Electron-impact ionization of hydrogen and lithiumlike systems

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The electron impact single ionization cross sections on a number of targets with atomic number \( Z = 1–92 \) in the H and Li isoelectronic sequences are calculated using a modified version of the recently propounded relativistic improved binary-encounter dipole (MRIBED) model [M. A. Uddin et al., Phys. Rev. A 70, 032706 (2004); 71, 032715 (2005)]. The modified RQIBED (MRIBED) model along with a \( Z \)-dependent factor in it is found remarkably successful in the applications to H-like and Li-like systems and also valid for the ionization of a filled \( s \) orbit including the He-like targets.

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I. INTRODUCTION

Electron impact (EI) is the major mode of ionization processes in fusion plasmas, besides being of fundamental interest in the atomic structure and collision mechanisms. In particular, the knowledge of ionization cross sections has wide applications in astrophysics, plasma physics, radiation physics, mass spectrometry, semiconductor physics, etc.

Both experiments and quantum-mechanical calculations generate cross-section data for selected targets at some discrete energies. On the other hand, the fields of applications require at least 20%–30% accurate cross sections for a wide range of targets and energies. This need can be best served by simple-to-use models that can provide a fast generation of reasonably accurate cross sections for any target over a wide domain of energies. This situation leads the practitioners in the applied fields to prefer the simple analytic models rather than the quantal calculations as the latter are arduous and not the applied fields to prefer the simple analytic models rather than the quantal calculations as the latter are arduous and not easy for the rapid generation of cross sections.

Reviews of EI ionization and associated empirical models are provided in Refs. [1–3]. A compilation of selected experimental and theoretical data are given by Tawara and Kato [4]. Among the various models, those of Thomson [5], Lotz [6,7] and Gryzinski [8] have historical interest. Recently, the empirical models of Bernstam, Ralchenko, and Maron (BRY) [9] and Deutsch and Mirk (DM) [10–17] and the binary-encounter-dipole (BED) model of Kim and Rudd [18] have enjoyed wide applications in their respective domains. In particular, the BED model has demonstrated reasonable successes in the description of the EI ionization of molecular targets [19–23]. However, the model has been applied to only a few one-electron atomic ions like He\(^+\) and Li\(^{2+}\) [18].

Uddin et al. [24] proposed the relativistic improved binary-encounter dipole (MRIBED) model with incorporation of ionic and relativistic ingredients into the structure of the simplified version of improved-binary-encounter-dipole (siBED) model of Huo [25] and applied with remarkable successes to the description of the EI ionization of He-like systems [24], K-shell [26] ionization, and Be-like targets [27]. All of these studies brought out the existence of a generic set of values of the two parameters of the MRIBED model, thereby indicating some relevance of these parameters to the electronic structure of the species. The constant values \( d_1 = d_2 = 0.0 \) have been found good for both the K-shell ionization and the ionization of Be-like targets, where only the \( s \) orbits remain filled. Although the experimental EI cross sections for the He-like systems have been described well using the parameter values \( d_1 = 0.0 \) and \( d_2 = 0.05 \) in [24], a reexamination indicates that all these experimental data can also be reproduced satisfactorily within 20%–30% using the \( d_1 = d_2 = 0.0 \) generic values. Thus all cases of ionization in the filled \( s \) orbit can be accounted for by these generic values.

It may be of interest to explore the MRIBED model to targets with an unfilled \( s \) subshell. Hydrogenlike and lithiumlike targets are of the simplest structure in this category and may serve as test cases for the aforesaid study of application of the MRIBED model to the EI ionization from the unfilled \( s \) subshell. In the course of our investigation, we could not find any generic set of values akin to these H- and Li-like targets. We then keep the values of the two parameters fixed at the \( d_1 = d_2 = 0.0 \) values for the \( s \) orbit and incorporate a \( Z \)-dependent factor following the procedure of Fontes et al. [28] for application to the \( s \)-orbit ionization. This choice makes the expression for \( G \) in Eq. (7) of [26] much simpler as compared to either the siBED [25] or MRIBED [24,26] model. The model so framed is, henceforth, referred to as the modified RQIBED (MRIBED) model.

We apply the MRIBED model to calculate the EI single ionization cross sections of He, Ne\(^{6+}\), and U\(^{90+}\) from the helium isoelectronic sequence H, He\(^+\), Mo\(^{31+}\), Dy\(^{65+}\), and U\(^{91+}\) from the hydrogenic isoelectronic sequence and of Li, N\(^{14+}\), Ti\(^{19+}\), V\(^{20+}\), Cr\(^{21+}\), Mn\(^{22+}\), Fe\(^{23+}\), and U\(^{89+}\) from the lithium
isoelectronic sequence. The prediction from the MRIBED model is compared with the available experimental data, the isoelectronic sequence. The prediction from the MRIBED model is compared with the available experimental data, the calculations of BRY [9], and the modified Hombourger empirical (MHEMP) [29] models and other theoretical results. The theoretical methods used for comparison are the distorted-wave Born approximation (DWBA) [30,31], relativistic DWBA (RDWBA) [32], convergent-closed-coupling (CCC) approximation [33], relativistic two-potential distorted-wave (TPDWA01) approximation [34], Coulomb-Born (CB) approximation [35], the analytic fit formula of Fontes et al. to the relativistic DWBA (FRDWA) [36], and the assessed data of Bell et al. [37].

