

Electron excitation of hydrogenlike ions in the Coulomb Born approximation

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We investigate the excitation of positive ions by charged-particle impact in the Coulomb Born approximation. We obtain closed-form expressions for the $1s-2s$ and $1s-2p$ amplitudes and present numerical results for the corresponding excitation cross sections. We also indicate how the matrix elements may be used to calculate excitation and ionization cross sections for many-electron ions.

I. INTRODUCTION

In this paper we study inelastic excitation processes of positive ions by electron impact. Since these processes have important applications in astrophysics and plasma physics, theoretical investigations of such problems are of practical interest. Such investigations are also of more fundamental interest since electron-ion scattering represents a situation where the distorted wave approximation must be used.

Excitation cross sections for hydrogenlike systems take a simple closed form in the plane-wave Born approximation (PBA) which, however, fails at lower energies (near threshold) and loses information regarding anisotropy for all energies. One can improve the calculations by substituting Coulomb wave functions for plane waves in the Born approximation.^{1,2} The resulting approximation is named the Coulomb Born approximation (CBA). In CBA, the long-range Coulomb field of the ion is taken care of properly and the incident and target electrons are subject to the same potential of the target core. (The distribution of the electrons in the ion is not affected in zeroth order by the incident electron.) Burgess¹ *et al.* evaluated the cross sections of $1s-2s$ and $1s-2p$ excitations for the e^- -He⁺ system in CBA, employing partial-wave analysis of the incident and scattered electrons. However, partial-wave treatments require a large number of partial waves at high energy and are not useful for impact by heavy particles. Mitra and Sil,² avoiding the partial-wave expansion, calculated the cross sections for $1s-2s$ transition also in CBA with full continuum waves for incident and scattered electrons; nevertheless, their matrix element is given as an integral requiring numerical computation. Gaillitis³ formulated closed form expressions for $1s-n_s$ and $1s-2p$ transitions; however, the $1s-2p$ amplitude was within a dipole approximation in which the fin-

ite size of atom is neglected.

We now obtain closed form expressions for the positive ion excitation amplitudes in both $1s-2s$ and $1s-2p$ transitions with full continuum wave functions without further approximation. The amplitudes are expressed as sums of hypergeometric functions. In the present work we do not consider the effect of rearrangement collision or interchange of spin between the incident and target electrons. If these effects become appreciable, the first Born approximation would not be sufficient to calculate the transition amplitude.

In Sec. II we derive the closed form of the excitation amplitude for the transitions $1s-2s$ and $1s-2p$, which are the ones of most interest. We calculate, in Sec. III, the total cross sections for excitation to $2s$ and $2p$ states of the helium ion and discuss the results and further applications of the present theory.

II. MATRIX ELEMENTS

In CBA the initial motion of the incident electron is described in zeroth approximation by an eigenstate of the Hamiltonian $H = T - (Z-1)e^2/r$. In the final state, the motion is again described by eigenstates of the same Hamiltonian. Consequently, in an inelastic collision the incident electron undergoes a transition from one eigenstate of H to another, owing to the residual interaction $V = (e^2/|\vec{r} - \vec{r}'|)$. Then the transition matrix element is given by

$$T_{fi} = -\frac{1}{2\pi} \iint d^3r d^3r' \psi_{\vec{k}}^{(-)*}(\vec{r}) \phi_f^*(\vec{r}') \times \frac{e^2}{|\vec{r} - \vec{r}'|} \phi_i(\vec{r}') \psi_{\vec{k}}^{(+)}(\vec{r}). \quad (1)$$

Here ϕ_i and ϕ_f are the initial- and final-bound-state wave functions of an ion with nuclear charge Z , and $\psi_{\vec{k}}^{(+)}$ and $\psi_{\vec{k}}^{(-)}$ represent the incident and outgoing electron states in the field of an ion with

charge $Z - 1$. The matrix element T can be written

$$T_{fi} = -\frac{1}{2\pi} \int d^3r \psi_{\mathbf{k}}^{(-)*}(\mathbf{r}) U_{i \rightarrow f}(\mathbf{r}) \psi_{\mathbf{k}}^{(+)}(\mathbf{r}) \quad (2)$$

with

$$U_{i \rightarrow f}(\mathbf{r}) = \int d^3r' \phi_f^*(\mathbf{r}') \frac{e^2}{|\mathbf{r} - \mathbf{r}'|} \phi_i^*(\mathbf{r}'), \quad (3)$$

where ϕ_i and ϕ_f are hydrogenic wave functions with nuclear charge Z . $\psi_{\mathbf{k}}^{(+)}$ and $\psi_{\mathbf{k}}^{(-)}$ are the full Coulomb continuum wave functions corresponding to charge $Z - 1$; explicitly

