Relativistic effects on the polarization of line radiation emitted from He-like and H-like ions following electron-impact excitation

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The radiation emitted from ions excited by a directed electron beam can be strongly linearly polarized. According to Itikawa, Srivastava, and Sakimoto [Phys. Rev. A. **44**, 7195 (1991)] the degree of polarization should be independent of atomic number in an isoelectronic sequence when expressed as a function of incident-electron energy in threshold units. We used a distorted-wave computer code to calculate cross sections for electron-impact excitation to specific magnetic sublevels of H- and He-like ions with $Z=13$, 18, 22, 42, 56, 79, and 92. We found that the polarization of the resulting radiation is indeed independent of atomic number in the nonrelativistic limit. But when relativistic effects are properly taken into account, the polarization is markedly Z dependent. We show how the differences between the relativistic and nonrelativistic results vary with the incident-electron energy, as well as with increasing atomic number.

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I. INTRODUCTION

In this paper we discuss the results of our investigation of relativistic effects on the polarization of radiation emitted following electron-impact excitation of highly charged He- and H-like ions. Recently Itikawa, Srivastava, and Sakimoto [1] reported calculations which indicated that the polarization is independent of atomic number for H-like and He-like ions when expressed as functions of incident-electron energy in the threshold units. They calculated the polarization for several low-Z ions and then determined the polarization for the case of the infinite-Z approximation. However, they neglected relativistic effects in their calculations. For low-Z ions at low collision energies relativistic effects are not significant. But for higher-Z ions, relativistic effects on the target atomic structure and the high-energy scattered waves are not negligible, and these effects can significantly affect the cross sections for electron-impact excitation. Since the polarization of the emitted radiation depends upon the cross sections for excitation to magnetic sublevels, one might expect that relativistic effects on the polarization could be significant for ions with high atomic number.

In a plasma the radiation emitted following electron collisional excitation can be polarized when the electron distribution is anisotropic. This occurs in some astrophysical plasmas [2] and also in laboratory plasmas under conditions where the ions are excited by a directed electron beam [3]. A notable example of this is the electron-beam ion trap (EBIT) at Lawrence Livermore National Laboratory [4]. In the EBIT, ions are confined in a small region and exposed to a vertically directed electron beam which can excite or further ionize the trapped ions. Under these circumstances, the magnetic sublevels of the excited states may not be populated statistically. The radiation emitted from the trap is observed from a direction perpendicular to the direction of the electron beam, and can be strongly polarized. The degree of polarization depends upon the cross sections for electron-impact excitation to specific magnetic sublevels of the ions.

In recent years there have been several theoretical studies of electron-impact excitation to specific magnetic sublevels of ions and polarization of the subsequent radiation [1,5–10]. There have also been recent experimental studies of polarization of radiation on EBIT [11,12]. In this work we made a systematic investigation of relativistic effects on the polarization of radiation emitted following electron-impact excitation of the $1s^2 \rightarrow 1s2p(^1P_1)$ transition in He-like ions of Si, A, Ti, Mo, Ba, Au, and U, and the $1s \rightarrow 2p_{3/2}$ transition in H-like ions of these same elements. We calculated the excitation cross sections and the polarization fractions in the nonrelativistic limit and then repeated the calculations with relativity included.

II. RESULTS AND DISCUSSION

A. He-like ions

The polarization for radiation emitted at 90° with respect to the electron beam has related to the excitation cross sections by

$$P=(\sigma_0-\sigma_1)/(\sigma_0+\sigma_1) , \quad (1)$$

where σ_0 and σ_1 are the cross sections for electron-impact excitation from the ground state to the $m=0$ and 1 magnetic sublevels, respectively. These excitation cross sections, σ_0 and σ_1, were calculated using a distorted-wave code developed by Zhang, Sampson, and Clark [8]. Configuration-interaction-type wave functions were used in the target structure calculations which were performed with a Dirac-Fock-Slater atomic structure code [13,14] developed for use with the scattering computer code in Ref. [8]. These codes can be used in a fully relativistic mode or in a nonrelativistic mode, and we made use of both of these modes in order to obtain the results neces-

TABLE I. Polarization of the $1s2p(^1P_1)\rightarrow 1s^2$ line in He-like ions. (The infinite-Z values are from Ref. [1].) X is the incident-electron energy in threshold units.

	Polarization							
X	Si	A	Ti	Mo	Ba	Au	U	$Z=\infty$
				Nonrelativistic				
2	53.80	53.66	53.62	53.56	52.97	53.47	53.51	53.4
4	35.73	35.36	35.44	35.42	36.06	35.26	35.25	35.3
5	28.96	28.95	28.93	28.97	27.09	28.87	28.81	28.7
				Relativistic				
2	52.44	53.81	53.81	53.87	54.23	54.31	53.40	53.4[a]
4	34.51	37.82	37.85	38.87	41.37	46.07	47.43	35.3
5	28.29	29.85	30.26	33.59	36.63	41.93	44.69	28.7

[a]The infinite-Z values shown here are nonrelativistic values.

sary to effect the comparisons made in this study.

In Table I we show the polarization of the $1s2p(^1P_1)\rightarrow 1s^2$ line for He-like ions with $13\leq Z\leq 92$. In the nonrelativistic case the polarization is nearly independent of Z and has approximately the same value as the polarization for infinite Z given in Ref. [1]. This holds true for incident-electron energies of two, three, and five times threshold and is consistent with the claim in Ref. [1] that the polarization should be independent of Z.

