Energy distribution of secondary electrons in electron-impact ionization of hydrogenic and heliumlike ions

D. Fang, W. Hu, J. Tang, Y. Wang, and F. Yang
Department of Nuclear Science, Fudan University, Shanghai 200433, People's Republic of China
(Received 22 June 1992)

The energy differential cross sections for electron-impact ionization of H- and He-like ions have been calculated using a distorted-wave Born exchange approximation. The calculated results are well fitted to a two-parameter Gaussian function. These results from the fitting, which reproduce the calculated cross sections with an average error of about 4%, are in good agreement with experimental results.

PACS number(s): 34.80.−i

I. INTRODUCTION

In the study of astrophysical plasmas such as the solar corona and laboratory plasmas such as those used in fusion research, knowledge of ionization balance curves giving the relative abundance of the different ionization stages of each element as a function of temperature is very important. There is much information available concerning the total cross section of electron-impact ionization of ions both experimentally and theoretically [1–4]. However, there is little information about the energy differential cross section of ionization, which indicates the energy distribution of secondary electrons during ionization, and which may be even more important in understanding the evolution and structure of high-temperature plasmas. In order to supply data for understanding and modeling the processes of high-temperature plasmas, we made many calculations of the energy differential cross sections of electron-impact ionization for H-like and He-like ions. In principle, other ion species and their isoelectronic series can be calculated in the same procedure, but in practice a large scale and detailed calculation of such cross sections is quite expensive computationally. Thus a simple fit to the theoretically calculated results by an analytic formula is desirable. Among many fitting procedures, Lotz plot [5] are frequently used to fit the total cross sections. Kim [6] analyzed the secondary-electron energy distribution by Platzman plot in which the ratio of measured cross section to the Rutherford cross section is plotted as a function of the energy loss of the impact electron. Clark, Abdallah, and Mann, Jr. [7] used nine parameters to fit the scaled hydrogenic total cross section and then obtained the total cross section for a complex ion by using screening parameters. They also fitted differential cross sections and the fitting procedure can reproduce all values for the Coulomb-Born exchange (CBX) differential cross sections with a maximum error of 20% and average error of 5%. They found that the fit form can be applied to more elaborate calculations such as distorted-wave approximation. In this paper we find that the energy differential cross sections calculated by distorted-wave Born exchange (DWBE) approximation can be well fitted by a Gaussian function with two adjustable parameters. The dependence of the two parameters on the nuclear charge of the target ion and on the energy of the incident electron, that is, the scaling laws of the parameters, are also given.

In Sec. II, we briefly describe the theory framework and numerical procedures. Section III presents the calculated results of energy differential cross sections along with the prescription of fitting procedures and the scaling law of the adjustable parameters. Discussions on the DWBE approximation and comparison with other calculations are made in Sec. IV, and a detailed check on our fitting procedure is also given in this section. Section V provides a brief summary.

II. DISTORTED-WAVE BORN EXCHANGE APPROXIMATION

The energy differential cross section of electron-impact ionization σ can be given by [8]

$$\sigma(E_i,E_e)=\frac{dQ}{dE_e}$$
$$=\frac{8}{\pi E_i}-\sum_{l_i,l_e,l_f,L}(2L+1)I_{l_i,l_e,l_f}(E_i,E_e)\ , \qquad (1)$$

where l_i, l_e, and l_f are the orbital angular momenta of the incident, ejected, and scattered electrons, L is the conserved total angular momentum of the whole system, and

$$I_{l_i,l_e,l_f,L}=|f|^2+|g|^2-\alpha|f||g|\ , \qquad (2)$$

where f and g are the direct and exchange scattering amplitudes, respectively, and α is a phase factor. In this paper, the "maximum interference" approximation of Peterkop [9] was used ($\alpha=1$). The scattering amplitudes can be written as

$$f=\sum_{\lambda}f_{\lambda}(l_b,l_i,l_e,l_f,L)\left[P_bP_i\left|\frac{1}{r_{12}}\right|P_eP_f\right]_{\lambda}\ , \qquad (3)$$

$$g=\sum_{\lambda}f_{\lambda}(l_b,l_i,l_f,l_e,L)\left[P_bP_i\left|\frac{1}{r_{12}}\right|P_fP_e\right]_{\lambda}\ , \qquad (4)$$

where l_b is the orbital angular momentum of the bound target electron, f_λ is an angular factor, r_{12} is the distance between the two electrons, and P_b, P_i, P_e, and P_f are the radial wave functions corresponding to the bound, incident, ejected, and scattered electrons, respectively. In the present work, the target ion wave functions are obtained by a single-configuration Hartree-Fock code [10]. For free-electron wave functions, the DWBE approximation was employed, in which the distortion of the nuclear Coulomb potential due to orbital electrons is taken into account. The potential $V(r)$ which the free electrons experienced is given by

