

### Calculation of *K*-vacancy production by relativistic projectiles

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Cross sections for the production of *K* vacancies by relativistic projectiles are calculated using the plane-wave Born approximation. Electronic 1s and continuum states are represented using semirelativistic Darwin wave functions. The calculated cross sections are in good agreement with measurements using 4.88-GeV protons, and also very high-energy (50–900-MeV) electrons. Simple formulas are given to calculate the cross section for projectile energies greater than  $\sim 3Mc^2$ .

#### I. INTRODUCTION

Recently there has been a growing interest in vacancy production by relativistic projectiles. *K*-vacancy production by electrons has most often been studied<sup>1-3</sup>; however two measurements with protons<sup>4,5</sup> and one using heavy ions<sup>6</sup> have also been made. The highest-energy heavy-projectile measurement was with 4.88-GeV protons.<sup>5</sup> The results were analyzed using the plane-wave Born approximation (PWBA),<sup>7-10</sup> and revealed the need to include the current-current interaction between the projectile and target electron, which is not included in the usual PWBA theory.<sup>7</sup> Although the inclusion of the current-current interaction considerably improved the agreement between theory and experiment, discrepancies remained for *K*-vacancy production in high- $Z_2$  targets. Meanwhile Davidović *et al.*<sup>11</sup> (henceforth referred to as DMN) made calculations using Moller's PWBA equations,<sup>12</sup> and the Pauli approximation to represent the electronic wave functions.<sup>13</sup> DMN's calculation for 4.88-GeV protons agree very nicely with experiments over the entire range of targets ( $28 < Z_2 < 92$ ). They claimed that the better agreement with experiment is obtained because the calculations of Anholt *et al.*<sup>5</sup> are only partially relativistic. However, we show in this paper that DMN's equations reduce to basically the same equations as Anholt's when terms of the order of  $m/M$  ( $m$  is the mass of the electron,  $M$  is the mass of the projectile) and  $(Z_2\alpha)^3, 4, \dots$  ( $\alpha = 137^{-1}$ ) are neglected. The main difference between the two calculations is due to an error in Anholt's equations.<sup>5</sup>

In this paper we present a simpler derivation of the cross section for the production of *K* vacancies by relativistic projectiles than that of DMN, expanding on the derivation in Anholt *et al.*<sup>5</sup> Screening, which was neglected by Anholt *et al.*,<sup>5</sup> is included. Also, we include the spin-flip term

(excitation of spin-down *K* electrons to spin-up continuum states and vice versa), the importance of which was pointed out by DMN.

In deriving these equations, we assume only that the momentum lost by the projectile in exciting the *K* electron is much less than its total momentum. Thus, the equations should be equally valid for electron and proton excitation as long as the electron's energy is greater than approximately 40 times the *K*-shell binding energy. The equivalence of electron and proton excitation cross sections has been suggested also by DMN, and demonstrated experimentally by Tawara.<sup>14</sup> Therefore, we also compare our calculations with 2-, 50-, 300-, and 900-MeV electron excitation cross sections.

Finally simple formulas are given to calculate *K*-vacancy production by relativistic projectiles with kinetic energies greater than  $\sim 3Mc^2$ .

We use atomic units throughout this paper.

#### II. THEORY

Our theory is based on the PWBA formulas of Moller.<sup>12</sup> The incident proton or electron with momentum  $\vec{k}_1$ , and spin  $\vec{s}_1$ , is represented by a Dirac plane wave

$$\psi_1 = N_1 a_{1s_1} \exp[i(\vec{k}_1 \cdot \vec{R} - \omega_1 t)], \tag{1}$$

where  $\omega_1$  is the projectile's total energy  $\gamma Mc^2$ ,  $M$  is the mass of the projectile,  $\vec{R}$  is the projectile coordinate, and  $a_{1s_1}$  is a four-vector given by

$$\begin{aligned} a_{1+1/2} &= (1, 0, k_{1z}/K_1, (k_{1x} - ik_{1y})/K_1), \\ a_{1-1/2} &= (0, 1, (k_{1x} + ik_{1y})/K_1, k_{1z}/K_1), \end{aligned} \tag{2}$$

with  $K_1 = (\gamma + 1)Mc$ .