However, the situation is quite different when relativistic effects are taken into account. At incident electron

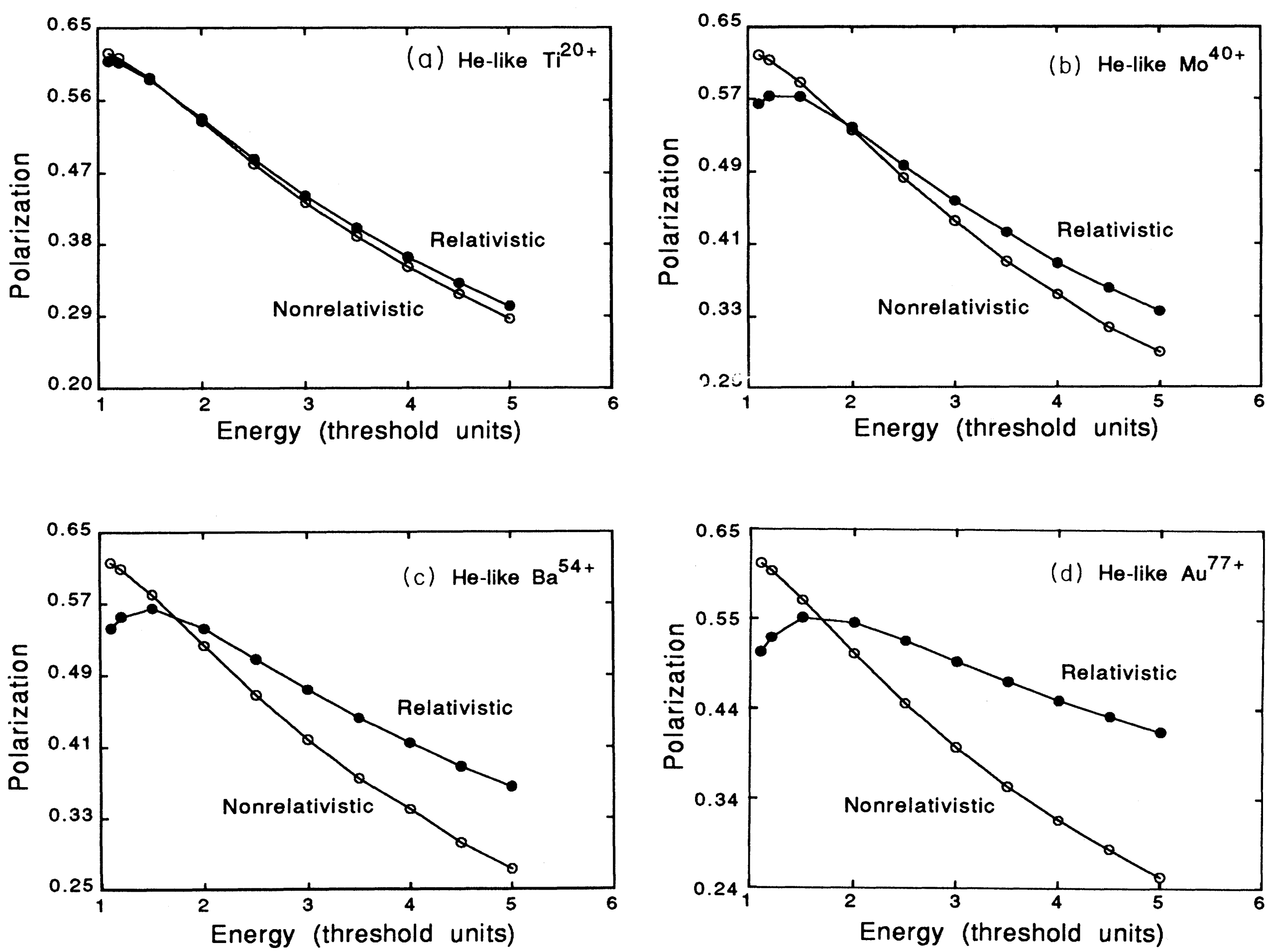

FIG. 1. Polarization for He-like ions as functions of incident-electron energy in threshold units. The dark circles represent the relativistic values and the open circles represent the nonrelativistic values.

energies of twice the threshold energy the polarization is 52.44 for Si and remains fairly constant for the whole range of Z. The nonrelativistic infinite-Z value is 53.4. At incident energies four times threshold, the polarization for Si is 34.51, which is close to the nonrelativistic infinite-Z value of 35.30. However, at these energies, the polarization rapidly increases with increasing Z, and at $Z=92$ it has increased to 47.43. At incident energies five times threshold the polarization for $Z=13$ is still close to the nonrelativistic infinite-Z value, but it increases even more rapidly with increasing Z. Thus for $Z=92$, at five times the threshold energy, the polarization is 44.69, which is quite different from the nonrelativistic infinite-Z value of 28.7.