$$\begin{aligned} \psi_{\mathbf{k}}^{(+)}(\mathbf{r}) &= \exp\left(\pi \frac{Z-1}{k}\right) \Gamma(1-a) e^{i\mathbf{k} \cdot \mathbf{r}} \\ &\quad \times {}_1F_1[a, 1; i(kr - \mathbf{k} \cdot \mathbf{r})] \\ &= N_{\mathbf{k}}^{(+)} e^{i\mathbf{k} \cdot \mathbf{r}} {}_1F_1[a, 1; i(kr - \mathbf{k} \cdot \mathbf{r})], \end{aligned} \quad (4)$$

and

$$\begin{aligned} \psi_{\mathbf{k}}^{(-)}(\mathbf{r}) &= \exp\left(\pi \frac{Z-1}{k'}\right) \Gamma(1+b) e^{i\mathbf{k}' \cdot \mathbf{r}} \\ &\quad \times {}_1F_1[-b, 1; -i(k'r + \mathbf{k}' \cdot \mathbf{r})] \\ &= N_{\mathbf{k}'}^{(-)} e^{i\mathbf{k}' \cdot \mathbf{r}} {}_1F_1[-b, 1; -i(k'r + \mathbf{k}' \cdot \mathbf{r})], \end{aligned}$$

where $a = i(Z-1)/k$ and $b = i(Z-1)/k'$.

The differential cross sections for the excitation are given by

$$\sigma_{\Omega} = (k'/k) |T_{fi}|^2. \quad (5)$$

In the present paper, the cross sections are scaled in units of $Z^4/(\pi a_0^2)$ and the energies are in units of the excitation energy, $\frac{3}{8}Z^2$.

A. 1s-2s excitation

$U_{1s \rightarrow 2s}$, the atomic potential occurring in the matrix element of Eq. (2), is spherically symmetric and is given by

$$U_{1s \rightarrow 2s} = -\frac{4}{27} \sqrt{2} Z \left(1 + \frac{3}{2} Zr\right) e^{-3Zr/2}. \quad (6)$$

Then the 1s-2s excitation amplitude can be written

$$\begin{aligned} T_{1s \rightarrow 2s} &= \frac{2\sqrt{2}Z}{27\pi} N_{\mathbf{k}}^{(+)} N_{\mathbf{k}'}^{(-)*} \left(1 - x \frac{\partial}{\partial x}\right) \frac{\partial}{\partial x} \\ &\quad \times \int d^3r e^{i(\mathbf{k} - \mathbf{k}') \cdot \mathbf{r}} \frac{e^{-x r}}{r} {}_1F_1[a, 1; i(kr - \mathbf{k} \cdot \mathbf{r})] \\ &\quad \times {}_1F_1[b, 1; i(k'r + \mathbf{k}' \cdot \mathbf{r})] \\ &= \frac{2\sqrt{2}Z}{27\pi} N_{\mathbf{k}}^{(+)} N_{\mathbf{k}'}^{(-)*} \left(1 - x \frac{\partial}{\partial x}\right) \frac{\partial}{\partial x} I_{ab}, \end{aligned} \quad (7)$$

where

$$\begin{aligned} I_{ab} &= \int d^3r e^{i(\mathbf{k} - \mathbf{k}') \cdot \mathbf{r}} \frac{e^{-x r}}{r} {}_1F_1[a, 1; i(kr - \mathbf{k} \cdot \mathbf{r})] \\ &\quad \times {}_1F_1[b, 1; i(k'r + \mathbf{k}' \cdot \mathbf{r})] \end{aligned}$$

and $x = \frac{3}{2}Z$. The integral I_{ab} in Eq. (7) is evaluated in closed form as a hypergeometric function in the Appendix. In general the term $e^{-i\mathbf{p} \cdot \mathbf{r}}$ is set to equal unity for the hydrogenlike excitation amplitudes, but may differ from unity in the calculations of the cross sections for many-electron ions.

I_{ab} , which is required in the calculations of excitation amplitudes is, from Eq. (A3) of the Appendix, with $\mathbf{p} = 0$, given by

$$\begin{aligned} I_{ab} &= 4\pi [x^2 + (\mathbf{k} - \mathbf{k}')^2]^{a+b-1} (x - ik - ik')^{-a-b} \\ &\quad \times (x - ik + ik')^{-a} (x + ik - ik')^{-b} \\ &\quad \times {}_2F_1\left(a, b; 1; 1 - \frac{x^2 + (\mathbf{k} - \mathbf{k}')^2}{x^2 + (k - k')^2}\right). \end{aligned} \quad (8)$$

Equation (8) with Eq. (7) then represents $T_{1s \rightarrow 2s}$ in terms of hypergeometric functions.