The paper is organized as follows. The MRIBED model is sketched in Sec. II. In Sec. III, we first revisit the EI ionization on He-like targets and then discuss the MRIBED results for the H- and Li-like systems in comparison with the available experimental cross sections and other theoretical findings. Section IV is devoted to the discussion of the results and the conclusions arrived at.

II. OUTLINE OF THE MRIBED MODEL

In the MRIBED model with both its parameters set to \(d_1 = d_2 = 0.0\), the expression for the EI ionization cross section, following [26,27], can be obtained as

\[
\sigma_{\text{MRIBED}} = \sigma_{\text{Mott}}^R + \sigma_{\text{Born}}^R,
\]

where

\[
\sigma_{\text{Mott}}^R = S^R H,
\]

and

\[
\sigma_{\text{Born}}^R = F^R G,
\]

\[
S^R = \frac{4 \pi N_0 \alpha^2}{\beta^2 Z^2} \left( \frac{\alpha^2}{\beta^2} + \frac{\alpha^2}{\beta^2_0} \right) (q + 1),
\]

\[
H = \left[ \frac{k_0^2 - \alpha_0^2}{k_0^2} \right] - \ln \left( \frac{k_0^2 \alpha_0^2}{k_0^2 + \alpha_0^2} \right),
\]

\[
F^R = \frac{64\beta_0^2 N_0}{\alpha \beta^2 Z^2},
\]

and

\[
G = \int_0^{(a_0^2 - \alpha_0^2)^2} k_p(k_p^2 + \alpha_0^2)^2 dE_p
\]

\[
\times \int_{K_{\text{min}}}^{K_{\text{max}}} \frac{1}{K[(K + k_p)^2 + \alpha_0^2][(K - k_p)^2 + \alpha_0^2]} dK.
\]

In the above equations, \(T = k_0^2 / 2\) is the energy of the incident electron, \(U = k_p^2 / 2\) the kinetic energy of the bound electron, \(I = \alpha_0^2 / 2\) the binding energy of the target electron, and \(E_p = k_p^2 / 2\) the energy of the ejected electron with \(\alpha_0\) having the dimension of momentum in atomic units [25]. \(K = k_0 + k_p\) denotes the momentum transfer vector with \(k_p\) representing the momentum of the electron after a collision in the atomic unit. The maximum and minimum values of \(K\) are given in [38]. \(N_0\) is the number of electrons in the orbit considered, and \(q\) denotes the ionic charge of the target.

Using \(m\) as the mass of the electron, \(c\) as the velocity of light in the free space, and \(\alpha\) as the fine structure constant, the quantities \(\beta_t, \beta_b,\) and \(\beta_a\) in Eqs. (4) and (6) are defined in terms of \(t' = k_0^2 / (2mc^2)\), \(b' = k_p^2 / (2mc^2)\), and \(a' = \alpha_0^2 / (2mc^2)\), respectively, as

\[
\beta_t^2 = 1 - \frac{1}{(1 + t')^2},
\]

\[
\beta_b^2 = 1 - \frac{1}{(1 + b')^2},
\]

and

\[
\beta_a^2 = 1 - \frac{1}{(1 + a')^2}.
\]

In line with the form of the Z-dependent factor \(F_F(Z)\) of Fontes et al. [28] given by

\[
F_F(Z) = [140 + (z/20)^5] / 141,
\]

the EI cross sections for an \(s\) orbit in the proposed MRIBED model can be evaluated by using

\[
\sigma_{\text{MRIBED}} = (\sigma_{\text{MRIBED}}) F(Z),
\]

with

\[
F(Z) = 1.0 \text{ for a filled } s \text{ orbit}
\]

\[
= 1 + m Z^n \text{ for an unfilled } s \text{ orbit}.
\]

The reduced cross sections defined by
with \( I \) in Rydberg units and \( a_0 \) as the Bohr radius, are found to be independent of \( Z \) for the H and Li isoelectronic sequences for low incident energies. This finding encourages us to construct the \( \sigma_{MRIBED} \) in Eq. (12) following the procedure of Fontes et al. [28].