In Figs. 1(a)–1(d) we show the polarization as a function of incident-electron energy for different He-like ions. For He-like Ti the relativistic and nonrelativistic curves stay close to one another at all energies. The nonrelativistic polarization is about 0.63 near threshold and rapidly decreases monotonically with increasing energy. The relativistic results are slightly below the nonrelativistic results at threshold, and increase slightly before starting to decrease at higher energies. This same pattern of a slight increase in the polarization after threshold, followed by a steady decrease in the polarization, was apparent in the intermediate coupling calculations for He-like Fe reported by Inal and Dubau [5]. The relativistic and nonrelativistic results are equal at about $1.5X$. (We use X to represent threshold energy.) The relativistic results decrease with increasing energy, but at a slightly lower rate than the decrease in the nonrelativistic curve, so the two curves become increasingly separated at higher energies.

The nonrelativistic curve for the He-like ions with higher atomic number is essentially the same as that for He-like titanium. But the near-threshold polarization decreases as Z increases when relativistic effects are taken into account, and at higher incident-electron energies the slope of the relativistic curve gets smaller with increasing Z. For all of the He-like ions the relativistic and nonrelativistic curves cross at incident energies near 1.8 times threshold. The differences between the relativistic and

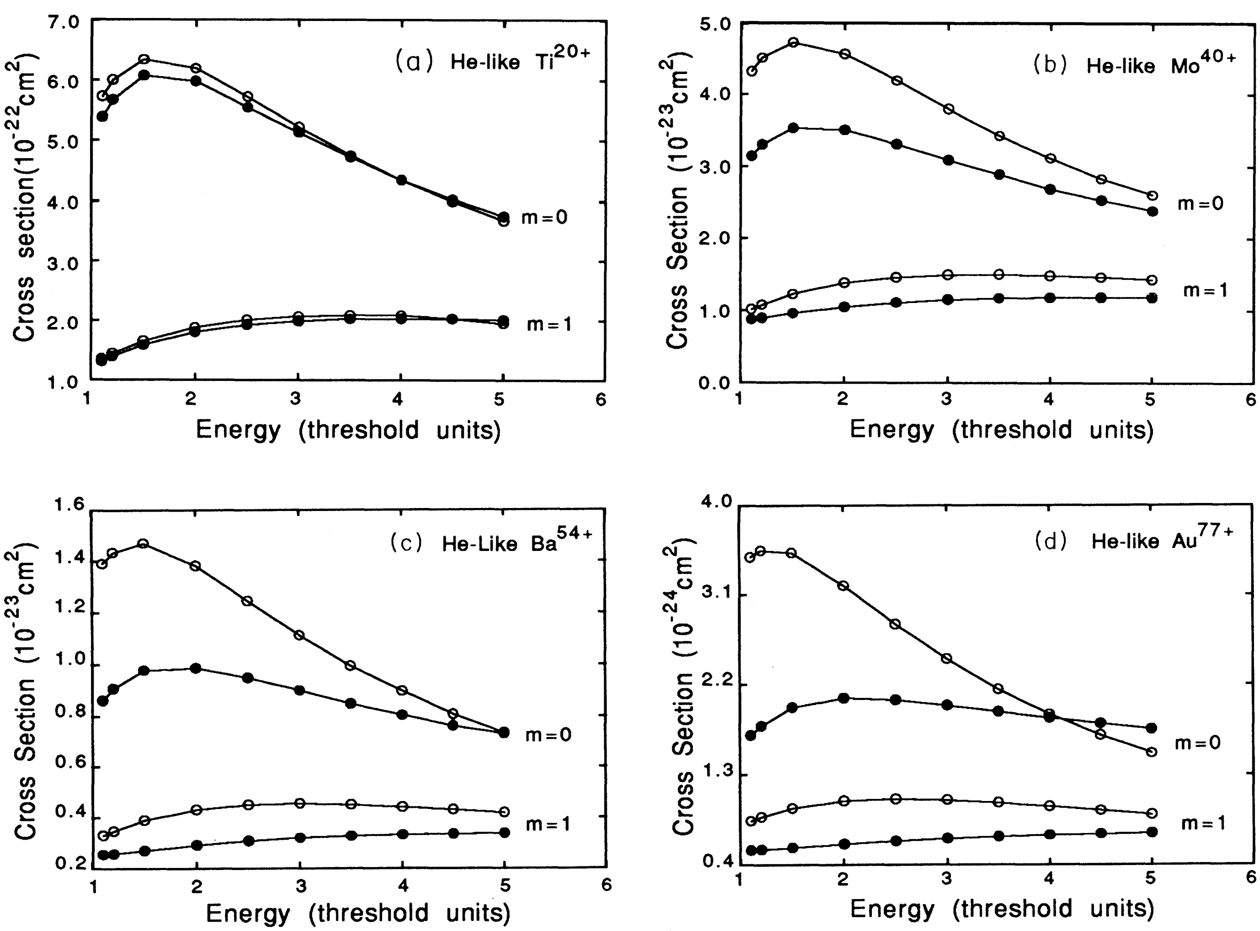

FIG. 2. Cross sections for electron-impact excitation to specific magnetic sublevels of He-like ions as functions of incident-electron energy in threshold units. The dark circles are the relativistic cross sections and the open circles are the nonrelativistic cross sections.

TABLE II. Polarization of the $2p_{3/2} \rightarrow 1s_{1/2}$ line in H-like ions. (Infinite-Z values from Ref. [1] have been multiplied by 1.5 as explained in text.) X is the incident-electron energy in threshold units.

