Some exact analytical results and a semi-empirical formula for single electron ionization induced by ultrarelativistic heavy ions

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Abstract

The delta function gauge of the electromagnetic potential allows semiclassical formulas to be obtained for the probability of exciting a single electron out of the ground state in an ultrarelativistic heavy ion reaction. Exact formulas have been obtained in the limits of zero impact parameter and large, perturbative, impact parameter. The perturbative impact parameter result can be exploited to obtain a semi-empirical cross section formula of the form $\sigma = A \ln \gamma + B$ for single electron ionization. A and B can be evaluated for any combination of target and projectile, and the resulting simple formula is good at all ultrarelativistic energies. The analytical form of A and B elucidates a result previously found in numerical calculations: scaled ionization cross sections decrease with increasing charge of the nucleus being ionized. The cross section values obtained from the present formula are in good agreement with recent CERN SPS data from a Pb beam on various nuclear targets.

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I. INTRODUCTION

In a recent work [1] ionization cross sections were calculalated for a number of representative cases of collisions involving ultrarelativistic Pb, Zr, Ca, Ne and H ions. The method of calculation (on a computer) involved an exact semiclassical solution of the Dirac equation in the ultrarelativistic limit [2]. A single electron was taken to be bound to one nucleus with the other nucleus completely stripped. The probability that the electron would be ionized in the collision was calculated as a function of impact parameter, and cross sections were then constructed by the usual integration of the probabilities over the impact parameter. The results of the probability calculations were used to construct cross sections for various ion-ion collision combinations in the form

$$\sigma = A \ln \gamma + B \tag{1}$$

where A and B are constants for a given ion-ion pair and γ $(= 1/\sqrt{1 - v^2})$ is the relativistic factor one of the ions seen from the rest frame of the other.

In Section II of this paper analytic results are derived for the probability that a single ground state electron will be excited in an ultrarelativistic heavy ion reaction. Exact semiclassical formulas are presented for the limits of zero impact parameter and perturbational impact parameters. In Section III the perturbational impact parameter analytical form is used as a basis to construct semi-empirical formulas for A and B. These formulas reproduce the previous numerical results for single particle ionization, and they illuminate the systematic behavior of A and B with changing target and projectile ion species. Ionization cross sections calculated with Eq.(1) are then compared with data.

II. IMPACT PARAMETER DEPENDENT PROBABILITIES

If one works in the appropriate gauge [3], then the Coulomb potential produced by an ultrarelativistic particle (such as a heavy ion) in uniform motion can be expressed in the following form [4]

$$V(\boldsymbol{\rho}, z, t) = -\alpha Z_1 (1 - \alpha_z) \delta(z - t) \ln \frac{(\mathbf{b} - \boldsymbol{\rho})^2}{b^2}. \tag{2}$$

$\mathbf{b}$ is the impact parameter, perpendicular to the z–axis along which the ion travels, $\boldsymbol{\rho}$, z, and t are the coordinates of the potential relative to a fixed target (or ion), α_z is the Dirac matrix,

α the fine structure constant, and Z_1 and v the charge and velocity of the moving ion. This is the physically relevant ultrarelativistic potential since it was obtained by ignoring terms in $(\mathbf{b}-\boldsymbol{\rho})/\gamma^2$ [4] [3]. Its multipole expansion is

$$
\begin{aligned}
V(\boldsymbol{\rho}, z, t) = \alpha Z_1 (1-\alpha_z)\delta(z-t) & \\
\Big\{ -\ln\frac{\rho^2}{b^2} & \qquad \rho > b \\
+ \sum_{m>0} \frac{2\cos m\phi}{m} & \\
\times \Big[\Big(\frac{\rho}{b}\Big)^m & \qquad \rho < b \\
+ \Big(\frac{b}{\rho}\Big)^m \Big] \Big\}. & \qquad \rho > b
\end{aligned}
\tag{3}
$$

