

\*Work supported in part by the U.S. Atomic Energy Commission.

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## Procedure for Computing Cross Sections for Single and Multiple Ionization of Atoms in the Binary-Encounter Approximation by the Impact of Heavy Charged Particles\*

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(Received 22 December 1972)

A procedure is developed for computing cross sections for the multiple ionization of atoms by the impact of protons or other fully stripped nuclei. The ionization probability, as a function of energy and impact parameter,  $P(E, b)$ , is computed at several beam energies in the binary-encounter approximation for a ground-state hydrogenic electron scattered by an incident proton. Scaling laws are given which may be used to extend these results to other projectiles, other targets, and other hydrogenlike filled atomic shells. It is shown that  $P(E, 0) = \langle \sigma(E, r) / 2\pi r^2 \rangle$  for isotropic, but otherwise arbitrary, electron-density distributions. A formulation for multiple-ionization cross sections is developed in terms of the single-electron probabilities  $P(E, b)$  for each atomic shell, assuming that both the electrons and the shells are mutually independent. Numerical calculations are compared to recent predictions in the semiclassical Coulomb approximation and to recent satellite and hypersatellite x-ray data. The discrepancies are generally within those resulting from uncertainties of 30–200% in the single-ionization cross sections, when the ionization probability is much less than one. Then, approximating  $P(Eb)$  vs  $b$  as a step function, the multiple-ionization cross sections are reduced to simple combinations of single-ionization cross sections. These single-ionization cross sections may be evaluated in the binary-encounter approximation by applying scaling laws to the usual universal curve that we tabulate. Multiple-ionization cross sections may thus be estimated without the aid of a computer.

### I. INTRODUCTION

In the past several years there has been a resurgence of interest in ionization phenomena, in part owing to advancing experimental technique and in part owing to applications in other fields. Considerable progress has been made in developing approximate calculations of cross sections for the single ionization of atoms by the impact of charged particles, even though exact calculations have not been done. The approximate calculations are

simple and may be applied to reasonably complex systems. Recently there have been observations of x-ray satellite<sup>1</sup> and hypersatellite<sup>2</sup> transitions corresponding to multiple ionization of atoms and molecules. Interpretations<sup>3</sup> and calculations<sup>4</sup> which have described the atomic data have quickly followed.

In this paper, simple formulas and tables are compiled which may be easily used to compute cross sections for the single ionization of atoms by the impact of charged particles in the binary-

encounter approximation.<sup>5-7</sup> These binary-encounter cross sections are then expressed in an impact-parameter formulation; and the probability for ionization  $P(E_i, b)$  is computed for several projectile energies  $E_i$ . This representation is extended to include multiple atomic ionization, i.e., arbitrary numbers of electrons may be removed from arbitrary atomic shells by the impact of a proton or other fully stripped ion. Full numerical calculations are compared to the recent predictions of Hansteen and Mosebekk<sup>4</sup> as well as to recent experimental data. Finally, the expressions for multiple-ionization cross sections are simplified so that estimates may be easily done.

#### A. Single-Ionization Theory

One of the earliest and most successful theories is the Coulomb-Born theory, first worked out by Bethe<sup>8</sup> in 1930. Simple Coulomb-Born calculations for arbitrary atomic systems may now be easily calculated with the tables of Merzbacher *et al.*,<sup>9</sup> using appropriate scaling laws. The dependence of the cross section on projectile velocity scales to the orbit velocity of the removed electron, and the projectile charge dependence of the cross section scales as  $z^2$ .

Other quantum-mechanical formulations of the ionization problem include the impulse approximation of Vainshtein, Presyakov, and Sobelman<sup>10</sup> and the high-energy Glauber approximation of McGuire, Hidalgo, Doolen, and Nuttall.<sup>11</sup> In all of these quantum-mechanical approximations, the projectile velocity is assumed to be somewhat greater than the velocity of the orbiting atomic electron that is removed.

#### B. Binary-Encounter Model

Some of the most successful, if not the best understood, calculations of atomic ionization have been those based on the binary-encounter model. The earliest binary-encounter calculation, represented in Fig. 1, was done by Gryzinski<sup>12</sup> who

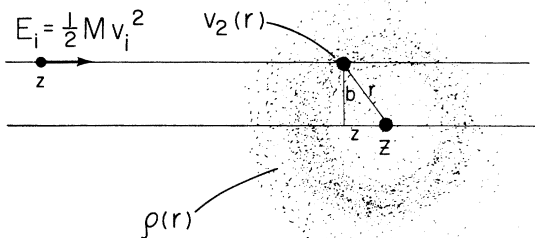


FIG. 1. Representation of the binary-encounter model. The incident projectile with velocity  $v_i$  scatters via a two-body Coulomb interaction from an electron with velocity  $v_2$ . The atomic electron is characterized by a density distribution  $\rho(v_2(r))$ .

used the model to compute atomic charge exchange and excitation, as well as ionization. These cross sections  $\sigma(E_i)$  were calculated from an approximate expression for the two-body Coulomb-scattering cross section  $\sigma(v_i, v_2, M, m) \cong \sigma(v_i, v_2)$  for particles of velocities  $\vec{v}_i$  and  $\vec{v}_2$ , isotropically averaged over the directions of the velocities. The cross section for the scattering of atomic electrons was found by integrating over a velocity distribution  $\rho(v_2, v_0)$  corresponding to the velocity of the atomic electron, namely,

$$\sigma(E_i) = N \int_0^\infty \sigma(v_i, v_2, M, m) \rho(v_2, v_0) 4\pi v_2^2 dv_2, \quad (1)$$

where  $N$  is the number of atomic electrons involved in the scattering, and  $\frac{1}{2} m v_0^2 = |U|$ , where  $U$  is the electron binding energy. The normalization of  $\rho(v_2, v_0)$  is given by

$$\int_0^\infty 4\pi v_2^2 \rho(v_2, v_0) dv_2 = 1. \quad (2)$$

In this calculation,  $\rho(v_2, v_0)$  does not change as the projectile passes through the atom (static approximation), and correlations between the atomic electrons are ignored.

The two-body Coulomb cross section was found approximately by integrating over the cross section per unit energy transfer, namely,

$$\sigma(v_i, v_2) = \int_{E_{\min}}^{E_{\max}} \frac{d\sigma(v_i, v_2, \Delta E)}{d\Delta E} d\Delta E. \quad (3)$$

The ionization, charge-exchange, and excitation cross sections differ only in the range of energy transfers over which one integrates. In the case of ionization, for example,  $E_{\min} = U$ , where  $U$  is the binding energy, and  $E_{\max} = E_i$ , the projectile energy.