B. 1s-2p excitation

The 2p state has the $m = 1, 0,$ and -1 magnetic substates, thus $U_{1s \rightarrow 2p}$ is not spherically symmetric, and we have

$$U_{1s \rightarrow 2p} = -\frac{4\sqrt{2}}{27} Z \left[x \left(1 - x \frac{\partial}{\partial x}\right) \frac{\partial}{\partial x} f(r) \right] \frac{\mathbf{r}}{r^3}, \quad (9)$$

with

$$f(r) = \int_0^r r'' e^{-x r''} dr''.$$

The commutator relation

$$\frac{\mathbf{r}}{r^3} = -\frac{1}{Z-1} [H, \vec{\nabla}],$$

allows us to express the transition amplitudes for the various 2p magnetic substates as components of a vector $\vec{T}_{1s \rightarrow 2p}$ given by

$$\begin{aligned} \vec{T}_{1s \rightarrow 2p} &= -\frac{2\sqrt{2}}{27\pi} N_{\mathbf{k}}^{(+)} N_{\mathbf{k}'}^{(-)*} \frac{Z}{Z-1} \\ &\quad \times \left(1 - x \frac{\partial}{\partial x}\right) \frac{\partial}{\partial x} \vec{I}, \end{aligned} \quad (10)$$

where

$$\vec{I} = \langle \mathbf{k}', b | [H, \vec{\nabla}] f(r) | \mathbf{k}, a \rangle. \quad (11)$$

We note that the 1s-2p amplitude of Eq. (10) is nearly the same as the 1s-2s; only the integral parts I_{ab} for 1s-2s and \vec{I} for 1s-2p are different.

Because $|\mathbf{k}, a\rangle$ and $|\mathbf{k}', b\rangle$ in \vec{I} are eigenstates of H , we can rewrite it

$$\begin{aligned} \vec{I} &= \frac{1}{2} (k^2 - k'^2) \langle \mathbf{k}', b | f(r) \vec{\nabla} | \mathbf{k}, a \rangle \\ &\quad - \frac{1}{2} \langle \mathbf{k}', b | [f(r), \nabla^2] \vec{\nabla} | \mathbf{k}, a \rangle. \end{aligned} \quad (12)$$

In evaluating Eqs. (10) and (11) we shall need functions $|\vec{k}, a+n\rangle$ and $|\vec{k}', b+n'\rangle$ defined as

$$|\vec{k}, a+n\rangle = e^{i\vec{k}\cdot\vec{r}} {}_1F_1[a+n, 1; i(kr - \vec{k}\cdot\vec{r})] \quad (13)$$

and

$$|\vec{k}', b+n'\rangle = e^{i\vec{k}'\cdot\vec{r}} {}_1F_1[-(b+n'), 1; -i(k'r + \vec{k}'\cdot\vec{r})].$$

These functions are eigenfunctions of the Hamiltonian H only if $n=0$.

Reflection symmetry in the plane of \vec{k} and \vec{k}' requires that \vec{I} has components only in that plane. Accordingly we select two components of \vec{I} , $\vec{I}\cdot\hat{k}$, and $\vec{I}\cdot\hat{k}'$. These components are identical if \vec{k} is parallel to \vec{k}' , however, in that case \vec{I} has only one component because of cylindrical symmetry. We present only the calculation of $\vec{I}\cdot\hat{k}$ since exactly the same steps are used to evaluate $\vec{I}\cdot\hat{k}'$.

The projection \hat{k} onto the gradient of $|\vec{k}, a\rangle$ gives $\hat{k}\cdot\vec{\nabla}|\vec{k}, a\rangle = ik|\vec{k}, a\rangle - (a/r)[|\vec{k}, a+1\rangle - |\vec{k}, a\rangle]$. (14)

Upon substituting Eq. (14) into Eq. (12), we find that contributions from the first term in (14) exactly cancel and $\vec{I}\cdot\hat{k}$ becomes

$$\begin{aligned} \vec{I}\cdot\hat{k} &= \frac{1}{2}a \left((k^2 - k'^2) \langle \vec{k}', b | \frac{f(r)}{r} (|\vec{k}, a+1\rangle - |\vec{k}, a\rangle) \right. \\ &\quad \left. + \langle \vec{k}', b | [f(r), \nabla^2] (1/r) (|\vec{k}, a+1\rangle - |\vec{k}, a\rangle) \right) \\ &= \frac{1}{2}a \{ (k^2 - k'^2) I_{1k} + I_{2k} \}. \end{aligned} \quad (15)$$

The first term I_{1k} is exactly written in terms of I_{ab} ; thus, we have

$$\begin{aligned} I_{1k} &= \frac{1}{x^2} \left((I_{a+1,b} - I_{ab})_{x=0} - (I_{a+1,b} - I_{ab}) \right. \\ &\quad \left. + x \frac{\partial}{\partial x} (I_{a+1,b} - I_{ab}) \right). \end{aligned} \quad (16)$$

