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Ionization of excited xenon atoms by electrons

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Measured cross sections for electron-impact ionization of excited Xe atoms are not presently available. Therefore, we combine in this work the formalisms of the binary encounter approximation and Sommerfeld's quantization of atomic orbits and derive from first-principles cross sections for ionization of excited atoms by electrons of low and moderate energies (up to a few hundred eV). The approach of this work can be used to calculate the cross sections for electron-impact ionization of excited atoms and atomic ions other than xenon.

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I. INTRODUCTION

Ionization of noble-gas atoms is important in many applications, including spacecraft thrusters, excimer lasers, and fusion plasmas. This work concentrates on xenon because of its current prominence as a propellant in ion engines and Hall thrusters. Studies of nonequilibrium processes in these devices requires knowledge of electron-impact ionization of xenon atoms from both ground and excited states. Electron-impact ionization of heavy atoms such as xenon is difficult to study experimentally as well as theoretically. As a result, measured cross sections are available only for ionization of the ground-state Xe atom [1–4] (see also references cited in [3]). Theoretical work [5–7] on electron-impact ionization of the ground state as well as excited states of xenon is scarce and limited in scope.

Ionization of the ground-state xenon atom by an electron of energy less than a few hundred eV can be reliably described by the "energy-corrected" binary encounter approximation (ECBEA) developed recently by the authors [8] for electron-impact ionization of rare-gas atoms with atomic number $Z \gtrsim 20$. This approach provides easy-to-calculate analytical ionization cross sections with accuracy acceptable in most applications. In this work, we modify the ECBEA approach in order to calculate the cross sections for electron-impact ionization of excited xenon atoms from outer as well as inner atomic shells.

The ECBEA approach combines the binary encounter approximation [9,10] of energy transfer between two electrons, Sommerfeld's theory of quantization of atomic orbits to describe the dynamics of the target's electrons, and a statistical description of the cumulative interactions of the atomic electrons. The atomic field of the target atom can significantly change the energy of the ionizing electron as it nears the target; this is taken into account by this approach. The energy change can be given by [8,11]

$$\epsilon' = \epsilon + E_e^{(nl)} + W_{nl}, \qquad (1)$$

where ϵ is the energy of the incident electron far from the target atom, ϵ' is the "corrected" energy of the incident electron at the point of its BEA collision with an electron of the nlth atomic shell, $E_e^{(nl)}$ is the kinetic energy, and W_{nl} is the mean binding energy of the nlth electron participating in the ionizing collision. In the above, n and l are the principal and the orbital angular momentum quantum numbers, respectively, of the shell (equivalent) electrons.

II. MEAN BINDING ENERGIES OF ATOMIC ELECTRONS

Estimating the binding energy W_{nl} of an electron of an nl shell in a many-electron atom is a complex and difficult problem [12]. The mean binding energy of each (equivalent) electron in each atomic shell is an average effect of many-body electron-electron and electron-nucleus interactions which depends of the atomic electronic configuration. This effect is estimated here by a statistical procedure able to predict reasonable values of the mean binding energies of electrons in a number of heavy atoms [11,13,14].

Since the collisional energies considered in this work are not large, we assume in our calculations that only electrons of two or three outermost atomic shells (5s and 5p shells in the configuration $5s^25p^6$; the 5s, 5p, and 6s shells in the configurations $5s^25p^56s$; or the 5s, 5p, and 6p shells in the configurations $5s^25p^56p$) contribute significantly to the electron-impact atomic ionization when the target xenon atom is either in its ground state or in one of the ten excited states listed in Table I. (These states are denoted below by subscripts i that range from the ground state, $i=1$, to $i=11$, the highest excited state considered.) Thus, according to the statistical procedure mentioned above and discussed in [8,11], the mean binding energy of an electron in one of the three outermost nlth shells of the atom can be given as [8,11,13]

$$W_{nl} = N_{nl}^{-1} \sum_{m}^{N_{nl}} U_m^{(nl)}, \qquad (2)$$

where N_{nl} is the number of the electrons in the shell, and $U_m^{(nl)}$ is the minimum energy (ionization energy) needed to move the mth electron of the shell to the continuum. In other words, the mean binding energy of an electron in one of the three outermost shells in xenon in the ith state is taken as the following [8,11,13]:

(a) The 5s shell in configurations $5s^25p^6$, $5s^25p^56s$, and $5s^25p^56p$ ($i \in \{1,\ldots,11\}$),