$$V(r)=-\frac{Z}{r}+\sum J_{nl}(r)\ , \tag{5}$$

where Z is the nuclear charge, $J_{nl}(r)$ represents the potential from one electron in state nl, and the summation is over all of the target electrons. J_{nl} is given by

$$J_{nl}(r)=\frac{1}{r}\int_0^r P_{nl}^2(\rho)d\rho+\int_r^\infty \frac{P_{nl}^2(\rho)}{\rho}d\rho\ . \tag{6}$$

We used a program based on Eqs. (1)–(6) to calculate the energy differential cross sections for electron-impact ionization of H- and He-like ions. The integrals in (3) and (4) were calculated with a block linear radial grid [11]. In the calculation, the summation of each partial wave was truncated when the increments were less than 0.2%. For impact-electron energy u (in unit of ionization threshold) lower than 2.25, the number of partial waves calculated were less than 20. For higher energies such as $u=10$, the partial waves were included up to 55. We plotted the L distribution of the cross sections in logarithmic scale and found that it can be well fitted to a straight line in the tail section. One can extrapolate the contributions from even higher partial waves. We also found that such an extrapolation added less than 1% of the cross section to the final results.

In calculations for He-like sequences, we found it important to include a semiclassical exchange (SCE) potential [12] in the distortion, which presents the exchange effects between bound and free electrons. Inclusion of SCE brings down the cross sections about 10–20 % for low-Z ions.

III. RESULTS

We selected several targets including the neutral atom to study: H, He^+, Li^{2+}, C^{5+}, S^{15+}, Fe^{25+}, and Pb^{81+} for the H-like isoelectronic series, and He, Li^+, B^{3+}, O^{6+}, Ar^{16+}, Fe^{24+}, and Pb^{80+} for the He-like isoelectronic series. As examples, we show one figure for the energy differential cross sections for different incident energies for ionization of He^+ (see Fig. 1), and another figure for ionization of B^{3+} (see Fig. 2). In order to present results of different incident energies in one figure, the reduced ejected energy x is introduced,

$$x=E_e/(E_i-I)=E_e/I(u-1)\ , \tag{7}$$

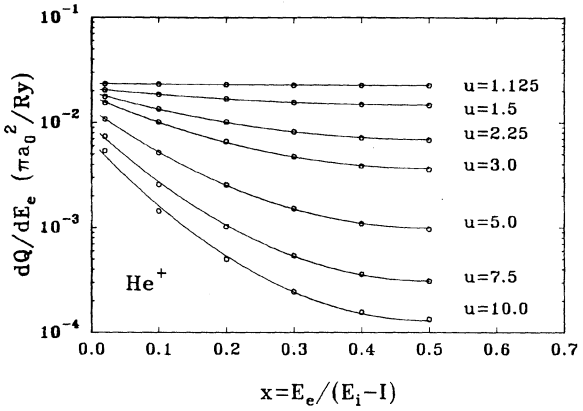

FIG. 1. The energy differential cross sections at different incident energies for ionization of He^+.

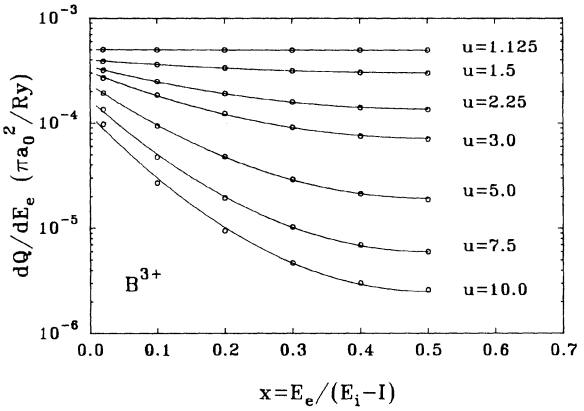

FIG. 2. The energy differential cross sections at different incident energies for ionization of B^{3+}.

TABLE I. Ionization potentials (in rydberg units).