Using isotropic-hydrogenic density distributions for closed shells, corresponding to

$$\rho(v_2, v_0) = \frac{8}{\pi^2} \frac{v_0^5}{(v_0^2 + v_2^2)^4}, \quad (4)$$

where  $\frac{1}{2} m v_0^2 = -U$ , Gryzinski<sup>12</sup> was able to compute the ionization cross section in a closed form, namely,

$$\sigma(E_i) = (Nz^2\sigma_0/U^2)G(V), \quad (5)$$

where  $N=2$  for the  $K$  shell,  $z$  is the projectile charge, and  $\sigma_0 = \pi e^4 = 6.56 \times 10^{-14} \text{ cm}^2 \text{ eV}^2$ . The term  $G(V)$  is a function of the scaled velocity  $V = v_i/v_0$ , which we give in Table I. For  $V > 0.206$ ,  $G(V)$  has been expressed algebraically<sup>12</sup> as

$$\begin{aligned} G(V) = & [V^2/(1+V^2)]^{3/2} V^{-2} \\ & \times [(V^2/1+V^2) + \frac{2}{3}(1+1/\alpha)\ln(2.7+V)] \\ & \times [1-1/\alpha][1-(1/\alpha)^{1+V^2}], \end{aligned} \quad (6a)$$

TABLE I.  $G(V)$  vs  $V$ . In the classical binary-encounter approximation, the ionization cross section may be found according to  $\sigma(V) = Nz^2\sigma_0 G(V)/U^2$ , where  $\sigma_0 = 6.56 \times 10^{-14} \text{ cm}^2 \text{ eV}^2$ ,  $U$  is the binding energy,  $z$  is the projectile charge, and  $N$  is the number of electrons in the shell from which the electron is removed. The scaled velocity  $V$  is equal to  $v_i/v_0$ , where  $v_i$  is the projectile velocity and  $v_0$  the velocity of the orbiting atomic electron. In principle, the Gerjuoy-Vriens-Garcia  $G(V)$  is more exact than Gryzinski's  $G(V)$ . Corrections for Coulomb deflection have not been included.

| Scaled velocity $V$ | Gerjuoy Vriens Garcia $G(V)$ | Gryzinski $G(V)$ |
|---------------------|------------------------------|------------------|
| 0.100               | 0.000 024 9                  | 0.000 026 6      |
| 0.120               | 0.000 099 7                  | 0.000 055 2      |
| 0.140               | 0.000 282                    | 0.000 102        |
| 0.160               | 0.000 694                    | 0.000 174        |
| 0.180               | 0.001 46                     | 0.000 279        |
| 0.200               | 0.002 89                     | 0.000 426        |
| 0.220               | 0.004 80                     | 0.001 43         |
| 0.240               | 0.008 36                     | 0.008 18         |
| 0.260               | 0.0133                       | 0.0187           |
| 0.280               | 0.0192                       | 0.0318           |
| 0.300               | 0.0273                       | 0.0466           |
| 0.320               | 0.0385                       | 0.0627           |
| 0.340               | 0.0519                       | 0.0795           |
| 0.360               | 0.0668                       | 0.0968           |
| 0.380               | 0.0842                       | 0.114            |
| 0.400               | 0.104                        | 0.132            |
| 0.420               | 0.127                        | 0.150            |
| 0.440               | 0.152                        | 0.167            |
| 0.460               | 0.178                        | 0.185            |
| 0.480               | 0.206                        | 0.202            |
| 0.500               | 0.235                        | 0.219            |
| 0.520               | 0.266                        | 0.236            |
| 0.540               | 0.297                        | 0.252            |
| 0.560               | 0.328                        | 0.268            |
| 0.580               | 0.358                        | 0.283            |
| 0.600               | 0.388                        | 0.297            |
| 0.620               | 0.418                        | 0.311            |
| 0.640               | 0.446                        | 0.325            |
| 0.660               | 0.474                        | 0.337            |
| 0.680               | 0.500                        | 0.349            |
| 0.700               | 0.524                        | 0.360            |
| 0.720               | 0.547                        | 0.371            |
| 0.740               | 0.568                        | 0.381            |
| 0.760               | 0.588                        | 0.390            |
| 0.780               | 0.606                        | 0.399            |
| 0.800               | 0.622                        | 0.406            |
| 0.820               | 0.636                        | 0.414            |
| 0.840               | 0.649                        | 0.420            |
| 0.860               | 0.660                        | 0.426            |
| 0.880               | 0.669                        | 0.431            |
| 0.900               | 0.677                        | 0.436            |
| 0.920               | 0.683                        | 0.440            |
| 0.940               | 0.688                        | 0.443            |
| 0.960               | 0.692                        | 0.446            |
| 0.980               | 0.694                        | 0.449            |

Table I(Continued)

| Scaled velocity $V$ | Gerjuoy Vriens Garcia $G(V)$ | Gryzinski $G(V)$ |
|---------------------|------------------------------|------------------|
| 1.000               | 0.696                        | 0.451            |
| 1.100               | 0.687                        | 0.454            |
| 1.200               | 0.662                        | 0.449            |
| 1.300               | 0.626                        | 0.439            |
| 1.400               | 0.585                        | 0.425            |
| 1.500               | 0.543                        | 0.409            |
| 1.600               | 0.502                        | 0.391            |
| 1.700               | 0.462                        | 0.373            |
| 1.800               | 0.426                        | 0.355            |
| 1.900               | 0.393                        | 0.338            |
| 2.000               | 0.362                        | 0.321            |
| 2.100               | 0.334                        | 0.305            |
| 2.200               | 0.309                        | 0.289            |
| 2.300               | 0.286                        | 0.274            |
| 2.400               | 0.266                        | 0.260            |
| 2.500               | 0.247                        | 0.247            |
| 2.600               | 0.230                        | 0.235            |
| 2.700               | 0.215                        | 0.224            |
| 2.800               | 0.201                        | 0.213            |
| 2.900               | 0.188                        | 0.203            |
| 3.000               | 0.177                        | 0.193            |
| 3.500               | 0.132                        | 0.154            |
| 4.000               | 0.102                        | 0.125            |
| 4.500               | 0.0810                       | 0.103            |
| 5.000               | 0.0658                       | 0.0872           |
| 6.000               | 0.0459                       | 0.0642           |
| 7.000               | 0.0338                       | 0.0493           |
| 8.000               | 0.0259                       | 0.0391           |
| 9.000               | 0.0205                       | 0.0318           |
| 10.000              | 0.0166                       | 0.0264           |
| 15.000              | 0.007 40                     | 0.0128           |
| 20.000              | 0.004 16                     | 0.007 66         |
| 25.000              | 0.002 66                     | 0.005 12         |
| 30.000              | 0.001 85                     | 0.003 68         |

where

$$\alpha = 4V^2(1 + 1/V). \quad (6b)$$

For  $V < 0.206$ ,  $G(V)$  is approximately given by

$$G(V) = \frac{4}{15}V^4. \quad (6c)$$

In 1964 Stabler<sup>13</sup> found an exact expression for  $\sigma(v_1, v_2)$  for particles of equal mass. In 1966 both Gerjuoy<sup>5</sup> and Vriens<sup>6</sup> independently derived exact expressions for arbitrary masses  $M$  and  $m$ . The classical two-body cross sections obtained depended on  $M/m$ , i.e.,  $\sigma(v_1, v_2) \rightarrow \sigma(v_1, v_2, M/m)$ . A number of calculations, notably those of Garcia,<sup>7</sup> followed, and it was found that for  $M \gg m$ , the ionization cross section could be cast into the form of Eq. (5), with  $G(V)$  given by Vriens<sup>6</sup> for  $V > \frac{1}{2}$  as

$$\begin{aligned}
G(V) = \frac{1}{4V^2} \left\{ \frac{35}{6} + \frac{35}{3\pi} \tan^{-1}c + \frac{128}{9\pi} (V^3b^3 - b^{3/2}) + \frac{cb}{3\pi} \left( 35 - \frac{58}{3}b - \frac{8}{3}b^2 \right) \right. \\
+ \frac{2}{3\pi} Vab \left[ (5 - 4V^2) \left( 3a^2 + \frac{3}{2}ab + b^2 \right) - cV \left( \frac{15}{2} + 9a + 5b \right) \right] \\
\left. - \frac{16}{\pi} Va^4 \ln(4V^2 + 1) - V^2a \left( 1 + \frac{2}{\pi} \tan^{-1}c \right) \left( \frac{5}{2} + 3a + 4a^2 + 8a^3 \right) \right\}, \quad (7a)
\end{aligned}$$

where

$$c = V - \frac{1}{4}V, \quad b = (1 + c^2)^{-1}, \quad a = (1 + V^2)^{-1}. \quad (7b)$$

We present the Gerjuoy-Vriens-Garcia  $G(V)$  over a large range of  $V$  in Table I.