	Polarization							
X	Si	A	Ti	Mo	Ba	Au	U	$Z=\infty$
				Nonrelativistic				
2	33.82	33.84	33.87	33.87	33.79	33.80	38.83	31.2
4	19.69	19.69	19.66	19.69	19.67	19.71	19.63	19.3
5	15.52	15.63	15.56	15.59	15.57	15.62	15.62	15.6
				Relativistic				
2	33.93	34.04	34.18	35.10	35.98	38.37	38.55	31.2[a]
4	19.93	20.21	20.76	22.14	23.92	27.29	29.31	19.3
5	15.84	16.17	16.49	18.57	20.60	23.58	26.76	15.6

[a]The infinite-Z values shown here are nonrelativistic values.

nonrelativistic curves become increasingly conspicuous as Z increases.

In Figs. 2(a)–2(d) we show the effects of relativity on the cross sections for excitation to the magnetic sublevels of the He-like ions. For all of the ions the cross section for excitation to the $m=0$ sublevels is significantly larger than the cross section for excitation to the $m=1$ sublevel in the nonrelativistic results, and in the relativistic results as well. Inal and Dubau also observed that the $m=0$ sublevel is preferentially populated in electron-impact excitation of He-like ions [5]. However, the differences between the $m=0$ and 1 cross sections diminish at higher incident-electron energies. This preferential excitation to the $m=0$ sublevel at lower incident energies occurs be-

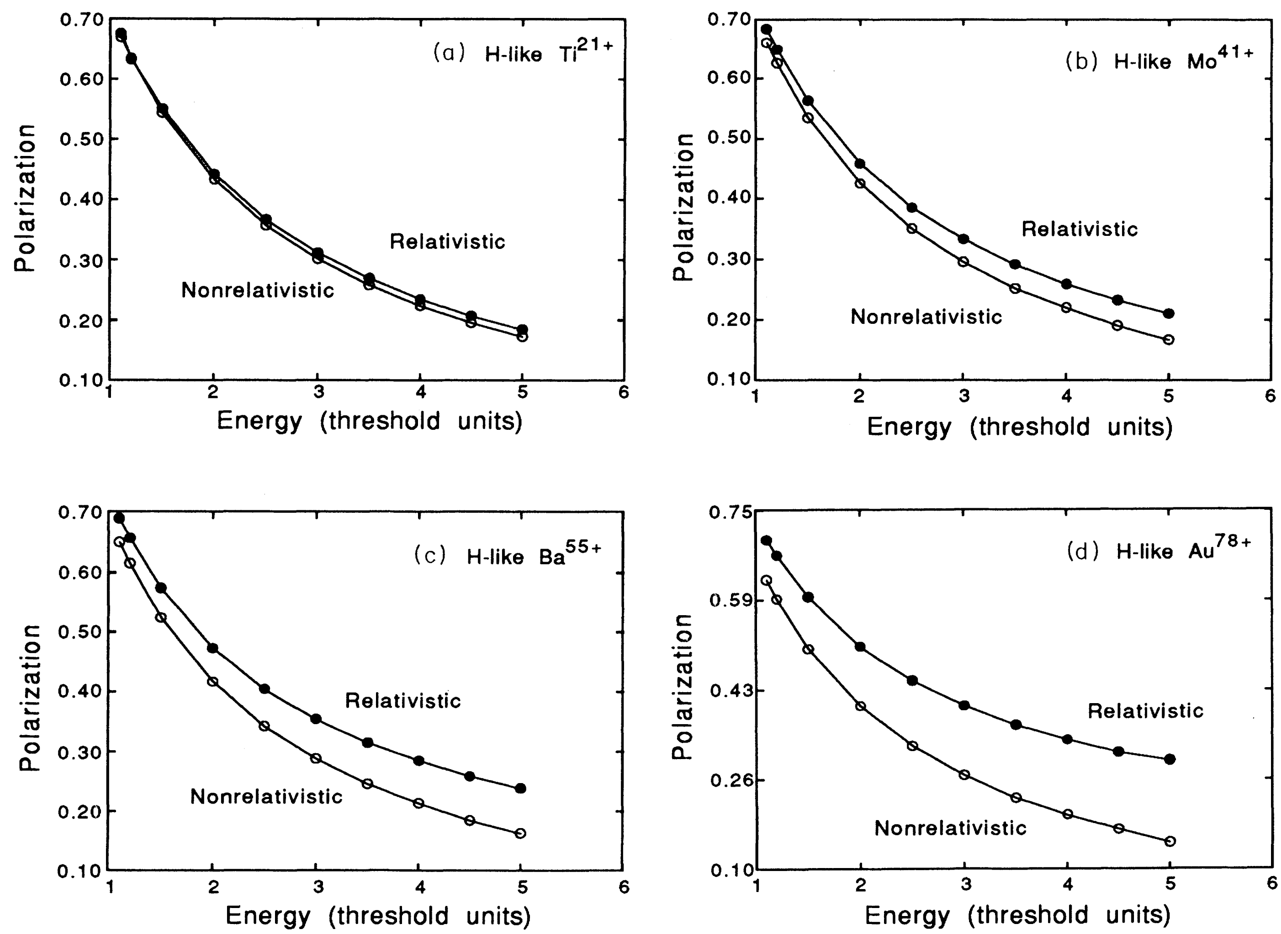

FIG. 3. The polarization fractions for H-like ions. The dark circles are the relativistic values and the open circles are the nonrelativistic values.

cause the momentum transfer is predominantly parallel to the direction of motion of the incident electron at lower collision energies [15–17]. Since this direction is also along the axis of quantization, the orbital momentum and its projection m are zero for the incident electron. These quantum numbers are also initially zero for the target ion. At much higher incident energies, the momentum transfer becomes predominantly transverse to this direction [16]. As a result the ratio of the $m=0$ cross section to the $m=1$ cross section begins to decrease rapidly at higher energies. We find that for both sublevels the differences between the relativistic and nonrelativistic results become increasingly pronounced as Z increases.