Moller and DMN have shown that the cross section for the excitation of an electron from state  $\psi_0$  to a continuum state with energy  $\epsilon$  with a momentum transfer  $q$  is given by

$$\frac{d^2\sigma}{d\epsilon dq} = \frac{2\pi Z_1^2}{c^2} \frac{K_1' K_1^0}{(k_1^0)^2} \frac{q}{(q^2 - q_z^2 \beta^2)^2} \frac{1}{4} \sum_{s_1^0 s_1^z s_2^0 s_2^z} \left| a_{1s_1^0}^* a_{1s_1^z}^0 \int \psi_{\epsilon s_2^0}^* \psi_{0s_2^0} e^{i\vec{q} \cdot \vec{r}} d^3 \vec{r} - a_{1s_1^z}^* \vec{\alpha}_1 a_{1s_1^0}^0 \int \psi_{\epsilon s_2^0}^* \vec{\alpha}_2 \psi_{0s_2^0} e^{i\vec{q} \cdot \vec{r}} d^3 \vec{r} \right|^2, \tag{3}$$

where  $q_x = \Delta E/v$  is the minimum momentum transfer needed to excite the electron to the continuum ( $\Delta E$  is the energy transfer,  $v$  is the projectile velocity),  $\vec{r}$  is the electronic coordinate,  $k_1^0$  is the initial projectile momentum,  $k_1'$  is the final momentum,  $Z_1$  is the projectile charge, and  $\psi_{\epsilon s_2}$  and  $\psi_{0s_2^0}$  are final and initial electronic wave functions with spin  $\vec{s}_2$ . The first term in the absolute square in this equation comes from the Coulomb interaction between the projectile and the target electron.<sup>7</sup> The second is between the current density of the projectile  $a_1'^* \vec{\alpha}_1 a_1^0$  and that of the electron  $\psi_{\epsilon} \vec{\alpha}_2 \psi_0$ , where  $\vec{\alpha}_1$  and  $\vec{\alpha}_2$  are Dirac matrices.

The essential approximation that we make is to set the initial momentum  $\vec{k}_1^0$  equal to  $\vec{k}_1'$ , thus  $a_1' = a_1^0$ . This assumes that the projectile's momentum is so large that the deflection due to the momentum transferred to excite the electron is negligible, which is certainly valid for relativistic protons or heavy ions, but is also a good approximation for very-high-energy electrons. Using this approximation, it is easy to show that

$$[K_1' K_1^0 / 4(k_1^0)^2]^{1/2} a_{1s_1}^* a_{1s_1}^0 = \beta^{-1} \delta_{s_1^0 s_1'},$$

and

$$[K_1' K_1^0 / 4(k_1^0)^2]^{1/2} a_{1s_1}^* \vec{\alpha}_1 a_{1s_1}^0 = (\vec{\beta}/\beta) \delta_{s_1^0 s_1'}, \quad (4)$$

where  $\vec{\beta} = \vec{v}/c$ . Thus the cross section is given by

$$\frac{d^2\sigma}{d\epsilon dq} = \frac{4\pi Z_1^2}{v^2} \frac{q}{(q^2 - q_x^2 \beta^2)^2} \times \sum_{s_2^0 s_2'} \left| \int \psi_{\epsilon s_2'}^* (1 - \vec{\beta} \cdot \vec{\alpha}_2) \psi_{0s_2^0} e^{i\vec{q} \cdot \vec{r}} d\vec{r} \right|^2. \quad (5)$$

To evaluate the electronic matrix elements, it is desirable to take  $q$  to be the polar axis, thus  $\vec{q} \cdot \vec{r} = qz$ . If the collision takes place in the  $xz$  plane, and  $\lambda$  is the angle between  $\vec{\beta}$  and  $\vec{q}$ , then

$$\vec{\beta} \cdot \vec{\alpha}_2 = \beta \cos \lambda \alpha_x + \beta \sin \lambda \alpha_z, \quad (6)$$

where  $\cos \lambda = q_x/q$ . Therefore

$$\left| \int \psi_{\epsilon s_2'}^* (1 - \vec{\beta} \cdot \vec{\alpha}_2) e^{i\vec{q} \cdot \vec{r}} \psi_{0s_2^0} d\vec{r} \right|^2 = |F - \beta \cos \lambda G_x|^2 + |\beta \sin \lambda G_x|^2, \quad (7)$$

where

$$F = \int \psi_{\epsilon s_2'}^* \psi_{0s_2^0} e^{iaz} d\vec{r}$$

and

$$G_x = \int \psi_{\epsilon s_2'}^* \alpha_x \psi_{0s_2^0} e^{iaz} d\vec{r}$$

with a similar equation for  $G_x$ . We are allowed to

square the two terms in Eq. (7) separately because  $\alpha_x$  connects different final electronic states to the 1s state than  $F$  or  $G_x$ . (For example,  $G_x$  excites 1s electrons to  $m_l = \pm 1$  continuum states, while  $F$  and  $G_x$  excites 1s electrons to  $m_l = 0$  continuum states.)