For $b >> \rho$

$$
V(\boldsymbol{\rho}, z, t) = \delta(z-t)\alpha Z_1 (1-\alpha_z) 2\frac{\rho}{b}\cos\phi. \tag{4}
$$

As will be shown in Section III, when $\mathbf{b}$ becomes large enough that expression Eq.(4) is inaccurate for use in calculating a probability, we match onto a Weizsacker-Williams expression which is valid for large b. Note that the b^2 in the denominator of the logarithm in Eq.(2) is removable by a gauge transformation, and we retain the option of keeping or removing it as convenient.

It was shown in Ref. [2] that the δ function allows the Dirac equation to be solved exactly at the point of interaction, $z = t$. Exact amplitudes then take the form

$$
\begin{aligned}
a_f^j(t=\infty) = \delta_{fj} + \int_{-\infty}^{\infty} dt e^{i(E_f - E_j)t} \langle \phi_f | \delta(z-t)(1-\alpha_z) & \\
\times (e^{-i\alpha Z_1 \ln(\mathbf{b}-\boldsymbol{\rho})^2} - 1) | \phi_j \rangle &
\end{aligned}
\tag{5}
$$

where j is the initial state and f the final state. This amplitude is in the same form as the perturbation theory amplitude, but with an effective potential to represent all the higher order effects exactly,

$$
V(\boldsymbol{\rho}, z, t) = -i\delta(z-t)(1-\alpha_z)(e^{-i\alpha Z_1 \ln(\mathbf{b}-\boldsymbol{\rho})^2} - 1), \tag{6}
$$

in place of the potential of Eq.(2).

Since an exact solution must be unitary, the ionization probability (the sum of probabilities of excitation from the single bound electron to particular continuum states) is equal to the deficit of the final bound state electron population

$$\sum_{ion} P(b) = 1 - \sum_{bound} P(b) \tag{7}$$

The sum of bound state probabilities includes the probability that the electron remains in the ground state plus the sum of probabilities that it ends up in an excited bound state. From Eq.(5) one may obtain in simple form the exact survival probability of an initial state

$$P_j(b) = |\langle\phi_j|(1-\alpha_z)e^{-i\alpha Z_1 \ln(\mathbf{b}-\boldsymbol{\rho})^2}|\phi_j\rangle|^2. \tag{8}$$

By symmetry the α_z term falls out and we are left with

$$P_j(b) = |\langle\phi_j|e^{-i\alpha Z_1 \ln(\mathbf{b}-\boldsymbol{\rho})^2}|\phi_j\rangle|^2. \tag{9}$$

The ground state wave function ϕ_j is the usual K shell Dirac spinor [5]

$$\phi_j = \begin{pmatrix} g(r)\chi^{\mu}_{\kappa} \\ if(r)\chi^{\mu}_{-\kappa} \end{pmatrix} \tag{10}$$

with upper and lower components wave functions g and f

$$\begin{aligned} g(r) &= N\sqrt{1+\gamma_2}\; r^{\gamma_2-1}\; e^{-\alpha Z_2 r} \\ f(r) &= -N\sqrt{1-\gamma_2}\; r^{\gamma_2-1}\; e^{-\alpha Z_2 r} \end{aligned} \tag{11}$$

where Z_2, is the charge of the nucleus that the electron is bound to, $\gamma_2 = \sqrt{1-\alpha^2 Z_2^2}$, and

$$N^2 = \frac{(2\alpha Z_2)^{2\gamma_2+1}}{2\Gamma(\gamma_2+1)}. \tag{12}$$

Let us first consider $b = 0$. We have

$$P_j(b=0) = |\langle\phi_j|e^{-2i\alpha Z_1 \ln\rho}|\phi_j\rangle|^2 = |\langle\phi_j|e^{-2i\alpha Z_1(\ln r+\ln(\sin\theta))}|\phi_j\rangle|^2. \tag{13}$$

