Atomic inner-shell ionization

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Cross sections for the K-shell ionization of medium-heavy atoms by relativistic electrons have been calculated in a relativistic framework in the Coulomb gauge to order α_0 $(=e^2/\hbar c)$ in the interaction Hamiltonian. Here exchange is neglected. The incident- and scattered-electron wave functions are described by Dirac plane waves. Only the bound- and ejected-electron wave functions are described nonrelativistically for a screened Coulomb potential, used earlier by the present authors. Thus the screening effect is taken into account in this calculation in a satisfactory manner. The calculation is a repetition of what has been published recently by the present authors with one important exception: Here, the ejected-electron continuum state wave function that is used is determined variationally for the above screened Coulomb potential. Thereby some perturbation approximation of *ad hoc* nature could be avoided. As a consequence, considerable improvement is noticed in the total cross-section results. Comparison with experimental results for ^{29}Cu, ^{47}Ag, and ^{79}Au shows a good agreement. The calculation may easily be extended to ionization from other shells.

I. INTRODUCTION

In most earlier theoretical investigations[1–5] of inner-shell ionization problems, screening effects on the atomic electrons were taken into account through the choice of the effective central potential in the form

$$V(r)=-\frac{\alpha_0 Z_{\text{eff}}}{r}+v_0 ,$$

where $Z_{\text{eff}}=Z-0.3$ for the K shell and v_0 is a constant term. This is satisfactory for describing the bound-state wave function. For the description of scattering states there arise major difficulties.[6] One of these is in assigning proper energies to the two outgoing electrons moving with velocities v and v_1, respectively. A second one is a conceptual one, closely linked with the first difficulty which forces one to suggest[4] certain virtual excitation to give rise to contributions to real ionizations. Moreover such virtual contributions very often are $\frac{1}{3}$ to $\frac{2}{3}$ of the real contributions. So a better way of treating the screening effect is warranted. Scofield[7] actually took such a step and calculated total ionization cross sections for a number of species using Dirac-Hartree-Slater atomic wave functions in the calculation. An alternative way of taking the screening effect into account is to use the Thomas-Fermi[8] model potential as the effective central potential for the atomic active electron. An approximation to this potential has actually been used by Fermi[9] in some other context. We also proposed[10] recently for the use of the above screened Coulomb potential

$$V(r)=-\frac{\alpha_0}{r}-\frac{\alpha_0(Z_1-1)}{r}e^{-\alpha_0\lambda r} \tag{1}$$

in the study of inner-shell ionization problems. One good thing with this potential is that the above-mentioned difficulties no longer arise. One needs in the inner-shell ionization calculation both the bound-state and the scattering-state solutions for this potential. Bound-state solutions are easily obtained by the variational method. In our earlier calculations[11] the scattering state wave function was taken corresponding to a certain Coulomb potential, a part of the above potential, and the effect of the remaining part was treated perturbatively. This gives rise to certain difficulties and the results do not always appear to be good. So in our present work we have calculated both the bound- and the scattering-state wave functions variationally, although nonrelativistically, for the above potential and used these in our earlier formulation of the problem to obtain a formula for the triply differential cross section for the K shell ionization. We computed both the differential and the total cross section results for a number of atoms and compared these with other theoretical and experimental results. In most cases our results closely agree with those of Scofield,[7] particularly for heavier atoms.

II. THEORY

In our relativistic formulation of the atomic inner-shell ionization problems we use the Coulomb gauge. In this gauge the interaction Hamiltonian separates into a "static" Coulomb part and into a part which involves interaction with the transverse electromagnetic field. This second part includes the retardation effect. In a central field approximation for the atomic active electron and in absence of exchange, the scattering amplitude to the order α_0 becomes

$$T=T_d+T_{\rm tr}\ , \tag{2}$$

where

$$T_d=\left\langle \Phi_f \left| \frac{\alpha_0}{r_{12}}+V(r_2) \right| \Phi_i \right\rangle$$

and where

$$\Phi_i(\mathbf{r}_1,\mathbf{r}_2;\sigma_1,\sigma_2)=\varphi_i(\mathbf{r}_1,\sigma_1)u_{\sigma_2}(\mathbf{r}_2)$$

and

$$\Phi_f(\mathbf{r}_1,\mathbf{r}_2;\sigma_1',\sigma_2')=\varphi_f(\mathbf{r}_1,\sigma_1')u_{\sigma_2'}(\mathbf{r}_2)\ ,$$

φ_i being the initial bound-state wave function for the K electron and φ_f the final scattering-state wave function for it. Because of orthogonality we may write as well for it the expression

$$T_d=\left\langle \Phi_f \left| \frac{\alpha_0}{r_{12}} \right| \Phi_i \right\rangle\ . \tag{3a}$$