In an absolute sense the change in cross sections due to relativistic interactions is much greater for excitation to the $m=0$ sublevel than for excitation to the $m=1$ sublevel. But there is little difference in the overall relative changes in the cross sections for the $m=0$ and 1 excitations. For example, in the case of He-like Mo, the largest change in the $m=0$ cross section is about 33%, while the largest change in the $m=1$ cross section is about 31%. In the case of He-like Ba, the largest change in the $m=0$ cross section is about 50% and the largest change in the $m=1$ cross section is about 48%. The maximum relative change, however, does not occur at the same energy for the two magnetic sublevels, and in general the relative change in the cross sections for the $m=0$ excitation at a particular energy may be significantly different from the relative change in the cross section for the $m=1$ excitation at that same energy. Since the polarization of the emitted radiation depends on the deviation from statistical population of the magnetic sublevels of the excited states, the unequal relative changes in the excitation cross sections at a given energy results in a change in the polarization at that energy.

In our results, the effect of relativistic interactions is to decrease the cross section for excitation to the $m=0$ sublevel at low and intermediate incident-electron energies. However, the relativistic and nonrelativistic curves eventually cross, and at the highest energies the relativistic cross sections are larger than the nonrelativistic cross sections. For He-like uranium, we see that the nonrelativistic cross section for excitation to the $m=0$ sublevel is more than a factor of 2 greater than the relativistic cross section in the lower-energy region. But the relativ-

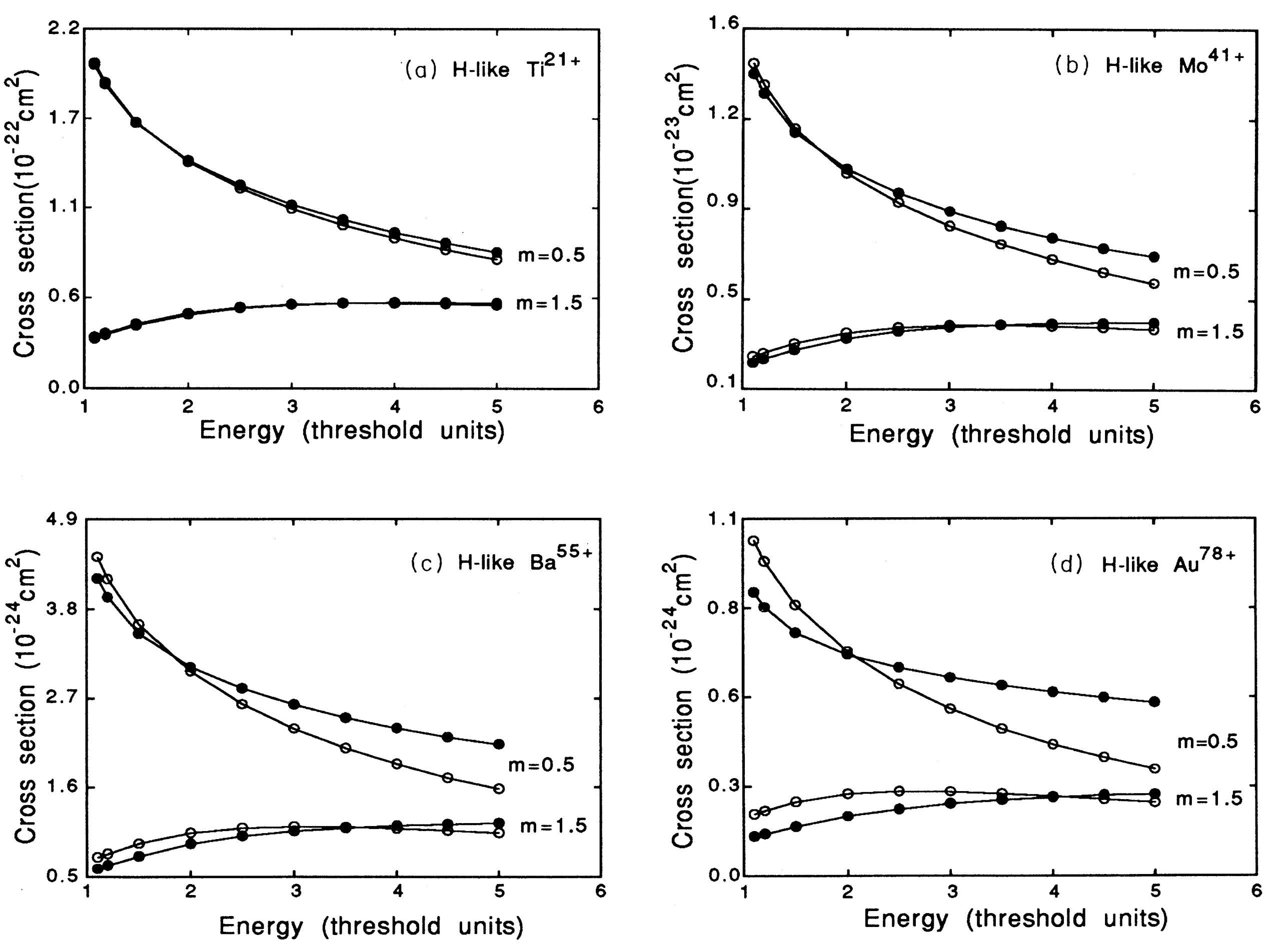

FIG. 4. Cross sections for electron-impact excitation to specific magnetic sublevels of H-like ions as functions of incident-electron energy in threshold units. The dark circles are relativistic cross sections and the open circles are nonrelativistic cross sections.