H-like sequence						
H	He^+	Li^{2+}	C^{5+}	S^{15+}	Fe^{25+}	Pb^{81+}
1.0	4.0	9.0	36.0	256.9	682.8	7578.0
He-like sequence						
He	Li^+	B^{3+}	O^{6+}	Ar^{16+}	Fe^{24+}	Pb^{80+}
1.79	5.55	19.06	54.35	303.2	650.2	7427.2

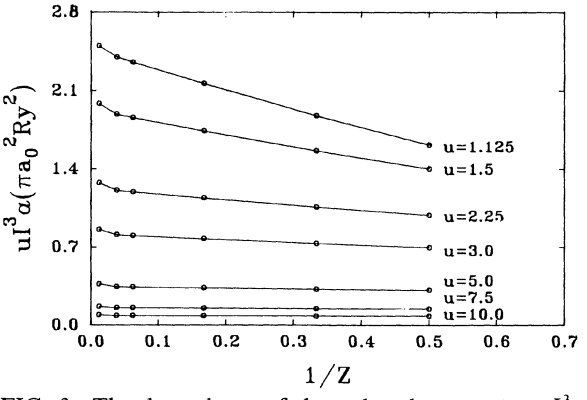

FIG. 3. The dependence of the reduced parameter uI^3a on $1/Z$ for different u in H-like sequences.

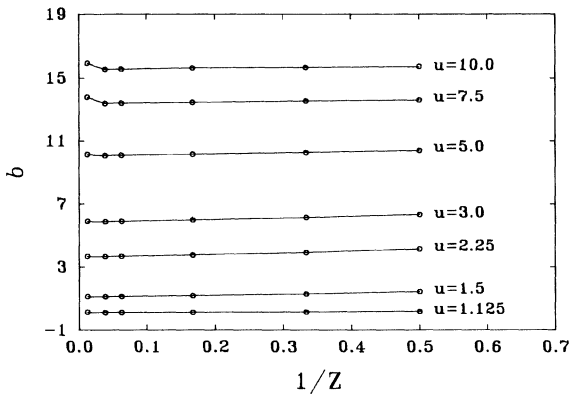

FIG. 4. The dependence of the parameter b on $1/Z$ for different u in H-like sequences.

where E_e and E_i are ejected and incident energies and I is the ionization potential. The values of I are listed in Table I. The quantity x is the ratio of ejected electron energy to assignable energy in the final state, and it has a range between 0 and 1. Since the energy differential cross section σ has the symmetry $\sigma(1-x)=\sigma(x)$, only the range of x from 0 to 0.5 is considered in our calculations. The open circles in Figs. 1 and 2 represent the calculated cross sections. We found these points can be well fitted to a Gaussian function with two parameters, i.e., the differential cross sections can be given in the form

$$\sigma(u,x)=\frac{dQ}{dE_e}=ae^{b(x-0.5)^2} . \tag{8}$$

The solid lines in Figs. 1 and 2 are our fits with Eq. (8).

The two parameters a and b of the Gaussian function are related to the size and shape of the energy differential cross sections. Figures 3 and 4 give the dependence of the two parameters on $1/Z$ for different u in H-like sequences. It should be noted that the reduced parameter uI^3a is introduced instead of a in order to suppress the large change of a due the change in Z. Using Eq. (8) and along with the parameters, we can reproduce the DWBE differential cross sections with a maximum error of 10% and average error of 4%.

The dependence of the two parameters in He-like series is similar to that in H-like series. We list these parameters for He-like series in the form of tables instead of figures (see Tables II and III).

TABLE II. Scaled parameter uI^3a (in units of πa_0^2) for He-like sequence.

Ions	He	Li^+	B^{3+}	O^{6+}	Ar^{16+}	Fe^{24+}	Pb^{80+}
$u=1.125$	0.355	2.246	3.848	4.239	4.631	4.725	4.954
$u=1.500$	1.056	2.100	3.118	3.409	3.671	3.739	3.944
$u=2.250$	1.233	1.654	2.110	2.251	2.368	2.400	2.541
$u=3.000$	1.050	1.268	1.479	1.545	1.603	1.618	1.717
$u=5.000$	0.566	0.662	0.663	0.676	0.688	0.693	0.744
$u=7.500$	0.282	0.329	0.308	0.311	0.314	0.315	0.339
$u=10.000$	0.164	0.189	0.172	0.173	0.174	0.174	0.188

TABLE III. Parameter b for He-like sequence.