The expression for the transverse term may be written as

$$T_{\rm tr}=-\frac{4\pi\alpha_0}{(t^2-w_{if}^2)}\sum_{\epsilon} u^*_{\sigma_2'}(\mathbf{p}_f)(\boldsymbol{\alpha}\cdot\boldsymbol{\epsilon})u_{\sigma_2}(\mathbf{p}_i)\int d^3r_1\varphi_f^*(\mathbf{r}_1,\sigma_1')(\boldsymbol{\alpha}\cdot\boldsymbol{\epsilon})e^{i\mathbf{t}\cdot\mathbf{r}_1}\varphi_i(\mathbf{r}_1,\sigma_1)\ . \tag{3b}$$

In all these expressions we use the same notations as those of Ref. 2 and natural systems of unit are used unless otherwise stated. The expression for the triply differential cross section then becomes

$$\frac{d^3\sigma}{dw_f\,d\Omega_p\,d\Omega_{p_f}}=r_0^2\left[\frac{pp_fww_iw_f}{(2\pi)^5p_i}\right]\frac{1}{\alpha_0^2}(|\overline{T_d}|^2+|\overline{T}_{\rm tr}|^2)\ , \tag{4}$$

where quantities with an overbar correspond to those in which spin averages are taken. Finally the result has to be multiplied by a factor of two corresponding to two electrons in the K shell. It may be noted here that the parameter λ in potential (1) is so chosen that the theoretical and experimental ionization energies become the same.

III. DETAILS OF CALCULATIONS

For ionization of not too heavy atoms one may use nonrelativistic wave functions for the atomic electron. So we determine the K-electron wave function variationally. The nonrelativistic variationally determined wave function and the corresponding energy for the K electron are given[10] by

$$\varphi_i(\mathbf{r}_1,\sigma_1)=\frac{1}{\sqrt{\pi/a_1^3}}e^{-a_1r_1}u_{\sigma_1}(0)\ , \tag{5a}$$

where

$$a_1=\alpha_0\left[Z-\frac{3\lambda^2}{4Z}\right]$$

and

$$\epsilon_i=-(\alpha_0Z)^2/2+\lambda\alpha_0^2(Z-1)\ . \tag{5b}$$

In our present calculation we determine the continuum state wave function for potential (1) also variationally. Actually we set

$$\varphi_f(\mathbf{r}_1,\sigma_1')=[\varphi_C(\mathbf{r}_1)+\varphi(\mathbf{r}_1)]u_{\sigma_1'}(\mathbf{p})\ , \tag{6}$$

where $\varphi_C(\mathbf{r}_1)$ is the nonrelativistic Coulomb wave function satisfying the equation

$$\left[-\tfrac{1}{2}\nabla_1^2-\frac{\alpha_0}{r_1}\right]\varphi_C(\mathbf{r}_1)=E\varphi_C(\mathbf{r}_1) \tag{7}$$

and the equation satisfied by $\varphi_f(\mathbf{r}_1,\sigma_1')$ is

$$[-\tfrac{1}{2}\nabla_1^2+V(r_1)]\varphi_f(\mathbf{r}_1,\sigma_1')=E\varphi_f(\mathbf{r}_1,\sigma_1')\ , \tag{8}$$

so that $\varphi(\mathbf{r}_1)$ vanishes at infinity and describes the continuum state at short distances. The equation satisfied by $\varphi(\mathbf{r}_1)$ is

$$[-\tfrac{1}{2}\nabla_1^2+V(r_1)-E]\varphi(\mathbf{r}_1)=\left[\frac{\alpha_0(Z-1)}{r_1}e^{-\alpha_0\lambda r_1}\right]\varphi_C(\mathbf{r}_1)\ . \tag{9}$$

We find $\varphi(\mathbf{r}_1)$ from this equation by the least-squares approximation. We choose $\varphi(\mathbf{r}_1)$ in the form

$$\varphi(\mathbf{r}_1)=(c_1+c_2r_1+c_3r_1^2+c_4r_1\cos\theta_1 +c_5r_1^2\cos^2\theta_1+\cdots)e^{-\mu r_1}\ , \tag{10}$$

where μ is set equal to α_0Z for ionization from the K shell and the complex parameters c_1, c_2, c_3, c_4, c_5, etc., are determined by minimizing the quantity

$$\int d^3r_1\,r_1^2\,|c_1\varphi_1+c_2\varphi_2+c_3\varphi_3+c_4\varphi_4+c_5\varphi_5-F|^2\ , \tag{11}$$

where

$$F=\frac{\alpha_0(Z-1)}{r_1}e^{-\alpha_0\lambda r_1}\varphi_C(\mathbf{r}_1)\ ,$$