More detailed and circuitous manipulations are needed to evaluate I_{2k} . Upon evaluating the commutator $[f, \nabla^2]$ we obtain

$$\begin{aligned} I_{2k} &= \langle \vec{k}', b | \frac{3-xr}{r} e^{-xr} (|\vec{k}, a+1\rangle - |\vec{k}, a\rangle) \\ &\quad + 2 \langle (\vec{k}'b)' | r^{-1} e^{-xr} (|\vec{k}, a+1\rangle - |\vec{k}, a\rangle), \end{aligned} \quad (17)$$

where

$$\begin{aligned} |(\vec{k}', b)'\rangle &= \vec{r}\cdot\vec{\nabla}|\vec{k}', b\rangle \\ &= -i\vec{k}'\cdot\vec{r}|\vec{k}', b\rangle + b(|\vec{k}', b+1\rangle - |\vec{k}', b\rangle). \end{aligned} \quad (18)$$

Substituting $\vec{k}'\cdot\vec{\nabla}_p e^{-i\vec{p}\cdot\vec{r}} = -i\vec{k}'\cdot\vec{r} e^{-i\vec{p}\cdot\vec{r}}$ into Eq. (18) and the result into Eq. (17) we obtain

$$\begin{aligned} I_{2k} &= 3(I_{a+1,b} - I_{ab}) + x \frac{\partial}{\partial x} (I_{a+1,b} - I_{ab}) \\ &\quad + 2\vec{k}'\cdot[\vec{\nabla}_p (I_{a+1,b} - I_{ab})]_{p=0} \\ &\quad + 2b(I_{a+1,b+1} - I_{a+1,b} - I_{a,b+1} + I_{ab}). \end{aligned} \quad (19)$$

Consider the gradient terms with respect to \vec{p} , namely, $(\vec{k}'\cdot\vec{\nabla}_p I_{ab})_{p=0}$. Using the recurrence relation

$$\begin{aligned} y {}_1F_1(b, 1; y) &= b {}_1F_1(b+1, 1; y) - (2b-1) {}_1F_1(b, 1; y) \\ &\quad + (1-b) {}_1F_1(b-1, 1; y), \end{aligned}$$

we write $\vec{k}'\cdot(\vec{\nabla}_p I_{ab})_{p=0}$,

$$\begin{aligned} \vec{k}'\cdot(\vec{\nabla} I_{ab})_{p=0} &= -b I_{a,b+1} + (2b-1) I_{ab} \\ &\quad + (1-b) I_{a,b-1} - ik' \frac{\partial}{\partial x} I_{ab}. \end{aligned} \quad (20)$$

Similarly

$$\begin{aligned} \vec{k}'\cdot(\vec{\nabla} I_{a+1,b})_{p=0} &= -b I_{a+1,b+1} + (2b-1) I_{a+1,b} \\ &\quad + (1-b) I_{a+1,b-1} - ik' \frac{\partial I_{ab}}{\partial x}. \end{aligned} \quad (21)$$

Differentiating I_{ab} with respect to x and using the relation

$$\begin{aligned} \frac{d}{dZ} Z^{1-a} (1-Z)^{a+b-1} {}_2F_1(a, b; 1; Z) \\ = (1-a) Z^{-a} (1-Z)^{a+b-2} {}_2F_1(a-1, b; 1; Z), \end{aligned} \quad (22)$$

we express the factors $I_{a,b-1}$ and $I_{a+1,b-1}$ as

$$(b-1) I_{a,b-1} = \frac{x^2 + k^2 - k'^2 - 2ik'x}{2x} \frac{\partial I_{a,b-1}}{\partial x} + b I_{ab} \quad (23)$$

and

$$\begin{aligned} (b-1) I_{a+1,b-1} &= \frac{x^2 + k^2 - k'^2 - 2ik'x}{2x} \\ &\quad \times \frac{\partial I_{a,b-1}}{\partial x} + \left(\frac{ik}{x} + b \right) I_{a+1,b}. \end{aligned} \quad (24)$$

Substituting Eqs. (23) and (24) into Eqs. (20) and (21), and the resultant into (19) we obtain the greatly simplified expression

$$\begin{aligned} I_{2k} &= I_{a+1,b} - I_{ab} - \frac{2ik}{x} I_{a+1,b} \\ &\quad - \frac{k^2 - k'^2}{x} \frac{\partial}{\partial x} (I_{a+1,b} - I_{ab}). \end{aligned} \quad (25)$$