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TABLE I. The ground state and ten excited states of the xenon atom considered in this work. The E_i are the states' excitation energies.

i	Paschen	Designation	E_i(eV)
1	p_0	$5p^6\ {}^1S^0$	0.00
2	$1s_5$	$6s[3/2]_2$	8.31
3	$1s_4$	$6s[3/2]_1$	8.44
4	$1s_3$	$6s'[1/2]_0$	9.45
5	$1s_2$	$6s'[1/2]_1$	9.57
6	$2p_{10}$	$6p[1/2]_1$	9.58
7	$2p_9$	$6p[5/2]_2$	9.68
8	$2p_8$	$6p[5/2]_3$	9.72
9	$2p_7$	$6p[3/2]_1$	9.79
10	$2p_6$	$6p[3/2]_2$	9.82
11	$2p_5$	$6p[1/2]_0$	9.93

$$W_{5s} = (U_1^{(5s)} + U_2^{(5s)})/2 = 110 \text{ eV}, \tag{3}$$

where $U_1^{(5s)}=100$ eV and $U_2^{(5s)}=120$ eV, respectively.

(b) The $5p$ shell in configuration $5s^2 5p^6$ $(i=1)$,

$$W_{5p} = (U_1^{(5p)} + U_2^{(5p)} + U_3^{(5p)} + U_4^{(5p)} + U_5^{(5p)} + U_6^{(5p)})/6 = 41.74 \text{ eV}, \tag{4}$$

where $U_1^{(5p)}=12.13$ eV, $U_2^{(5p)}=21.21$ eV , $U_3^{(5p)}=32.12$ eV, $U_4^{(5p)}=46$ eV, $U_5^{(5p)}=57$ eV , and $U_6^{(5p)}=82$ eV, respectively.

(c) The $5p$ shell in configurations $5s^2 5p^5 6s$ and $5s^2 5p^5 6p$ $(i \in \{2,\ldots,11\})$:

$$W_{5p} = (U_2^{(5p)} + U_3^{(5p)} + U_4^{(5p)} + U_5^{(5p)} + U_6^{(5p)})/5 = 47.67 \text{ eV}. \tag{5}$$

(d) The $6s$ shell in configurations $5s^2 5p^5 6s$ $(i \in \{2,3,4,5\})$: $W_{6s}=U_1^{(6s)}/1=3.81$ eV, 3.69 eV, 2.68 eV, and 2.56 eV for states $i=2,3,4$ and 5, respectively.

(e) The $6p$ shell in configurations $5s^2 5p^5 6p$ $(i \in \{6,\ldots,11\})$: $W_{6p}=U_1^{(6p)}/1=2.55$ eV, 2.44 eV, 2.41 eV, 2.34 eV, 2.31 eV, and 2.20 eV for states $i=6$, 7, 8, 9, 10, and 11, respectively.

We introduce a "shell parameter" k_{nl} for each shell under consideration [8,11],

$$k_{nl} = W_{nl}/U_1^{(nl)}, \tag{6}$$

where, as before, $U_1^{(nl)}$ is the first ionization potential of the shell. Using relationship (6), one has $k_{5s}=1.1$, $k_{5p}=2.25$ (in the configurations $5s^2 5p^5 6s$ and $5s^2 5p^5 6p$ with $i \in \{2,\ldots,11\}$), or $k_{5p}=3.44$ (in the configuration $5s^2 5p^6$ with $i=1$), $k_{6s}=1$ (in the configurations $5s^2 5p^5 6s$ with $i \in \{2,3,4,5\}$), and $k_{6p}=1$ (in the configurations $5s^2 5p^5 6p$ with $i \in \{6,\ldots,11\}$).

III. IONIZATION CROSS SECTIONS

The cross section for ionization of the nl atomic shell of a xenon atom excited to the ith state by an incident electron of energy ϵ can be given by the following expression: (a) n arbitrary, $l=0$ [11],

$$Q_{nl}(k_{nl},U_1^{(nl)},\lambda) = \frac{N_{nl}\sigma_0(1-\lambda^{-2})}{[U_1^{(nl)}]^2[1+(\lambda^2+k_{nl})^{1/2}]^2} \times \left[1 + \frac{2}{(\lambda^2+k_{nl})^{1/2}} + \frac{2}{3}(1+\lambda^{-2})\right], \tag{7}$$