Since the quantity  $U^2\sigma(E_i)/Nz^2$  does not vary with target or projectile, this quantity is referred to as a "universal curve." The agreement with experiments for the  $K$ -shell ionization of atomic electrons by the impact of protons is generally within a factor of 2, and the energy dependence  $E_i$  reflects the data very well.

The ionization cross section maximizes as the velocity of the projectile approaches the velocity of the atomic electron, i.e., near  $V=1$ . Since the

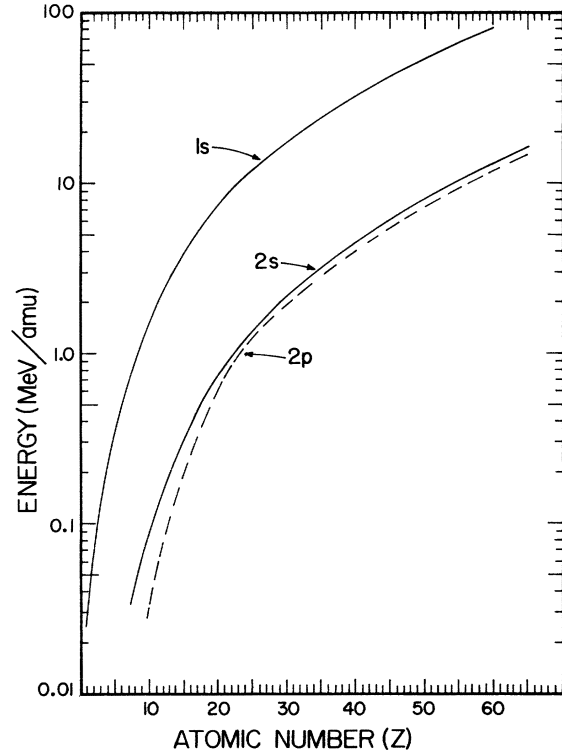


FIG. 2. Energy for maximum ionization for various targets. Both the cross section and probability for ionization peak when the velocity of the projectile and velocity of the atomic electron are nearly the same. The projectile energy required for maximum ionization is plotted for both  $K$ - and  $L$ -shell electrons for atoms from  $Z=10$  to  $Z=60$ .

orbit velocity varies from atom to atom, the beam energy required for maximum ionization varies with the atomic nuclear charge  $Z$ , as is shown for  $K$  and  $L$  shells in Fig. 2.

Thomas and Garcia<sup>14</sup> have derived a correction to  $\sigma(E_i)$  corresponding to the Coulomb deflection of the projectile by the atomic nucleus. The correction is less than 1% for  $U/E_i \leq 10^{-3}$  and  $V \geq 0.5$ . Experimental deviations from the  $z^2$  projectile dependence predicted by the Born and binary-encounter approximations have been observed,<sup>15,16</sup> and a number of explanations<sup>16,17</sup> have been proposed.

## II. IMPACT-PARAMETER FORMULATION

It is common to consider the scattering of particles as a function of impact parameter  $b$  and to express the total cross section as an integral over impact parameters, namely,

$$\sigma(E_i) = N \int_0^R 2\pi b P(E_i, b) db. \quad (8)$$

Here  $P(E_i, b)$  is the scattering probability per electron in a given shell,  $N$  is the number of participating electrons, and  $R$  is the distance at which  $P(E_i, b)$  goes to zero.

In order to express  $\sigma(E_i)$  in the form of Eq. (8), we begin with the expression defined by the binary-encounter approximation, namely,

$$\begin{aligned}
\sigma(E_i) = N \int d\Delta E \int d^3v_2 \rho(\vec{v}_2) \\
\times \frac{d\sigma}{d\Delta E} \left( v_i, \vec{v}_2, \frac{M}{m}, \Delta E \right), \quad (9)
\end{aligned}$$

where  $(d\sigma/d\Delta E)(v_i, \vec{v}_2, M/m, \Delta E)$  corresponds to the two-body Coulomb cross section per unit energy transfer effectively<sup>5</sup> averaged over the direction of  $\vec{v}_i$ . We now assume a relationship between the velocity  $\vec{v}_2$  and position  $\vec{r}$  of the atomic electron. Classically, this is easily done using conservation of energy, namely,

$$\frac{1}{2} m v_2^2 - Ze^2/r = U = -\frac{1}{2} m v_0^2. \quad (10)$$

Solving for  $v_2(r)$  we have,

$$v_2(r)/v_0 = [(2a/r) - 1]^{1/2}, \quad (11)$$

where  $a$  is the orbital radius of the atomic electron. For a  $K$ -shell electron in hydrogen  $a = a_0 = 0.529 \times 10^{-8}$  cm is the Bohr radius.

We assume that the ionization cross section is strongly peaked when the projectile and target are close together,<sup>18</sup> so that  $\vec{r}$  corresponds to both the position of the electron and projectile in the following development. Further assuming that  $\rho(\vec{v}_2(\vec{r}))$  is isotropic in  $\vec{v}_2$  at each  $\vec{r}$ , we write Eq. (9) as

$$\sigma(E_i) = N \int d\Delta E \int dr 4\pi r^2 \rho(r) \times \int \frac{d\sigma}{d\Delta E}(v_i, v_2(r), M/m, \Delta E, \hat{v}_2) d\hat{v}_2, \quad (12)$$

and consider a projectile with a well-defined impact parameter incident on an isotropic electron cloud, as depicted in Fig. 1. At any given point in an isotropic electron cloud the result of integrating over  $\hat{v}_2$  does not depend<sup>5</sup> on the direction of the projectile velocity  $\hat{v}_i$  but only on the magnitude of  $\vec{v}_i$  and  $\vec{v}_2$ . Assuming  $v_i$  is constant, the only variation of the integration over  $\hat{v}_2$  is the  $v_2$  dependence, established by Gerjuoy.<sup>5</sup> Since  $v_2$  depends only on  $r$  (and not  $\hat{r}$ ), we may use Gerjuoy's results for  $d\sigma/d\Delta E(v_i, v_2(r), \Delta E)$  and write,

$$\sigma(E_i) = N \int dr \left( 4\pi r^2 \rho(r) \int d(\Delta E) \frac{d\sigma}{d\Delta E} \times (v_i, v_2(r), M/m, \Delta E) \right). \quad (13)$$

