first term on the right-hand side in the above equation is just the matrix element of the unit operator: **1**. The second term includes the transition operator $\mathcal{T}$.

If we use Eq. (16) for the matrix elements of the $\mathcal{S}$ operator in Eq. (15), then we shall obtain four terms for the reduced density matrix of the final atomic state. In the calculation of those terms we shall use the fact that the $A(\boldsymbol{k})$ function is strongly peaked at $\boldsymbol{k}_{\mathrm{in}}$ along with the technique described by Rodberg and Thaler ([35], p. 194) and by the present authors [20].

We define now the quantity dP/dS (following Rodberg and Thaler [35], p.195), by the formula

$$\frac{dP}{dS} = 2\pi\hbar v_{\mathrm{in}} \int \frac{d\boldsymbol{k}_1}{(2\pi)^3} \int \frac{d\boldsymbol{k}_2}{(2\pi)^3} A(\boldsymbol{k}_1) A^*(\boldsymbol{k}_2) \delta(E_{k_1}^{\alpha J} - E_{k_2}^{\alpha J}), \quad (17)$$

where v_{in} is the initial speed of the center of the wave packet, $v_{\mathrm{in}} = \hbar k_{\mathrm{in}}/m$. It can be easily shown that dP/dS is the probability that the incident wave packet (with a given spin projection) crosses a unit area perpendicular to the direction of propagation (the z axis).

Let us now introduce the scattering amplitude by the definition

$$f_{\alpha' J' M', \alpha J M}^{m_s' m_s}(\theta, \phi) = -\frac{m}{2\pi\hbar^2} \langle \boldsymbol{k}_2 m_s'; \alpha' J' M' | \mathcal{T} | \boldsymbol{k}_1 m_s; \alpha J M\rangle, \quad (18)$$

where θ and ϕ refer to the polar and azimuthal angles, respectively, of $\boldsymbol{k}_2$ relative to $\boldsymbol{k}_1$. Magnitudes $k_1 = |\boldsymbol{k}_1|$ and $k_2 = |\boldsymbol{k}_2|$ are related by the energy conservation relation

$$\frac{\hbar^2 k_1^2}{2m} + E_{\alpha J} = \frac{\hbar^2 k_2^2}{2m} + E_{\alpha' J'}, \quad (19)$$

i.e., the $\mathcal{T}$ matrix element is calculated on the energy shell between the initial state $|\boldsymbol{k}_1 m_s; \alpha J M_1\rangle$ and the final state $\langle \boldsymbol{k}_2 m_s'; \alpha' J' M'|$.

We then obtain for the asymptotic form of the density matrix the result [63]

$$\begin{aligned}\rho_{M_1' M_2'}^{\mathrm{out}} = {} & \delta_{\alpha\alpha'} \delta_{JJ'} \delta_{M_1' M'} \delta_{M M_2'} \\ & - \frac{dP}{dS} \frac{2\pi}{k_{\mathrm{in}}} i \delta_{\alpha\alpha'} \delta_{JJ'} \frac{1}{2} \sum_{m_s} [f_{\alpha J M_2', \alpha J M}^{m_s m_s^*}(0,0) \delta_{M_1' M'} \\ & - f_{\alpha J M_1', \alpha J M'}^{m_s m_s}(0,0) \delta_{M M_2'}] + \frac{dP}{dS} \frac{1}{2} \frac{k_{\mathrm{out}}}{k_{\mathrm{in}}} \\ & \times \sum_{m_s m_{s_0}} \int d\Omega f_{\alpha' J' M_1', \alpha J M'}^{m_{s_0} m_s}(\theta, \phi) f_{\alpha' J' M_2', \alpha J M}^{m_{s_0} m_s^*}(\theta, \phi). \end{aligned} \quad (20)$$

For inelastic scattering the first and second terms in Eq. (20) are absent, however they play an important role in analysis of elastic scattering. We note here that the scattering amplitude, introduced by Eq. (18), factorizes in the form [38]

$$\begin{aligned} f_{\alpha' J' M', \alpha J M}^{m_{s_0} m_s}(\theta, \phi) = {} & f_{\alpha' J' M', \alpha J M}^{m_{s_0} m_s}(\theta) \\ & \times \exp[i(M + m_s - M' - m_{s_0})\phi]. \end{aligned} \quad (21)$$

Let us assume now a completely arbitrary form for the density matrix of level αJ. The density operator representing that state can be expended in terms of state multipoles (see, e.g., Blum [36], p. 95) in the form,

$$\boldsymbol{\rho}_{\alpha J}^{\mathrm{in}} = \sum_{kq} \langle T_q^{(k)}(\alpha J)^\dagger \rangle^{\mathrm{in}} T_q^{(k)}(\alpha J), \quad (22)$$

where the $T_q^{(k)}(\alpha J)$ operator is defined as

$$T_q^{(k)}(\alpha J) = \sum_{M'M} (-1)^{J-M'}(2k+1)^{1/2}\begin{pmatrix} J & J & k \\ M' & -M & -q \end{pmatrix} \times |\alpha JM'\rangle\langle \alpha JM| \tag{23}$$

with

$$\begin{pmatrix} J & J & k \\ M' & -M & -q \end{pmatrix}$$

referring to the 3-j symbol, and $\langle T_q^{(k)}(\alpha J)^\dagger\rangle^{\text{in}}$ is given by the formula

$$\langle T_q^{(k)}(\alpha J)^\dagger\rangle^{\text{in}} = \text{Tr}[\boldsymbol{\rho}_{\alpha J}^{\text{in}} T_q^{(k)}(\alpha J)^\dagger]. \tag{24}$$

III. INCORPORATION OF THE EXCHANGE

The account of the exchange of the incident electron with the target electrons is not trivial within a wave-packet formulation. We follow the general approach of Goldberger and Watson [39] and present here only the result with detailed derivation being given in Appendix A.

Since the incident electron is identical to the target electrons and is a fermion, the total $N+1$ electron wave function must be antisymmetrical in the electron coordinates at any time. Since an antisymmetric wave function can evolve only from an antisymmetric one (since the total Hamiltonian is symmetric in the electron coordinates), the initial wave packet also must be an anti-symmetric function in the electron coordinates and can be given in the form ([39], Chap. 4) [40]

$$\Phi_s(t) = (N+1)^{1/2}\mathcal{A}\Phi(t), \tag{25}$$

where we used $\mathcal{A}$ to denote the antisymmetrization operator which can be given as (the same operator was denoted as $\boldsymbol{S}$ by Kelly [40])

$$\mathcal{A} = (N+1)^{-1}\sum_{j=1}^{N+1} \delta_j Q_j \tag{26}$$

with $\delta_{N+1}=1$, $\delta_{j\neq N+1}=-1$, $Q_{N+1}=1$ and $Q_{j\neq N+1}$ interchanges the coordinates of the incident electron with those of the jth electron ($j=1,\ldots,N$). In Eq. (25) $\Phi(t)=\Phi(\mathbf{r},\sigma,t)$ is given by Eq. (8). Using Eq. (8) in Eq. (25) and the linearity of the $\mathcal{A}$ operator, we obtain

$$\Phi_s(t) = (N+1)^{1/2}(2\pi)^{-3}\int d\boldsymbol{k}A(\boldsymbol{k})\mathcal{A}[e^{i\boldsymbol{k}\cdot\boldsymbol{r}_{N+1}}\eta_{m_s}(\sigma_{N+1}) \times \Psi_{\alpha JM}(\boldsymbol{r}_1\sigma_1,\ldots,\boldsymbol{r}_N\sigma_N)]\exp\left(-\frac{i}{\hbar}E_k^{\alpha J}t\right), \tag{27}$$

where the $A(\boldsymbol{k})$ function is strongly peaked around the value of $\boldsymbol{k}_{\text{in}}$. If we introduce now the notation

$$\begin{aligned}\chi_{s(\boldsymbol{k},m_s;\alpha JM)}(\boldsymbol{r}_1\sigma_1,\ldots,\boldsymbol{r}_{N+1}\sigma_{N+1}) &= (N+1)^{1/2}\mathcal{A}\chi_{\boldsymbol{k},m_s;\alpha JM}(\boldsymbol{r}_1,\sigma_1,\ldots,\boldsymbol{r}_{N+1},\sigma_{N+1}) \\ &\equiv (N+1)^{1/2}\mathcal{A}[\exp(i\boldsymbol{k}\cdot\boldsymbol{r}_{N+1})\eta_{m_s}(\sigma_{N+1}) \\ &\quad\times\Psi_{\alpha JM}(\boldsymbol{r}_1\sigma_1,\ldots,\boldsymbol{r}_N\sigma_N)]\end{aligned} \tag{28}$$

then we can write

$$\Phi_s(t) = (2\pi)^{-3}\int d\boldsymbol{k}A(\boldsymbol{k})\chi_{s(\boldsymbol{k},m_s;\alpha JM)}\exp\left(-\frac{i}{\hbar}E_k^{\alpha J}t\right). \tag{29}$$

If we denote now by $|\Phi_s(t)\rangle_{\text{out}}$ the state in the asymptotic future which evolved from the $|\Phi_s(t)\rangle$ state in the asymptotic past then one can see easily (see, e.g., [39,40]) that

$$|\Phi_s(t)\rangle_{\text{out}} = \mathcal{A}|\Phi(t)\rangle_{\text{out}}, \tag{30}$$

where $|\Phi(t)\rangle_{\text{out}}$ is given by Eq. (11).