and (b) n arbitrary, $l>0$ [8],

$$Q_{nl}(\xi_{nl},k_{nl},U_1^{(nl)},\lambda) = \frac{N_{nl}\sigma_0(\lambda^2-1)[3\lambda^2+2k_{nl}(1+\lambda^2)z_{nl}]}{3[U_1^{(nl)}]^2\lambda^4[\lambda^2+k_{nl}(1+z_{nl})]}, \tag{8}$$

or, somewhat more accurately,

$$Q_{nl}(\xi_{nl},k_{nl},U_1^{(nl)},\lambda) = \frac{N_{nl}\sigma_0(\lambda^2-1)}{3[U_1^{(nl)}]^2\lambda^8} \times \left[4k_{nl}^2 + 4k_{nl}(k_{nl}-1)\lambda^2 + (3+2k_{nl})\lambda^4 - \frac{4k_{nl}^2(2k_{nl}-\lambda^2+2k_{nl}\lambda^2+2\lambda^4)}{\sqrt{4k_{nl}(k_{nl}+\lambda^2)+\xi_{nl}\lambda^4}}\right]. \tag{9}$$

Here $\sigma_0=\pi e^4$; when $U_1^{(nl)}$ is given in eV, the appropriate numerical value is $\sigma_0=6.56\times10^{-18}$ eV^2 m^2. Defining

$$\lambda \equiv [\epsilon/U_1^{(nl)}]^{1/2}, \quad \xi_{nl} \equiv (l/n)^2, \quad \text{and } \psi_{nl} \equiv \sqrt{1-\xi_{nl}}, \tag{10}$$

we have

$$z_{nl} = \frac{\psi_{nl}^{1/2}}{2}\left[\frac{[2-\psi_{nl}(\xi_{nl}-2)-2\xi_{nl}]^{1/2}}{1+\psi_{nl}-\xi_{nl}} - \frac{\xi_{nl}\psi_{nl}^{1/2}}{(2\psi_{nl}+2-\xi_{nl})^{1/2}(1-\psi_{nl}-\xi_{nl})}\right], \tag{11}$$

or (with accuracy better than 1%)

$$z_{nl} \simeq [1-(\xi_{nl}/4)^2]^{1/4}. \tag{12}$$

The cross section for electron-impact single ionization of a xenon atom excited to state i $(i \in \{1,\ldots,11\})$ can be given as a sum of the ionization cross sections for all the atomic shells important for the process,

$$Q_{at} = \sum_{nl} Q_{nl}. \tag{13}$$

In other words, in the energy range considered in this work, the cross section (in m^2) for electron-impact ionization of a xenon atom excited to the ith state is

$$Q_{at}^{(i=1)} = Q_{5s}^{(i=1)} + Q_{5p}^{(i=1)}, \tag{14}$$

$$Q_{at}^{(i=2-5)} = Q_{5s}^{(i=2-5)} + Q_{5p}^{(i=2-5)} + Q_{6s}^{(i=2-5)}, \tag{15}$$

$$Q_{at}^{(i=6-11)} = Q_{5s}^{(i=6-11)} + Q_{5p}^{(i=6-11)} + Q_{6p}^{(i=6-11)}, \tag{16}$$

where

$$Q_{5s}^{(i=1)} = Q_{5s}^{(i=2-5)} = Q_{5s}^{(i=6-11)} = 1.31 \times 10^{-21} \frac{1-\lambda^{-2}}{(1+\sqrt{1.1+\lambda^2})^2} \times \left(\frac{5}{3} + \frac{2}{3\lambda^2} + \frac{2}{\sqrt{1.1+\lambda^2}} \right), \quad (17)$$

$$Q_{5p}^{(i=1)} = 8.92 \times 10^{-20} \frac{\lambda^2-1}{\lambda^8} \left[47.33 + 33.57\lambda^2 + 9.88\lambda^4 - \frac{47.33(6.88+5.88\lambda^2+2\lambda^4)}{\sqrt{47.33+13.76\lambda^2+\lambda^4/25}} \right], \quad (18)$$

$$Q_{5p}^{(i=2-5)} = Q_{5p}^{(i=6-11)} = 2.43 \times 10^{-20} \frac{\lambda^2-1}{\lambda^8} \left(20.25 + 11.25\lambda^2 + 7.5\lambda^4 - \frac{455.62+354.37\lambda^2+202.50\lambda^4}{\sqrt{506.25+225\lambda^2+\lambda^4}} \right), \quad (19)$$

