Ionization of one-electron ions penetrating a target at relativistic energies

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It is argued that the cross section for ionization of a hydrogenlike ion penetrating a target at relativistic speed $v=\beta c$ saturates already at moderate values of $\gamma\equiv 1/\sqrt{1-\beta^2}$. This is at variance with results published previously [R. Anholt and U. Becker, Phys. Rev. A **36**, 4628 (1987)]. A simple model is developed and shown to yield cross sections in accordance with those of the only two experiments performed so far.
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I. INTRODUCTION

The present paper has been prompted by the recent publication of two different experimental investigations of the ionization of relativistic one-electron ions as they penetrate a target [1,2]. In these articles, experimental findings are compared to the extensive theoretical results presented by Anholt and Becker [3]. The experimental data of Claytor *et al.* [1] were recorded at the Alternating Gradient Synchrotron (AGS) at Brookhaven National Laboratory at a relatively moderate energy of the incoming ion corresponding to $\gamma \equiv 1/\sqrt{1-v^2/c^2}=12.6$; here v denotes the ion velocity. The measured cross sections are reported to be in agreement with the theoretical results of [3]. The data of Krause *et al.* [2] were recorded at the CERN Super Proton Synchrotron at $\gamma=168$. The extracted cross sections are reported to be somewhat below the theoretical values of Anholt and Becker.

In the following I shall argue that the most likely cause of the discrepancy at the higher energy is an erroneous dependence of the ionization cross section on projectile energy in the theoretical work [3]. Simple estimates of the ionization cross section will be performed and actual numbers will be computed and compared to the experimental data. Throughout I shall set $\beta\equiv v/c=1$ (when it appears as a factor).

II. STRUCTURE OF CROSS SECTIONS

For any given combination of target and projectile atomic numbers, Anholt and Becker [3] state that cross sections have the structure

$$\sigma^{\mathrm{AB}}=\sigma_1^{\mathrm{AB}}+\sigma_2^{\mathrm{AB}}(\ln\gamma-\tfrac{1}{2}). \qquad (1)$$

Here the partial cross sections that I have labeled σ_1^{AB} and σ_2^{AB} are energy independent. Values for these are given in [3] for the case where the target particle is a bare charge, that is, a bare target nucleus, as well as for the case where the target object is a neutral atom. The latter ‘‘screening-included’’ case is covered through extensive tabulation of values of σ_1^{AB} and σ_2^{AB} for a wide range of projectile-target combinations.

As is obvious from Eq. (1), Anholt and Becker [3] predict that the projectile ionization cross section grows with $\ln\gamma$ both with and without screening included; Figs. 4 and 5 in [3] provide an illustration. As I shall now argue, this cannot be. Instead of showing the behavior (1), the cross section will actually saturate already at moderate projectile energies for any collision system when screening is included.

The structure of the projectile ionization cross section is roughly

$$\sigma=\sigma_1+\sigma_2\ln(b_{\max}/b_{\min}). \qquad (2)$$

Here $b_{\max}$ is some maximum impact parameter beyond which ionization does not occur, whereas the minimum $b_{\min}$ and the contribution σ_1 are linked together by the requirement that σ_1 accounts for contributions for impact parameters smaller than $b_{\min}$. The estimates to be presented in Sec. III are of exactly this form with essentially energy-independent results for σ_1 and σ_2.

To get an idea of how the cross section behaves we have to decide on the relevant lengths. There are three. One is the radius of the K shell of the projectile ion. I shall use this as $b_{\min}$ as it allows for simple estimates of the close and distant collision contributions to the ionization cross section, that is,

$$b_{\min}\sim a_K\sim a_0/Z_p, \qquad (3)$$

where Z_p is the atomic number for the incoming ion and $a_0=\lambda\!\!\!^{-}_C/\alpha$ is the Bohr radius for hydrogen (α being the fine-structure constant and $\lambda\!\!\!^{-}_C=\hbar/mc$ the Compton wavelength of the electron).