Putting in the explicit form of the upper and lower components for the K shell lowest bound state Dirac wave function and carrying out the integration we have

$$P_j(b=0) = \frac{\pi}{4}\left|\frac{\Gamma(2\gamma_2 + 1 - 2i\alpha Z_1)\Gamma(1 - i\alpha Z_1)}{\Gamma(2\gamma_2 + 1)\Gamma(\frac{3}{2} - i\alpha Z_1)}\right|^2, \tag{14}$$

or

$$P_j(b=0) = \frac{\pi\alpha Z_1 \,\mathrm{ctnh}(\pi\alpha Z_1)}{(1 + 4\alpha^2 Z_1^2)}\left|\frac{\Gamma(2\gamma_2 + 1 - 2i\alpha Z_1)}{\Gamma(2\gamma_2 + 1)}\right|^2. \tag{15}$$

It is interesting to compare this result with a previous calculation of the probability of ionization in "close collisions" by Bertulani and Baur [6]. For a one electron atom they find

$$P_{ion}(b < \lambda_c/\alpha Z_2) = 1.8\ \alpha^2 Z_1^2, \tag{16}$$

where $\lambda_c = \hbar/m_e c$ is the electron Compton wavelength. If we take the low Z_1 limit of our expression Eq.(15) and then subtract it from one we obtain

$$P_{ion}(b=0) = (\frac{\pi^2}{3} - 1)\alpha^2 Z_1^2 = 2.29\ \alpha^2 Z_1^2 \tag{17}$$

However our expression Eq.(15) only gives the flux lost from the initial state; some of that flux goes into excited bound states and is not ionized. From our previous numerical calculations we find that the actual ionization probabilities obtained either by summing up final continuum states or else by subtracting all the final bound states from unity were 76% – 80% respectively of the flux lost from the initial state. Thus if we multiply the constant in Eq.(17) by such a percentage we are in remarkable agreement with Bertulani and Baur for the perturbative limit.

Now let us consider the case of $b >> \rho$. From Eq.(4) and Eq.(9) we have

$$P_j(b) = |\langle\phi_j|e^{-2i\alpha Z_1 \cos(\phi)(\rho/b)}|\phi_j\rangle|^2. \tag{18}$$

Expanding the exponential up to ρ^2/b^2 we have

$$P_j(b) = |\langle\phi_j|1 - 2i\alpha Z_1 \cos(\phi)\frac{\rho}{b} - 2\alpha^2 Z_1^2 \cos^2(\phi)\frac{\rho^2}{b^2}|\phi_j\rangle|^2 \tag{19}$$

The term in $\cos(\phi)$ vanishes by symmetry, and integrating, we obtain

$$P_j(b) = 1 - 2\frac{Z_1^2}{Z_2^2}\frac{(1 + 3\gamma_2 + 2\gamma_2^2)}{3}\frac{\lambda_c^2}{b^2} \tag{20}$$

by ignoring the term in $1/b^4$.

Both limits, Eq.(15) for $b = 0$ and Eq.(20) for $b >> \rho$, are relativistically correct and thus correct for all Z_1 and Z_2 since exact Dirac wave functions were used.

III. A SEMI-EMPIRICAL FORMULA FOR SINGLE ELECTRON IONIZATION

It is well known that the cross section for ionization of any pair of projectile and target species can be expressed as a sum of a constant term and a term going as the log of the relativistic γ of the beam as seen in the target rest frame [6] [7] [1]

$$\sigma_{ion} = A \ln \gamma + B. \tag{21}$$

The cross section of this form is constructed from an impact parameter integral

$$\sigma_{ion} = 2\pi \int P(b)_{ion}\ b\ db \tag{22}$$

where $P(b)$ is the probability of ionization at a given impact parameter. If all the flux lost from the initial state went into the continuum then Eq.(20) would provide the ionization probability at moderately large b

$$P_{ion}(b) = 2\frac{Z_1^2}{Z_2^2}\frac{(1 + 3\gamma_2 + 2\gamma_2^2)}{3}\frac{\lambda_c^2}{b^2}. \tag{23}$$