Following Goldberger and Watson [39] one can show that the antisymmetrized state (30) can be represented as (details of the derivation are given in Appendix A)

$$\begin{aligned}|\Phi_s(t)\rangle_{\text{out}} &= (2\pi)^{-6}\int d\boldsymbol{k}'\sum_{\alpha'J'M'}\chi_{s(\boldsymbol{k}',m_s',\alpha',J',M')} \\ &\quad\times\exp(-iE_{\boldsymbol{k}'}^{\alpha'J'}t)\int d\boldsymbol{k}A(\boldsymbol{k}) \\ &\quad\times\langle\chi_{s(\boldsymbol{k}',m_s';\alpha'J'M')}|\mathcal{S}|\chi_{s(\boldsymbol{k},m_s;\alpha JM)}\rangle.\end{aligned} \tag{31}$$

This result implies that all formulas obtained in the preceding section hold under the inclusion of exchange if the approprite matrix elements of the $\mathcal{S}$ and $\mathcal{T}$ operators and consequently all scattering amplitudes are calculated from theoretical schemes that include exchange.

IV. COMPUTATIONAL METHOD

The CCC method has been previously extensively used to study electron scattering from hydrogen [21] and barium atoms [22]. The CCC method solves a system of momentum-space Lippmann-Schwinger equations for the $\mathcal{T}$-matrix which is obtained upon multichannel expansion of the total wave function of the scattering system. The CCC method uses a square integrable representation of both the discrete and continuous spectrum of the target atom and/or ion. This allows us to take into account not only interchannel coupling within the target discrete spectrum but also coupling to ionization channels.

We performed calculations for e-H and e-Ba scattering in order to illustrate the general properties of the various cross sections for creation, destruction, and transfer of atomic multipole moments. The choice of these scattering systems was dictated by the following considerations. For the e-H system the CCC method solves the scattering problem without any approximations and the results of CCC calculations have been verified against accurate experimental results for elastic scattering, excitations and total and differential ionization processes [41,42]. In calculation of e-Ba scattering the Ba

atom is modeled as a quasi-two-electron system with an inert Hartree-Fock core. This model proved to be successful in describing elastic electron scattering and electron impact excitations from the Ba ground state [22,43]. Electron scattering from the Ba $6s6p\ ^1P_1$ and $6s5d\ ^1D_2$ excited states has been studied in a series of experiments at the Jet Propulsion Laboratory and the University of Manitoba. These experiments included measurements of differential cross sections and electron-photon coincidence parameters for elastic scattering and electron impact excitations from $6s6p\ ^1P_1$ and $6s5d\ ^1D_2$ excited states [44–46]. Good agreement was obtained between these experimental results and the CCC calculations.

The details of the present CCC calculations are as follows. In the case of e-H scattering the close-coupling expansion consists of 65 states with 15 S, 14 P, 13 D, 12 F, and 11 G states. This model has 15 negative energy states with the remaining 50 states providing square-integrable representation of the target continuum. For e-Ba scattering the close-coupling expansion consists of 245 states with 17 ^1S, 14 ^3S, 24 $^{1,3}S$, 24 ^1D, 2 ^3D, 16 $^{1,3}F$, 8 ^1G, 7 ^3G, 3 $^{1,3}H$ states. These states were obtained by diagonalization of the Ba atom Hamiltonian in a set of two-electron configurations where one of the electrons is constrained to $6s$, $6p$ or $5d$ orbitals while the other electron can occupy $l=0$, 1, 2, 3 orbitals. Such a Ba structure model allows us to capture the most important electron-electron correlations in the Ba spectrum while keeping the size of the calculations feasible.

Our CCC results will be compared in some cases with our first-order Born approximation (FBA) results for the same quantity. It is quite interesting that for integrated cross sections and for inelastic transitions it was shown by Frame [47] that the FBA results agree numerically with the straight-line trajectory semiclassical results, the approximation scheme adopted by Fujimoto *et al.*[14] and Fujimoto and Kazantsev [15] for PPS applications. (For a discussion of the Frame theorem, see Bethe and Jackiw [48], pp. 326–328.) Thus we can make a clear assessment about the difference between the quantum-mechanical formulation along with the CCC numerical implementation on the one hand, and the semiclassical straight-line trajectory approximation and numerical implementation on the other hand. We note here that, from the special symmetry of the scattering amplitude that holds in the semiclassical approximation it immediately follows that alignment cannot be created by elastic scattering in the semiclassical straight-line trajectory approximation. Thus again in that case we can make a comparison of our CCC results with the semiclassical results (identically zero).

V. CREATION, DESTRUCTION, TRANSFER OF ATOMIC MULTIPOLE MOMENTS VIA TRANSITIONS BETWEEN DIFFERENT LEVELS (INELASTIC SCATTERING)

In this section we shall consider in detail only inelastic scattering processes, i.e., processes for which $\alpha \neq \alpha'$ or $J \neq J'$. The next section will consider the change in multipole moments for scattering on a given level, $\alpha=\alpha'$ and $J=J'$.

For inelastic scattering processes we can write the final density matrix in the form

$$\rho^{\text{out}}_{M'_1M'_2} = \frac{dP}{dS}\frac{1}{2}\frac{k_{\text{out}}}{k_{\text{in}}}\sum_{m_s m_{s_0}} \times \int d\Omega f^{m_{s_0}m_s}_{\alpha' J' M'_1,\alpha J M'}(\theta,\phi) f^{m_{s_0}m_s *}_{\alpha' J' M'_2,\alpha J M}(\theta,\phi) \tag{32}$$

for the case when the initial density matrix was given by Eq. (12). In general, the initial density matrix will be given by Eqs. (22) and (23) where the multipole moments $\langle T^{(k)}_q(\alpha J)^\dagger\rangle$ can take arbitrary values. Due to the linearity of the relevant quantum-mechanical equations we then obtain in this latter case for the final density matrix the formula

$$\rho^{\text{out}}_{M'_1M'_2} = \frac{dP}{dS}\sum_k \langle T^{(k)}_q(\alpha J)^\dagger\rangle^{\text{in}} \times \sum_{M'M} (-1)^{J-M'}(2k+1)^{1/2}\begin{pmatrix} J & J & k \\ M' & -M & -q \end{pmatrix}\frac{1}{2}\frac{k_{\text{out}}}{k_{\text{in}}} \times \sum_{m_s m_{s_0}} \int d\Omega f^{m_{s_0}m_s}_{\alpha' J' M'_1,\alpha J M'}(\theta,\phi) f^{m_{s_0}m_s *}_{\alpha' J' M'_2,\alpha J M}(\theta,\phi). \tag{33}$$

Here we have used the factorization of the scattering amplitude, given by Eq. (21) which due to integration over the azimuthal angle in Eq. (33) leads to $M'_1-M'_2=M'-M=q$. For the state multipoles of this final density matrix we obtain

$$\langle T^{(k')}_q(\alpha' J')^\dagger\rangle^{\text{out}} = \text{Tr}[\rho^{\text{out}}_{\alpha' J'} T^{(k')}_q(\alpha' J')^\dagger] = \sum_{M'_1M'_2}(-1)^{J'-M'_1}(2k'+1)^{1/2} \times \begin{pmatrix} J' & J' & k' \\ M'_1 & -M'_2 & -q \end{pmatrix}\rho^{\text{out}}_{M'_1M'_2}. \tag{34}$$

Using Eq. (33) in Eq. (34) we obtain the final-state state multipoles in terms of the initial-state state multipoles, the scattering amplitudes, and dP/dS, the probability that the incident wave packet with a given spin projection crosses a unit area perpendicular to the direction of propagation,

$$\langle T^{(k')}_q(\alpha' J')^\dagger\rangle^{\text{out}} = \frac{dP}{dS}\sum_k \langle T^{(k)}_q(\alpha J)^\dagger\rangle^{\text{in}} \times \sum_{M'_1M'_2}(-1)^{J'-M'_1}(2k'+1)^{1/2}\begin{pmatrix} J' & J' & k' \\ M'_1 & -M'_2 & -q \end{pmatrix} \times \sum_{M'M}(-1)^{J-M'}(2k+1)^{1/2}\begin{pmatrix} J & J & k \\ M' & -M & -q \end{pmatrix}\frac{1}{2}\frac{k_{\text{out}}}{k_{\text{in}}} \times \sum_{m_s m_{s_0}} \int d\Omega f^{m_{s_0}m_s}_{\alpha' J' M'_1,\alpha J M'}(\theta,\phi) f^{m_{s_0}m_s *}_{\alpha' J' M'_2,\alpha J M}(\theta,\phi). \tag{35}$$

This is the principal result of this section. In the following

we shall specialize this general formula to certain particular cases.