It may be shown that<sup>15</sup>

$$G_x = \Delta EF/qc, \quad (8)$$

therefore

$$F \cos \lambda G_x = F(1 - \beta^2 q_x^2/q^2), \quad (9)$$

and Eq. (5) becomes

$$\frac{d^2\sigma}{d\epsilon dq} = \frac{4\pi Z_1^2 q}{v^2} \sum_{s_2^0 s_2'} \left( \frac{|F_{s_2^0 s_2'}|^2}{q^4} + \frac{|\beta \sin \lambda G_{xs_2^0 s_2'}|^2}{(q^2 - q_x^2 \beta^2)^2} \right), \quad (10)$$

which is essentially identical to Anholt *et al.*<sup>5</sup> and Fano.<sup>10</sup>

Following DMN, we evaluate the electronic matrix elements  $F$  and  $G_x$  using Darwin or Pauli wave functions<sup>13</sup>

$$\psi_{ns_2} = N_2 a_{s_2} \psi_n^0, \quad (11)$$

where  $\psi_n^0$  is the normalized eigenfunction of the nonrelativistic Hamiltonian for the 1s ( $\psi_0^0$ ) or continuum ( $\psi_\epsilon^0$ ) state,  $N_2$  is a normalization factor, and  $a_{s_2}$  is the electronic four-vector given by

$$a_{1/2} = \left( \frac{i}{K_2} \left( \frac{\partial}{\partial x} - i \frac{\partial}{\partial y} \right), -\frac{i}{K_2} \frac{\partial}{\partial z}, 0, 1 \right),$$

and

$$a_{-1/2} = \left( \frac{i}{K_2} \frac{\partial}{\partial z}, \frac{i}{K_2} \left( \frac{\partial}{\partial x} + i \frac{\partial}{\partial y} \right), 1, 0 \right). \quad (12)$$

Here  $K_2 = c(\gamma_2 + 1) = c(2 - E_2/c^2)$ , where  $E_2$  is the binding energy  $\frac{1}{2}Z^2$  or  $-\epsilon = -\frac{1}{2}k^2$ , and  $k$  is the electronic momentum (we assume in writing  $\epsilon = \frac{1}{2}k^2$  that the major contribution to  $\sigma_K$  comes from continuum states with  $\epsilon \ll c^2$ ).

In this work, we will neglect all terms of the order of  $(Z\alpha)^3, 4, \dots$ , where  $\alpha = 1/c$ . Thus we put  $K_2^0 = K_2^2 = 2c$ . The normalization factors are given by

$$N_2^0 = [1 + (Z\alpha/2)^2]^{-1/2}$$

and

$$N_2' = [1 + (k\alpha/2)^2]^{-1/2}. \quad (13)$$

Inserting Eqs. (11)–(13) into Eq. (10) we obtain the following matrix elements:

$$\begin{aligned}
F_{(1/2)(1/2)} &= F_{-(1/2)-(1/2)} \\
&= d \int [\psi_\epsilon^{0*} \psi_0^0 + (2c)^{-2} \vec{\nabla} \psi_\epsilon^{0*} \cdot \vec{\nabla} \psi_0^0] e^{i\alpha z} d\vec{r} \\
&\approx d \int \psi_\epsilon^{0*} \psi_0^0 e^{i\alpha z} d\vec{r} = dI_0,
\end{aligned} \tag{14}$$

$$\begin{aligned}
F_{(1/2)-(1/2)} &= F_{-(1/2)(1/2)} \\
&= \frac{qd}{4c^2} \int \psi_\epsilon^{0*} \frac{\partial \psi_0^0}{\partial x} e^{i\alpha z} d^3\vec{r} = \frac{qd}{4c^2} I_x,
\end{aligned}$$

$$G_{x(1/2)(1/2)} = G_{x-(1/2)-(1/2)} = \frac{id}{c} I_x,$$

$$G_{x(1/2)-(1/2)} = G_{x-(1/2)(1/2)} = -\frac{dq}{2c} I_0,$$

where  $d = N_2^0 N_2^0$ ,<sup>7, 17, 18</sup>

$$|I_0|^2 d\epsilon = (3q^2 + Z^2 + k^2) q^2 A_3 d\epsilon,$$

$$|I_x|^2 d\epsilon = (Z^2 + k^2) / 4A_2 d\epsilon$$

and

$$A_n = \frac{2^8 Z \exp\{-2Z/k \tan^{-1}[2Zk/(Z^2 + q^2 - k^2)]\}}{3[1 - \exp(-2\pi/k)] [(q+k)^2 + Z^2]^n [(q-k)^2 + Z^2]^n}. \tag{15}$$

Following DMN, for  $F_{(1/2)(1/2)}$  we have dropped the  $(2c)^{-2} \vec{\nabla} \psi_\epsilon^{0*} \cdot \vec{\nabla} \psi_0^0$  terms. These terms are of the order of  $\sim ikZ \psi_\epsilon^{0*} \psi_0^0$ , thus when  $F_{(1/2)(1/2)}$  is squared, including these terms gives a factor  $1 + (Zk\alpha^2/4)^2$ , which is a correction of the order of  $(Z\alpha)^4$  which we have already neglected elsewhere. Also,  $F_{(1/2)-(1/2)}$  is a  $(Z\alpha)^4$  term which is negligible.