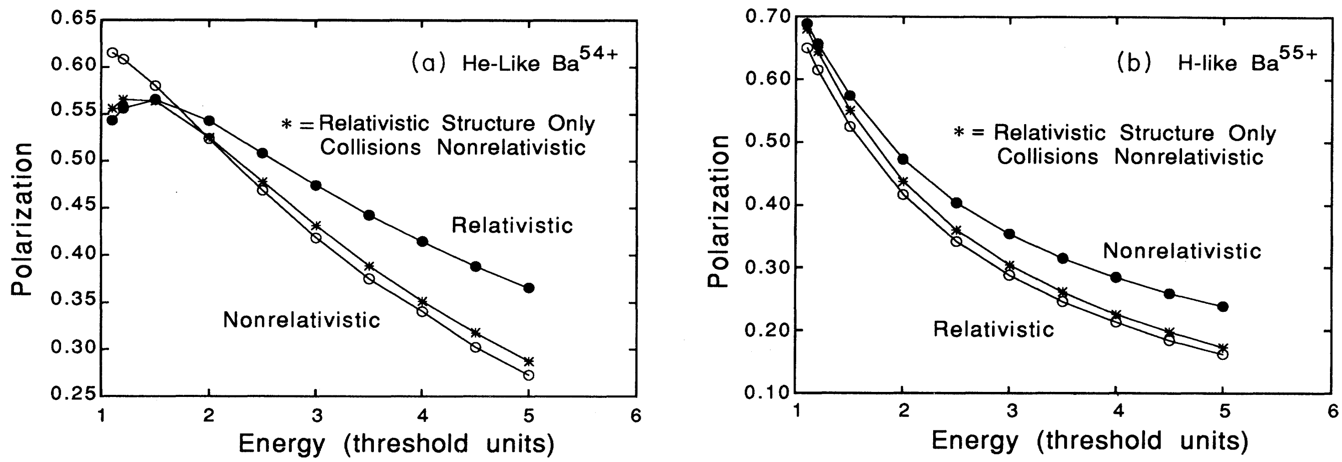

FIG. 5. Polarization for (a) He-like Ba and (b) H-like Ba as functions of impact electron energy in threshold units. The dark circles are relativistic values, the open circles are the nonrelativistic values, and the asterisks are the values obtained from a calculation in which the atomic structure calculation is relativistic but the scattering electron is treated nonrelativistically.