Equation (35) can be written in the form

$$\langle T_q^{(k')}(\alpha' J')^\dagger\rangle^{\text{out}} = \frac{dP}{dS}\sum_k \langle T_q^{(k)}(\alpha J)^\dagger\rangle^{\text{in}} g(k'q,\alpha' J';kq,\alpha J), \tag{36}$$

where the g-matrix transforms the $\langle T_q^{(k)}(\alpha J)^\dagger\rangle^{\text{in}}$ initial multipoles into the final $\langle T_q^{(k')}(\alpha' J')^\dagger\rangle^{\text{out}}$ multipole. We shall call the (kq) term of the sum on the right-hand side (rhs) of Eq. (37) the connecting term with the final (k',q) multipole and we shall use that notation,

$$\langle T_q^{(k')}(\alpha' J')^\dagger\rangle^{\text{out}} \Leftrightarrow \frac{dP}{dS}\langle T_q^{(k)}(\alpha J)^\dagger\rangle^{\text{in}} g(k'q,\alpha' J';kq,\alpha J). \tag{37}$$

Let us consider the special case of the connecting term (denoted by the $\Leftrightarrow$ symbol) of $k'=0$, $q'=0$ with $k=0$, $q=0$. Equation (35) gives for this case,

$$\langle T_0^{(0)}(\alpha' J')^\dagger\rangle^{\text{out}} \Leftrightarrow \frac{dP}{dS}\langle T_0^{(0)}(\alpha J)^\dagger\rangle^{\text{in}} \times (2J'+1)^{-1/2}(2J+1)^{-1/2}\sum_{MM'} \sigma_{\alpha JM,\alpha' J' M'}, \tag{38}$$

where we have introduced the magnetic sublevel excitation cross section for the $\alpha JM \to \alpha' J' M'$ electron-impact induced transition by the definition,

$$\sigma^{m_s m_{s_0}}_{\alpha JM,\alpha' J' M'} = \frac{k_{\text{out}}}{k_{\text{in}}}\int d\Omega |f^{m_{s_0} m_s}_{\alpha' J' M',\alpha JM}(\theta,\phi)|^2 \tag{39}$$

and the spin-averaged-summed magnetic sublevel excitation cross section by the formula

$$\sigma_{\alpha JM,\alpha' J' M'} = \frac{1}{2}\sum_{m_s,m_{s_0}} \sigma^{m_s,m_{s_0}}_{\alpha JM,\alpha' J' M'}. \tag{40}$$

If we now use the relationship between the zeroth multipole and the atomic density (see, e.g., Blum [36], p. 97), and introduce the level-to-level integral cross section by the definition

$$\sigma_{\alpha J,\alpha' J'} = \frac{1}{2J+1}\sum_{MM'} \sigma_{\alpha JM,\alpha' J' M'}, \tag{41}$$

and if we denote by $n(\alpha J)$ and $n(\alpha' J')$ the relative number of atoms in a selected volume in the initial αJ level and the final $\alpha' J'$ level, respectively, then it can be shown that Eq. (38) can be written in the form

$$n(\alpha' J') \Leftrightarrow n(\alpha J)\frac{dP}{dS}Q_0^{0,0}, \tag{42}$$

where

$$Q_0^{0,0}(\alpha J,\alpha' J') = \sigma_{\alpha J,\alpha' J'}. \tag{43}$$

It expresses the relationship between the number of atoms produced by the incident electron with a given dP/dS value with cross section $\sigma_{\alpha J,\alpha' J'}$ from the initial level and the number of electrons occupying the initial level. This is just the traditional definition of the integrated electron impact excitation cross section.

As a second example we shall consider the case when $k'=2, q'=0$ and $k=0, q=0$. Equation (35) gives for this case a result of the form

$$\langle T_0^{(2)}(\alpha' J')^\dagger\rangle^{\text{out}} \Leftrightarrow \frac{dP}{dS}n(\alpha J)Q^{0,2}(\alpha J,\alpha' J'), \tag{44}$$

where the alignment creation cross section, $Q_0^{0,2}(\alpha J,\alpha' J')$ is obtained in the form

$$Q_0^{0,2}(\alpha J,\alpha' J') = \sum_{M'}\frac{(-1)^{J'-M'}}{2J+1}\langle J' J' M' - M'|20\rangle \sum_M \sigma_{\alpha JM,\alpha' J' M'} \tag{45}$$

in which $\langle J' J' M' - M'|20\rangle$ refers to a Clebsch-Gordan coefficient. The expression given by Eq. (45) for the alignment creation cross section is identical to the formula used by Kazantsev *et al.* [17,18] for the same quantity and also formally identical to the semiclassical expression given by Fujimoto *et al.* [14], and by Fujimoto and Kazantsev [15] except here the cross sections are calculated quantum mechanically.

For the third example we consider the case when $k'=0, q'=0$ and $k=2, q=0$. This gives the relationship

$$n(\alpha' J') \Leftrightarrow \frac{dP}{dS}\langle T_0^{(2)}(\alpha J)^\dagger\rangle^{\text{in}} Q_0^{2,0}(\alpha J,\alpha',J'), \tag{46}$$

where the alignment destruction cross section (called alignment-to-population cross section by Fujimoto and Kazantsev [15]), is obtained in the form

$$Q_0^{2,0}(\alpha J,\alpha',J') = \sum_{MM'}(-1)^{J-M}\langle JJM-M|20\rangle \sigma_{\alpha JM,\alpha' J' M'}. \tag{47}$$

This form agrees with the one given by Fujimoto and Kazantsev [15], except here the cross sections are calculated quantum mechanically.

For our final example we consider the $k'=2$ and $k=2$ case. In the special case of $q=0$ we obtain

$$\langle T_0^{(2)}(\alpha' J')^\dagger\rangle^{\text{out}} \Leftrightarrow 5\frac{dP}{dS}\langle T_0^{(2)}(\alpha J)^\dagger\rangle^{\text{in}} \times \sum_{M'}(-1)^{J'-M'}\begin{pmatrix} J' & J' & 2 \\ M' & -M' & 0\end{pmatrix} \times \sum_M (-1)^{J-M}\begin{pmatrix} J & J & 2 \\ M & -M & 0\end{pmatrix}\sigma_{\alpha JM,\alpha' J' M'}. \tag{48}$$

If we now define the alignment-transfer cross section, $Q_0^{2,2}(\alpha J,\alpha' J')$, by the formula

$$\langle T_0^{(2)}(\alpha' J')^\dagger\rangle^{\text{out}} \Leftrightarrow \frac{dP}{dS} Q_0^{2,2}(\alpha J, \alpha' J')\langle T_0^{(2)}(\alpha J)^\dagger\rangle^{\text{in}}, \quad (49)$$

then we obtain for it, from Eq. (48),

$$Q_0^{2,2}(\alpha J, \alpha' J') = \sum_{M'} (-1)^{J'-M'}\langle J' J' M' - M' | 20\rangle \times \sum_{M} (-1)^{J-M}\langle JJM - M | 20\rangle \sigma_{\alpha JM, \alpha' J' M'}. \quad (50)$$

This latter form is identical to that given by Fujimoto *et al.* [14] and Fujimoto and Kazantsev [15], except that here it is formulated fully quantum mechanically.

Analogously to Eq. (49) we can define the coherence-transfer cross section, $Q_q^{2,2}(\alpha J, \alpha' J')$ $(q=-2,-1,1,2)$, by the formula

$$\langle T_q^{(2)}(\alpha' J')^\dagger\rangle^{\text{out}} \Leftrightarrow \frac{dP}{dS} Q_q^{2,2}(\alpha J, \alpha' J')\langle T_q^{(2)}(\alpha J)^\dagger\rangle^{\text{in}}, \quad (51)$$

then we obtain

$$Q_q^{2,2}(\alpha J, \alpha' J') = \sum_{M_1' M_2'} (-1)^{J'-M_1'}\langle J' J' M_1' - M_2' | 2q\rangle \times \sum_{M' M} (-1)^{J-M'}\langle JJM' - M | 2q\rangle \times \frac{1}{2}\frac{k_{\text{out}}}{k_{\text{in}}} \sum_{m_s m_{s_0}} \int d\Omega f^{m_{s_0} m_s}_{\alpha' J' M_1', \alpha J M'}(\theta, \phi) \times f^{m_{s_0} m_s *}_{\alpha' J' M_2', \alpha J M}(\theta, \phi). \quad (52)$$

This is the quantum-mechanical version of the expression for the coherence transfer cross section given by Fujimoto *et al.* [14] and Fujimoto and Kazantsev [15] who have defined it within the semiclassical impact-parameter formalism. In the quantum-mechanical case, just as in the semiclassical one, the coherence transfer cross section is expressed directly in terms of the scattering amplitudes and the formula cannot be simplified to one expressed in terms of cross sections.

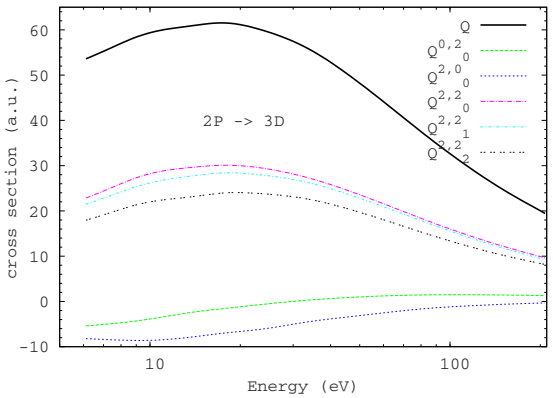

FIG. 1. (Color online) Electron impact excitation cross section, alignment creation, transfer, and destruction cross sections, and coherence transfer cross sections for the electron impact excitation of the hydrogen $2P$ state to the $3D$ state.