The term in large parentheses is an isotropic function of  $r$ . Consequently, we write

$$\sigma(E_i) = N \int d^3r \rho(r) \sigma(v_i, v_2(r), M/m) = \int_0^R db 2\pi b \int_{-(R^2-b^2)^{1/2}}^{+(R^2-b^2)^{1/2}} dz \rho([b^2+z^2]^{1/2}) \times \sigma(v_i, v_2([b^2+z^2]^{1/2}), M/m), \quad (14)$$

where the integrand is zero for  $r > R$ . We now identify

$$P(E_i, b) = 2 \int_0^{(R^2-b^2)^{1/2}} \rho([b^2+z^2]^{1/2}) \times \sigma(v_i, v_2([b^2+z^2]^{1/2}), M/m) dz \quad (15)$$

as the scattering probability. It immediately follows that the probability at zero-impact parameter is given by

$$P(E_i, 0) = \langle \sigma(v_i, v_2(r), M/m) \rangle / 2\pi r^2. \quad (16)$$

Our expression for  $P(E_i, 0)$  has a simple physical interpretation, namely, that  $P(E_i, b)$  corresponds to the average value of the cross-sectional area for ionization divided by twice the projected area of the target electron. For  $b \neq 0$ ,  $P(E_i, b)$  is proportional to the density of the electron cloud seen by the projectile weighted by the ionization cross

section appropriate to  $v_2(r)$ . The total cross section  $\sigma(E_i)$  is, of course, identical to that computed from Eq. (1). Furthermore, the shape of  $P(E_i, b)$  as a function of  $b$  is in agreement with results based on the semiclassical approximation.<sup>19</sup>

It is important to note that our expression for  $P(E_i, b)$  is not unique, since neither  $\vec{v}_2(\vec{r})$  nor  $\rho(r)$  is uniquely defined, for example. For a given atomic target one could choose  $\rho(r) = |\Psi(r)|^2$  or  $\rho(v_2(r)) = |\Psi(v_2)|^2$ . Fortunately, for hydrogenic density distributions, both density distributions lead to  $P(E_i, b)$  that are identical at  $b = 0$ , and similar elsewhere.

#### A. Results for Hydrogenic Density Distributions

The density distribution corresponding to identical electrons in a filled hydrogenic shell follows from Eq. (4) and (10), namely,

$$\rho(v_2(r)) = [(2a/r) - 1]^{1/2} / 2\pi a^3, \quad r \leq 2a, \\ = 0, \quad r \geq 2a. \quad (17)$$

The scattering probability may now be expressed, using Eq. (10), as,

$$P(E_i, b) = \int_0^{(4a^2-b^2)^{1/2}} \frac{v_2(r)}{v_0} \times \frac{\sigma(v_i, v_2(r), M/m)}{\pi a^2} \frac{dz}{a}, \quad (18)$$

where  $r = (b^2 + z^2)^{1/2}$ ,  $v_2(r)$  is given by Eq. (11),  $v_0$  is the rms velocity and  $a$  the scaled Bohr radius of the atomic electron. For  $M/m > 10^3$  and  $E_i/U \geq 76$ ,  $P(E_i, b)$  is essentially independent of  $M$ , i.e.,  $P(E_i, b) = P(V, b)$ , where  $V = v_i/v_0$  is the scaled velocity. For example, at  $E_i/U \cong 10^3$  and  $M = 1840m$ , increasing  $M$  by a factor of 4 changes  $P(E_i, b)$  by less than 1%.

There are several useful scaling laws for filled shell hydrogenic distributions which we now consider:

(i) Projectile scaling

$$P_z(V, b) = z^2 P_{z=1}(V, b). \quad (19)$$

Since  $P(V, b)$  does not depend on the mass of the projectile, only the  $z^2$  charge dependence contributes at fixed  $V$ .

(ii) Target scaling

$$P_z(V, b) = Z^{-2} P_{Z=1}(V, b). \quad (20)$$

Here  $Z$  is the effective nuclear charge seen by the projectile at the point of impact with the atomic electron. Note that  $V = v_i/v_0$  changes with  $Z$  due to the change in the target binding energy. Therefore for fixed  $V$  different projectile velocities are required. In practice, one first computes  $V$  corresponding to the target of interest, one then computes  $P_{Z=1}(V, b)$  (or uses Fig. 3), and one then

scales by multiplying  $P_{Z^{-1}}(V, b)$  by  $Z^{-2}$ . An example is worked out in Sec. III.

(iii) Level scaling

$$P_n(V, b/a_n) = P_{n-1}(V, b/a_1). \quad (21)$$

Here  $a_n$  is the radius of the  $n$ th atomic level.

These scaling laws may be quickly confirmed by using either the Gerjuoy<sup>6</sup> or Vriens<sup>7</sup> expression for  $\sigma(v_1, v_2, M/m)$ , along with the scaling rules,  $a \rightarrow n^2 a/Z$ ,  $v_0 \rightarrow v_0 Z/n$  for hydrogenic electrons.

The results of calculations of  $P(V, b)$  for protons on hydrogen are shown in Fig. 3. As a function of  $b$ ,  $P(V, b)$  is flat near the origin and is monotonically decreasing. Near  $V=1$ , the probability  $P(V, 0)$  is greater than 1, suggesting that this calculation overestimates  $P(V, b)$ . The proton-hydrogen ionization cross section obtained from the binary-encounter calculation itself is a factor of 1.85 times greater than the experiment at  $V=1$ . This overestimate is, in part, due to the fact that the influence of the projectile on the binding energy of the electron has been ignored. If the increase in this binding energy were included, the probability would decrease. This effect is overestimated by assuming that the projectile is united with the atomic nucleus when ionization occurs, so that

$$U \rightarrow U(1+z/Z)^2. \quad (22)$$

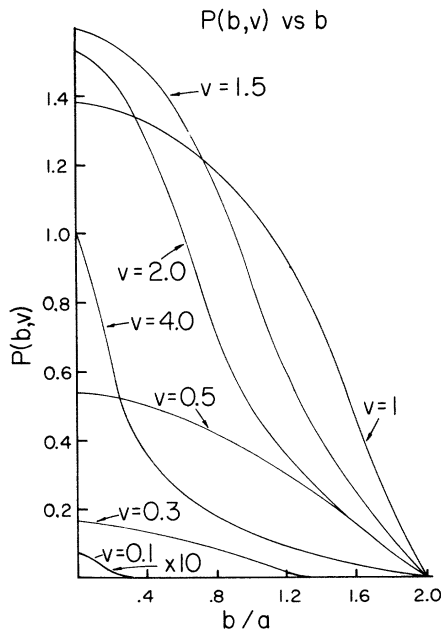


FIG. 3. Ionization probability  $P(V, b)$  vs  $b$  at various scaled velocities  $V$ . The scaled velocity  $V$  is equal to  $v_i/v_0$ , where  $v_i$  is the velocity of the incident projectile, and  $v_0$  is the orbit velocity of the atomic electron. The impact parameter  $b$  is measured in units of the radius  $a$  of the orbiting electrons.