Combining I_{2k} from Eq. (25) and I_{1k} from Eq. (16) as required in Eq. (15) we have

$$\begin{aligned} \vec{I}\cdot\hat{k} &= \frac{a}{2} \left(\frac{k^2 - k'^2}{x^2} [(I_{a+1,b} - I_{ab})_{x=0} - (I_{a+1,b} - I_{ab})] \right. \\ &\quad \left. + I_{a+1,b} - I_{ab} - \frac{2ik}{x} I_{a+1,b} \right). \end{aligned} \quad (26)$$

Similarly

$$\vec{\Gamma} \cdot \hat{k}' = \frac{b}{2} \left(\frac{k^2 - k'^2}{x^2} [(I_{a,b+1} - I_{ab})_{x=0} - (I_{a,b+1} - I_{ab}) - I_{a,b+1} + I_{ab} + \frac{2ik'}{x} I_{a,b+1}] \right). \quad (27)$$

The first terms, those with $x=0$, in Eqs. (26) and (27) are equivalent to the bremsstrahlung amplitude first given by Sommerfeld.⁴ The Sommerfeld amplitude was used by Guth and Mullin⁵ to evaluate nuclear dipole transitions in the point-nucleus approximation. When only the $\vec{\Gamma}/r^3$ term of U_{1s-2p} in Eq. (9) is kept, our results reduce to those of Guth and Mullin. The remaining terms with $x \neq 0$ may be regarded as the effect due to the finite size of the target atom. Note that in Eqs. (26) and (27) $\vec{\Gamma} \cdot \hat{k}$ and $\vec{\Gamma} \cdot \hat{k}'$ are antisymmetric under the change of \vec{k} into $-\vec{k}'$, as required by the relation, $\psi_{\vec{k}}^{(+)*} = \psi_{-\vec{k}}^{(-)}$ between incoming and outgoing wave functions. In the forward direction, where \vec{k} is parallel to \vec{k}' , $\vec{\Gamma} \cdot \hat{k} = \vec{\Gamma} \cdot \hat{k}'$, since for $\hat{k} \cdot \hat{k}' = 1$, $a(I_{a+1,b} - I_{ab}) = b(I_{a,b+1} - I_{ab})$. As a further check on our results, we recover the plane-wave Born expressions by setting the multiplicative factors a in Eq. (26) and b in Eq. (27) equal to $i(Z-1)/k$ and $i(Z-1)/k'$, respectively, and then setting $a=b=0$ elsewhere.

The amplitude $\vec{T}_{1s \rightarrow 2p}$ can be alternatively represented by two components along orthogonal directions T_z and T_x , where T_z is the component along the direction of the incident electron and T_x is along an axis in the scattering plane;

$$\vec{T}_{1s \rightarrow 2p} = T_z \hat{k} + T_x \hat{x}, \quad (28)$$

Accordingly T_z and T_x are given by

$$T_z = -\frac{2\sqrt{2}}{27\pi} \frac{Z}{Z-1} x \left(1 - x \frac{\partial}{\partial x} \right) \frac{\partial}{\partial x} \vec{\Gamma} \cdot \hat{k}, \quad (29)$$

$$T_x = -\frac{2\sqrt{2}}{27\pi} \frac{Z}{Z-1} x \left(1 - x \frac{\partial}{\partial x} \right) \frac{\partial}{\partial x} \times (\vec{\Gamma} \cdot \hat{k}' - \cos\theta \vec{\Gamma} \cdot \hat{k}) \frac{1}{\sin\theta},$$

with $\cos\theta = \hat{k} \cdot \hat{k}'$.

Equations (28) and (29) are needed to compute the polarization of collision excited fluorescence. Rather than tabulate the polarization of collision excited fluorescence, which depends upon such details a fine and hyperfine structure, we parameterize the anisotropy in terms of A_0^{col} , the Fano-Macek alignment parameters,^{6,7} given by

$$A_0^{\text{col}} = (\sigma_0 - \sigma_1) / (\sigma_0 + 2\sigma_1), \quad (30)$$

where

$$\sigma_0 = \frac{k'}{k} \int |T_z|^2 d\hat{k},$$

and

$$2\sigma_1 = \frac{k'}{k} \int |T_x|^2 d\hat{k}. \quad (31)$$

The quantity A_0 depends only upon the properties of the excited state, not upon how it decays, in contrast to the polarization of fluorescence.

III. RESULTS AND DISCUSSIONS

The scaled cross sections for transitions $1s-2s$ and $1s-2p$ are shown in Figs. 1 and 2 together with PBA prediction and experimental data.⁸⁻¹⁰ We find excellent agreement with the results of Refs. 1 and 2 in CBA for all energies where comparison is possible. Our analytic results for the $1s-2s$ excitation agree with the experimental data of Dolder and Peart,⁸ and of Dance *et al.*⁹ within 1% at 10 times the threshold energy and within 10% at 5 times the threshold energy. We also compared the $1s-2p$ excitation cross section with the experimental data of Dashchenko *et al.*¹⁰ and obtained similar results.