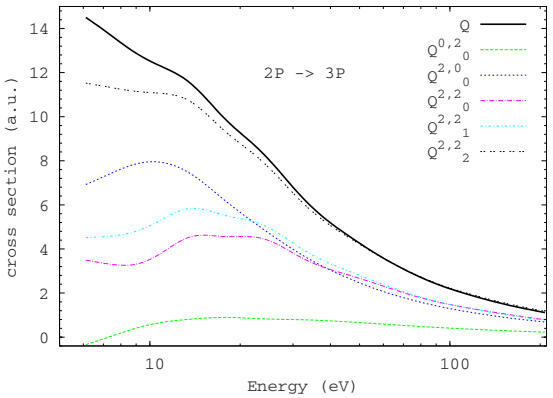

FIG. 2. (Color online) Same as Fig. 1 but for the electron impact excitation of the hydrogen $2P$ state to the $3P$ state.

In order to be consistent with terminology used in the field of PPS we refer to the $Q_q^{kk'}$ quantities as cross sections. Note, however, that these alignment creation, destruction, transfer, and coherence transfer cross sections can be both positive and negative while the standard excitation cross section $\sigma_{\alpha J, \alpha' J'}$ [Eq. (41)] is positive.

We have used the CCC method to produce numerical results illustrating the energy dependence of these various cross sections. In Figs. 1 and 2 we present results for selected excitation processes for the electron-hydrogen scattering system ($2P$ to $3D$ and $3P$) and in Fig. 3 for the electron-barium system ($6s5d\ ^1D_2$ to $6s6p\ ^1P_1$). The choice of nonzero angular momentum of the initial and final states allows for nontrivial result for all $Q_q^{kk'}$ cross sections. (In these figures the electron impact excitation cross section for the specific transition is denoted by Q.)

The alignment creation cross section, $Q_0^{0,2}(\alpha J, \alpha' J')$, can be expressed in terms of the excitation cross section $Q_0^{0,0}(\alpha J, \alpha' J') = \sigma_{\alpha J, \alpha' J'}$ and the polarization fraction P of the radiation emitted from the $(\alpha' J')$ level to the lower level $(\alpha'' J'')$ in the form [14],

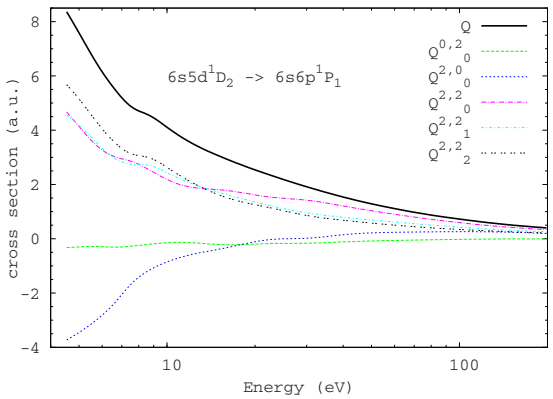

FIG. 3. (Color online) Same as Fig. 1 but for the electron impact excitations of the barium $6s5d\ ^1D_2$ state to the $6s6p\ ^1P_1$ state.

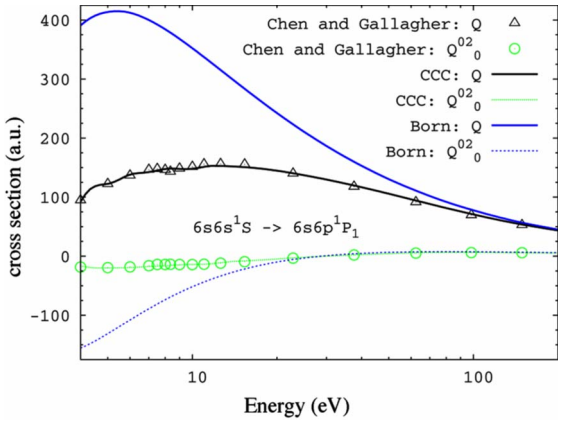

FIG. 4. (Color online) Electron impact excitation and alignment creation cross sections for the electron impact excitation of barium ground state ($6s6s\ ^1S$ state) to the $6s6p\ ^1P_1$ state. Experiment is due to Chen and Gallager [53].

$$Q_0^{0,2}(\alpha J,\alpha' J') = (-1)^{J'+J''}\sqrt{\frac{2}{3}}\begin{Bmatrix} J' & J' & 2 \\ 1 & 1' & J'' \end{Bmatrix} \times Q_0^{0,0}(\alpha J,\alpha' J')2P/(3-P). \quad (53)$$

A large body of experimental data for the polarization fraction, P, is available. Most of such measurements have been done for the states excited by electron impact on the ground state which is normally an S state. Such excitation processes normally create an aligned excited state. Thus, together with excitation cross sections $Q_0^{0,0}(\alpha J,\alpha' J')$ the alignment creation cross sections $Q_0^{0,2}(\alpha J,\alpha' J')$ are the only nontrivial cross sections available for measurement for such transitions.

The CCC method [49] has been used extensively to study the alignment creation cross sections for e-He scattering for a number of $2\ ^{1,3}S$-$n\ ^{1,3}P$ and $2\ ^{1,3}S$-$n\ ^{1,3}D$ transitions [50] and Fujimoto [51] presented a number of examples from CCC calculations for $1\ ^1S$-$n\ ^1P$ transitions. (See Fig. 6.2 in Fujimoto [51]). In those cases the CCC results showed excellent agreement with experiment. Furthermore, Iwamae *et al.* [52] have used the CCC e-He CCC calculation results in the population-alignment collisional-radiative model to describe anisotropic electron velocity distribution in an ECR helium plasma.

In Fig. 4 we compare the results of the present CCC and FBA calculations with the experimental results for the alignment creation cross section that were obtained by the use of the Eq. (53) from measurements of the optical excitation function (apparent cross section) and polarization fraction for the Ba resonance line ($6s6s\ ^1S$ to $6s6p\ ^1P_1$) by Chen and Gallagher [53]. The alignment creation cross section $Q_0^{0,2}$ has been obtained via Eq. (53). The measured apparent cross section and polarization fraction, P, have contributions due to cascading from high lying levels which have been taken into account in the CCC results. The present CCC results are in agreement with previous results from Fursa and Bray [22] CCC(115) model and with experiment. We also note that the experimental apparent cross section has been renormalized by multiplying it by a factor of 1.06, see, for more details, Fursa and Bray [22].

Figure 4 shows excellent agreement between the CCC results and the experiment for the integrated electron impact excitation cross section and for the alignment creation cross section, while the FBA results show very poor agreement with the experiment for $E<10$ eV incident electron energy. According to the theorem of Frame [47] the FBA results for the above quantities agree numerically with the semiclassical straight-line trajectory results for these quantities. Thus, the latter results show very poor agreement with the experiment in the same energy range, a range which is of great importance for plasma kinetic studies.

It is interesting to note that alignment-creation cross section Q_0^{02} which is most often used in PPS related analyses is one of the smallest especially when compared with the alignment-transfer $Q_0^{2,2}$ and coherence-transfer $Q_1^{2,2}$, $Q_2^{2,2}$ cross sections. This could have important implications for the modeling of anisotropic plasmas [52,54].

VI. CREATION, DESTRUCTION, AND CHANGE OF ATOMIC MULTIPOLE MOMENTS ON A GIVEN LEVEL

Let us consider now changes of multipole moments of a level which are induced by electron scattering, i.e., when $\alpha'=\alpha$ and $J'=J$. In this sections we shall use the abbreviation for the scattering amplitude,

$$f_{MM'}^{m_s m_{s_0}} \equiv f_{\alpha JM,\alpha JM'}^{m_s m_{s_0}} \quad (54)$$

and similarly for the cross sections

$$\sigma_{MM'} \equiv \sigma_{\alpha JM,\alpha JM'}. \quad (55)$$

For this case we obtain from the general equation, Eq. (20),

$$\rho_{M_1' M_2'}^{\text{out}} = \delta_{M_1' M'}\delta_{MM_2'} - \frac{dP}{dS}\frac{2\pi}{k_{\text{in}}} i \frac{1}{2}\sum_{m_s} \times [f_{M_2',M}^{m_s m_s^*}(0,0)\delta_{M_1' M'} - f_{M_1',M'}^{m_s m_s}(0,0)\delta_{MM_2'}] + \frac{dP}{dS}\frac{1}{2}\sum_{m_s m_{s_0}} \int d\Omega f_{M_1',M'}^{m_{s_0} m_s}(\theta,\phi) f_{M_2',M}^{m_{s_0} m_s^*}(\theta,\phi). \quad (56)$$

If we use now the factorization of the forward scattering amplitude proven in Appendix B, then we obtain for the change of the density matrix elements on a given level by electron scattering,

$$\Delta\rho_{M_1' M_2'} \equiv \rho_{M_1' M_2'}^{\text{out}} - \delta_{M_1' M'}\delta_{MM_2'} = -\frac{dP}{dS}\frac{2\pi}{k_{\text{in}}} i \frac{1}{2}\sum_{m_s} \times [f_{M,M}^{m_s m_s^*}(0,0) - f_{M',M'}^{m_s m_s}(0,0)]\delta_{MM_2'}\delta_{M_1' M'} + \frac{dP}{dS}\frac{1}{2}\sum_{m_s m_{s_0}} \int d\Omega f_{M_1',M'}^{m_{s_0} m_s}(\theta,\phi) f_{M_2',M}^{m_{s_0} m_s^*}(\theta,\phi). \quad (57)$$