In proton-hydrogen ionization at  $v=1.0$ ,  $P(V, b)$  is reduced by a factor of 4. Only when  $z/Z \ll 1$  does this effect become negligible. It is also interesting to note, from Fig. 3, that  $P(V, 0)$  peaks at  $V \approx 1.5$  whereas the cross section itself peaks near  $V=1.0$ .

### III. MULTIPLE IONIZATION

As early as 1927 calculations of double-ionization<sup>20</sup> cross sections by charged-particle impact were being done<sup>21</sup> in the Born approximation, and compared to experiment.<sup>22</sup> Little additional work was done until the 60's when Mittleman<sup>23</sup> performed calculations with an impulse approximation, and Russek<sup>24</sup> introduced a statistical model. In 1965 Gryzinski<sup>13</sup> first computed double-ionization cross sections from probabilities estimated using the binary-encounter model.

Recently a number of authors<sup>3,4</sup> have independently proposed the use of a binomial distribution of probabilities for the multiple ionization of one  $K$ - and  $nL$ -shell electrons in a single-target atom ( $n=0, 1, 2, 3, 4, 5, 6, 7$ , or 8). Experimentally one finds that under high resolution the  $K\alpha$  x-ray line splits into a number of satellite lines,<sup>1</sup> corresponding to

$$\sigma_K = \sum_n \sigma_{1K, nL}. \quad (23)$$

Since the energies of the satellite x rays observed correspond to levels of atoms with  $n$  electrons missing in the  $L$  shell (in addition to a single  $K$ -shell vacancy),  $\sigma_{1K, nL}$  is taken to be the cross section for removing one  $K$ - and  $n$   $L$ -shell electrons. In terms of probabilities  $P_K$  and  $P_L$  for  $K$ - and  $L$ -shell ionization,<sup>25</sup> we may express this idea by writing

$$\begin{aligned} P_K &= P_K [P_L + (1 - P_L)]^8 \\ &= P_K \sum_{n=0}^8 \binom{8}{n} P_L^n (1 - P_L)^{8-n}, \end{aligned}$$

where  $\binom{8}{n}$  is the binomial coefficient. It is assumed that  $P_K^2 \ll P_K \ll 1$ . It is now evident that

$$\begin{aligned} \sigma_{1K, nL}(E_i) &= 2 \int_0^\infty 2\pi b P_K(E_i, b) \binom{8}{n} P_L^n(E_i, b) \\ &\quad \times [(1 - P_L(E_i, b))]^{8-n} db \quad (24) \end{aligned}$$

corresponds to the cross section for removing one  $K$ - and  $n$   $L$ -shell electrons. Since interference terms are ignored, the calculation is classical.

#### A. Full Results

Calculations of cross sections for multiple  $K, L$  ionization in copper produced by the impact of a proton are presented in Fig. 4. Below 5 MeV our

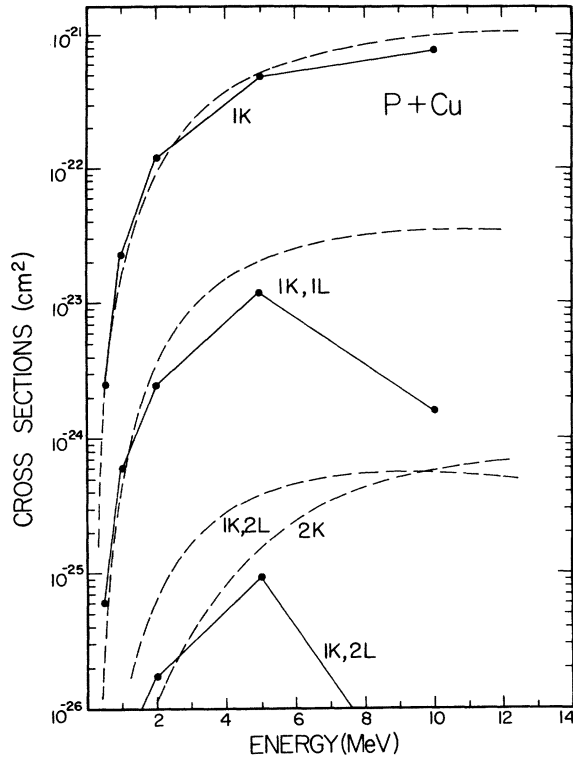


FIG. 4. Theoretical Coulomb ionization cross sections vs energy for  $p + \text{Cu}$ . Dashed curves represent classical binary-encounter calculations for removing  $n$   $K$ -shell and  $m$   $L$ -shell electrons. The points computed by Hansteen and Mosebekk in a SCA approximation are joined by straight lines. For  $p + \text{Cu}$ ,  $\sigma_{1K} \equiv \sum \sigma_{1K,nL} \approx \sigma_{1K,0L}$ .

results are in reasonable agreement with those of Hansteen and Mosebekk,<sup>4</sup> although it is apparent (e.g., at 5 MeV) that a difference in  $P_L$  can produce an avalanche of difference in going to successively higher states of  $L$ -shell ionization. The striking discrepancy at 10 MeV is primarily due to the difference in total  $L$ -shell ionization cross sections predicted by the two theories ( $1.3 \times 10^{-19}$

TABLE II. Double to single ionization cross-section ratios for 0.8-MeV protons on atoms near  $Z = 20$ . The experimental (Ref. 27) values include statistical fluorescence-yield corrections for each state of atomic ionization (0.8 MeV  $p + \text{atom}$ ).

| Target atom | $\sigma_{1K,1L}/\sigma_{1K,0L}$ |        |
|-------------|---------------------------------|--------|
|             | Expt.                           | Theory |
| Ca          | 0.095                           | 0.097  |
| Sc          | 0.087                           | 0.083  |
| Ti          | 0.076                           | 0.071  |
| V           | 0.044                           | 0.058  |
| Cr          | 0.032                           | 0.048  |
| Mn          | 0.022                           | 0.043  |

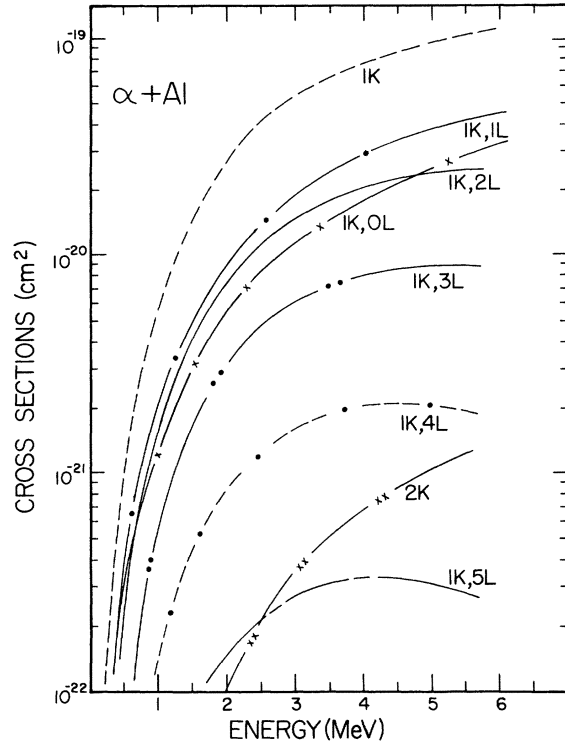


FIG. 5. Coulomb ionization cross sections vs energy for  $\alpha + \text{Al}$  computed in the classical binary-encounter approximation.