and

$$Q_{6s}^{(i=2-5)} = a_i \frac{1-\lambda^{-2}}{(1+\sqrt{1+\lambda^2})^2} \left(\frac{5}{3} + \frac{2}{3\lambda^2} + \frac{2}{\sqrt{1+\lambda^2}} \right), \quad (20)$$

$$Q_{6p}^{(i=6-11)} = b_i \frac{\lambda^2-1}{\lambda^8} \left(4 + 5\lambda^4 - \frac{4(2+\lambda^2+2\lambda^4)}{\sqrt{4+4\lambda^2+\lambda^4/36}} \right). \quad (21)$$

Here $a_i = 4.52\times10^{-19}, 4.82\times10^{-19}, 9.13\times10^{-19}, 10^{-18}$ for $i=2,3,4$, and 5, respectively, and $b_i = 3.36\times10^{-19}, 3.67\times10^{-19}, 3.76\times10^{-19}, 3.99\times10^{-19}, 4.10\times10^{-19}, 4.52\times10^{-19}$ for $i=6,7,8,9,10$, and 11, respectively. [Note that each of the 11 cross sections defined in relationships (17)–(21) has a different energy threshold $\epsilon_{th}=U_1^{(nl)}$, and that the magnitude of this threshold for ionization of the $5p$, $6s$, and $6p$ shells depends on the atomic state number i.]

The electronic configurations and excitation energies E_i of the considered 11 states of the xenon atom are given in Table I. We calculate below, as examples, the cross sections for electron-impact ionization of the Xe atom from $i=1$ (the ground state p_0), $i=2(1s_5)$, $i=4(1s_3)$, and $i=9(2p_7)$ states taking into account the contributions of the following outermost shells of the states: the $5s^2$ and $5p^6$ shells of the atom in the $i=1$ state, the $5s^2$, $5p^5$, and $6s$ shells of the atom in the $i=2$ state, the $5s^2$, $5p^5$, and $6s$ shells of the atom in the $i=4$ state, and the $5s^2$, $5p^5$, and $6p$ shells of the atom in the $i=9$ state. The cross sections for electron-impact ionization of Xe excited to the $i=1$, $i=2$, $i=4$, and $i=9$ state are shown in Figs. 1–4, respectively, and a comparison of the cross sections is made in Fig. 5.

The reader should remember, while viewing Fig. 5, that the assumptions of the present approach are well justified at impact energies less than about 100 eV (see discussion in [8]). Thus, the values of the cross sections shown in Fig. 5 at energies greater than 100 eV should be used with caution. (However, as discussed in [8], the accuracy of the cross sections at energies between 100 and 1000 eV should not be worse than a factor of 2.)

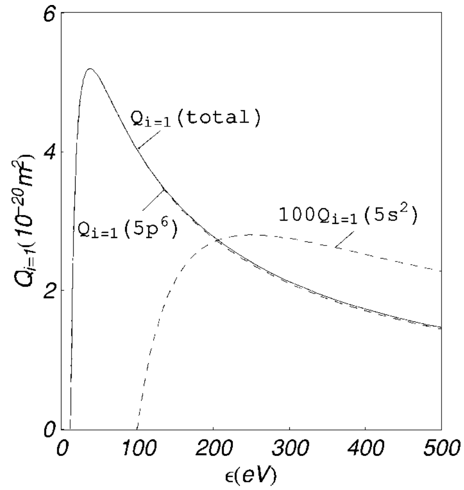

FIG. 1. The present cross sections for ionization of the ground-state ($i=1$, p_0) xenon atom by an electron of energy ϵ. The dashed curves represent contributions of the outermost atomic shells to the total ionization cross section (the solid curve).