We define now by the following formula the change of the atomic multipole moment on a given level by electron scattering:

$$\Delta\langle T_q^{(k')}(\alpha J)^\dagger\rangle = \mathrm{Tr}[\Delta\rho_{\alpha J} T_q^{(k')}(\alpha J)^\dagger] = \sum_{M_1' M_2'} (-1)^{J-M_1'}(2k'+1)^{1/2}\begin{pmatrix} J & J & k' \\ M_1' & -M_2' & -q \end{pmatrix} \times \Delta\rho_{M_1' M_2'}. \quad (58)$$

Using now Eq. (57) in Eq. (58), we obtain

$$\begin{aligned}\Delta\langle T_q^{(k')}(\alpha J)^\dagger\rangle = &-\frac{dP}{dS}\frac{2\pi}{k_{\mathrm{in}}} i \frac{1}{2}\sum_{m_s} [f_{M,M}^{m_s m_s^*}(0,0) - f_{M',M'}^{m_s m_s}(0,0)] \\ &\times (-1)^{J-M'}(2k'+1)^{1/2}\begin{pmatrix} J & J & k' \\ M' & -M & -q \end{pmatrix} \\ &+ \frac{dP}{dS}\frac{1}{2}\sum_{m_s m_{s_0}}\sum_{M_1' M_2'} (-1)^{J-M_1'}(2k'+1)^{1/2} \\ &\times \begin{pmatrix} J & J & k' \\ M_1' & -M_2' & -q \end{pmatrix} \int d\Omega f_{M_1',M'}^{m_{s_0} m_s}(\theta,\phi) \\ &\times f_{M_2',M}^{m_{s_0} m_s^*}(\theta,\phi). \end{aligned} \quad (59)$$

This formula holds for the case when the density operator of the initial atomic state, $\boldsymbol{\rho}^{\mathrm{in}}$, is given by Eq. (12).

Let us assume now that the density operator of the initial state is given by Eq. (22). Then, due to the linearity of the fundamental equations of quantum mechanics, we obtain

$$\begin{aligned}\Delta\langle T_q^{(k')}(\alpha J)^\dagger\rangle = &-\frac{dP}{dS}\frac{2\pi}{k_{\mathrm{in}}} i \frac{1}{2}\sum_{m_s}\sum_{MM'}\sum_{k} (2k+1)^{1/2} \\ &\times \begin{pmatrix} J & J & k \\ M' & -M & -q \end{pmatrix}\langle T_q^{(k)}(\alpha J)^\dagger\rangle^{\mathrm{in}} \\ &\times (2k'+1)^{1/2}\begin{pmatrix} J & J & k' \\ M' & -M & -q \end{pmatrix} \\ &\times [f_{M,M}^{m_s m_s^*}(0,0) - f_{M',M'}^{m_s m_s}(0,0)] \\ &+ \frac{dP}{dS}\frac{1}{2}\sum_{m_s m_{s_0}}\sum_{k}\sum_{MM'} (-1)^{J-M'}(2k+1)^{1/2} \\ &\times \begin{pmatrix} J & J & k \\ M' & -M & -q \end{pmatrix}\langle T_q^{(k)}(\alpha J)^\dagger\rangle^{\mathrm{in}} \\ &\times \sum_{M_1' M_2'} (-1)^{J-M_1'}(2k'+1)^{1/2} \\ &\times \begin{pmatrix} J & J & k' \\ M_1' & -M_2' & -q \end{pmatrix} \\ &\times \int d\Omega f_{M_1',M'}^{m_{s_0} m_s}(\theta,\phi) f_{M_2',M}^{m_{s_0} m_s^*}(\theta,\phi), \end{aligned} \quad (60)$$

where we used the factorization property of the scattering amplitude Eq. (21) which together with integration over azimuthal angles leads to $M'-M=M_1'-M_2'=q'$.

The first term on the right-hand side of Eq. (60) requires the value of the forward scattering elastic amplitude. At intermediate and high incident electron energies the accurate evaluation of $f_{M,M}^{m_s m_s}(0,0)$ requires a very large partial wave expansion. Instead, we use the optical theorem (see, e.g., Bransden [37], p. 145) to express this term via total scattering cross sections which can be calculated accurately using the analytical Born subtraction techique. This approach also allows us to elucidate the physical meaning of the first term in Eq. (60) and relate the derived cross sections to those familiar in plasma modeling semiclasical results.

In the following we shall use the mathematical identity,

$$f_{MM}^{m_s m_s}(0,0) - f_{MM}^{m_s m_s^*}(0,0) = 2i\,\mathrm{Im}\, f_{MM}^{m_s m_s}(0,0) \quad (61)$$

along with the optical theorem,

$$\mathrm{Im}\, f_{MM}^{m_s m_s}(0,0) = \frac{k_{\mathrm{in}}}{4\pi}\sigma_{\alpha JM,m_s}^{\mathrm{tot}}, \quad (62)$$

where $\sigma_{\alpha JM,m_s}^{\mathrm{tot}}$ refers to the total electron scattering cross section by the $|\alpha JM\rangle$ state with incident electron spin m_s,

$$\sigma_{\alpha JM,m_s}^{\mathrm{tot}} = \sum_{m_{s_0}}\sum_{\alpha' J' M'} \sigma_{\alpha JM,\alpha' J' M'}^{m_s m_{s_0}}. \quad (63)$$

We also define the spin-averaged quantity,

$$\sigma_{\alpha JM}^{\mathrm{tot}} = \frac{1}{2}\sum_{m_s}\sigma_{\alpha JM,m_s}^{\mathrm{tot}}. \quad (64)$$

A. Alignment creation on a given level by electron scattering

Alignment creation on a given level by heavy particle scattering has been studied for many years by Omont [1], by D'yakonov and Perel [2], by Petrashen, Rebane, and Rebane [3–6], and by Kazantsev, Petrashen, and Rebane [55]. The technique has been adapted for arbitrary perturbers (including electrons) by Fujimoto *et al.* [14] and by Fujimoto and Kazantsev [15]. In the case of heavy particle perturbers (e.g., ions) there was an argument by Petrashen, Rebane, and Rebane [4] that under certain conditions (namely only elastic scattering is possible and the semiclassical straight-line trajectory assumption holds) in the case of an isolated level, alignment cannot be created on a given level. On the other hand, Dashevskaya and Nikitin [8] argued that the above conclusion of Petrashen *et al.* [4] is due to an extra symmetry introduced into the problem by the straight-line trajectory approximation (which introduces detailed balance for magnetic sublevel to magnetic sublevel transitions) and if a more accurate approximation is made alignment creation can be obtained on a given level. (See the discussion in Fujimoto *et al.* [14].) In the case of inelastic scattering Kazantsev *et al.* [17,18] gave a quantum-mechanical definition of the alignment creation cross section. In earlier works, Trajmar *et al.* [56] and Csanak *et al.* [57] adopted the inelastic alignment creation cross-section definition of Kazantsev *et al.* [17,18] for elastic electron scattering and reported results for Ba [56] and OV ions [57] based on that formula.

Here we shall specify the general equation obtained in the preceding section to the problem of alignment creation on a given level by electron scattering and we will show that the formula is different from the one that holds for inelastic scattering. We will also show that alignment creation on a given level by electron scattering is possible.

First we start with the specification of the general formula given by Eq. (60) for alignment creation by elastic scattering. This corresponds to the $k'=2$, $k=0$, and $q=0$ connecting terms,

$$\begin{aligned}\Delta\langle T_0^{(2)}(\alpha J)^\dagger\rangle \Leftrightarrow & -\frac{dP}{dS}\frac{2\pi}{k_{\rm in}} i\frac{1}{2}\sum_{m_s}\sum_M (-1)^{J-M}(2J+1)^{-1/2} \\ & \times\langle T_0^{(0)}(\alpha J)^\dagger\rangle^{\rm in}\langle JJM-M|20\rangle[f^{m_s m_s}_{M,M}(0,0)-f^{m_s m_s}_{M,M}(0,0)] \\ & +\frac{dP}{dS}\frac{1}{2}\sum_{m_s m_{s_0}}\sum_M (2J+1)^{-1/2}\langle T_0^{(0)}(\alpha J)^\dagger\rangle^{\rm in} \\ & \times\sum_{M'}(-1)^{J-M'}\langle JJM'-M'|20\rangle\int d\Omega \\ & \times f^{m_{s_0} m_s}_{M',M}(\theta,\phi) f^{m_{s_0} m_s^*}_{M',M}(\theta,\phi). \end{aligned} \tag{65}$$

We can define the given level alignment creation cross section by the formula

$$\Delta\langle T_0^{(2)}(\alpha J)^\dagger\rangle \Leftrightarrow -\frac{dP}{dS}Q_0^{0,2}(\alpha J,\alpha J)n(\alpha J). \tag{66}$$

Then we obtain from Eq. (65) for $Q_0^{0,2}(\alpha J,\alpha J)$,

$$\begin{aligned} Q_0^{0,2}(\alpha J,\alpha J) = & \frac{1}{2J+1}\sum_M (-1)^{J-M}\langle JJM-M|20\rangle \\ & \times\left(\sigma^{\rm inel}_{\alpha JM}-\sum_{M'}(\sigma_{M'M}-\sigma_{MM'})\right), \end{aligned} \tag{67}$$

where $\sigma^{\rm inel}_{\alpha JM}$ refers to the sum of all inelastic cross sections of excitations and deexcitations out of the state $|\alpha JM\rangle$ by an unpolarized electron beam, and is given by the formula

$$\sigma^{\rm inel}_{\alpha JM}=\frac{1}{2}\sum_{m_s,m_{s_0}}\sum_{\alpha' J' M'(\alpha'\neq\alpha \text{ or } J'\neq J)}\sigma^{m_s m_{s_0}}_{\alpha JM,\alpha' J' M'}. \tag{68}$$

We note here that the first term in the large parentheses in Eq. (67) gives the contribution from inelastic scattering while the second term gives the elastic scattering contribution.