The two other lengths are candidates for $b_{\max}$. In the rest frame $\mathcal{R}$ of the incident ion, the time duration of the electric pulse produced by a target particle such as a target nucleus that passes by at distance b is $\Delta t\sim b/\gamma c$ and to liberate the electron bound to the ion at frequency $\omega_K=E_B/\hbar$, where $E_B=[1-\sqrt{1-(\alpha Z_p)^2}]mc^2$ is the binding energy, Δt^{-1} needs to be in excess of ω_K. This gives an effective maximum impact parameter of

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$$b_{\mathrm{ad}} \sim \gamma c/\omega_K \tag{4}$$

beyond which the interaction is adiabatic. Obviously, if Eqs. (3) and (4) are combined in Eq. (2), a cross section with the structure of that given in [3], Eq. (1), is obtained.

The third length follows from the simple observation that the target particles causing the ionization of the projectile are organized in neutral atoms. Hence the effective range of the field of a target nucleus as viewed in $\mathcal{R}$ can never exceed the atomic screening distance of target atoms. This leads to a maximum impact parameter of

$$b_{\mathrm{sc}} \sim a_{\mathrm{TF}} = 0.89 a_0 Z_t^{-1/3}, \tag{5}$$

where Z_t denotes the target atomic number and a_{TF} is the corresponding Thomas-Fermi screening length.

From the above discussion it follows that for the effective maximum impact parameter to enter Eq. (2) we should choose the smaller of b_{ad} and b_{sc}, that is,

$$b_{\mathrm{max}} \sim \min\left\{ \frac{\gamma c}{\omega_K}, 0.89 a_0 Z_t^{-1/3} \right\}. \tag{6}$$

With Eq. (6), the structure of the projectile ionization cross section is as given by Anholt and Becker, Eq. (1), but only until b_{ad} grows beyond b_{sc} where the cross section saturates, that is, becomes independent of projectile energy. An estimate of the value γ_c of γ beyond which saturation appears is obtained by setting $b_{\mathrm{sc}} = b_{\mathrm{ad}}$, i.e.,

$$\gamma_c \sim 60(\alpha Z_p)^2 / Z_t^{1/3} \tag{7}$$

(read 1 if the right-hand side comes out smaller than 1). This is a very low number; it is as low as ~ 5 for $Z_p = 82 = Z_t$.

Before turning to actual estimates of cross sections, it is worth noting that the above type of behavior with a $\ln\gamma$ dependence until a certain γ_c followed by saturation is well known for other processes. We may mention (a) the so-called density effect in ionization and ionization energy loss (see, e.g., [4,5]) and (b) bremsstrahlung and pair creation. The latter case (b) is closest to what we have here. By consulting, e.g., Heitler [6], it is obvious that arguments used to estimate effects of atomic screening on bremsstrahlung emitted by an electron deflecting in an atomic field are exactly as those used above. Furthermore, if bremsstrahlung were to be determined in a virtual photon calculation as discussed by Jackson [7], but now for a screened atomic nucleus [8], then the calculation to be performed would be very similar to the one I shall discuss next.

III. SIMPLE MODEL

To obtain some estimates of the projectile ionization cross section I shall use the Weizsäcker-Williams approach; see [7] or [9]. For the specific case of K-shell ionization, some useful hints may also be found in [5]. In this approach, the total cross section is separated into a close and a distant collision contribution as

$$\sigma = \sigma_{\mathrm{close}} + \sigma_{\mathrm{distant}} \tag{8}$$

at a dividing distance d.

For the dividing distance we choose

$$d = \lambda\!\!\!^{-}_C \sqrt{\frac{mc^2}{2\hbar\omega_K}}, \tag{9}$$

which essentially is the K-shell radius [cf. Eq. (3); the nonrelativistic expression for the binding energy is $(\alpha Z_p)^2 mc^2/2$]. The reason for this choice is twofold. First, the very application of an impact parameter b between (the center of) a given target object and the hydrogenlike projectile ion in the evaluation below of the distant collision contribution according to the virtual photon scheme demands that b be in excess of the latter struck system. The photon flux impinging on the extended hydrogenlike ion is calculated from the electromagnetic field strength of the target object at a distance b from (the center of) the object and considered uniform over the extent of the struck system. Second, for closer collisions the momentum transfer is greater than or equal to $\hbar/d$, which with Eq. (9) translates into energy transfers in excess of the binding energy; hence binding may be neglected in the estimate of the close-collision contribution to the ionization cross section.