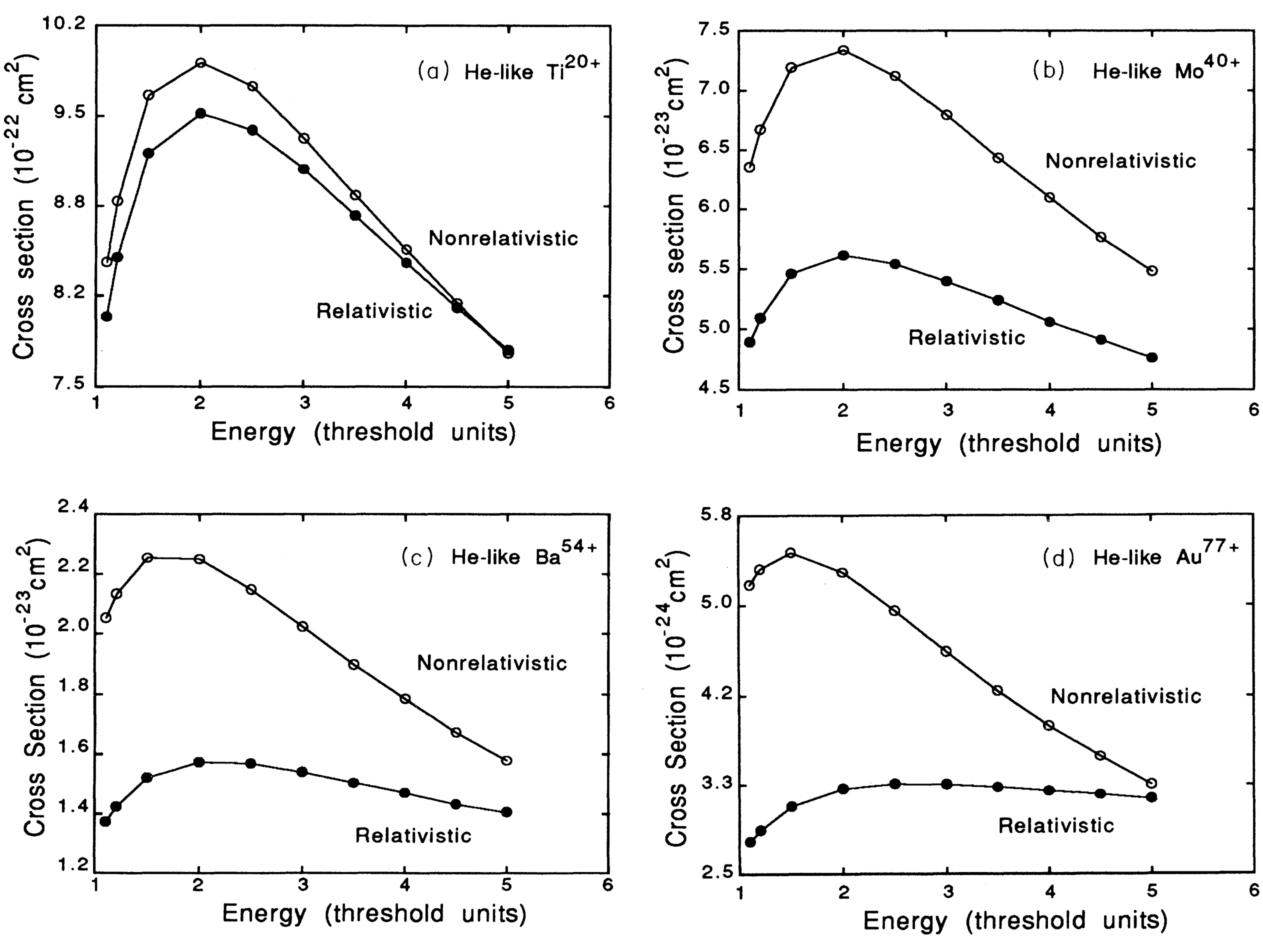

FIG. 6. Total electron-impact excitation cross sections for He-like ions. The symbols are the same as in Fig. 4.

istic and nonrelativistic results approach each other at higher incident-electron energies and are nearly equal at energies between four and five times threshold. This pattern persists for all Z. There is also a noticeable decrease in the $m=1$ cross sections as a result of relativistic effects, and this decrease also becomes increasingly significant with increasing Z.

B. H-like ions

For H-like ions the polarization of the $2p_{3/2} \rightarrow 1s_{1/2}$ is given by

$$P = -3B_0/(4-B_0) , \quad (2)$$

where

$$B_0 = (\sigma_{3/2} - \sigma_{1/2})/(\sigma_{3/2} + \sigma_{1/2}) . \quad (3)$$

Table II shows relativistic and nonrelativistic polarization for the $2p_{3/2} \rightarrow 1s_{1/2}$ line in H-like ions for impact electron energies of two, four, and five times threshold. As in the case of He-like ions the nonrelativistic results are fairly independent of Z and in close agreement with the infinite-Z results from Ref. [1]. Note that we have multiplied the infinite-Z results from Ref. [1] by 1.5 to account for the fact that Itikawa, Srivastava, and Sakimoto used spin-averaged $2p$ cross sections, while we used $2p_{3/2}$ cross sections in our calculations.

In Figs. 3(a)–3(d), we show the polarization as a function of incident-electron energy for H-like ions. In contrast to the He-like ions, the relativistic and nonrelativistic curves for H-like ions are all monotonically decreasing with increasing incident-electron energy and the curves do not intersect. However, the trends are similar to those observed for the He-like ions in that the relativistic curves are above the non-relativistic curves for all ions at higher incident-electron energies and the differences become more apparent with increasing Z. Also, for each particular ion the relativistic effects become more apparent with increasing incident-electron energy.

Figures 4(a)–4(d) show the cross sections for excitation to the $m=0.5$ and 1.5 magnetic sublevels of the H-like ions. In both the relativistic and nonrelativistic cases, the $m=0.5$ sublevel is preferentially populated in all of the H-like ions. The differences between the cross sections for the two magnetic sublevels decrease with increasing incident-electron energy. This is similar to the case of the He-like ions where the magnetic sublevel with the smaller magnetic quantum number also is preferentially