### III. RESULTS AND DISCUSSIONS

We have used published results for the ionization potentials given by Desclaux [39] for the neutral targets. The kinetic energies of all targets and ionization potentials of the ionic targets are calculated using the Dirac-Hartree-Fock code [40]. Using the 64-point Gauss-Legendre rule [41], the two-dimensional integrations over \( K \) and \( E_p \) [see Eq. (7)] are carried out numerically and the convergences are tested with increasing the Gaussian points. As mentioned earlier the parameters \( d_1 \) and \( d_2 \) are fixed at \( d_1=d_2=0.0 \). The values of the parameters \( m=0.365 \) and \( n=0.050 \) in Eq. (13) are determined from optimizing the overall fits of the MRIBED calculations with the experimental cross sections of all the targets in the H and Li isoelectronic sequences considered as well as Li2+, Be3+, B2+, C3+, N4+, O5+, N5+, O6+, Ne7+, Ar15+, Fe17+, and Ce3+ not included herein. Figure 1 compares the experimental cross sections for H with the calculated results using the factor \( F_Z \) of [28] in Eq. (12) and the proposed factor \( F_Z \) in the MRIBED model with \( m=0.365 \) and \( n=0.050 \). An inclusion of a quadratic term in \( F_Z \) does not improve the fits. Figure 2 displays the reduced cross sections \( Q_U \) in Eq. (14) for C5+, N4+,6+, O5+, and Ne7+ and shows that the cross sections are almost \( Z \) independent at low energies. The calculated cross sections are summed over all the subshells.
In Figs. 3–5 we compare the MRIBED predictions for the He, Ne$^{8+}$ and U$^{90+}$ with the experimental EI cross section data of Rejoub et al.\cite{rejoub1985}, Duponchelle et al.\cite{duponchelle1985}, Donets and Ovsyannikov\cite{donets1985}, and Marrs et al.\cite{marrs1985} with the theoretical results from the MRIBED model using $d_1=0.0$ and $d_2=0.05$\cite{uddin2005}, the present MRIBED model using $F(Z)=1.0$, the DWBA of Younger\cite{younger1985}, TPDW01\cite{ko1985}, and RDWBA of\cite{fontes1985}. Since the MRIBED calculations with $F(Z)=1.0$ are equivalent to those of MRIBED with $d_1=d_2=0.0$, it is evident from the figures that the MRIBED results using $d_2=0.05$ and those employing $d_2=0.0$ with $d_1=0.0$ in both cases are almost identical. Hence one can expect that the good performance of the MRIBED model on the He-like targets in\cite{uddin2005} using $d_1=0.0$ and $d_2=0.05$ should also be achieved with $d_1=d_2=0.0$, the same optimum parameter values for the K-shell ionization\cite{uddin2005_1} and ionization of the Be-like systems\cite{uddin2005_2}. Thus in all the three cases with ionization from a filled $s$ orbit, the appropriate values of the two parameters of the MRIBED model are $d_1=d_2=0.0$.

In Figs. 6–10 we compare the MRIBED predictions for the H, He$^+$, Mo$^{41+}$, Dy$^{65+}$, and U$^{91+}$ targets in the H isoelectronic sequence with the experimental EI cross-section data of Shah et al.\cite{shah1985}, Peart et al.\cite{peart1985}, Marrs et al.\cite{marrs1985}, and Watanabe et al.\cite{watanabe1985}; the results from the MHEMP\cite{coen1985}; and the assessed data Bell et al.\cite{bell1985}. The other theoretical calculations used for comparison in these figures are TPDW01 of Kuo and Huang\cite{ko1985}, RDWBA of Moores and Reed\cite{moore1985}, and FRDWBA of Fontes et al.\cite{fontes1985}. The RDWBA calculations include the Møller interaction\cite{moller1985} with consideration of exchange and interference effects. The DWBA calculations are the results from the fitting formula representing the...
quantal calculations. As evident in Figs. 6–10 the MRIBED model provides a satisfactory description of the experimental results for H–U91+ in the whole energy range and good agreement with the RDWBA and TPDW01 predictions, except for H and He+ where the latter results overestimate the experimental cross sections in the low-energy region. The MHEMP model gives reasonable fits to the data except the cases of H and He+. The assessed data generated from the Bell’s formula [37], with parameters being species dependent, are close to the experimental cross sections. The MRIBED model, with its simple structure, gives the best fit to the data in the overall assessment with all the targets in the H-like series. The TPDW01 and MHEMP results overestimate the experimental data for the cases of H and He+. For Dy65+, the MRIBED cross sections disagree with those calculated from the FRDWBA but agree closely with the RDWBA and MHEMP results. In the case of U91+, the FRDWBA underestimates the experimental value as well as the predicted cross sections from the RDWBA theory and the MRIBED and MHEMP models. The MRIBED model disagrees with MHEMP for Mo41+ (Fig. 8) and with both RDWBA and MHEMP for U91+ (Fig. 10) in predicting the cross sections at higher energies.