With the choice (9), the close-collision contribution is evaluated as

$$\sigma_{\mathrm{close}} = \int_{\hbar\omega_K}^{T_{\mathrm{max}}} dT \frac{d\sigma}{dT}, \tag{10}$$

where T is the energy transfer to the K-shell electron with a maximum $T_{\mathrm{max}} \gg \hbar\omega_K$ determined by kinematics. The energy transfer cross section $d\sigma/dT$ is computed as if the electron were free, that is, $d\sigma/dT$ is essentially the Rutherford cross section that is proportional to $1/T^2$. By neglecting higher-order terms in the cross section, the estimate for the close-collision contribution to the ionization cross section by an unscreened target nucleus hence is [10]

$$\sigma_{\mathrm{close}} \simeq 2\pi r_0^2 Z_t^2/\eta, \quad \eta \equiv \hbar\omega_K/mc^2. \tag{11}$$

Here $r_0 = \alpha \lambda\!\!\!^{-}_C$ is the classical electron radius; it may be remembered that up to an error of 0.2% only, $4\pi r_0^2$ equals 1 b.

The distant-collision contribution to the ionization cross section is determined as the interaction of a bunch of equivalent of photons with the hydrogenlike ion, that is,

$$\sigma_{\mathrm{distant}} = \int_{\omega_K}^{\infty} d\omega\, \sigma_\gamma(\omega) \frac{1}{\hbar\omega} \frac{dI}{d\omega}. \tag{12}$$

Here σ_γ is the atomic photoabsorption cross section for the projectile ion and $dI/d\omega$ is the intensity of the virtual-photon bunch whose spectrum is constructed in such a way that the individual frequency components of the electromagnetic field very closely resemble those of the target object perturbing the ion. We shall now discuss each of the factors entering the integrand in Eq. (12).

The virtual photon spectrum is determined in $\mathcal{R}$. A target object is flying by at an impact parameter b. Imagine two different cases. In the first case a bare ion of charge $Z_t e$ is passing by. Neglecting contributions of order $1/\gamma^2$, the electromagnetic field as observed at the position of the ion corresponds to a photon intensity of

$$\frac{dI}{d\omega d^2b}=\hbar\alpha Z_t^2\frac{1}{\pi^2 b^2}[xK_1(x)]^2, \tag{13}$$

where the quantity x is given as

$$x=\frac{\omega b}{\gamma c}. \tag{14}$$

In the second case the target object passing by is a screened nucleus. The virtual photon intensity is then approximately given by the same expression (13), but with x substituted by

$$x=\left[\left(\frac{\omega b}{\gamma c}\right)^2+\left(\frac{b}{a_{\mathrm{TF}}}\right)^2\right]^{1/2}, \tag{15}$$

cf. [11]. Since the modified Bessel function K_1 falls off exponentially for arguments larger than 1, the effective maximum impact parameter alluded to in Eq. (6) is immediately apparent. Integration of Eq. (13) over impact parameters b beyond d yields

$$\frac{dI}{d\hbar\omega}=\frac{2}{\pi}\alpha Z_t^2\left\{\xi K_0(\xi)K_1(\xi)+\frac{1}{2}\xi^2[K_0^2(\xi)-K_1^2(\xi)]\right\}, \tag{16}$$

where ξ is defined as x in Eqs. (14) and (15) but with d substituted for b, that is,

$$\xi=\frac{\omega d}{\gamma c}\times\begin{cases}1 & \text{for the bare nucleus}\\ \left[1+\left(\frac{\gamma c}{\omega a_{\mathrm{TF}}}\right)^2\right]^{1/2} & \text{for the screened nucleus.}\end{cases} \tag{17}$$

By application of the asymptotic expansions of the modified Bessel functions K_0 and K_1, Eq. (16) is seen to reduce to

$$\frac{dI}{d\hbar\omega}=\frac{2}{\pi}\alpha Z_t^2\left\{\ln\frac{1.123}{\xi}-\frac{1}{2}\right\} \tag{18}$$

in the limit of small arguments $\xi \ll 1$. The combination of Eq. (17) for the Coulomb case and Eq. (18) again makes the Anholt-Becker cross section (1) a familiar result, but not a general one.