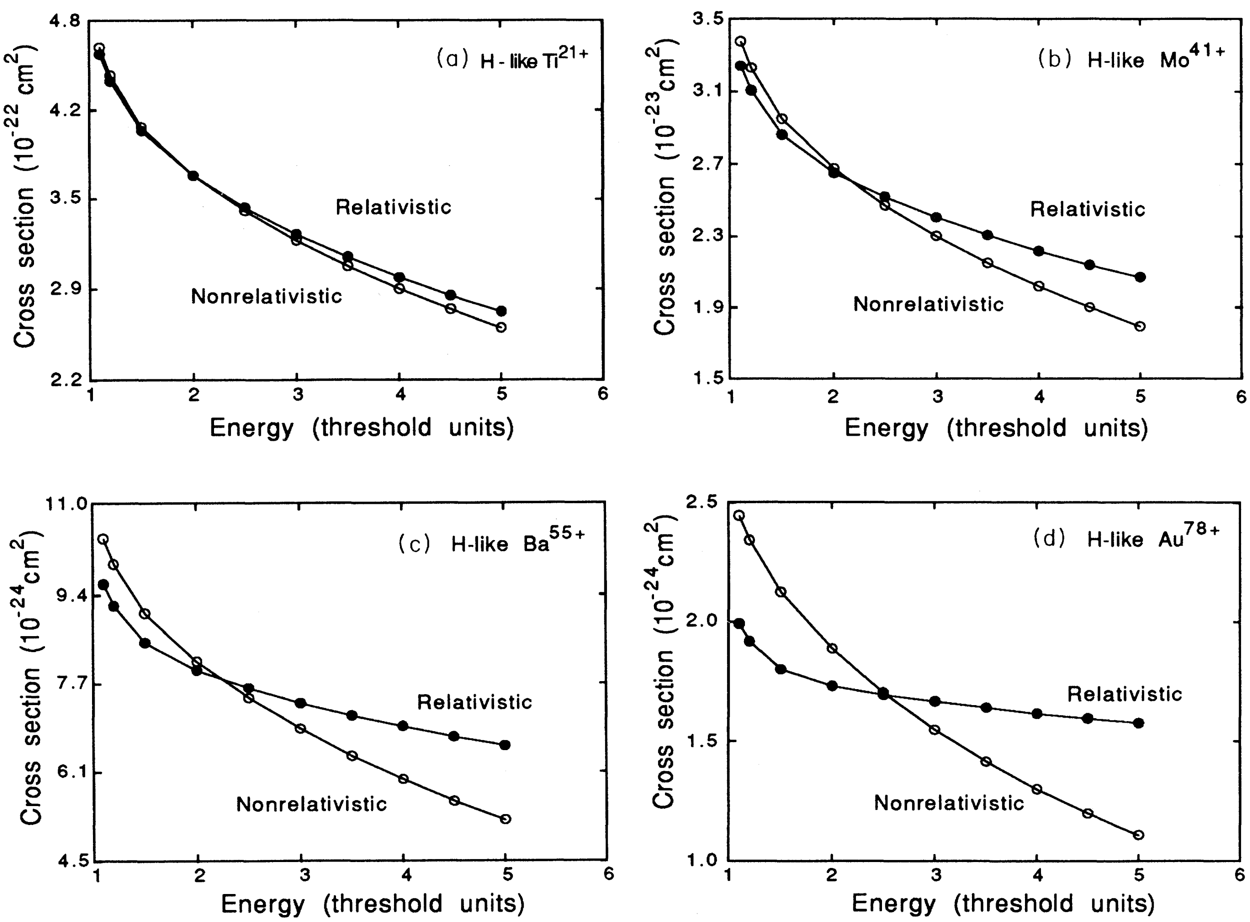

FIG. 7. Total electron-impact excitation cross sections for H-like ions. The symbols are the same as in Fig. 4.

populated. The effect of the relativistic interactions is to increase the cross sections at higher energies and to decrease them at lower energies for excitations to both the $m=0.5$ and the $m=1.5$ sublevels. But for the H-like ions, the relativistic and nonrelativistic curves cross at much lower incident-electron energies than in the case of He-like ions. For both magnetic sublevels the differences between relativistic and nonrelativistic results increase with increasing atomic number.

While it appears that the greatest relativistic effects in our calculations might be due to relativistic effects on the atomic structure of the target ions, there does seem to be some important kinematic effect also since, for a given ion, the differences between the relativistic and nonrelativistic results increase with increasing incident-electron energy. In order to test this we repeated the calculations for Ba with the atomic structure calculation done relativistically, but with the scattering calculation carried out nonrelativistically. In Fig. 5(a) we show the polarization for He-like Ba obtained in this manner. Near threshold and for low incident energies, the curve is closer to the relativistic curve. However, at higher incident energies the curve closely tracks the nonrelativistic curve. Similarly, in the case of H-like Ba [see Fig. 5(b)] we find that these results are nearly identical to the relativistic results near threshold, while they are closer to the nonrelativistic results at higher energies. Hence, for low collision energies, the relativistic effect on target structure is the most important factor while the relativistic effect on the scattering calculations becomes the dominant factor at high incident-electron energies.

Figures 6 and 7 show the total cross sections for He- and H-like ions, respectively. The total cross sections follow a pattern very similar to the patterns followed by the cross sections for excitation to the $m=0$ and 0.5 magnetic sublevels in He-like and H-like ions, respectively, with the relativistic cross sections being less than the nonrelativistic cross sections and becoming increasingly smaller than the nonrelativistic cross sections for ions with higher atomic number. The decrease in the cross sections due to relativity is a general feature of excitation resulting from spin-orbit effects and relativistic orbital contraction in the target ion [18,19].

III. CONCLUSION

We used distorted-wave methods to calculate cross sections for electron-impact excitation to the $m=0$ and 1 magnetic sublevels of the $1s^2 \rightarrow 1s2p(^1P_1)$ transition for He-like ions with $13 \leq Z \leq 92$, and for excitation to the $m=0.5$ and 1.5 magnetic sublevels for the $1s \rightarrow 2p_{3/2}$ transition for H-like ions of the same elements. We used these cross sections to calculate the polarization of radiation emitted following excitation. We determined how the cross sections for excitation to the specific magnetic sublevels are changed by the effects of relativity. In the nonrelativistic limit the polarization is independent of atomic number in an isoelectronic sequence, as predicted previously by other authors. We found, however, that relativistic effects considerably alter the polarization, and that the changes resulting from relativistic effects become progressively more significant as the incident-electron energy or the atomic number increases. Some of the effects discussed in this paper may be observable in planned experiments on the electron-beam ion trap at Lawrence Livermore National Laboratory [20].

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