We will take this form as a physical basis to build a semi-empirical formula for ionization. In any case we need to integrate the probability up to a natural energy cutoff. In order to do this we match the delta function solution Eq.(23) at some moderately large b onto the known Weizsacker-Williams probability for larger b by noting that if $b\omega << \gamma$ then

$$K_1^2(\frac{\omega b}{\gamma}) = \frac{\gamma^2}{\omega^2 b^2}, \tag{24}$$

and we can rewrite Eq.(24) in the Weizsacker-Williams form for large b

$$P_{ion}(b) = 2\frac{Z_1^2}{Z_2^2}\frac{(1 + 3\gamma_2 + 2\gamma_2^2)}{3}\frac{\lambda_c^2\omega^2}{\gamma^2}K_1^2(\frac{\omega b}{\gamma}). \tag{25}$$

To perform the large b cutoff recall that to high degree of accuracy

$$\frac{\omega^2}{\gamma^2}\int_{b_0}^{\infty} K_1^2(\frac{\omega b}{\gamma}) b\, db = \ln(\frac{0.681\gamma}{\omega b_0}) = \ln\gamma + \ln(\frac{0.681}{\omega b_0}). \tag{26}$$

We immediately obtain the following expression for A

$$A = \frac{4\pi\lambda_c^2}{3}\frac{Z_1^2}{Z_2^2}(1+3\gamma_2+2\gamma_2^2), \tag{27}$$

where λ_c^2, the square of the electron Compton wave length, is 1491 barns. However, as it turns out, uniformly for all species of heavy ion reactions, at perturbational impact parameters a little over 70% of the flux lost from the initial state goes into excited bound states and does not contribute to ionization. But since the ratio of flux going into continuum states to the total flux lost is so uniform we can use a fit to previously published numerical results [1] to obtain a semi-analytical form for A:

$$A = (0.2869)\frac{4\pi\lambda_c^2}{3}\frac{Z_1^2}{Z_2^2}(1+3\gamma_2+2\gamma_2^2), \tag{28}$$

or in barns

$$A = 1792\frac{Z_1^2}{Z_2^2}(1+3\gamma_2+2\gamma_2^2). \tag{29}$$

Now one can use the second term in Eq.(26) to obtain a provisional expression for B

$$B = A\ln(\frac{0.681}{\omega b_0}). \tag{30}$$

Obviously we need to evaluate ω and to discuss b_0. ω can be taken as the minimum ionization energy, $1-\gamma_2$, times a constant a little larger than one. One next observes that if $P_{ion}(b)$ varies as $1/b^2$ the impact parameter integral has to be cut off on the low side at some value b_0 to avoid divergence. In fact the $1/b^2$ dependence continues down to the surface of the atom where other terms evident in Eq.(3) begin to contribute. The atomic size is just the electron Compton wave length divided by αZ_2. In this region $P_{ion}(b)$ first rises faster than $1/b^2$ and then levels off to approach a constant change with b at $b=0$ [1]. One could try to add a low impact paramenter contribution to A based on Eq.(15) to our provisional form Eq.(30), but that turns out to unduly complicate things without improving the phenomenology. Our approach will be to set b_0 to an empirical constant divided by αZ_2

Eq.(30) now takes the form

$$B = A \ln(\frac{C\alpha Z_2}{1-\gamma_2}). \tag{31}$$

Putting in two analytical fine tuning factors and fitting the remaining constant to the numerical results of Ref. [1] we obtain a semi-analytical form for B:

$$B = A\gamma_1^{1/10}(1-\alpha^2 Z_1 Z_2)^{1/4} \ln(\frac{2.37\alpha Z_2}{1-\gamma_2}). \tag{32}$$