Thus, summing over spins, the  $K$  vacancy cross section *per atom* is given by

$$\begin{aligned}
\frac{d^2\sigma}{d\epsilon dq} &= \frac{16\pi Z^2 q d^2}{v^2} \left\{ \frac{|I_0|^2}{q^4} + \left| \frac{\beta \sin \lambda I_x}{c(q^2 - q_z^2 \beta^2)} \right|^2 \right. \\
&\quad \left. + \left| \frac{\beta \sin \lambda I_0 q}{2c(q^2 - q_z^2 \beta^2)} \right|^2 \right\}. \tag{16}
\end{aligned}$$

The first term inside the curly brackets is the usual term that appears in nonrelativistic PWBA theory.<sup>7</sup> It is called the longitudinal contribution. The second is the transverse contribution that appeared in Anholt's equations. The third is the spin-flip term.

To conclude this section, we re-express Eqs. (15) and (16) in a form suitable for numerical integration. We find it convenient to use the same integration variable as Merzbacher and Lewis,<sup>7</sup> Khandelwal *et al.*,<sup>8</sup> and Walske.<sup>9</sup> Letting  $W = \epsilon/I_K + 1$ , where  $I_K = \frac{1}{2} Z^2$ , and  $Q = q^2/Z^2$ ,

$$\begin{aligned}
\sigma_K &= \frac{8\pi Z^2}{\eta_K Z^4} \int_{W_{\min}}^{\infty} d^2 dW \int_{Q_{\min}}^{\infty} \frac{dQ}{Q^2} \\
&\quad \times \left( F_K + \frac{(\beta Z \alpha)^2 (1 - Q_{\min}/Q)}{(1 - \beta^2 Q_{\min}/Q)^2} \right. \\
&\quad \left. \times (G_K + \frac{1}{4} Q F_K) \right), \tag{17}
\end{aligned}$$

where

$$F_K = Z^2 I_0^2 = (3Q + W) Q A'_3,$$

$$G_K = I_x^2 = \frac{1}{4} W A'_2,$$

$$A'_n = \frac{2^7 \exp\{-2/k \tan^{-1}[2k/(Q + 1 - k^2)]\}}{3[1 - \exp(-2\pi/k)] [(Q - k^2 + 1)^2 + 4k^2]^n}, \tag{18}$$

$$d^2 = [1 + (Z\alpha/2)^2]^{-1} [1 + (W - 1)(Z\alpha/2)^2]^{-1},$$

$W = k^2 + 1$ ,  $W_{\min} = \Theta_K = 2U_K/Z^2$ ,  $Q_{\min} = W^2/4\eta_K$ ,  $\eta_K = v^2/Z^2$ ,  $Z = Z_2 - 0.3$ , and  $U_K$  is the  $K$ -electron binding energy. Evaluation of these equations when  $W < 1$  is described by Merzbacher and Lewis<sup>7</sup> and Walske.<sup>9</sup> For the transverse and spin terms, because the integrand becomes very large for  $Q \approx Q_{\min}$  when  $\beta^2 \approx 1$ , it is necessary to integrate the first step,  $Q_{\min} \rightarrow 1.3Q_{\min}$  analytically, keeping  $F$  and  $G$  constant over the interval. The remaining part of the integral is done using straightforward quadrature techniques.

### III. RESULTS AND DISCUSSION

Figure 1 compares our theoretical calculations with measured cross sections for the production of  $K$  vacancies by 4.88-GeV protons.<sup>5</sup> As noted previously, the measured cross sections are a factor

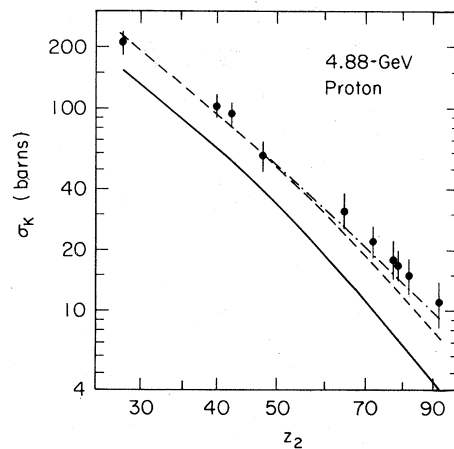


FIG. 1.  $K$ -vacancy production by 4.88-GeV protons versus target atomic number (Ref. 5). Solid line: longitudinal (Coulomb interaction) contribution; dashed line: longitudinal and transverse (current-current interaction); dash-dot: total cross section including spin-flip contribution.

of 1.5–2.5 larger than the longitudinal Coulomb-interaction contribution, which is the only contribution in the theory of Merzbacher and Lewis<sup>7</sup> and others.<sup>8,9</sup> The transverse (current-current) contribution increases the calculated cross sections by a factor of 1.5–2. Also the spin-flip contribution increases the high- $Z_2$  cross sections by another factor of 1.3. For low- $Z$  targets, the spin-flip contribution is a factor of the order of  $Q^2$  smaller than the transverse contribution [see Eqs. (17) and (18)]. The calculated cross sections are in good agreement with experiment, except possibly for the high- $Z$  targets.