The formula obtained for the given level alignment creation cross section, Eq. (67), agrees in form with that obtained using the semiclassical straightline trajectory approach, see Eq. (4.22b) in Fujimoto [16].

For the $J=1$ case, which is relevant to the experiment of Trajmar *et al.* [56], we obtain after inserting the expression for the appropriate Clebsch-Gordan coefficient,

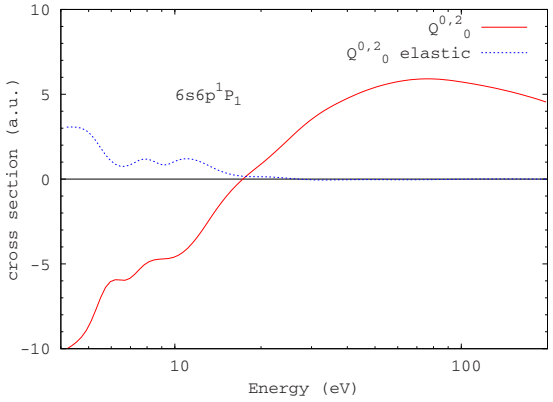

FIG. 5. (Color online) Alignment creation cross section for the barium $6s6p\ ^1P_1$ level and alignment creation cross section by elastic scattering by the same level.

$$\begin{aligned} Q_0^{0,2}(\alpha J=1,\alpha J=1) & \\ =\left(\tfrac{2}{3}\right)^{1/2}\left[(\sigma_{10}-\sigma_{01})+\tfrac{1}{3}(\sigma^{\rm inel}_{\alpha J=1,M=1}-\sigma^{\rm inel}_{\alpha J=1,M=0})\right]. & \end{aligned} \tag{69}$$

If we ignore the contribution to $Q_0^{0,2}$ from inelastic processes, then we obtain $Q_0^{0,2}(\alpha J=1,\alpha J=1)\approx(2/3)^{1/2}(\sigma_{10}-\sigma_{01})$, a result essentially identical to the one used by Dashevskaya *et al.* [7].

Here we have obtained a formula by quantum-mechanical methods for the alignment creation cross section by electron scattering on a given level. The formula obtained differs from the analogous formula relevant for inelastic electron scattering. The key difference originates from the interference effect between the incident beam and the forward scattered beam and leads to an additional term containing the forward scattering elastic amplitude. The latter term can be conveniently evaluated via use of the optical theorem. The alignment creation cross section (as well as other cross sections discussed in the next section) on a given level by electron scattering is, therefore, dependent on the excitation cross sections for inelastic scattering. It consists of two parts, the inelastic part and the elastic part. They agree in form with the formula obtained by the semiclassical straight-line trajectory method.

In Figs. 5 and 6 we have presented the cross sections for the creation of alignment on a given level and the alignment creation cross sections by elastic scattering from the $6s6p\ ^1P_1$ and $6s5d\ ^1D_2$ states. The elastic part of the alignment creation cross section is small and as incident electron energy increases it fast approaches zero. This can be explained as follows. As the incident electron energy increases the FBA becomes a progressively good approximation with the additional symmetry that is valid for the FBA magnetic sublevel elastic cross sections, $\sigma^{\rm FBA}_{M'M}=\sigma^{\rm FBA}_{MM'}$, leading to zero alignment creation cross section in the FBA. Similarly, in the straight-line trajectory semiclassical results the elastic part of the alignment creation cross section is identically zero, which is the reason for the long-held belief that alignment cannot be created by elastic scattering. However, it can be seen from Figs. 5 and 6 that the elastic part of the alignment

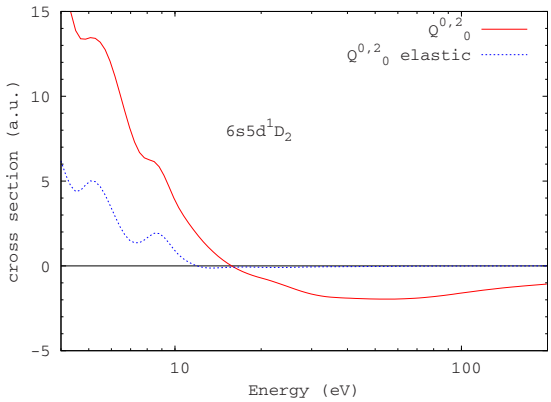

FIG. 6. (Color online) Alignment creation cross section for the barium $6s5d\ ^1D_2$ level and alignment creation cross section by elastic scattering by the same level.

creation cross section is not zero at low energies demonstrating that alignment can be created by elastic scattering. We can also see from Figs. 5 and 6 that the given level alignment creation cross section (containing both elastic and inelastic parts) is largest for low energies (<10 eV). Since the temperature of most plasmas falls into that region, these cross sections must be incorporated into modeling anisotropic plasmas which has not been done in the past.

B. Specification of the general formula for given-level transitions

Here we shall discuss the general equation for given-level multipole-moment changes given by Eq. (60), for specific combinations of the (k,q) and $(k'q)$ multipole indices.

First we shall consider the $k=0$, $k'=0$, and $q=0$ combination. After a calculation very similar to the one described in the preceding section, we obtain the result

$$\Delta n(\alpha J) \Leftrightarrow -n(\alpha J)\frac{dP}{dS}\frac{1}{2J+1}\sum_M \sigma^{\text{inel}}_{\alpha JM}, \tag{70}$$

where $\Delta n(\alpha J)$ refers to the change in the relative number of atoms occupying level αJ in a selected volume upon the passing of the wave packet. The above result is exactly what was expected: the change in occupation number of a given level is due only to inelastic (excitation and deexcitation) processes. If we define the given level electron scattering density transfer cross section $Q_0^{0,0}$ by the formula,

$$\Delta n(\alpha J) = -n(\alpha J)Q_0^{0,0}(\alpha J,\alpha J)\frac{dP}{dS} \tag{71}$$

then we obtain the expression

$$Q_0^{0,0}(\alpha J,\alpha J) = \frac{1}{2J+1}\sum_M \sigma^{\text{inel}}_{\alpha JM}, \tag{72}$$

a formula identical to that obtained semiclassically by Fujimoto *et al.* [14] and Fujimoto and Kazantsev [15] except here the cross sections are calculated quantum mechanically.

Alignment creation, i.e., the special case of $k'=2$, $k=0$ and $q=0$ has been discussed in the preceding section. Next we shall consider an alignment-to-population process, i.e., the special case of $k'=0$, $k=2$, and $q=0$. A simple calculation, similar to the previous case, gives the result

$$\Delta n(\alpha J) \Leftrightarrow -\frac{dP}{dS}\langle T_0^2(\alpha J)^\dagger\rangle^{\text{in}} Q_0^{2,0}(\alpha J,\alpha J), \tag{73}$$

where the alignment-to-population cross section, $Q_0^{2,0}$, is given by the formula

$$Q_0^{2,0} = \sum_M (-1)^{J-M}\langle JJM-M|20\rangle\sigma^{\text{inel}}_{\alpha JM}. \tag{74}$$

This formula agrees with the formulas obtained semiclassically by Fujimoto *et al.* [14] and by Fujimoto and Kazantsev [15] except here the cross sections are calculated quantum-mechanically.

The final case we will consider is that of $k=2$ and $k'=2$. For the special case of $q=0$ we obtain after some algebraic manipulations,

$$\begin{aligned}\Delta\langle T_0^{(2)}(\alpha J)^\dagger\rangle \Leftrightarrow & -\frac{5}{2}\frac{dP}{dS}\sum_M\sum_{m_s}\begin{pmatrix} J & J & 2\\ M & -M & 0\end{pmatrix}^2\\ & \times\langle T_0^{(2)}(\alpha J)^\dagger\rangle^{\text{in}}\sigma^{\text{tot}}_{\alpha JM,m_s} + 5\frac{dP}{dS}\\ & \times\sum_{M,M'}(-1)^{2J-M-M'}\begin{pmatrix} J & J & 2\\ M & -M & 0\end{pmatrix}\\ & \times\begin{pmatrix} J & J & 2\\ M' & -M' & 0\end{pmatrix}\sigma_{M,M'}\end{aligned} \tag{75}$$

which can be written in the form

$$\Delta\langle T_0^{(2)}(\alpha J)^\dagger\rangle = -\frac{dP}{dS}Q_0^{2,2}\langle T_0^{(2)}(\alpha J)^\dagger\rangle^{\text{in}}, \tag{76}$$

where $Q_0^{2,2}$ refers to the alignment destruction cross section and is given by the formula

$$\begin{aligned}Q_0^{2,2}(\alpha J,\alpha J) = & \sum_M \langle JJM-M|20\rangle^2\sigma^{\text{inel}}_{\alpha JM} + \sum_{M'\neq M}[\langle JJM\\ & -M|20\rangle^2 - (-1)^{M'-M}\langle JJM-M|20\rangle\\ & \times\langle JJM'-M'|20\rangle]\sigma_{MM'}.\end{aligned} \tag{77}$$