In the $1s-2p$ transition, one may neglect the effect due to the finite size of the atom at high energies. The matrix element $U_{1s \rightarrow 2p}(\vec{r})$ in this dipole approximation (DA) becomes $(\vec{r}/r^3)d_{fi}$ where d_{fi} is the matrix element of the dipole moment.³ Then the transition amplitude can be written

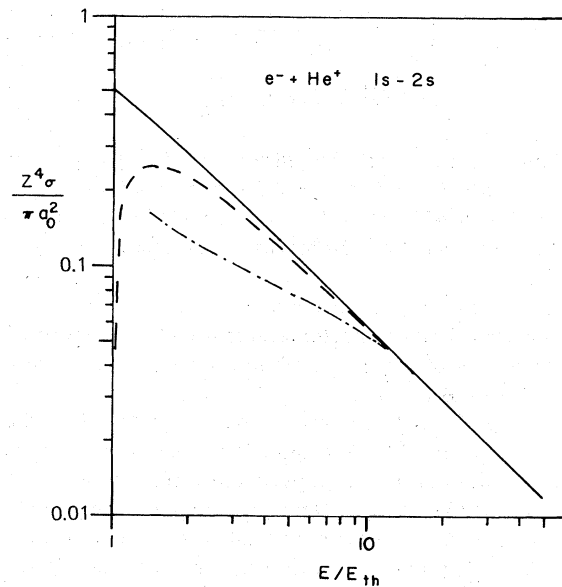


FIG. 1. Total cross sections for $e^- + \text{He}^+(1s) \rightarrow e^- + \text{He}^+(2s)$. The solid curve is the CBA result, the dashed line is the PBA result, and the broken curve is the experimental result of Dolder and Peart.

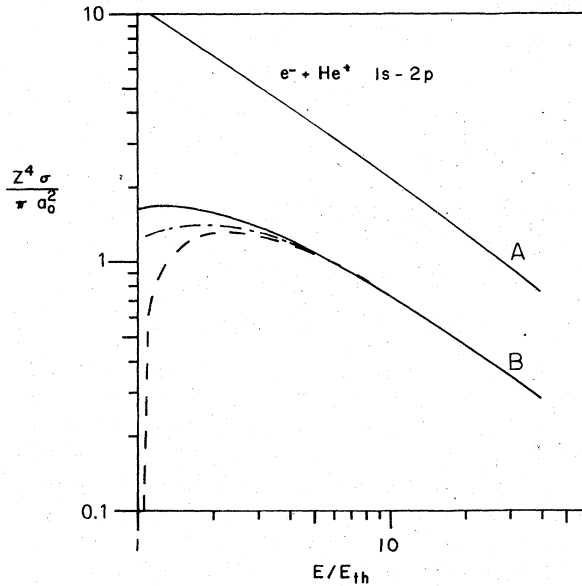


FIG 2. Total cross section for $e^- + \text{He}^+(1s) \rightarrow e^- + \text{He}^+(2p)$, where curve *A* is the DA result. The curves labeled *B* are the same as Fig. 1, where the broken curve is the experimental result of Dashchenko *et al.*

$$T_{1s \rightarrow 2p}^{\text{DA}} = -\frac{1}{2\pi} d_{fi} \int d^3r \psi_{\mathbf{k}}^{(-)*}(\mathbf{r}) \frac{\mathbf{r}}{r^3} \psi_{\mathbf{k}}^{(+)}(\mathbf{r}), \dots \quad (32)$$

which corresponds to the terms with $x=0$ in Eqs. (26) and (27). The total cross section can be calculated analytically as done in Bremsstrahlung cross section.¹¹ One finds

$$\sigma_{1s \rightarrow 2p}^{\text{DA}} = \frac{2\pi(Z-1)^2}{E_{th}} \frac{f}{E} \frac{\pi^2 Z_0}{(e^{2\pi(Z-1)/k} - 1)(1 - e^{-2\pi(Z-1)/k'})} \times \frac{d}{dZ'} |F(a, b, 1, z')|_{z'=Z_0}^2. \quad (33)$$

Here f is the oscillator strength, E the energy of the incident electron, E_{th} the excitation energy, and $Z_0 = -[4kk'/(k-k')^2]$. Gailitis²³ result differs from Eq. (33) by a factor of π , an apparent mistake.

At sufficiently high energies, one expects that both Coulomb deflection and finite-size effects become less significant. Then the total cross sections in CBA, PBA, and DA converge to $4\pi(f/E_{th})(\log E/E)$. However, as shown in Fig. (2), the cross section in DA converges more slowly to this limit than one might expect and differs drastically in the whole range of energies. This may be because the finite size contributions are coherent with the dipole term in the cross section. We find that the finite-size contribution is more important than the Coulomb deflection and DA is an inadequate method in the electron-ion excitation process.