IV. THE CROSS SECTIONS FOR IONIZATION OF THE ATOMIC LEVELS $5s^2 5p^6$, $5s^2 5p^5 6s$, AND $5s^2 5p^5 6p$

Younger [7] studied theoretically the contribution of the atomic shells to ionization of the ground-state xenon atom by electrons. The study concentrated on many-electron effects on the cross section. The author used in his study several different modifications of the distorted-wave Born-exchange approximation where Hartree-Fock wave functions were employed to describe the target. All the modifications yielded ionization cross sections that were greater at energies below 100 eV, by a factor of up to 2 or 3, than the corresponding measured cross sections. This discrepancy was explained by Younger as resulting mainly from the inedequacy of the distorted-wave approximation, rather than from the contribution of many-electron effects. Younger's most accurate atomic cross section was the one obtained when the $5p$-shell

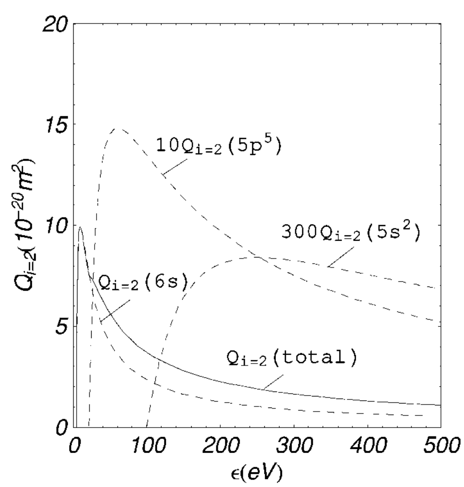

FIG. 2. The present cross sections for electron-impact ionization of the xenon atom excited to the $i=2$ $(1s_5)$ state. The meaning of the symbols is the same as in Fig. 1.

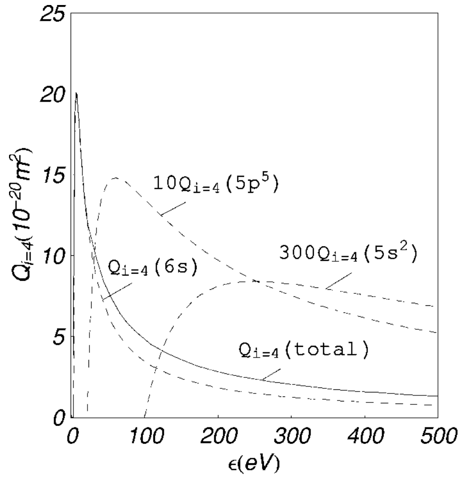

FIG. 3. The present cross sections for electron-impact ionization of the xenon atom excited to the $i=4$ ($1s_3$) state. The meaning of the symbols is the same as in Fig. 1.

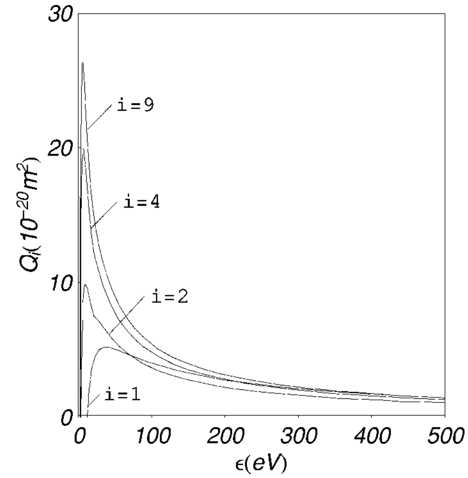

FIG. 5. Comparison of the present cross sections for electron-impact ionization of the xenon atom excited to states $i=1,2,4$, or 9.

contribution was treated within the frame of the distorted-wave Born-exchange approximation that included ground-state electron correlations. [This cross section was up to an order of magnitude greater than the 5*s*-shell contribution, obtained from the distorted-wave Born-exchange approximation using semiclassical exchange (SCE) partial waves [7], and up to about 30 times greater than the contribution of the 4*d* shell.] This atomic cross section was up to two times larger than the corresponding measured cross section and than the theoretical cross section of the present work, as seen in Fig. 6.

Even though Younger's distorted-wave approximation cross sections for ionization of the individual shells of the ground-state xenon atom are too high, they show a general trend which is similar to the trend of the present cross sections: the contributions of the inner shells of the Xe atom to the atomic ionization by electrons of energies considered in this work are much smaller than the contribution of the atomic outer shell.

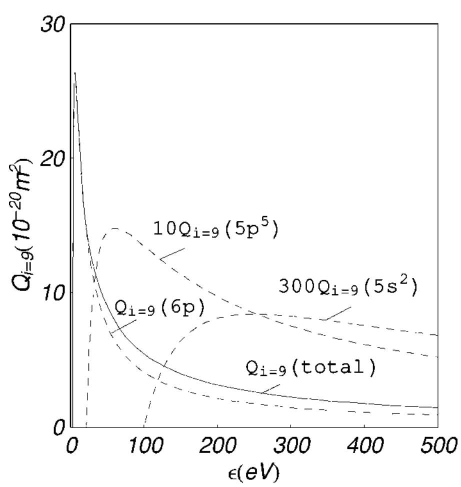

FIG. 4. The present cross sections for electron-impact ionization of the xenon atom excited to the $i=9$ ($2p_7$) state. The meaning of the symbols is the same as in Fig. 1.