As long as the projectile's momentum  $\vec{k}_1$  is much greater than the momentum  $\Delta\vec{k}_1$  transferred to excite the  $K$  electron, our equations should be valid for any projectile. Therefore in Fig. 2 are shown 2-, 50-, 300-, and 900-MeV electron excitation cross sections.<sup>1-3</sup> Also shown are the total calculated cross sections (sum of longitudinal, transverse, and spin-flip contributions). For the high-energy electron bombardments, agreement between theory and experiment is excellent. However, for excitation of high- $Z$  targets by 2-MeV electrons, the requirement  $|\Delta\vec{k}_1/\vec{k}_1| \ll 1$  is not accurately fulfilled, and one sees that the calculated cross sections are greater than experiment. In our calculations, the upper limit to the continuum energy  $\epsilon_{\max}$  was set to infinity, but if  $k_1$  is small, one can only integrate to a finite  $\epsilon_{\max}$ , losing a significant contribution to the integral if  $U_K$  and  $\epsilon_{\max}$  are of comparable magnitude.

Figure 3 shows calculated  $U_K$ -vacancy production cross sections as a function of the total pro-

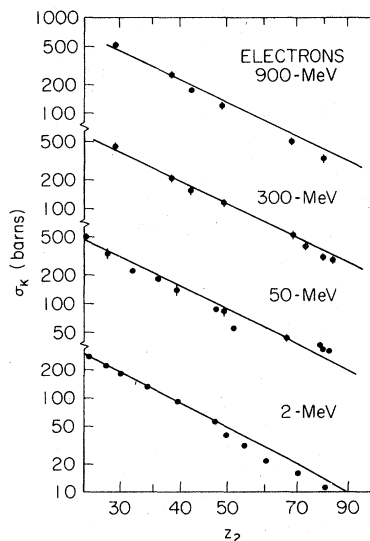


FIG. 2.  $K$ -vacancy production by 2-MeV (Ref. 1), 50-MeV (Ref. 2), and 300- and 900-MeV (Ref. 3) electrons. Solid lines: total calculated cross section.

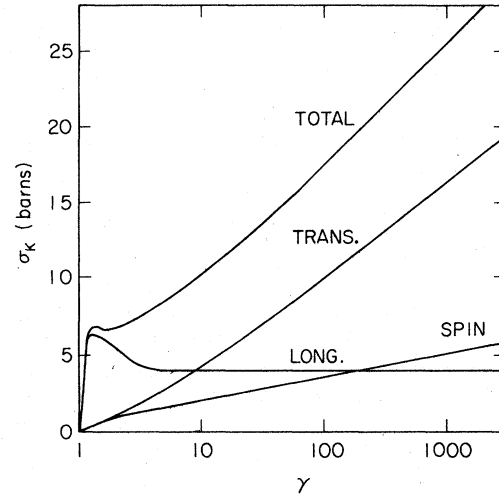


FIG. 3.  $U_K$ -vacancy production by projectiles with kinetic energies  $(\gamma - 1)Mc^2$ . The calculated longitudinal, transverse, and spin-flip contributions are shown separately as well as the total cross section.

jectile energy  $E_1$  in units of  $Mc^2$ . [The projectile's kinetic energy is  $(\gamma - 1)Mc^2$ .] For  $\gamma \geq 4$ , the projectile's velocity is constant and equal to  $c$ . Since the longitudinal contribution depends only on the projectile velocity, it is constant for  $\gamma \geq 4$ . The transverse and spin-flip contributions both increase as the  $\ln \gamma$ , the spin-flip contribution increasing less steeply. For  $\gamma < 1.3$ , (proton excitation energies less than 250 MeV/amu) the cross section is completely dominated by the longitudinal term; thus it is valid to use the tables of Khandelwal *et al.*<sup>8</sup> to calculate  $K$  vacancy cross sections for those energies.

The main difference between the present equations and Anholt's previous ones<sup>5</sup> is the inclusion of the spin-flip term here and the correction of an error in the previous equations. In the denominator of  $A_2$  [Eq. (15)], a factor

$$[(q+k)^2 + Z^2][(q-k)^2 + Z^2] = [q^2 + k^2 + Z^2]^2 - 4q^2k^2 \quad (19)$$

appears. In Ref. 5,  $-4q^2k^2$  was incorrectly written as  $-2q^2k^2$ . For  $q \approx 0$ , or  $Z_2 \approx 30$ , the difference between the two expressions is negligible, but when  $q/Z \approx 1$  or  $Z_2 \approx 92$ , the calculated cross sections differ significantly from one another. Thus Anholt's calculations<sup>5</sup> agreed poorly with experiment only for the high- $Z$  targets.