$\text{cm}^2$  vs  $0.25 \times 10^{-19} \text{ cm}^2$ ). Data for  $L_{III}$  ionization of Cu by protons from 0.4 to 1.8 MeV tend to support<sup>9</sup> the higher values calculated by the binary-encounter model.

Next we compare with experiment. In Table II we present the ratio of  $\sigma_{1K,1L}/\sigma_{1K,0L}$  for 0.8-MeV protons<sup>26</sup> incident on targets from  $Z = 20$  to  $Z = 25$ . Predictions for the multiple ionization of aluminum by  $\alpha$  particle impact over a wide energy range are presented in Fig. 5. In Table III, these results

TABLE III. Multiple-ionization cross-section ratios for  $\alpha$  particles on aluminum at several energies. The experimental (Ref. 28) values include statistical fluorescence-yield corrections for each state of atomic ionization ( $\alpha + \text{Al}$ ).

| Energy (MeV) | $\frac{\sigma_{1K,1L}}{\sigma_{1K,0L}}$ |        | $\frac{\sigma_{1K,2L}}{\sigma_{1K,1L}}$ |        | $\frac{\sigma_{1K,3L}}{\sigma_{1K,2L}}$ |        |
|--------------|---|--------|---|--------|---|--------|
|              | Expt.                                   | Theory | Expt.                                   | Theory | Expt.                                   | Theory |
| 3.0          | 1.15                                    | 1.70   | 0.28                                    | 0.74   | 0.14                                    | 0.42   |
| 2.4          | 1.50                                    | 1.72   | 0.35                                    | 0.75   | 0.12                                    | 0.43   |
| 2.0          | 1.65                                    | 1.75   | 0.41                                    | 0.76   | 0.13                                    | 0.44   |
| 1.6          | 1.91                                    | 1.73   | 0.51                                    | 0.76   | 0.18                                    | 0.43   |
| 1.0          | 2.25                                    | 1.57   | 0.57                                    | 0.68   | 0.15                                    | 0.39   |
| 0.8          | 2.09                                    | 1.42   | 0.53                                    | 0.62   | 0.19                                    | 0.35   |
| 0.5          | 1.39                                    | 1.08   | 0.40                                    | 0.47   | 0.11                                    | 0.27   |

are compared to data<sup>27</sup> recently taken at several energies about 1 MeV. The relative intensities given will be in better agreement than absolute cross sections since the theoretical error in  $P_L$  is cumulative. From Tables II and III we see that our average value of  $P_L$  is typically within a factor of 2 above experiment. This is comparable to the accuracy typically found is comparing total experimental and theoretical  $K$ - and  $L$ -shell cross sections. Our error may in part be due to ignoring the influence of the projectile on the binding energies of the atomic electrons, and in part due to the influence of  $L$ -shell vacancies on the binding energies (both effects tend to raise the effective nuclear charge and lower  $P_L$ ).

A number of hypersatellite transitions (double  $K$ -shell vacancy) have also been observed<sup>2</sup> in atoms near  $Z=20$  under the impact of 30 -MeV oxygen ions. Arbitrarily choosing the effective charge (+6) of 30 -MeV oxygen ions rather than the nuclear charge (+8), we computed the cross sections for the hypersatellite transitions, as well as the satellite transitions, in calcium. The relative intensities are compared to experiment in Table IV. The poor agreement in the intensity distributions is due to the fact that the intensity ratio goes as  $\bar{P}_L/(1 - \bar{P}_L)$ ,  $\bar{P}_L$  (the average value of  $P_L$ ) is near unity, and  $\bar{P}_L$  is a factor of 2 too large.

In theory the relative intensity distribution of the hypersatellite peaks closely resembles the distribution of the satellite peaks. This similarity, which is independent of the normalization of  $P_L$  or  $P_K$ , has been evident for all targets and all projectiles at all energies which we have considered in this paper. The absence of this similarity in the data may be due to experimental background and possible misidentification of the hypersatellite peaks.

## B. Approximate Results

### 1. Gryzinski and Kessel Models

Gryzinski<sup>13</sup> has computed the average ionization probability per electron in a very simple way by dividing the ionization cross section per electron by  $4\pi\bar{r}^2$ , where  $\bar{r}$  is the mean distance between electrons, i.e.,

$$P(E_i) \cong \sigma(E_i)/4\pi\bar{r}^2 N. \quad (25)$$

In other words, the probability for ionizing a single  $L$ -shell electron is simply equal to the area of the  $L$ -shell ionization cross section divided by the surface area of the total sphere at distance  $\bar{r}$  from the previous collision, illustrated in Fig. 6. Since the projectile crosses the sphere twice, the total probability is twice the value given by Eq. (25).

TABLE IV. Multiple-ionization cross-section ratios for 30-MeV oxygen on calcium. Some of the experimental values (Ref. 2) include statistical fluorescence-yield corrections for each state of atomic ionization (30 MeV O + Ca).

|   | $\frac{\sigma_{nK,1L}}{\sigma_{nK,0L}}$ | $\frac{\sigma_{nK,2L}}{\sigma_{nK,1L}}$ | $\frac{\sigma_{nK,3L}}{\sigma_{nK,2L}}$ | $\frac{\sigma_{nK,4L}}{\sigma_{nK,3L}}$ | $\frac{\sigma_{nK,5L}}{\sigma_{nK,4L}}$ | $\bar{P}_L$ |
|---|---|---|---|---|---|-------------|
| Satellite ( $n=1$ )                           |   |   |   |   |   |             |
| Experiment                                    | 3.10                                    | 1.52                                    | 0.82                                    | 0.41                                    | 0.58                                    | 0.28        |
| Theory  | 7.23                                    | 3.17                                    | 1.81                                    | 1.13                                    | 0.72                                    | 0.47        |
| Hypersatellite ( $n=2$ )                      |   |   |   |   |   |             |
| Experiment                                    | ...                                     | ...                                     | ...                                     | 2.5                                     | 1.2                                     | ...         |
| Theory  | 7.29                                    | 3.19                                    | 1.82                                    | 1.14                                    | 0.73                                    | 0.47        |
|   | Experiment                              |   |   | Theory                                  |   |             |
| $\frac{2K, \text{ total}}{1K, \text{ total}}$ | $\leq 0.007$                            |   |   | 0.022                                   |   |             |

Unfortunately, this approach does not work very well when used to compute  $P(E_i, b)$ . Gryzinski's assumption is that  $\sigma(v_i, v_2, M/m)$  is more or less independent of  $v_2$ , and therefore from Eqs. (1) and (2) is equal to  $\sigma(E_i)/N$ . In order to test this assumption, we computed  $P(E_i, b)$  from Eq. (18) using this assumption and compared it to the more exact result where  $\sigma(v_i, v_2, M/m)$  varies with  $v_2$ . The results are shown in Fig. 7. The shapes are quite different, especially near  $b=0$ . Furthermore, the Gryzinski result is a factor of 2 too large at  $b=0$ .