and φ_i's are the terms obtained by operating $[-\frac{1}{2}\nabla_1^2+V(r_1)-E]$ on the ith term in expansion (10). In our calculation it was found that the first four or five terms in the expansion are sufficient for converged results. So we recorded all our numerical results corresponding to five terms in expansion (10). Subsequent calculation is straightforward and leads to an expression for the triply differential cross section. Integrating this we get results for the doubly differential cross section and further integrations give the total cross section. One may note in this connection that here the energy conservation relation is

$$w_f + w = w_i + [1-(\alpha_0 Z)^2/2 + \alpha_0^2 \lambda (Z-1)] , \quad (12)$$

where w_i, w_j, and w are the energies of the incident electron, scattered electron, and ejected electron, the corresponding kinetic energies are E_0, E_f, and E, respectively.

IV. RESULTS

Differential as well as total cross sections have been calculated following the steps indicated in the last section. The present calculation is most suitable for the study of the total cross section, particularly for medium-heavy atoms, in view of the approximations used. So we present here a considerable amount of results for the total cross section. Contrary to this we present one set of results for a doubly differential cross section just to illustrate the quality of results obtained for this from the present calculation.

We present our computed total cross section results for ^{29}Cu, ^{47}Ag, and ^{79}Au in Figs. 1(a)—1(c), respectively. Results for ^{28}Ni, ^{47}Ag, and ^{79}Au and some other atoms are presented in the Table I. In the above figures we also present the experimental results of Davis *et al.*[14] and of Rester and Dance[15] and in case of ^{47}Ag an additional result of Fischer and Hoffmann.[16] The theoretical results of Scofield[7] and of Das[3] are also included for comparison, whenever available. The reason for inclusion of these two sets of results and not some others[1,4,17–19] is that the corresponding calculations are closely related to the present one in some respect or other.

In the case of ^{79}Au our results agree better with the experimental results compared to those of Scofield,[7] or of Das[3] (or of any other calculation). In the case of ^{29}Cu the agreement of our results with the measured values of Davis *et al.*[14] is also good. But in the case of ^{47}Ag, the experimental results of Rester and Dance[15] better fit with the results of Scofield for 200, 250, and 300 keV energies. Below 200 keV energy and for 2 MeV energy our results agree satisfactorily with the experimental results and some times in a better way. If we compare our present results for ^{79}Au with those of Das[3] it will be clear that the screening effect is most important at lower energies and that the present way of taking this effect into account is

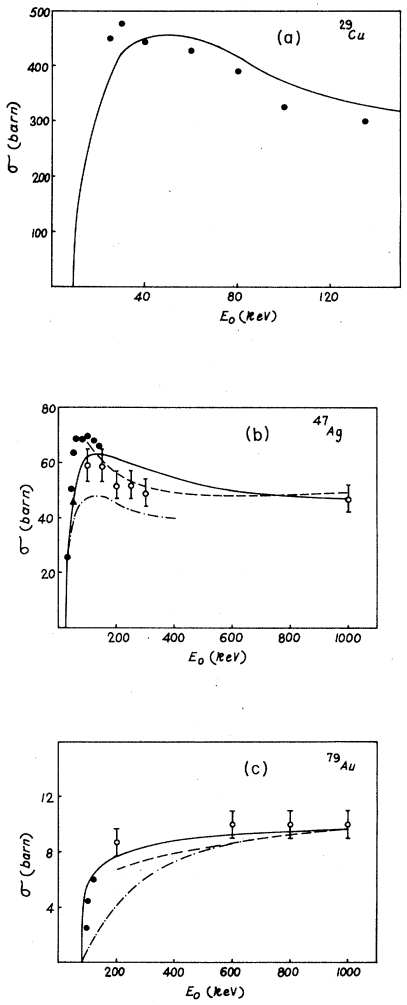

FIG. 1. Comparison of the total cross section for the K-shell ionization of (a) ^{29}Cu, (b) ^{47}Ag, and (c) ^{79}Au for different energies of the incident electron. Theory: ——, present calculation; – – – –, Scofield (Ref. 7); —·—·—, Das (Ref. 3). Experiment: ♀, Rester and Dance (Ref. 15); ●, Davis *et al.* (Ref. 14); ▲, Fischer and Hoffmann (Ref. 16).

TABLE I. Comparison of the present (P) cross section for the approximate Thomas-Fermi calculation with those of the Dirac-Hartree-Slater calculation of Scofield (Ref. 7) (S) for the K-shell ionization of atoms by electrons (cross sections are in barns).