Ions	He	Li^+	B^{3+}	O^{6+}	Ar^{16+}	Fe^{24+}	Pb^{80+}
$u=1.125$	3.21	0.102	0.062	0.148	0.118	0.121	0.159
$u=1.500$	3.78	1.07	1.14	1.13	1.10	1.08	1.08
$u=2.250$	5.34	3.35	3.75	3.67	3.64	3.63	3.66
$u=3.000$	6.97	5.35	5.86	5.86	5.83	5.83	5.88
$u=5.000$	10.53	9.00	10.02	10.02	10.00	10.00	10.10
$u=7.500$	13.84	12.43	13.34	13.34	13.35	13.35	13.75
$u=10.000$	15.95	14.69	15.50	15.50	15.51	15.51	15.92

IV. DISCUSSION

Although the DWBE calculation of differential cross section can be well fitted with the Gaussian function, there are two points to be made. The first concerns the accuracy of the DWBE calculation. In most of the early calculations, a variety of the Coulomb-Born (CB) approximation and the scaled hydrogenic method have been used. A recent calculation by Attaourti *et al.* [13] shows that the CBX approximation can provide quite good results for some heliumlike ions. More elaborately Younger and many others [14,15] have calculated several isoelectronic series of ions using distorted-wave approximation and indicated that, in general, the electron-impact ionization cross sections for ions can be well described by the DWBE in the range $u=1.0$–5.0. We repeated some calculations of the total cross section and compared with the previous calculations and experimental data. Our results differ from Younger's calculation by about 2% and agree with experimental data [16,17] reasonably well. The second point is that the Gaussian function can generate the correct total cross sections. To verify this, one can obtain the parameters by interpolating for any ion with $Z \leq 82$ in H-like or He-like series. As an example, we used linear interpolation and obtained the two parameters for N^{5+} at $u=1.5$. Following Eq. (8) we integrated the Gaussian function over x (E_e) and obtained the total cross section $\sigma=6.59\times10^{-20}$ cm^2. This result shows excellent agreement with Younger's calculation [14], which gives $\sigma=6.60\times10^{-20}$ cm^2. Since the variations of parameters are smooth, as shown in Figs. 3 and 4, the uncertainty due to interpolation should be small.

We have not yet discussed the variation of the two parameters with incident energy u. In this case, linear interpolation may not always be able to satisfy the accuracy requirement. Here a three-point Lagrangian interpolation seems suitable. We use this interpolation to calculate the total cross section for Li^+ at several incident energies. The results and comparison with experimental data [18,19] are given in Table IV. Our results are consistent with experimental data within the error range.

As a more detailed check, we need to compare the calculated energy differential cross section directly with experimental results. In general, the Born approximation method we used in the calculation is more accurate for

TABLE IV. Total cross section (10^{-18} cm^2) for Li^+.

E_i (eV)	Present value	Peart *et al.* [18]	Lineberger *et al.* [19]
100	1.61	1.52(15)	1.69(12)
200	3.94	3.92(6)	4.28(8)
300	4.24	4.14(6)	4.50(8)
400	4.02	4.10(6)	4.25(8)
500	3.83	3.90(6)	3.98(8)
600	3.53		3.62(8)
750	3.19	3.32(6)	

ions than for neutral atoms. However, we could not find experimental energy differential cross sections of electron-impact ionization for ions. In order to have some experimental data with which to compare, we performed our fitting procedure for neutral helium atom as an example, though our main interest is in ions. From interpolation, we obtained the two parameters a and b for the helium atom at an incident energy of 200 eV: $a=4.91\times10^{-3}$ (πa_0^2/Ry) and $b=14.56$. Figure 5 gives the comparison of energy differential cross sections between our Gaussian curve calculated from above parameters and experimental data. The experimental points are from Refs. [20–23]. We see that the simple calculation agrees very well with the experimental data. This supports our Gaussian function fitting method. We note that, in Fig. 5, the curve has been multiplied by a factor of 2. Since the experimental measurements do not distinguish between ejected and scattered electrons, our calculated results should be doubled in order to compare directly with measured values. After these checking procedures, we can say with confidence that the differential cross sections and the total cross sections can be obtained by parameter interpolation.

Clark, Abdallah, and Mann, Jr. [7] fitted the CBX differential cross sections with a formula,

$$\frac{dQ}{dE_e}=C_1+C_2(x-0.5)^4\ , \tag{9}$$

where C_1 and C_2 are parameters. In comparison with their fit, we found that the Taylor expansion of Eq. (8) includes the terms given by them. It seems that the exponential form is better.

V. CONCLUSION

In this paper, we have calculated the energy differential cross section of electron-impact ionization for some ions in H- and He-like sequence and fitted these results by a Gaussian function. The fit can reproduce the differential cross sections with an average error of about 4%. The comparison with experimental results and the total cross section calculations show that the Gaussian function can describe the differential cross sections very well.

The scaling of two parameters in the Gaussian function are also given, in the form of figures (for H-like sequence) or tables (for He-like sequence). Based on these figures or tables, one can obtain the needed values by interpolation and calculate the differential cross section by a very simple procedure. The total cross sections also can be obtained simply by integrating over the differential cross sections.