As to the photo cross section σ_γ appearing in Eq. (12), a rather simple choice is made. The choice is based on the nonrelativistic photo cross section obtained by Stobbe by application of the dipole approximation and exact Coulomb waves. It is identified in the following as σ_{Stobbe}; see, e.g., [6] for the actual expression. For high photon energies $\sigma_{\mathrm{Stobbe}} \propto \omega^{-7/2}$, whereas the true behavior of the photo cross section for $\hbar\omega \gtrsim mc^2$ is a much slower falloff $\sigma_\gamma \propto \omega^{-1}$. To account for this, the following expression is used:

$$\sigma_\gamma=(\sigma_{\mathrm{Stobbe}}^2+\sigma_{\mathrm{Pratt}}^2)^{1/2}, \tag{19}$$

where σ_{Pratt} is the high-energy result obtained by Pratt, cf. [12]. A check against tabulated atomic photo cross sections [13] shows reasonable agreement after reduction of the tabulated values to a single K electron has been made. For lead, for instance, it is found that values computed according to Eq. (19) are slightly lower, by 5–10 %, than the tabulated ones in the most important region just above the absorption edge. The overall accuracy of the entire scheme with the split (8) and the approximate treatment of each of the two contributions of course cannot be expected to be any better than this.

TABLE I. Results of the AGS experiment [1] compared to theory. The table gives cross sections, all in kb, for the ionization of a hydrogenlike gold ion as it penetrates various solid targets at $\gamma = 12.6$. Upon incidence, the ion is in its ground state. The first column gives the atomic number of the target. The second column gives the cross section measured in the experiment. The third column gives the theoretical prediction of Anholt and Becker [3] with screening included. The last two columns list results obtained in the present work for ionization by a bare target nucleus (fourth column) and a neutral atom (fifth column).

			Present work	
Z_t	Experiment	Anholt and Becker	Bare nucleus	Atom
6	0.310	0.310	0.243	0.271
13	1.18	1.28	1.14	1.15
29	5.26	5.80	5.73	5.37
47	16.2	14.4	15.5	13.7
79	38.2	38.8	43.4	38.0

IV. RESULTS

Table I shows a comparison between the experimental findings by Claytor *et al.* [1] and theoretical results as obtained by Anholt and Becker [3] as well as in the present work. The results of Anholt and Becker include screening. The results of the present work, obtained by the combination of formulas (8), (9), (11), (12), (16), (17), and (19), are shown for ionization by both a bare target nucleus and a neutral atom; in the last case contributions from target electrons have been included approximately by multiplying the result obtained for a screened nucleus by $1+Z_t^{-1}$.

The overall agreement between experimental results, the cross sections of Anholt and Becker, and those computed here with allowance for screening is quite good. Despite the result of the present calculation for $Z_t=6$ and the experimental finding for $Z_t=47$ fall somewhat outside the rest, no differences can be claimed to be significant in view of the accuracy of both experiment and applied theoretical models.

Table II similarly shows a comparison between the experimental findings by Krause *et al.* [2] and theoretical results as obtained by Anholt and Becker [3] as well as in the present work. Contributions from target electrons have again been included approximately in the last column by multiplying the result obtained for a screened nucleus by $1+Z_t^{-1}$.

In the high-energy case, there is a significant deviation between the two sets of theoretical values. The experimental data fall in between. For lower values of the target atomic number, the experimental data are closer to the theoretical values computed here; for $Z_t \geqslant 29$ the matter is less clear. The experimental cross sections were extracted from a ''capture experiment'' (the larger cross section listed at given Z_t)

TABLE II. Results of the CERN experiment [2] compared to theory. The table gives cross sections, all in kb, for the ionization of a hydrogenlike lead ion as it penetrates various solid targets at $\gamma = 168$. Upon incidence, the ion is in its ground state. Columns are as in Table I.