In Figs. 11–14 comparisons are made of the MRIBED predictions for the Li, N4+, Ti19+, V20+, Cr21+, Mn22+, Fe23+, and U89+ targets in the Li isoelectronic sequence, with the experimental data from Zapesochnyl and Aleksakhin [48, 49], McFarland and Kinney [52], Jalil et al. [53], Crandall et al. [54, 55], Donets and Ovsyannikov [45], and Rester and Dance [57]. The theoretical calculations, compared with the MRIBED results for the Li-like systems, are CCC of Bray [33], CB of Jacobowicz and Moores [35], DWBA of Wong et al. [56], and the model predictions from BRY [9]. As apparent from Fig. 11, although the MRIBED predictions for Li show discrepancies with the experimental data, it seems to perform better than the CCC calculations [33]. The calculated peak position from MRIBED is shifted towards the higher energies relative to those resulting from both the BRY and Bell predictions, which are close to each other. Figure 12 shows that the MRIBED model produces a satisfactory fit to the experimental data of N4+.
Figure 13 compares the calculated $2s$-orbit ionization cross sections for $\text{U}^{89+}$ from the present MRIBED model with the RDWBA results of [32]. The MRIBED cross sections are determined by the ionization potential $I$ and kinetic energy $U$ of the bound electron in addition to the incident energy. The $I(1s) = 29.38$ keV and $U(1s) = 33.31$ keV values for the $K$-shell ionization of Sn are close to the $I(2s) = 32.90$ keV and $U(2s) = 27.87$ keV for the $2s$ orbit of $\text{U}^{89+}$ and, in consequence, the EI cross sections for the latter are expected to be very similar to the half of the $K$-shell ionization cross sections for Sn. The MRIBED results agree very well with the experimental cross sections (reduced by a factor of 0.5) for Sn from Rester and Dance [57]. The RDWBA and MRIBED results are close to each other up to about 100 keV, and beyond that the former decrease more rapidly in contradiction to the experimental cross sections.

In Fig. 14, the MRIBED predictions for $\text{Ti}^{19+}$, $\text{V}^{20+}$, $\text{Cr}^{21+}$, $\text{Mn}^{22+}$, and $\text{Fe}^{23+}$, at the incident energy approximately 2.3 times the respective threshold energy, are compared with the experimental EI cross sections and DWBA calculations of Wong et al. [56] as well as the BRY [9] results. The DWBA calculations have been done using the code of [31]. The agreement among the MRIBED predictions, the experimental data, and the DWBA and BRY results is excellent.

IV. CONCLUSIONS

The MRIBED model is seen to provide a good description of the experimental EI cross-section data for hydrogen and...
Mn$^{22+}$, and Fe$^{23+}$ at the incident energy of approximately 2.3 times the threshold. The experimental data and the DWBA results are from [56]. The present MRIBED predictions are shown as the solid curve.

lithium isoelectronic series except for the lone case of atomic Li. The description has been accomplished for 16 targets in the range $Z=1$–92 using a single set of parameters $m =0.365$ and $n=0.050$. In the case of Li, the overall performance of the MRIBED model is comparable to other theoretical calculations (Fig. 10). In some of the species—e.g., H and Li isoelectronic sequences coupled with that achieved with the MRIBED model on members of He [24] and Be [27] isoelectronic series as well as on the $K$-shell ionization of atoms [26] indicates that the parameters $d_1$ and $d_2$, which are dependent on the electronic structure of the targets, play a pivotal role. The values $d_1=d_2=0.0$ are seemingly locked to the cases of ionization from an $s$ orbit. The form of $F(Z)$ for a filled $s$ orbit is $F(Z)=1$, and the MRIBED model reduces to the MRIBED one of [26,27].

The MRIBED model, in its performance to describe the EI ionization of the H- and Li-like species, is seen to be comparable to and even better, in some cases, than sophisticated theories like the DWBA, CB, RDWBA, and CCC. It is demonstrated that the present MRIBED model produces very encouraging and reliable results for ionization from any filled and unfilled $s$-orbital targets. In order to decide the predictive role of our method, it is our intention to extend this model to other open-subshell targets, especially the $p$-orbit target, since the open-subshell systems remain a challenge. The MRIBED model with its simple structure may turn out to be a very lucrative alternative for generating accurate data for plasma modeling codes.

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(38) M. Inokuti, Rev. Mod. Phys. 43, 297 (1971).
(40) M. Y. Amusia and L. V. Chernysheva, Computations of Atomic Processes (Institute of Physics, Bristol, 1997).
(50) C. Møller, Z. Phys. 70, 786 (1931).