For the case of $q=2,1,-1,-2$ we can use the same definition of the coherence transfer cross section, $Q_q^{2,2}$, as was used for inelastic scattering and given by Eq. (51). Then we obtain for it the formula

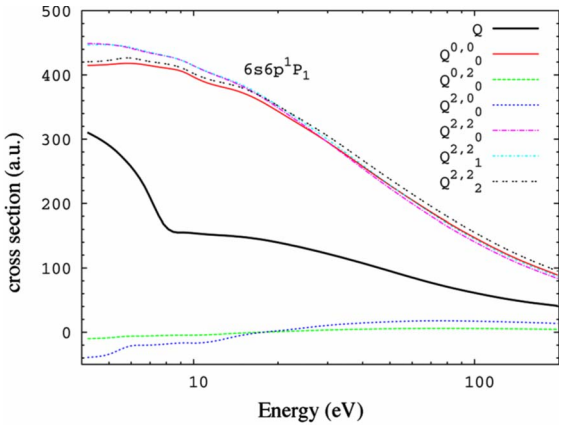

FIG. 7. (Color online) Elastic scattering cross section, alignment creation, transfer, destruction cross sections, and coherence transfer cross sections for the barium $6s6p\ ^1P_1$ level.

$$Q_q^{2,2}(\alpha J,\alpha,J)=\frac{2\pi}{k_{\rm in}}i\frac{5}{2}\sum_{m_s}\sum_{MM'}\begin{pmatrix}J & J & 2\\ M' & -M & -q\end{pmatrix}^2 \times[f^{m_s m_s^*}_{M,M}(0,0)-f^{m_s m_s}_{M',M'}(0,0)]-\frac{5}{2} \times\sum_{m_s m_{s_0}}\sum_{MM'}(-1)^{J-M'}\begin{pmatrix}J & J & 2\\ M' & -M & -q\end{pmatrix} \times\sum_{M_1'M_2'}(-1)^{J-M_1'}\begin{pmatrix}J & J & 2\\ M_1' & -M_2' & -q\end{pmatrix} \times\int d\Omega f^{m_{s_0}m_s}_{M_1',M'}(\theta,\phi)f^{m_{s_0}m_s^*}_{M_2',M}(\theta,\phi). \quad (78)$$

The first term in Eq. (78) can be expressed via magnetic sublevel total cross sections with the help of the optical theorem (62) and symmetry properties of the scattering amplitudes with respect to reflection in the scattering plane [58]. We present the results for elastic scattering from P and D states in Appendix C. The second term in Eq. (78) in general cannot be expressed via magnetic sublevel cross sections similarly to the case of inelastic scattering considered in Sec. IV.

Examples of given-level scattering cross sections obtained using the CCC method are presented in Figs. 7 and 8 for electron scattering from barium $6s6p\ ^1p_1$ and $6s5d\ ^1D_2$ states. (In these figures the elastic scattering cross section is denoted by Q.) The interesting feature of these results is that the density transfer cross section, $Q_0^{0,0}$, and the alignment destruction and coherence-transfer cross sections, $Q_q^{2,2}$ ($q=1,2$), are of similar magnitudes, especially at large energies. In order to explain this we note that the FBA amplitude becomes a good approximation for elastic scattering as the incident electron energy increases, especially for the small scattering angles. The FBA amplitude can be written in the usual way [39],

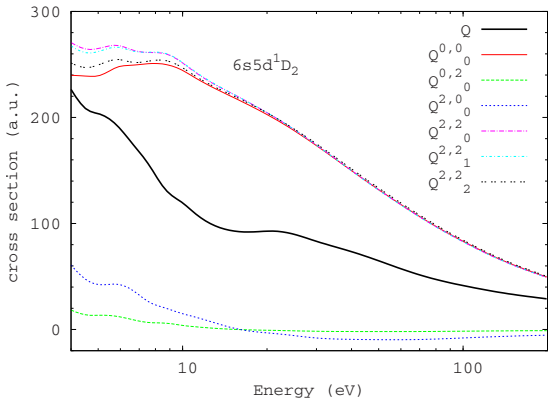

FIG. 8. (Color online) Same as Fig. 7 except for the barium $6s5d\ ^1D_2$ level.

$$f^{\rm Born}_{M'M}(\theta,\phi)\sim\frac{1}{q^2}\sum_{\lambda}Y^*_{\lambda,M'-M}(\hat{\boldsymbol{q}})\mathcal{F}_\lambda(q), \quad (79)$$

where $\boldsymbol{q}$ is the momentum transfer vector, $Y_{\lambda,\mu}$ are the spherical harmonics, and $\mathcal{F}_\lambda(q)$ is the form factor. In the limit of small momentum transfer q, the largest term on the rhs of Eq. (79) is the $\lambda=0$ term of the sum and it is proportional to q^2. Therefore, the amplitudes for transitions without change of magnetic sublevel, $M'=M$, will be by far the largest, and in addition, the forward scattering amplitudes corresponding to different magnetic sublevels will be of similar magnitude. This leads to simplification in Eq. (78), with the first term becoming proportional [see Eqs. (C2)–(C5)] to the total cross section, and the second term to the elastic scattering cross section with their difference equal to the total cross section for inelastic scattering or density transfer cross section $Q_0^{0,0}$. As a result, the density transfer cross section, $Q_0^{0,0}$, and the alignment destruction and coherence-transfer cross sections, $Q_q^{2,2}$, become of similar magnitude.

While the above consideration is accurate for elastic scattering FBA amplitudes only, similar properties hold for the results of our CCC calculations also. We find that magnetic sublevel total cross sections, $\sigma_M^{\rm tot}$, are of similar magnitudes for different magnetic sublevels (M values) which along with the results of Appendix C leads to approximate reduction of the first term in Eq. (78) to the total cross section. The second term in Eq. (78) requires integration over the product of scattering amplitudes $f^{m_{s_0}m_s}_{M_1',M'}(\theta,\phi)f^{m_{s_0}m_s^*}_{M_2',M}(\theta,\phi)$. We find that $M_1'=M'$ and $M_2'=M$ terms are of similar magnitude and substantially larger compared to other terms. This leads to the approximate reduction of the second term to the elastic scattering cross section.

We see from the above consideration that density transfer cross section, $Q_0^{0,0}$, and alignment destruction and coherence-transfer cross sections, $Q_q^{2,2}$, effectively contain summation over magnetic sublevel total and elastic cross sections, however, the alignment creation $Q_0^{0,2}$ and alignment-to-population $Q_0^{2,0}$ cross sections involve subtraction of the same total and elastic magnetic sublevel cross sections. As a result we observe that they are significantly smaller in magnitude. Therefore, it will be important in future modeling of

anisotropic plasmas that along with the alignment-creation and alignment-to-population cross sections, the density transfer cross section and the alignment destruction and coherence transfer cross sections be also included into the calculation.

VII. CONCLUSIONS

Here, as well as in our earlier presentation [20], we used the scientifically correct and physically transparent definition of multipole creation, destruction, and transfer cross sections via the use of the wave-packet propagation scheme, used by, e.g., Rodberg and Thaler [35] and by Goldberger and Watson [39] for the definition of conventional cross sections. We note however, that a compact definition of these cross sections, used for the definition of conventional cross sections, e.g., by Sitenko [58], is also possible, whose results agree with those presented here. This compact definition is in fact justified by our wave-packet procedure as discussed in the conventional case by Bjorken and Drell [59]. This compact formulation along with an exact, but more abstract formulation will be discussed in a future presentation [60].

One of the important conclusions of this work is that here we have demonstrated via the implementation of the CCC scheme that alignment can be created by elastic electron scattering. We have also shown that the CCC scheme gives excellent agreement with the experiment for the alignment-creation cross section out of the ground state of the Ba atom target. Future work will be directed to the implementation of the CCC scheme for the calculation and physical analysis of cross sections discussed in this work for important atomic targets that exist in anisotropic plasmas.

ACKNOWLEDGMENTS

The authors want to thank Professor T. Fujimoto, Professor Al Stauffer, and Professor Klaus Bartschat and Dr. Jon Weisheit, Dr. Suxing Hu, and especially Dr. Peter Hakel for reading and criticizing the original paper, and Dr. Chris Fontes for assistance with the preparation of the paper. This work was partially conducted under the auspices of the U.S. Department of Energy. Support of the Australian Research Council is also acknowledged.