Light-intensity observations frequently serve to

measure $2p$ excitation experimentally. The polarization and angular distribution of the radiation is then of some practical interest.

The polarization of decay radiation is given by⁶

$$p = \frac{3h^{(2)} \bar{G} A_0^{\text{col}}}{2 - h^{(2)} \bar{G} A_0^{\text{col}}}, \quad (34)$$

where \bar{G} is a constant, less than or equal to unity, which incorporates the effect of fine structure and hyperfine structure precession. If hyperfine structure is negligible and only fine structure is present, \bar{G} is given by

$$\bar{G} = \sum_{JJ'} \frac{(2J+1)(2J'+1)}{2S+1} \left\{ \begin{matrix} J' & J & 2 \\ S & S & L \end{matrix} \right\}^2 \frac{1}{1 + (W_{JJ'}\tau)^2}, \quad (35)$$

where τ is the atomic mean life, $W_{JJ'} = (E_J - E_{J'})/h$, $S = \frac{1}{2}$ for hydrogenlike ions, and $L = 1$ for p states. The constant $h^{(2)}$ incorporates details of the radiative transitions. It is given by⁶

$$h^{(2)}(L_i L_f) = (-1)^{L_i - L_f} \begin{Bmatrix} L_i & L_i & 2 \\ 1 & 1 & L_f \end{Bmatrix} \begin{Bmatrix} L_i & L_i & 2 \\ 1 & 1 & L_i \end{Bmatrix} \quad (36)$$

and is equal to -2 for $L_i = 1$ and $L_f = 0$.

The alignment is shown in Fig. 3. Note that, except for electron energies near threshold, total cross sections and alignments are in good agreement with predictions of PBA, but that the alignment deviates somewhat more than the cross section does, although the deviations are not large except at threshold. Such good agreement with the more approximate Born calculation is surprising, and presumably indicates a near cancellation of two effects. The Coulomb wave function incorpor-

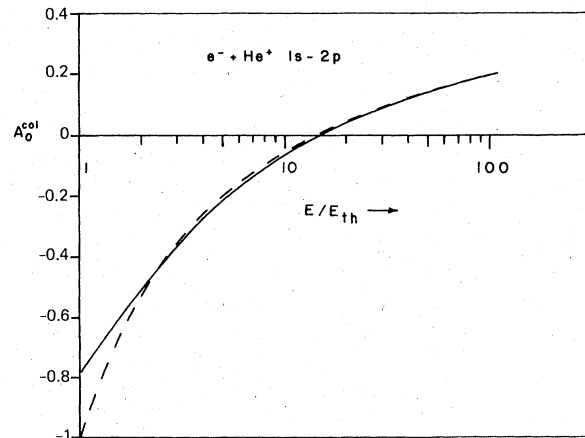


FIG. 3. Alignment A_0^{col} vs energy in the $2p$ transitions.

TABLE I. Total cross sections ($\pi a_0^2/Z^4$) and A_0^{sol} at energies E (in threshold units) for He^* .

E/E_{th}	$\sigma_{1s \rightarrow 2s}$	$\sigma_{1s \rightarrow 2p}$	A_0^{sol}
1.0	0.502 8	1.653	-0.782
1.05	0.484 6	1.669	-0.763
1.1	0.467 3	1.679	-0.744
1.2	0.435 4	1.688	-0.710
1.5	0.359 4	1.665	-0.622
2.0	0.277 2	1.574	-0.510
3.0	0.189 6	1.379	-0.365
4.0	0.143 9	1.221	-0.275
6.0	0.096 94	0.9980	-0.167
10.0	0.058 62	0.7434	-0.060
14.0	0.042 00	0.6006	-0.004
20.0	0.029 46	0.4726	0.045
24.0	0.024 57	0.4162	0.068
30.0	0.019 67	0.3549	0.092
34.0	0.017 37	0.3240	0.105
40.0	0.014 77	0.2874	0.121

ates an increased electron density of the incident and scattered electrons near the atomic nucleus, which increases the cross section as compared to PBA and is responsible for the nonzero-threshold cross section. It also incorporates an acceleration of the incident electron by the long-range Coulomb potential, which presumably decreases the cross section. Our results indicate that two effects almost exactly cancel over whole energy range except near threshold, although the reasons for the near cancellation are not clear.

For completeness, we tabulate cross sections and alignment parameters in Table I. These values were used to construct Figs. 1-3.