A more reasonable approximation is that credited to Kessel,<sup>28</sup> where  $P(E_i, b)$  is represented by a step function, namely,

$$P(E_i, b) \cong P_0(E_i), \quad b < R, \\ = 0 \quad b > R. \quad (27)$$

For the ionization of  $1K, nL$  atomic electrons, this seems quite reasonable since  $P(E_i, b)$  is quite flat near  $b=0$ . In the region near  $b=0$ , where  $P_K(E_i, b)$  is nonzero,  $P_L(E_i, b)$  is flat, so that only the value of  $P_L(E_i, b)$  near  $b=0$  is important. Using the Kessel model in Eq. (8), we have,

$$P_0(E_i) = \frac{\sigma(E_i)/N}{\pi R^2}. \quad (28)$$

It is interesting to note from Fig. 3 that near  $V=1$  it is quite reasonable to take  $R \cong (\sqrt{2})a$ . Con-

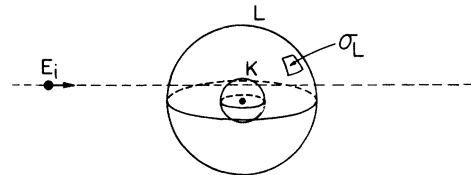


FIG. 6. Gryzinski's probability estimate. The probability for ionization is equal to the ionization cross section divided by the total area of the sphere. Since the projectile crosses the sphere twice, this estimate should be doubled.



sequently, the Kessel model gives the same average value of  $P_0(E_i)$  as Gryzinski, using  $\bar{r}$  equal to  $a$ . As the projectile velocity goes further from the orbit velocity of the atomic electron (i.e., as  $V$  goes further from unity), the value of  $R$  decreases.

## 2. Multiple-Ionization Recipes

In this section we give a procedure for computing cross sections for the multiple ionization of atoms by the impact of fully stripped ions. This procedure may be applied without the use of a computer using the graphs and tables contained herein.

We begin by assuming that each electron shell of the atom is independent, and by expanding the total probability for all processes, namely,

$$\begin{aligned} 1 &= [P_K + (1 - P_K)]^{n_K} [P_L + (1 - P_L)]^{n_L} \\ &\quad \times [P_M + (1 - P_M)]^{n_M} \dots [P_J + (1 - P_J)]^{n_J}, \\ &= \prod [P_I + (1 - P_I)]^{n_I}. \end{aligned} \quad (29)$$

Here  $P_I$  is the probability per electron for ionization in the  $I$ th shell and  $n_I$  are the number of electrons in the  $I$ th shell. Expanding in binomial coefficients,  $\binom{n_I}{n_K}$ , we identify

$$\begin{aligned} \sigma_{n_K, n_L, n_M, \dots, n_J} &= \int db \, 2\pi b \binom{n_K}{n_K} P_K^{n_K} (1 - P_K)^{n_K - n_K} \\ &\quad \times \binom{n_L}{n_L} P_L^{n_L} (1 - P_L)^{n_L - n_L} \\ &\quad \times \binom{n_M}{n_M} P_M^{n_M} (1 - P_M)^{n_M - n_M} \\ &\quad \times \dots \binom{n_J}{n_J} P_J^{n_J} (1 - P_J)^{n_J - n_J} \end{aligned} \quad (30)$$

as the cross section for removing  $n_K$   $K$ -shell electrons,  $n_L$   $L$ -shell electrons,  $n_M$   $M$ -shell electrons,  $\dots$ , and  $n_J$   $J$ -shell electrons.

The probabilities  $P_I(E_i, b)$  may now be computed in either the semiclassical approximation,<sup>4</sup> or in the binary-encounter model<sup>5</sup> using Eq. (15). If the isotropic hydrogenic density distribution for a closed-electron shell is used, then  $P(E_i, b)$  may be computed from Eq. (16) for one case and the scaling laws [Eqs. (14-21)] may be used to generate the other cases. The influence of the projectile charge may be overestimated using Eq. (22) to increase the binding energy of the atomic electrons.

The simplest estimate of the multiple ionization probabilities is found by taking

$$\begin{aligned} P(E_i, b) &\cong \frac{\sigma(E_i)/N}{\pi R^2}, \quad b \leq R \\ &= 0, \quad b > R. \end{aligned} \quad (31)$$

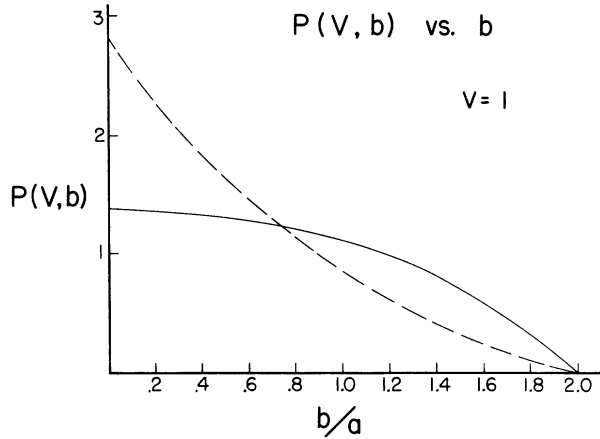


FIG. 7.  $P(V, b)$  vs  $b$ . The dashed curve corresponds to Gryzinski's estimate where the two-body Coulomb cross section  $\sigma(v_i, v_j)$  is approximated by the average ionization cross section  $\sigma(v_i)$ . The solid curve represents a more exact calculation, where  $\sigma(v_i, v_j)$  is integrated with a hydrogenic density distribution  $\rho(v_j)$ . In both cases the total cross section is the same.

Here  $R \leq (\sqrt{2})a$ , where  $a$  is the orbital radius of the electron; the equality sign holds when the projectile velocity is close to the orbit velocity of the atomic electron being ionized, i.e., the scaled velocity,  $V = v_{inc}/v_{orb}$  is near unity. For  $V$  not near unity,  $R$  may be estimated from Fig. 3.

The cross section  $\sigma(E_i)/N$  may be easily evaluated from Eq. (5). The  $G(V)$  functions for both Gryzinski, and Gerjuoy, Vriens, and Garcia are given in the table. The Gerjuoy, Vriens, Garcia results are the more rigorous, although Gryzinski's results are often closer to experimental data.

The approximation used in Eq. (31) is best justified for single ionization in the  $I$ th shell and multiple ionization in shells higher than the  $I$ th shell. Then, except for the  $I$ th electron, all the probabilities will tend to be flat (unless the orbit velocities differ by an order of magnitude or more from the  $I$ th orbit velocity) over the region of nonzero  $P_I(E_i, b)$ . In this case, Eq. (30) reduces to

$$\begin{aligned} \sigma_{n_I, n_R, n_S, \dots, n_J} &= \binom{n_R}{n_R} P_R^{n_R} (1 - P_R)^{n_R - n_R} \\ &\quad \times \binom{n_S}{n_S} P_S^{n_S} (1 - P_S)^{n_S - n_S} \\ &\quad \times \dots \binom{n_J}{n_J} P_J^{n_J} (1 - P_J)^{n_J - n_J} \sigma_I, \end{aligned} \quad (32)$$

where

$$\sigma_I = N_I \int 2\pi b P_I(b) db \quad (P_I \ll 1) \quad (33)$$

is the cross section for ionizing a single  $I$ -shell electron.