Equations (42) and (43) of DMN reduce to ours when one sets  $K_2 = K'_2 = 2c$  and, in the first line of Eq. (42), sets  $\frac{1}{2}(Z^2 + k^2) = U_K + \epsilon$ . The latter approximation is discussed below. DMN argue against setting  $K_2 = K'_2 = 2c$ , claiming that when one integrates over the continuum energy  $\epsilon$  or the final

electron momentum  $k$ , one obtains for 4.88-GeV protons a spurious contribution to the cross sections from the region near  $k_{\max}$ , where  $k_{\max}$  is given by

$$k_{\max}^2 = [Mc(\gamma - 1) + m - I_K/c]^2 - m^2 \approx [Mc(\gamma - 1)]^2. \quad (20)$$

This corresponds to transferring the projectile's entire momentum to the electron, so  $k_{\max}$  is extremely large. As is well known in PWBA calculations for nonrelativistic projectiles,<sup>7</sup> one can effectively put  $k_{\max} = \infty$ , and integrate over  $\epsilon$  or  $k$  until the integral converges, generally near  $\epsilon_{\max} \approx 40 I_K$ . DMN point out that if one keeps the exact value of  $K_z$ , this spurious contribution is removed. We find it easier to integrate only to  $\epsilon_{\max} \approx 40 I_K$ , thus the region near  $k_{\max}$  is ignored.

Finally we wish to point out that the evaluation of Eq. (7) for very high-projectile energies using inexact wave functions can be very inaccurate. The relation  $G_z = \Delta EF/qc$  [Eq. (8)] is exact for ideal wave functions. If one has  $G_z = a\Delta EF/qc$ , where  $a \neq 1$ , the longitudinal contribution to the cross sections would be given by integrating

$$\frac{d\sigma}{d\epsilon} = \frac{16\pi Z_1^2 d^2}{v^2} \int_{q_z}^{\infty} \frac{dq |F|^2}{q^4} \frac{(1 - a\beta^2 q_z^2/q^2)^2}{(1 - \beta^2 q_z^2/q^2)^2}. \quad (21)$$

For  $\beta \approx 1$  and  $a \neq 1$ , one has a large contribution to the integral near  $q = q_z$ . The error, due to having  $a \neq 1$ , is given approximately by

$$\sigma_K(a) = \sigma_K(a=1)[1 + (1-a)^2\gamma^2 + \text{terms in } (1-a)\gamma \text{ and } \ln\gamma]. \quad (22)$$

Thus, for excitation by 1000-GeV protons or 500-MeV electrons where  $\gamma = 1000$ , one must have  $a > 0.999$  to obtain an accurate result. Since DMN

evaluated Eq. (7) using one-electron wave functions, they obtain  $G_z = \frac{1}{2}(Z^2 + k^2)F/qc$ , not  $(U_K + \epsilon)F/qc$ , which for  $k = \epsilon = 0$ , means  $a = \Theta_K$ . Thus one should not expect very accurate results for  $\gamma \gtrsim 10$ . For 900-MeV electron excitation ( $\gamma = 1800$ ) of  $Ni(\Theta_K = 0.8)$  and  $U(\Theta_K = 1.01)$ , we obtain  $3 \times 10^6$  and 340 b for the longitudinal contribution using DMN's equations, but only 150 and 4.9 b using Eq. (10). In view of the good agreement between our calculations and experiment for these energies, the use of Eq. (10) is clearly the best way to evaluate  $\sigma_K$ .

#### IV. RECIPE FOR $K$ -VACANCY CROSS SECTIONS

Although numerical evaluation of Eqs. (17)–(18) is not difficult, we recognize that it is occasionally desirable to be able to calculate the  $K$ -vacancy production cross sections on the back of an envelope. In this section we derive simple formulas for the transverse and spin-flip contributions to the  $K$ -vacancy production cross section, for projectiles with  $\gamma \gtrsim 3$ . The longitudinal contribution  $\sigma_{kl}$  can be calculated using the tables of Khandelwal *et al.*<sup>8</sup> or Rice *et al.*<sup>19</sup> However, in their work, the normalization of factor  $d^2$  [Eq. (8)] was not included. One can correct for this by multiplying their cross section by

$$d_0^2 = [1 + (Z\alpha/2)^2]^{-2}. \quad (23)$$

Our numerical calculations of  $\sigma_{kl}$  agree within 5% with Khandelwal's multiplied by  $d_0^2$ .

The transverse contribution can be evaluated analytically if one makes the following approximations to Eqs. (17)–(18): (i) neglect  $Q$  with respect to  $1 - k^2$  (dipole approximation), (ii) set  $1 - \exp(-2\pi/k) = 1$ , (iii) set

$$\exp\{-2/k \tan^{-1}[2k/(1 - k^2)]\} = e^{-4}(4/3W - 1/3)$$

(Ref. 20), and (iv) set  $d^2 = d_0^2$ . One then obtains

TABLE I. Comparison of numerically calculated transverse contribution  $\sigma_{Kt\text{num}}$  to Eq. (24).