APPENDIX A: ACCOUNT OF THE EXCHANGE

In order to prove Eq. (31) we need to use an important theorem proven by Kelly [40]. Kelly has shown that even though the $\chi_{s(a)}(a \equiv \boldsymbol{k}, m_s; \alpha JM)$ functions for all possible values of the a quantum numbers do not form a complete set, however a function f_s still can be expanded in terms of them if f_s has the form

$$f_s = (N+1)^{1/2} \mathcal{A} f, \tag{A1}$$

where f is an unsymmetrized wave function of the coordinates of the $N+1$ electrons in which the incident electron is localized far from the origin (the location of the nucleus). Since the $\Phi_s(t)_{\text{out}}$ function satisfies the requirement of the Kelly theorem, we can write

$$|\Phi_s(t)\rangle_{\text{out}} = \sum_a |\chi_{s(a)}\rangle\langle\chi_{s(a)}|\Phi_s(t)\rangle_{\text{out}}. \tag{A2}$$

The $\langle\chi_{s(a)}|\Phi_s(t)\rangle_{\text{out}}$ coefficient has been obtained by Goldberger and Watson ([39], pp. 146 and 147) in the form,

$$\langle\chi_{s(b)}|\Phi_s(t)\rangle_{\text{out}} = (2\pi)^{-9/2} \exp\left(-\frac{i}{\hbar} E_{k'}^{\alpha' J'} t\right) \int d\boldsymbol{k} A(\boldsymbol{k}) \langle \mathcal{A}(b) \times |\mathcal{S}| \mathcal{A}(a)\rangle, \tag{A3}$$

where $\langle\mathcal{A}(b)|\mathcal{S}|\mathcal{A}(a)\rangle$ refers to the $\mathcal{S}$-matrix element between antisymmetrized states $\langle\chi_{s(b)}|$ and $|\chi_{s(a)}\rangle$. This matrix element was defined in general terms by Goldberger and Watson ([39], p. 147). For electron-atom scattering Goldberger and Watson [39] have shown that $\langle\mathcal{A}(b)|\mathcal{S}|\mathcal{A}(a)\rangle$ can be written in the form

$$\langle\mathcal{A}(b)|\mathcal{S}|\mathcal{A}(a)\rangle = \delta_{ba} - 2\pi i \delta(E_b - E_a)\langle\mathcal{A}(b)|\mathcal{T}|\mathcal{A}(a)\rangle, \tag{A4}$$

where

$$\langle\mathcal{A}(b)|\mathcal{T}|\mathcal{A}(a)\rangle = \langle b|\mathcal{T}|a\rangle - N\langle Q_j(b)|\mathcal{T}|a\rangle \tag{A5}$$

with Q_j, $(j=1,\ldots,N)$ referring to the permutation operator of the coordinates of the jth electron with that of the scattering (the $N+1$st) electron,

$$\langle Q_j(b)|\boldsymbol{r}_1, \ldots, \boldsymbol{r}_j, \ldots, \boldsymbol{r}_{N+1}\rangle = \langle b|\boldsymbol{r}_1, \ldots, \boldsymbol{r}_{N+1}, \ldots, \boldsymbol{r}_j\rangle. \tag{A6}$$

The first term on the right-hand side of Eq. (A5) is referred to as the direct term, it is the one which appeared in the earlier development when the electron was treated as a distinguishable particle. The second term is the exchange term and appears here because the identity of the incident electron with the target electrons was taken into account giving rise for the possibility of an exchange. Now using Eq. (A3) in Eq. (A2), we obtain,

$$|\Phi_s(t)\rangle_{\text{out}} = (2\pi)^{-6} \int d\boldsymbol{k}' \sum_{\alpha' J' M'} \chi_{s(\boldsymbol{k}', m_s', \alpha', J', M')} \times \exp(-iE_{k'}^{\alpha' J'} t) \int d\boldsymbol{k} A(\boldsymbol{k}) \langle\mathcal{A}(b)|\mathcal{S}|\mathcal{A}(a)\rangle. \tag{A7}$$

Since in the expression for $\langle\mathcal{A}(b)|\mathcal{S}|\mathcal{A}(a)\rangle$ given by Eq. (A4) both in the first and second term there is a factor of a δ function in the energies, $\delta(E_{k'}^{\alpha' J'} - E_k^{\alpha J})$, the $\exp(-E_{k'}^{\alpha' J'} t)$ factor can be substituted by $\exp(-E_k^{\alpha J} t)$ in Eq. (A6) and obtain a generalization of Eq. (11). We can see that the only difference between the above equation and Eq. (11) is that the matrix elements of the $\mathcal{S}$ operator now are calculated with the inclusion of an exchange term as given by Eq. (A5). The same conclusion was also reached by Kelly [40].

APPENDIX B: FACTORIZATION OF THE FORWARD SCATTERING AMPLITUDE

Here we want to prove the factorization of the forward scattering amplitude in the δ function. Since according to Eq.

(18) the scattering amplitude is proportional to the appropriate matrix element of the transition operator $\mathcal{T}$, we shall prove the factorization for the appropriate matrix element of $\mathcal{T}$.

As discussed in Sec. III and Appendix A the matrix elements of the $\mathcal{T}$ operator can be given by Eq. (A5) as a sum of a direct term and an exchange term. Here we are interested in forward scattering, i.e., when $\boldsymbol{k}=\boldsymbol{k}'$.

If we choose the z axis, the axis of quantization, along the $\boldsymbol{k}$ vector, then we can write, [see Rodberg and Thaler [35], p. 241, Eq. (2.36)]

$$|\boldsymbol{k},m_s\rangle = \sum_{l=0}^{\infty} i^l[4\pi(2l+1)]^{1/2}|k,l,m_l=0,m_s\rangle, \tag{B1}$$

where

$$\langle \boldsymbol{r},\sigma|k,l,m_l,m_s\rangle = j_l(kr)Y_{lm}(\theta,\phi)\chi_{m_s}(\sigma) \tag{B2}$$

with $j_l(x)$ referring to the lth spherical Bessel function and $Y_{lm}(\theta,\phi)$ to the spherical harmonic, using the notation and definitions of Rodberg and Thaler [35].

Using Eq. (B1) in the matrix element of the $\mathcal{T}$ operator, we obtain

$$\begin{aligned}\langle \boldsymbol{k},m_s;\alpha JM_1|\mathcal{T}|\boldsymbol{k},m_s;\alpha JM_2\rangle &= \sum_{l=0}^{\infty} i^{l'-l}4\pi[(2l+1)(2l'+1)]^{1/2}\langle k,l,m_l \\ &= 0,m_s;\alpha JM_1|\mathcal{T}|k,l',m_{l'}=0,m_s;\alpha JM_2\rangle.\end{aligned} \tag{B3}$$

If we denote by j_z the total one-electron angular momentum projection opearator along the z axis, then we have

$$j_z|k,l,m_l=0,m_s\rangle = \hbar m_s|k,l,m_l=0,m_s\rangle. \tag{B4}$$

If we denote now by J_z the total angular momentum projection operator along z for the electron plus atom system, then we have

$$J_z|k,l,m_l=0,m_s;\alpha JM\rangle = \hbar(m_s+M)|k,l,m_l=0,m_s;\alpha JM\rangle. \tag{B5}$$

J_z commutes with the total Hamiltonian of the electron plus atom system, H, and with V, the electron atom interaction potential. Therefore, the J_z operator also commutes with the $\mathcal{T}$ operator since the latter depends only on the H and V operators. As a consequence the following factorization holds:

$$\begin{aligned}\langle k,l,m_l=0,m_s;\alpha JM_1|\mathcal{T}|k,l',m_{l'}=0,m_s;\alpha JM_2\rangle &= \langle k,l,m_l=0,m_s;\alpha JM_1|\mathcal{T}|k,l',m_{l'}=0,m_s;\alpha JM_1\rangle \\ &\times \delta_{M_1M_2}.\end{aligned} \tag{B6}$$

Using now Eq. (B6) in Eq. (B3) we obtain the desired factorization for the direct term. Now we must show that the same factorization holds for the second term on the right-hand side of Eq. (A5), for the exchange term. This can be accomplished quite easily if one looks at the spatial representation of the state vector $\langle Q_j(b)|$ given by Eq. (31). This latter equation clearly shows that Q_j is indeed a permutation operator. Since the J_z operator is a symmetric operator (it is the sum of the one-electron total angular momentum projection operators), therefore J_z commutes with Q_j and thus if $\langle b|$ was an eigenstate of the J_z operator, the $\langle Q_j(b)|$ state will also have the same eigenvalue. As a consequence the desired factorization will hold also for the exchange term.

APPENDIX C: REDUCTION OF THE FORWARD SCATTERING TERM IN EQ. (78)

Expression of the first term in Eq. (78) via magnetic sublevel total cross sections requires application of the optical theorem (62) together with the symmetry property of the elastic scattering amplitude due to reflection in the scattering plane [58],

$$f^{m_s,m_s}_{M,M}(0,0) = f^{-m_s,-m_s}_{-M,-M}(0,0). \tag{C1}$$

For the elastic scattering from a P state we obtain for the first term in Eq. (78),

$$Q_1^{22} = \tfrac{1}{2}(\sigma_0^{\mathrm{tot}} + \sigma_1^{\mathrm{tot}}), \tag{C2}$$

$$Q_2^{22} = \sigma_1^{\mathrm{tot}}, \tag{C3}$$

and for the elastic scattering from a D state,

$$Q_1^{22} = \tfrac{1}{14}\sigma_0^{\mathrm{tot}} + \tfrac{1}{2}\sigma_1^{\mathrm{tot}} + \tfrac{3}{7}\sigma_2^{\mathrm{tot}}, \tag{C4}$$

$$Q_2^{22} = \tfrac{2}{7}(\sigma_0^{\mathrm{tot}} + \sigma_2^{\mathrm{tot}}) + \tfrac{3}{7}\sigma_1^{\mathrm{tot}}. \tag{C5}$$

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[61] Our approach here is based on the wave-packet formalism of Rodberg and Thaler [35].
[62] Our treatment can be easily generalized for spin-polarized incident electron beam by the inclusion of the appropriate spin-polarization function.
[63] The details of this calculation can be found in our earlier presentation [20].