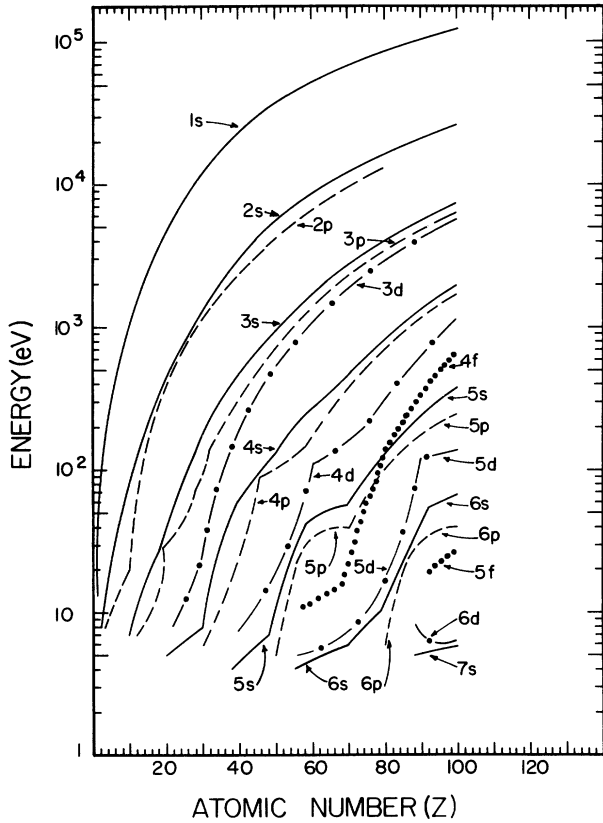


FIG. 8. Atomic binding energy vs atomic number. The binding energies for various atomic shells and subshells are plotted for all atoms from  $Z = 1$  to  $Z = 100$ . This figure is based on the variational calculations of Herman and Skillman.

The only parameters required to do a calculation are the binding energies  $U$  and the radii  $R$  of the electrons that are removed from the atom. The binding energies for all shells in all atoms are given in Fig. 8, based on the variational calculations of Herman and Skillman.<sup>29</sup> The cutoff radii may be estimated from Fig. 3 in terms of the atomic radii  $a$ . These may in turn be estimated by using  $a = n^2 a_0 / Z$ , where  $n$  designates the electron shell,  $Z$  is the effective nuclear charge at that shell, and  $a_0 = 0.529 \times 10^{-8}$  cm.

As an example, let us estimate the cross section for the ionization of one  $K$ -shell and several  $L$ -shell electrons for 3.2-MeV  $\alpha$  particles incident on titanium. In order to compute  $\sigma_{1K,nL}$  we use Eqs. (5), (30), and (31) with  $N_K = 2$  and  $N_L = 8$ . We take the binding energies for  $K$ - and  $L$ -shell electrons in titanium ( $Z = 22$ ) from Fig. 8 as 5000 and 500 eV, respectively. In choosing the  $L$ -shell binding energy we have chosen an average  $L$ -shell binding energy, ignoring the differences between subshells as well as the fact that  $U$  changes for each state of ionization. We use  $(Z/n)^2 = |U|/13.6$ .

Now  $V = [(E/U)(m/M)]^{1/2} = 0.3$  for the  $K$  shell and 0.9 for the  $L$  shell. Consequently, we take  $R = (\sqrt{2})a = (\sqrt{2})(2)^2 a_0 / 12 = 2.5 \times 10^{-9}$  cm for the  $L$ -shell cutoff, since  $V \approx 1$ . We now find from Eqs. (5) and (31) that  $P_L \approx 0.036$  using the tabulated Gerjuoy, Vriens, and Garcia  $G(V)$ . The cross section may be evaluated according to

$$\sigma_{1K,nL} = \binom{8}{n} P_L^n (1 - P_L)^{8-n} \sigma_K, \quad (34)$$

where the value of  $\sigma_K$  may be quickly found from Eq. (5). The ratios  $\sigma_{1K,1L}/\sigma_{1K,0L}$  and  $\sigma_{1K,2L}/\sigma_{1K,0L}$  are 0.29 and 0.039, respectively. The corresponding experimental values<sup>28</sup> are 0.218 and 0.026, respectively, while the full BEA calculations give 0.29 and 0.038.

It is much easier to evaluate  $P_L(V, 0)$  by using Fig. 3 and the scaling laws corresponding to Eqs. (17–19). At  $V = 0.9$ ,  $P_L(V, 0) \approx z^2/Z^2 P(1, 0) \approx (2/12)^2 1.4 \approx 0.039$ , in reasonable agreement with the previous estimate of 0.036.

In the current applications of this procedure, primarily estimating cross sections for removing one  $K$ - and  $nL$ -shell electrons, the estimates of  $P_L$  are typically within a factor of 2 of the value which best fits the data, and usually the estimates are too large.

Finally, let us compare our estimates to the results of Hansteen and Mosebekk for the ratio of  $\sigma_{1K,1L}/\sigma_{1K,0L}$  for 0.5–10 MeV protons on copper. Since  $0.5 \leq V \leq 2.5$ , we take  $R = (\sqrt{2})a$  in Eq. (31). In atomic units ( $e^2 = \hbar = m_e = 1$ ),  $P_L$  may then be expressed as

$$P_L \approx 2(z/Z)^2 G(V). \quad (34)$$

Taking  $Z^2 = 4|U_L|/13.6 = 294$ , the results given in Table V may be quickly confirmed. Except at 10 MeV, they are in good agreement with Hansteen and Mosebekk. At 10 MeV the total  $L$ -shell ionization cross sections predicted by the binary-encounter approximation is five times that predicted by the semiclassical approximation, so that the large discrepancy in  $\sigma_{1K,1L}/\sigma_{1K,0L}$  is to be

TABLE V. Comparison of double-to-single-ionization cross sections for  $p + \text{Cu}$ . Our present estimates are compared to those of Hansteen and Mosebekk, who integrate over probabilities computed in the semiclassical approximation.

| Energy (MeV) | $\sigma_{1K,1L}/\sigma_{1K,0L}$ |                   |
|--------------|---------------------------------|-------------------|
|              | McGuire-Richard                 | Hansteen-Mosebekk |
| 0.5          | 1.5%                            | 2.4%              |
| 1.0          | 3.1                             | 2.6               |
| 2.0          | 3.8                             | 1.2               |
| 5.0          | 2.6                             | 2.5               |
| 10.0         | 1.5                             | 0.2               |

expected. The full binary-encounter results in Fig. 4 are within 10% at low energies and a factor of ~2 at high energies of the binary-encounter estimates in Table V.

#### IV. CONCLUSION

The theory of multiple ionization based on the binary-encounter approximation gives relative intensities which are usually within a factor of 2 of experiment for heavy, fully stripped projectiles, when the probability for atomic ionization is much

smaller than one. Simple estimates, easily done using tables and scaling laws, give about the same accuracy.

#### ACKNOWLEDGMENTS

We wish to acknowledge J. S. Hansen, who contributed substantially to the early development of this work, and E. Merzbacher, C. P. Bhalla, J. R. Macdonald, C. L. Cocke, O. L. Weaver, M. H. Mittleman, and J. D. Garcia for stimulating discussions.

\*Work supported in part by the Atomic Energy Commission.

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