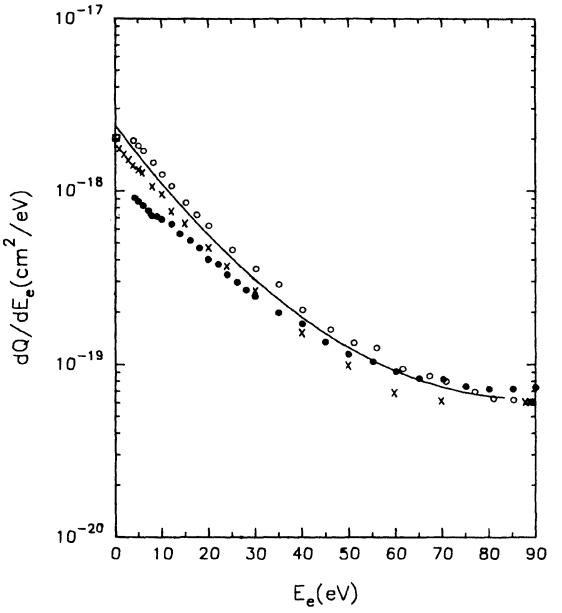

FIG. 5. The energy differential cross sections for ionization of helium atom by 200 ev electron impact. Theoretical value: —— present calculation. Experimental data: ×, Shyn *et al.* [20]; ○, Opal *et al.* [21]; ●, Rudd and Dubois [22]; □, Grisson *et al.* [23].

ACKNOWLEDGMENTS

This work is supported by Natural Science Foundation of China and partially supported by Fok Ying Tung Education Foundation.

[1] D. H. Crandall, R. A. Phaneuf, B. E. Hasselpuist, and D. C. Gregory, J. Phys. B **12**, L249 (1979).
[2] S. Rachafi, D. S. Belic, M. Duponchelle, J. Jureta, M. Zambra, Zhang Hui, and P. Defrance, J. Phys. B **24**, 1037 (1991).
[3] S. M. Younger, Phys. Rev. A **26**, 3177 (1982).
[4] N. R. Badnell, D. C. Griffin, and M. S. Pindzola, J. Phys. B **24**, L275 (1991).
[5] W. Lotz, Z. Phys. **206**, 205 (1967).
[6] Y.-K. Kim, Radiat. Res. **61**, 21 (1975); **64**, 96 (1975).
[7] R. E. H. Clark, J. Abdallah, and J. B. Mann, Jr., Astrophys. J. **381**, 597 (1991).
[8] S. M. Younger, Phys. Rev. A **22**, 111 (1980).
[9] R. K. Peterkop, Zh. Eksp. Teor. Fiz. **41**, 1938 (1961) [Sov. Phys. JETP **14**, 1377 (1962)].
[10] R. D. Cowan, *The Theory of Atomic Structure and Spectra* (University of California Press, Berkeley, 1981).
[11] D. F. Fang and Y. S. Wang, J. Phys. B **24**, 1749 (1991).

[12] M. E. Riley and D. G. Truhlar, J. Chem. Phys. **63**, 2182 (1975).
[13] Y. Attaourti, P. Defrance, A. Makhoute, and C. J. Joachain, Phys. Scr. (Sweden) **43**, 578 (1991).
[14] S. M. Younger, Phys. Rev. A **22**, 1425 (1980).
[15] See references in *Electron Impact Ionization*, edited by T. D. Mark and G. H. Dunn (Springer-Verlag, Berlin, 1986).
[16] H. Tawara and T. KaTo, At. Data Nucl. Data Tables **36**, 167 (1987).
[17] M. A. Lennon, K. L. Bell, H. B. Gilbody, J. G. Hughes, A. E. Kingston, M. J. Murray, and F. J. Smith, J. Phys. Chem. Ref. Data **17**, 1285 (1988).
[18] B. Peart and K. T. Dolder, J. Phys. B **1**, 872 (1968).
[19] W. C. Lineberger, J. W. Hooper, and E. W. McDaniel, Phys. Rev. **141**, 151 (1966).
[20] T. W. Shyn and W. E. Sharp, Phys. Rev. A **19**, 557 (1979).
[21] C. B. Opal, E. C. Beaty, and W. K. Peterson, At. Data **4**, 209 (1971).
[22] M. E. Rudd and R. D. Dubois, Phys. Rev. A **16**, 26 (1977).
[23] J. T. Grisson, R. N. Compton, and W. R. Garrett, Phys. Rev. A **6**, 977 (1971).