Table I expands a corresponding table from Ref. [1] by adding cross sections of symmetric ion-ion pairs calculated with the formulas for A and B. There is good agreement between the formula values for the cross sections (first rows) and the numerical cross sections calculated by subtracting the bound state probabilities from unity (second rows) or calculated by summing continuum electron final states (third rows). For both A and B the agreement is also good with the Anholt and Becker calculations [7] in the literature for the lighter ion species. However with increasing mass of the ions the perturbative energy dependent term A decreases in the formula calculations and in our previous numerical calculations, whereas it increases in the Anholt and Becker calculations. The greatest discrepancy is for Pb + Pb, with Anholt and Becker being about 60% higher. The reason that the A should decrease with increasing mass (actually Z) of the ions is explained by the

$$(1+3\gamma_2+2\gamma_2^2) = 3 - 2\alpha^2 Z_2^2 + 3\sqrt{1-\alpha^2 Z_2^2} \tag{33}$$

factor in the formula for A (and thereby B also). As we noted before, perhaps the discrepancy between our A decreasing with Z and the Anholt and Becker A increasing with Z is due to the fact that Anholt and Becker use approximate relativistic bound state wave functions and the present calculations utilize exact Dirac wave functions for the bound states. For the term B (which has the non-perturbative component) the agreement is relatively good between all the calculations.

In the perturbative limit (small Z_1, Z_2) the cross section formula goes over to

$$\sigma = (0.2869) 8\pi\lambda_c^2 \frac{Z_1^2}{Z_2^2} \ln\frac{2.37\gamma}{\alpha Z_2} = 7.21\lambda_c^2 \frac{Z_1^2}{Z_2^2} \ln\frac{2.37\gamma}{\alpha Z_2}. \tag{34}$$

By way of comparison, Bertulani and Baur [6] using the equivalent photon method and taking the contribution of $b \geq \lambda_c/\alpha Z_2$ found

$$\sigma = 4.9\lambda_c^2 \frac{Z_1^2}{Z_2^2} \ln \frac{2\gamma}{\alpha Z_2} \tag{35}$$

for this case of ionization of a single electron.

Table II shows results of the calculation of B (multiplied by Z_2^2/Z_1^2) for a number of representative non-symmetric ion-ion pairs. (Since A is perturbative, scaling as Z_1^2, its value can be taken from Table I for the various pairs here.) Once again there is good agreement between the formula values for the cross sections (first rows) and the numerical cross sections calculated by subtracting the bound state probabilities from unity (second rows) or calculated by summing continuum electron final states (third rows). The only notable disagreement is with Anholt and Becker for Pb targets.

The availabilty of the present semi-empirical formula facilitates a comparison with available CERN SPS data. Calculations with the formula are in considerably better agreement with the data of Krause et al. [8] for a Pb beam on various targets than are the Anholt and Becker numbers with or without screening. Note that in this case the role of target and beam are reversed. It is the single electron Pb ion in the beam that is ionized by the various nuclei in the fixed targets. The formula numbers do not include screening, which should in principle be included for a fixed target case. However, one might infer from the Anholt and Becker calculations that the effect of screening is smaller than the error induced by using an approximate rather than proper relativistic wave function for the electron bound in Pb.

Note that the formula has not been fit to experimental data. It is compared with experimental data. The "empirical" aspect of this formula refers to adjusting the formula to previous numerical calculations of Ref. [1]

At RHIC the relativistic γ of one ion seen in the rest frame of the other is 23,000, and of course there is no screening, so the present formula should be completely applicable. The present formula predicts a single electron ionization cross section of 101 kilobarns for Au + Au at RHIC. The corresponding cross section from Anholt and Becker is 150 kilobarns.