4.88-GeV protons						
Cross sections (in b)						
$Z_2$	$\sigma_{Kt\text{num}}$	Eq. (24)	Ratio <sup>a</sup>	Eq. (24)	$d_0^2 = 1$	Ratio <sup>a</sup>
28	71	68	1.04	69		1.03
47	21	18.8	1.09	20		1.03
65	9.1	7.9	1.15	8.8		1.04
92	3.3	2.7	1.24	3.3		1.00
50-MeV electrons				900-MeV electrons		
$Z_2$	$\sigma_{Kt\text{num}}$	Eq. (24)	Ratio <sup>a</sup>	$\sigma_{Kt\text{num}}$	Eq. (24)	Ratio <sup>a</sup>
		$d_0^2 = 1$			$d_0^2 = 1$	
28	209	206	1.01	358	351	1.02
47	61	60	1.01	104	101	1.03
65	27	26	1.04	47	45	1.04
92	10	9.9	1.04	17	16.9	1.04

<sup>a</sup>Ratio =  $\sigma_{Kt\text{num}}/\sigma_{Kt}$  [Eq. (24)].

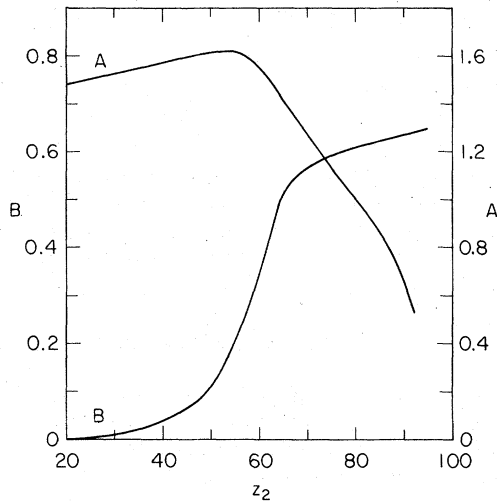


FIG. 4. Fitted constants  $A$  and  $B$  (in b) appearing in Eq. (25) versus target atomic number.

$$\sigma_{\kappa t} = 2.9 \times 10^4 (Z_1 d_0 / Z_2 \beta \Theta_K^2)^2 \times \left(\frac{4}{9} \Theta_K - \frac{1}{12}\right) [\ln(\gamma^2) - \beta^2] \quad (\text{b}). \quad (24)$$

Table I compares Eq. (24) with the numerically calculated transverse cross sections. For 4.88-GeV proton bombardments of high- $Z$  targets, the numerically calculated cross sections are larger than the values from Eq. (24). This is mainly due to a failure of the dipole approximation; for high- $Z_2$ ,  $\eta_K \approx 1$ , hence  $Q$  is not negligible with respect to  $1 - k^2$ . One can compensate for this by setting  $d_0^2 = 1$  in Eq. (24). With  $d_0^2 = 1$ , Eq. (24) gives the correct transverse cross section to within 5% for all projectile energies with  $\gamma \geq 3$  as Table I shows. It is purely accidental that setting  $d_0^2 = 1$  compensates for making the dipole approximation.

We have also attempted to derive a simple formula for the spin-flip cross section  $\sigma_{\kappa s}$  using the same approximations. The resulting formulas are quite complicated, and not very accurate. Figure 3 suggests that  $\sigma_{\kappa s}$  might be given by

$$\sigma_{\kappa s} = A + B \ln \gamma, \quad (25)$$

where, for  $\gamma \geq 3$ ,  $A$  and  $B$  are  $Z_2$  dependent, energy-independent constants. We find that the calculated spin-flip cross sections can be fit accurately using this simple equation. The constants  $A$  and  $B$  are shown in Fig. 4. Their dependence

TABLE II. Constants  $A$  and  $B$  in Eq. (25) (in b).

$Z_2$	$A$	$B$	$Z_2$	$A$	$B$
28	1.52	0.012	65	1.40	0.51
35	1.56	0.023	75	1.12	0.60
47	1.60	0.080	85	0.85	0.62
55	1.62	0.200	92	0.54	0.66

on  $Z_2$  suggests a complicated dependence on  $Z\alpha$ ,  $\Theta_K$ , and  $\eta_K$ . Since  $\sigma_{\kappa s}$  makes a small contribution to the total  $K$ -vacancy cross section, the spin-flip contribution can be obtained to sufficient accuracy (5%–10%) by directly interpolating from Table II or Fig. 4.

## V. CONCLUSIONS

$K$ -vacancy production by relativistic projectiles can be accurately calculated using the relativistic PWBA for all targets with  $20 < Z_2 < 92$ . In this paper we have shown how the equations of Anholt *et al.*<sup>5</sup> and Fano<sup>10</sup> are derived from the theory of Moller,<sup>12</sup> and how these equations are more accurate than DMN's (Ref. 11) at extremely high projectile energies.