APPENDIX: INTEGRAL OF I_{ab}

I_{ab} in (7) can be evaluated with the term $e^{-i\vec{p}\cdot\vec{r}}$ for wider use such as further ionizations by impact, although the calculations of the excitation transition do not necessitate it. Then I_{ab} is written

$$I_{ab} = \int d^3r \exp[i(\vec{k} - \vec{k}' - \vec{p}) \cdot \vec{r}] \frac{e^{-xr}}{r} {}_1F_1[a, 1; i(kr - \vec{k} \cdot \vec{r})] {}_1F_1[b, 1; i(k'r + \vec{k}' \cdot \vec{r})]. \quad (\text{A1})$$

With the integral representation for confluent hypergeometric functions, Eq. (A1) can be expressed as

$$I_{ab} = \frac{1}{B(a, 1-a)} \frac{1}{B(b, 1-b)} \int_{-1}^1 dt (1-t)^{-a} (1+t)^{a-1} \int_0^1 du u^{b-1} (1-u)^{-b} \int d^3r r^{-1} \exp[-\lambda r + ik'ur + i(u\vec{k}' - \vec{k}' - \vec{p}') \cdot \vec{r}]. \quad (\text{A2})$$

Here $\lambda = x - \frac{1}{2}i(1+t)k$ and $\vec{p}' = \vec{p} - (1-t)\frac{1}{2}\vec{k}$. Integrating over the r variables, then setting $u = (v+1)^{-1}$ we easily evaluate the integral over u to obtain

$$I_{ab} = \frac{4}{B(a, 1-a)} \int_{-1}^1 dt (1-t)^{-a} (1+t)^{a-1} \frac{[\lambda^2 + (\vec{p}' + \vec{k}')^2]^{b-1}}{[p'^2 + (\lambda - ik')^2]^b} = \frac{4\pi C^{a+b-1}}{A^b A'^a} {}_2F_1(a, b; 1; z), \quad (\text{A3})$$

where

Fano and Inokuti¹² advocate Coulomb Born calculations employing a method incorporating a six-dimensional integral over a product of the atomic form factor $F_{ij}(\vec{P} - \vec{P}')$ times $|\vec{P} - \vec{P}'|^{-2}$ and a function W depending only on the Coulomb distortion of incident and scattered waves. This procedure has the advantage that it separates the atomic dynamics, represented by $F(\vec{P} - \vec{P}')$, from dynamics of a single electron in a Coulomb potential, represented by W . This separation, while useful, requires analysis and numerical computation of a six-dimensional integral with δ -function-like singularities. Our expression for I_{ab} in the Appendix simplifies the Fano-Inokuti approach.

By Fourier transforming the interaction potential $|\mathbf{r} - \mathbf{r}'|^{-1}$ we easily obtain the expression for Coulomb excitation of a many-electron ion. Specifically we have

$$T_{fi} = \int d^3p F_{if}(\vec{p}) \frac{1}{p^2} \langle \psi_{\vec{k}'}^{(-)} | e^{-i\vec{p}\cdot\vec{r}} | \psi_{\vec{k}}^{(+)} \rangle. \quad (\text{37})$$

The matrix element in Eq. (37) is given by

$$\langle \psi_{\vec{k}'}^{(-)} | e^{-i\vec{p}\cdot\vec{r}} | \psi_{\vec{k}}^{(+)} \rangle = - \left(\frac{\partial}{\partial x} I_{ab}(X, \vec{p}) \right)_{x=0}. \quad (\text{38})$$

where $I_{ab}(X, \vec{p})$ is given by Eq. (A3) of the Appendix. In using Eqs. (37) and (38), one must properly recognize the various δ -function terms, such as

$$\frac{1}{2\pi^2} \lim_{x \rightarrow 0} \frac{d}{dx} \frac{1}{x^2 + (\vec{p} - \vec{q})^2} = -\delta(\vec{p} - \vec{q}).$$

Note that Eq. (37) involves only a three-dimensional integration and could prove useful for numerical computation. Computer codes for calculating $F_{if}(\vec{q})$ already exist, thus evaluation of a triple integral is the main remaining task.

$$A = (x - ik')^2 + (\vec{p} - \vec{k})^2,$$

$$A' = (x - ik)^2 + (\vec{p} + \vec{k}')^2,$$

$$C = x^2 + (\vec{p} - \vec{k} + \vec{k}')^2,$$

and

$$Z = 2 \frac{A[\vec{k} \cdot (\vec{p} - \vec{k} + \vec{k}') - ikx] - C(\vec{p} \cdot \vec{k} - k^2 - ikx - kk')}{AA'}.$$

When $\vec{p} = 0$, as required for most of our work,

we have

$$A = (x - ik')^2 + k^2,$$

$$A' = (x - ik)^2 + k'^2,$$

$$C = x^2 + (\vec{k} - \vec{k}')^2,$$

and

$$z = 1 - \frac{x^2 + (\vec{k} - \vec{k}')^2}{x^2 + (k - k')^2}.$$

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