IV. ACKNOWLEDGMENTS

After this work was completed, a paper by Voitkiv, Müller and Grün [9], which includes screening in ionization of relativistic projectiles, was brought to my attention. I would like to thank Carlos Bertulani for pointing out this paper to me and for reading the present manuscript. This manuscript has been authored under Contract No. DE-AC02-98CH10886 with the U. S. Department of Energy.

REFERENCES

[1] A. J. Baltz, Phys. Rev. **A 61**, 042701 (2000).

[2] A. J. Baltz, Phys. Rev. Lett. **78**, 1231 (1997).

[3] A. J. Baltz, M. J. Rhoades-Brown, and J. Weneser, Phys. Rev. **A 44**, 5568 (1991).

[4] A. J. Baltz, Phys. Rev. **A 52**, 4970 (1995).

[5] M. E. Rose, *Relativistic Electron Theory* (Wiley, New York, 1961).

[6] Carlos A. Bertulani and Gerhard Baur, Physics Reports **163**, 301 (1988).

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

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

[9] A. B. Voitkiv, C. Müller, and N. Grün, Phys. Rev. **A 62**, 062701 (2000).

TABLE I. Calculated Ionization Cross Sections Expressed in the Form $A \ln \gamma + B$ (in barns)

		Pb + Pb	Zr + Zr	Ca + Ca	Ne + Ne	H + H
A	Formula	8400	10,212	10,618	10,718	10,752
	$1 - \sum_{bnd} e^-$	8680	10,240	10,620	10,730	10,770
	$\sum_{cont} e^-$	8450	9970	10,340	10,440	10,480
	Anholt & Becker [7]	13,800	11,600	10,800	10,600	10,540
B	Formula	14,133	27,375	36,623	44,638	69,629
	$1 - \sum_{bnd} e^-$	14,190	28,450	38,010	46,080	71,090
	$\sum_{cont} e^-$	12,920	27,110	36,530	44,430	68,780
	Anholt & Becker	13,000	27,800	37,400	45,400	70,000

TABLE II. Calculated values of the scaled quantity $(Z_2^2/Z_1^2)B$ for non-symmetric combinations of colliding particles. The second nucleus (Z_2) is taken to be the one with the single electron to be ionized. Since Anholt and Becker cross sections without screening are completely perturbative, their values of of B also can be taken from Table IV, and are repeated here for convenient comparison.

	H + Ne	H + Ca	Ca + H	H + Zr	H + Pb	Pb + H
Formula	44,716	36,890	69,462	28,226	16,487	66,539
$1 - \sum_{bnd} e^-$	46,150	38,270	70,820	29,440	17,090	67,550
$\sum_{cont} e^-$	44,490	36,790	68,520	28,070	15,680	65,330
Anholt & Becker [7]	45,400	37,400	70,000	27,800	13,000	70,000
	Pb +Ne	Ne + Pb	Pb + Ca	Ca + Pb	Pb + Zr	Zr + Pb
Formula	42,308	16,313	34,503	16,097	25,751	15,592
$1 - \sum_{bnd} e^-$	42,560	17,030	34,720	16,870	26,010	16,250
$\sum_{cont} e^-$	41,000	15,690	33,330	15,530	24,730	14,930
Anholt & Becker	45,400	13,000	37,400	13,000	27,800	13,000

TABLE III. Cross sections for the ionization of a 160 GeV/A one electron Pb projectile (Z_2) by various fixed nuclear targets (Z_1). Unlike in Table II, here the appropriate (Z_1^2/Z_2^2) factor has been included. Cross sections are given in kilobarns to match the format of the CERN SPS data.

Target	Z_1	Formula	SPS Data	Anholt & Becker (with screening)	Anholt & Becker (no screening)
Be	4	0.14	0.14	0.24	0.20
C	6	0.32	0.31	0.49	0.45
Al	13	1.5	1.3	2.0	2.1
Cu	29	7.4	6.9	9.0	10.5
Sn	50	22	15	25	31
Au	79	53	42	60	78