Neither measured nor theoretical cross sections are available in the literature for electron-impact ionization of xenon atoms excited to the individual states listed in Table I. However, some theoretical results exist for ionization of two (6*s* and 6*p*) atomic levels. These levels each consist of several states, with the level properties obtained from averaging over the properties of the level's states [5,6]. Ton-That and Flannery [5] have calculated the cross section for ionization of the Xe level that is a state-averaged conglomerate of the two lowest atomic metastable states, $5s^25p^56s[3/2]_2$ ($i=2$) and $5s^25p^56s[1/2]_0$ ($i=4$). The cross section was calculated using the Born "half-range" approximation (BH) [15] and the symmetric binary encounter approximation (BE) [16] assuming identical orbitals for both states of the combined $5s^25p^56s$ level and identical effective potential for the target electrons. The quantal speed distribution of each target electron was obtained from a transformation of the electron spatial wave function. At impact energies less than 20–30 eV,

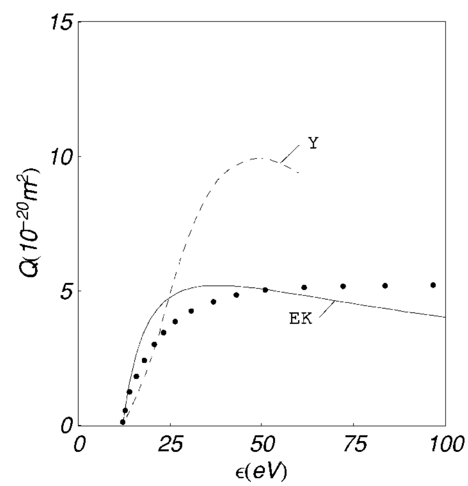

FIG. 6. The cross sections for electron-impact ionization of the $5s^25p^6$ level of the xenon atom. The solid curve EK is the cross section of the present work, while the dashed curve Y is the cross section of Younger [7]. The dots represent the measured values of the cross section [1–3].

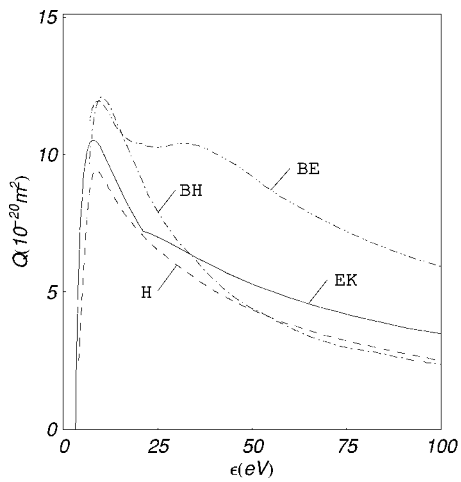

FIG. 7. The cross sections for electron-impact ionization of the state-averaged level $5s^25p^56s$ of the xenon atom. The solid curve EK is the cross section of the present work; the dash-dot curve BH and the double dash-dot curve BE represent the cross sections of Ton-That and Flannery [5], respectively; and the dashed curve H is the cross section of Hyman [6].

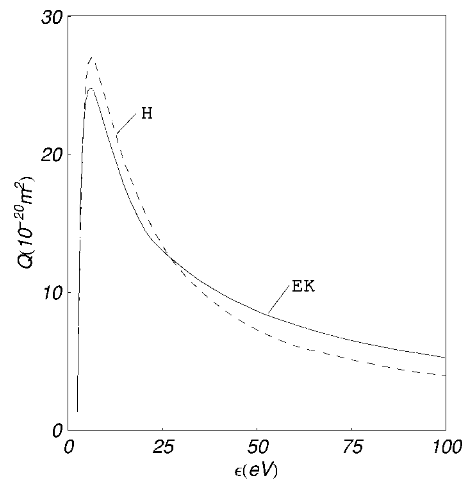

FIG. 8. The cross sections for ionization of the state-averaged level $5s^25p^56p$ of the xenon atom. The solid curve EK is the cross section of the present work, and the dashed curve H represents the cross section of Hyman [6].

the BH cross section, shows better agreement with the measured cross sections for electron-impact ionization of the low metastable level of the neon atom (no measurements exist for the xenon atom) than the BE cross section, which accounts for the contribution of the atomic inner shells. The same is true for argon at energies up to about 20–30 eV, but at higher energies the measured argon cross section is between the BE and BH results.