			Present work	
Z_t	Experiment	Anholt and Becker	Bare nucleus	Atom
4	0.15–0.14	0.24	0.15	0.14
6	0.31	0.49	0.33	0.28
13	1.4–1.3	2.0	1.6	1.1
29	8.0–6.9	9.0	7.8	5.2
50	21–15	25	23	15
79	53–42	60	58	35

and an ''ionization experiment'' (the smaller cross section listed at given Z_t). According to the authors, systematic uncertainties (unknown contributions from ionization of excited states) are such that the results of the ionization experiment are believed to most nearly represent the true ground-state ionization of the lead ion [14]. The results of the ionization experiment strongly favor the theoretical values computed here. Note that the difference between experimental results and our theoretical estimates is nowhere beyond the combination of the inaccuracies with which either one is produced. As to the theoretical estimates, it may be mentioned that all the current fifth-column results receive about equal contributions from distant and close collisions (with a slight dominance of the distant collision contribution). In view of this, as well as in view of the quite rough treatment of the contributions from the two classes of collisions, the decision of how to combine the two, and the choice of photo cross section, the numbers produced here should not be trusted better than to within 10–20 %.

It may be noted that in the CERN case as opposed to the AGS case, all the results produced here for the Coulomb case (no screening) are below the results of Anholt and Becker with screening included. The reason may well be the current use of a nonperturbative photo cross section (although through a simple fit): While the scheme applied here certainly is perturbative in the action of the target constituents, this is not so for the action of $Z_p e$ on the liberated electron. As is well known, the nonrelativistic photo cross section of Stobbe is only 0.12 times the plane-wave Born value in the immediate neighborhood of the absorption edge. This type of effect shows for the projectile ionization by a bare charge more clearly at higher energies simply because the distant-collision contribution in this case increases with γ. See also [15].

V. CONCLUDING REMARKS

We have shown above that the cross section for ionizing a hydrogenlike projectile as it penetrates matter saturates already at moderate values of the Lorentz factor γ. This is in contrast to the results and supposedly general formulas published previously by Anholt and Becker [3] and showing a $\ln\gamma$ dependence. It may be noted that Anholt and Becker shoot for energies beyond 10 GeV/amu. As the study above shows, saturation has actually set in for virtually all collision systems at such energies.

We have constructed a simple model and computed cross sections that are in agreement with experimental data. It is furthermore important to note that the cross sections computed here agree with those of Anholt and Becker at low to moderate values of γ but fall significantly below at high values of γ. Our discussion in Sec. II explains the physics behind this difference.

Although the primary purpose of the present contribution is to explain the energy dependence of the ionization cross section rather than to compute very accurate numbers, we may mention a few ways in which the quality of the components of the simple model presented in Sec. III may be improved. Obviously, one may try to find a more accurate photo cross section. For instance, the cross section could be extracted from measured values. Or, since we are dealing with a hydrogenlike system, relatively simple, though relativistic, calculations could be performed along the lines of [16]. See also [17]. In addition to that, the Compton effect could be added. Another obvious improvement would be to compute accurately an expression for the photon intensity $dI/d\omega db$ corresponding to actual atomic potentials.

The work by Krause *et al.* [2] contains a remark concerning coherent addition of amplitudes or, similarly, interference between what is called Coulomb and transverse contributions. Such effects, which have been reported recently for projectile excitation [18], are not an issue in the approach followed in the present paper: As long as the notion of an impact parameter makes sense, all ''interferences'' are included via the photo cross section σ_γ and the photon intensities, determining the distant-collision contribution σ_{distant}, Eq. (12), and the collision cross section $d\sigma/dT$ entering the integrand in Eq. (10) and determining the close-collision contribution σ_{close}.

A final remark regards a conclusion in the paper by Krause *et al.* [2] that in electron-positron pair creation with capture of the electron to the projectile bare lead ion at $\gamma = 168$, experimental values indicate 15–20 % going to excited states, whereas calculations suggest a significantly higher number of the order of (or beyond) 30%; cf. [16]. It should be noted that the $2s$ state contributes 12.5% to the latter number (the total for all s states being roughly 20%). Since the $2s$ state has difficulties decaying radiatively to the ground state, the lack of observation of the $2s$ contribution in the experiment may well explain the difference.