The main improvement which could be made to the theory is to use Dirac or relativistic Hartree-Fock (RHF) wave functions instead of the Pauli wave functions, retaining all terms in  $Z\alpha$ . To estimate the influence this has on  $K$  vacancy production one can compare with photoelectric cross sections calculated using RHF wave functions.<sup>20</sup> Using Pauli wave functions, the photoelectric cross section is given by

$$\sigma_p = (8\pi\alpha^2 / \Delta E) d^2 |I_x(q_z)|^2, \quad (26)$$

with  $\beta^2 = 1$ . For  $U$ , Eq. (26) and (15) agree within 8% with RHF calculations<sup>20</sup> for  $120 < q_z < 400$  keV/ $c$  or  $0 < \epsilon \approx 3U_K$ . Thus use of Dirac or RHF wave functions appears to have a small effect on the transverse contribution to  $\sigma_K$ . Although this only demonstrates the effect of using relativistic wave functions on  $\sigma_{\kappa t}$ , we expect approximately the same effect on  $\sigma_{\kappa l}$  and  $\sigma_{\kappa s}$ , since the main contribution to  $F_K$  [Eq. (17)] is a dipole one.

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<sup>1</sup>A. Li-Scholz, R. Collé, I. L. Preiss, and W. Scholz, Phys. Rev. A **7**, 1957 (1973).

<sup>2</sup>D. H. H. Hoffman, H. Genz, W. Löw, and A. Richter, Phys. Lett. A **65**, 304 (1978).

<sup>3</sup>L. M. Middleman, R. L. Ford, and R. Hofstadter, Phys. Rev. A **2**, 1429 (1970).

<sup>4</sup>O. N. Jarvis, C. Whitehead, and M. Shah, Phys. Rev. A **5**, 1198 (1972).

- <sup>5</sup>R. Anholt, S. Nagamiya, J. O. Rasmussen, H. Bowman, J. G. Ioannou, and E. Rauscher, *Phys. Rev. A* **14**, 2103 (1976).
- <sup>6</sup>R. Anholt, J. Ioannou, H. Bowman, E. Rauscher, S. Nagamiya, J. O. Rasmussen, T. Shibata, and H. Ejiri, *Phys. Lett. A* **59**, 429 (1977).
- <sup>7</sup>E. Merzbacher and H. Lewis, *Encyclopedia of Physics* (Springer-Verlag, Berlin, 1958), Vol. 34, p. 166.
- <sup>8</sup>G. S. Khandelwal, B. H. Choi, and E. Merzbacher, *At. Data* **1**, 103 (1969).
- <sup>9</sup>M. C. Walske, *Phys. Rev.* **101**, 940 (1956).
- <sup>10</sup>U. Fano, *Annu. Rev. Nucl. Sci.* **13**, 1 (1963).
- <sup>11</sup>D. M. Davidović, B. L. Moiseiwitsch, and P. H. Norrington, *J. Phys. B* **11**, 847 (1978) (referred to as DMN).
- <sup>12</sup>C. Möller, *Ann. Phys. (Leipz.)* **14**, 531 (1932).
- <sup>13</sup>C. G. Darwin, *Proc. Roy. Soc. London, Ser. A* **118**, 654 (1928).
- <sup>14</sup>H. Tawara, *Phys. Lett. A* **59**, 199 (1976).
- <sup>15</sup>Proof of this follows similar lines as proofs that mat-

rix elements of  $\vec{p}$  are equal to matrix elements of  $\Delta E\vec{r}$ .

$$\begin{aligned}\Delta EF &= \int \psi_{\epsilon}^* (He^{iqz} - e^{iqz}H)\psi_0 d\vec{r} \\ &= c \int \psi_{\epsilon}^* (\vec{\alpha} \cdot \vec{p}e^{iqz} - e^{iqz}\vec{\alpha} \cdot \vec{p})\psi_0 d\vec{r} \\ &= qc \int \psi_{\epsilon}^* \alpha_x e^{iqz} \psi_0 d\vec{r}.\end{aligned}$$

- <sup>16</sup>Several misprints appeared in Ref. 5. In Eq. (6),  $4\pi$  should be replaced with  $8\pi$ . In Eq. (8)  $(Z^2+k^2)^{-1}$  should appear on the right-hand side. The error mentioned in the text should be corrected by replacing the  $-2q^2k^2$  factor in Eq. (8) by  $-4q^2k^2$  and the  $-2yP$  factors in Eqs. (10) and (11) by  $-4yP$ .
- <sup>17</sup>J. Fischer, *Ann. Phys. (Leipz.)* **8**, 821 (1931).
- <sup>18</sup>D. M. Davidović and B. L. Moiseiwitsch, *J. Phys. B* **8**, 947 (1975).
- <sup>19</sup>R. Rice, G. Basbas, and F. D. McDaniel, *At. Data. Nucl. Data Tables* **20**, 503 (1977).
- <sup>20</sup>J. H. Scofield as quoted by R. H. Pratt, A. Ron, and H. K. Tseng, *Rev. Mod. Phys.* **45**, 320 (1973).