E_0 (keV) \ Z	28		47		56		67		79		83		92	
	P	S	P	S	P	S	P	S	P	S	P	S	P	S
50	459	525	46.4											
100	478	368	62.8	67.6	33.2	32.3			6.52					
150	403	302	62.7	61.0		32.0		14.6						
200	359	267	61.2	56.5	31.4	30.7	15.7	15.1	7.64	6.77	5.32	5.07		
300		232	58.7	51.6		29.1		15.2	8.24	7.56		5.95	3.82	3.38
400	288	216	56.4	49.4	29.3	28.4	16.1	15.3	8.77	7.98	6.83	6.41	4.13	3.86
500		208		48.5		28.3		15.5		8.32		6.76		4.20
600	236	203	49.7	48.3		28.4	16.4	15.8	9.32	8.64	7.34	7.08	4.75	4.49
800		200		48.6	28.5	28.9	16.8	16.5		9.24	7.73	7.64	5.16	4.97
1000	218	201	47.5	49.5	30.1	29.7	17.2	17.1	9.74	9.78	8.18	8.14	5.51	5.39
2000	214	214			32.2	33.6	20.1	19.9	11.4	11.9	9.63	10.0	6.27	6.90

better. Here it may be recalled that the present calculation and the calculation of Das[3] are the same except in the treatment of the screening effect. A look at Table I will convince one that the present results compare favorably with the results of Scofield for heavier elements, say for $Z \geq 56$. At lower energies the present results are a little larger and are expected to be a little better compared to those of Scofield [cf. Fig. 1(c)]. It may be noted further that our results for ^{29}Cu agree satisfactorily with the experimental results of Davis. But in this case there are no results of Scofield. However, for ^{28}Ni for which the value of Z is just less by unity our results significantly differ from those of Scofield. Unfortunately in this case there exists no recent measurements, say by Davis. The old experimental results are disfavored by both the calculations. So new measurements are needed to clarify the situation. The 2 MeV energy for the electron is quite high. At this energy one may expect very little effect of screening. As a result the present calculation, the calculations of Scofield[7] and of Ndefru, Wills, and Malik,[5] and of Davidović and Moiseiwitsch[4] give nearly identical results (cf. Table I). The agreement with the measurements of Li-Scholz *et al.*[20] is also very good. In the above theoretical calculations exchange has not been included. When this is included, the results at lower energies will be a little less, say by 10% or less.

Differential cross sections depend sensitively on the quality of the wave function used in the calculation. In certain cases the effect of exchange is also very important. Our present calculation is not expected to give a highly accurate differential cross section except at small angles, since on the one hand exchange is neglected and on the other relativistic effects have been neglected when the bound and ejected electron wave functions are calculated. So in general we get results for differential cross sections whose accuracies are similar to those of Das[2] except for the changes which occur due to the different way of treating the screening effect. Thus the results for the doubly differential cross section $d^2\sigma/dE_1 d\cos\theta_1$ for ^{79}Au for 300 keV electron energy and 20° scattering angle, presented in Fig. 2, show a peculiar depression around 180 keV energy, not present in previous theoretical results of Das[2] or of Das and Chakraborty,[10] but give better agreement with the experimental results of Komma and Nakel[21] for intermediate and lower energies. For high energies the results of Das and Chakraborty[10] give better agreement. This last calculation uses a relativistic Sommerfeld-Maue[22] wave function for an approximate Coulomb potential.

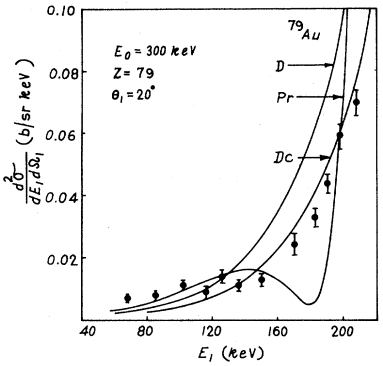

FIG. 2. Comparison of the doubly differential cross section for the K-shell ionization of ^{79}Au for different energies of the detected electron. Theory: Pr, present calculation; D, Das (Ref. 2); DC, Das and Chakraborty (Ref. 10). Experiment: ⧫, Komma and Nakel (Ref. 21).

V. CONCLUSIONS

From the discussion of the last section it is more or less clear that the present calculation gives good results for total cross sections, especially for medium-heavy elements. The close agreement between the present results and the results of Scofield is also highly encouraging. Thus the way in which the screening effect is taken into account is quite satisfactory. Moreover we do not face the sort of difficulties mentioned in the Introduction. During our calculation of the continuum-state ejected electron wave function by the least-squares method we also face no trouble and find very quick convergence with four or five terms in expansion (10), at most. Salient relativistic effects have been included in our calculation. For better results for differential cross sections one needs to include the exchange effect properly, and secondly, the bound and ejected electron wave function need to be calculated including the relativistic effects properly, possibly by solving the relevant equations variationally for the screened Coulomb potential (2), especially for heavier atoms. Finally it may be stated that the calculation may be easily extended for ionization from other shells.

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