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[1] N. Claytor, A. Belkacem, T. Dinneen, B. Feinberg, and Harvey Gould, Phys. Rev. A **55**, R842 (1997).

[2] H. F. Krause, C. R. Vane, S. Datz, P. Grafström, H. Knudsen, C. Scheidenberger, and R. H. Schuch, Phys. Rev. Lett. **80**, 1190 (1998).

[3] R. Anholt and U. Becker, Phys. Rev. A **36**, 4628 (1987).

[4] A. H. Sørensen and E. Uggerhøj, Comments At. Mol. Phys. **17**, 285 (1986).

[5] Allan H. Sørensen, Phys. Rev. A **36**, 3125 (1987).

[6] W. Heitler, *The Quantum Theory of Radiation* (Dover, New York, 1984).

[7] J. D. Jackson, *Classical Electrodynamics* (Wiley, New York, 1975).

[8] The reader may want to check out the problem section in Jackson's book [7].

[9] E. J. Williams, K. Dan. Vidensk. Selsk. Mat. Fys. Medd. **13**, No. 4 (1935).

[10] For the close-collision contribution screening is only important if Z_p is very small while at the same time Z_t is very large. Roughly, something like $Z_p < Z_t^{1/3}$ is required. Such cases shall not be considered in the following; throughout I assume the screening length of target atoms to be in excess of the radius of the projectile ion.

[11] The result is an approximation, which is made simply for convenience. For a nucleus screened exponentially such as to yield the potential $Z_t e \exp(-r/a_{\mathrm{TF}})r$ in the laboratory, the combination of formulas (13) and (15) actually overestimates the spectrum. However, while stating this it should be remembered that actual atomic screening is somewhat less dramatic than $\exp(-r/a_{\mathrm{TF}})$. (The fact that the construction leads to an overestimate of photon intensities for the Yukawa case of course implies that the conclusion I shall reach concerning cross sections being lower than those of Anholt and Becker is not at danger.)

[12] R. H. Pratt, Akiva Ron, and H. K. Tseng, Rev. Mod. Phys. **45**, 273 (1973); cf. Eq. (6.1.8). The inclusion of the correct high-energy tail is actually not very crucial for the present purpose. If σ_γ was chosen simply as σ_{Stobbe}, the results for the case of screening included would only be approximately 2% lower than those actually appearing in the last column of the two tables. In view of the smallness of this correction, we have not attempted to include also the Compton effect (or other effects relevant only at very high photon energies); for a hydrogenlike lead ion it will not exceed the photoeffect before energies in excess of, roughly, $10^2 mc^2$.

[13] Wm. J. Veigele, At. Data **5**, 51 (1973); J. H. Hubbell, Wm. J. Veigele, E. A. Briggs, R. T. Brown, D. T. Cromer, and R. J. Howerton, J. Phys. Chem. Ref. Data **4**, 471 (1975).

[14] Randy Vane (private communication).

[15] In [2] there is a reference to unpublished work by Baltz dealing with an exact time-dependent solution of the Dirac equation for a hydrogenic lead ion colliding with a bare lead ion. For $\gamma = 168$ he finds 70% of the value of Anholt and Becker (unscreened). This may well reflect the remark on the effect of a nonperturbative photo cross section in the present construction.

[16] C. K. Agger and A. H. Sørensen, Phys. Rev. A **55**, 402 (1997).

[17] A. Ichihara, T. Shirai, and J. Eichler, Phys. Rev. A **49**, 1875 (1994); **54**, 4954 (1996).

[18] Th. Stöhlker, D. C. Ionescu, P. Rymuza, F. Bosch, H. Geissel, C. Kozhuharov, T. Ludziejewski, P. H. Mokler, C. Scheidenberger, Z. Stachura, A. Warczak, and R. W. Dunford, Phys. Lett. A **238**, 43 (1998).