Hyman [6] calculated, using the symmetric binary encounter approximation [16], the electron-impact ionization cross sections for the $5s^25p^56s$ and $6p$ xenon levels with properties averaged over each level's states. His approximation used the quantum-mechanical momentum distribution function of the target electron determined from a semiempirical "scaled-effective-charge" method [17,18].

The state-averaged cross sections of Ton-That and Flannery and of Hyman for ionization of the $6s$ and $6p$ levels of xenon atoms are compared in Figs. 7 and 8 with the corresponding cross sections of the present work.

One can see in Fig. 7 that our state-averaged cross section for the ionization of the $6s$ level of xenon atoms (the solid curve EK) at impact energies less than about 20 eV is closer to the cross section of Hyman (the dashed curve H) than to the cross sections of Ton-That and Flannery (the dot-dash curve BH and the double-dash-dot curve BE). At higher energies, our cross section and the BE cross section show an expected qualitative contribution of the inner shells, but the two cross sections differ up to 50%. It seems that the contribution of the inner shell in the BE calculations is too big for several reasons. The first is that the BE cross section is almost twice as big as the BH cross section at energies as low as 35 eV, and this difference seems to be unrealistically large at such a low energy. Secondly, it seems clear that inclusion of the inner-shell contribution in Hyman's calculations for energies greater than 20 eV would give a cross section substantially lower than the corresponding BE cross section and, most likely, closer to our cross section than to the BE cross section. Also, the present approach gives a cross section for ionization of the ground-state xenon atom that is not much different from the corresponding measured values (see Fig. 6). Thus, the present cross section for ionization of xenon atoms excited to the $6s$ level seems to more accurately represent reality at low and medium energies than do either the cross sections of Ton-That and Flannery or those of Hyman. A more authoritative statement on the accuracy will of course be possible when measurements of the cross sections are available.

Figure 8 shows a comparison of Hyman's cross section (the dashed curve H) and the present cross section (the solid curve EK) for ionization of the $6p$ level of the xenon atom. Again, the cross sections are close to one another at energies below 30 eV. The present cross section correctly becomes larger than Hyman's cross section, a result of the inner shells' contribution being taken into account in our calculations.

V. FINAL REMARKS

Since neither measured nor theoretical cross sections for electron-impact ionization of Xe atoms excited to the individual states listed in Table I are available, it is impossible to judge the accuracy of the cross sections of the present work. However, the discussion given above of the results shown in Figs. 6–8, and the fact that our approach is derived from first principles, suggest that the accuracy of the present cross sections at impact energies less than a few hundred eV is similar to that of our cross sections for electron-impact ionization of ground-state xenon atoms [8]. The accuracy of the present cross sections at high energies (200–1000 eV) should therefore be worse (but by no more than a factor of 2) than those of the low-energy cross sections. At very high impact energies ($\epsilon > 1$ keV), the present approach has the traditional weakness of the binary encounter formalisms, i.e., the departure of the cross sections from their measured energy dependence. However, at these high energies, quite accurate cross sections for the electron-impact ionization of the excited xenon atoms can be obtained from the Bethe-Born approximation [19].

One should notice that the energy dependence of the present cross sections close to the ionization threshold differs from the corresponding dependence of Wannier's threshold law [20,21]. The former dependence is practically linear, while the latter law is $Q_i \sim (E_q - U_i)^{1.127}$ (see the discussion on this subject in [8]).

At the low and medium collision energies considered in this work, the present cross sections for direct electron-impact ionization of xenon atoms are not much different from the corresponding total ionization cross sections, since at such energies the corrections to the excited atomic states due to exchange, core polarization, etc., are not large [6,7].

Finally, we add that the present approach to ionization of atoms by low- and medium-energy electrons is a general one, derived from first principles. Therefore, the approach appears very promising for description of the electron-impact ionization of excited atoms and atomic ions other than xenon atoms if the collision energy is not high and if the number of the electrons in the target particle is large $(Z \gtrsim 20)$.

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