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[1]K. T. Tang, Phys. Rev. 187, 122 (1969).

[2]K. T. Tang and M. Karplus, J. Chem. Phys. 49, 1676 (1968).

[3]A. Dalgarno, R. J. W. Henry, and C. S. Roberts, Proc. Phys. Soc. (London) 88, 611 (1966).

[4]A. C. Allison and A. Dalgarno, Proc. Phys. Soc. (London) 90, 609 (1967).

[5]A. M. Arthurs and A. Dalgarno, Proc. Phys. Soc. (London) A256, 540 (1960).

[6]W. N. Sams and D. J. Kouri, J. Chem. Phys. 51, 4809 (1969); 51, 4815 (1969).

[7]J. M. Blatt and L. C. Biedenharn, Rev. Mod. Phys. 24, 258 (1952).

[8]G. Racah, Phys. Rev. 61, 186 (1942); 62, 438 (1942); 63, 367 (1943). Also, L. C. Biedenharn, J. M. Blatt, and M. E. Rose, Rev. Mod. Phys. 24, 249 (1952).

[9]B. R. Johnson and D. Secrest, J. Chem. Phys. 48, 4682 (1968).

[10]The precise values of σ_{tot}^{cc} are 1.107 bohr^2 at $E=0.1$ eV, 1.278 bohr^2 at $E=0.15$ eV, and 1.183 bohr^2 at $E=0.25$ eV.

[11]There does not appear to be a constant scale factor which would bring the distorted-wave and close-coupling results for $\sigma(\theta)$ into agreement for all values of θ. Further, agreement of σ_{tot}^{cc} and σ_{tot}^{Tang} requires only agreement of the B_0 coefficient, while the B_λ for $\lambda \neq 0$ may still differ significantly.

[12]If the potential is expressed in the multipole form $V(\vec{R}) = V_0(R) + V_2(R) P_2(\cos\theta)$, then for the $j=0$ elastic scattering, the matrix element of $P_2(\cos\theta)$ is zero so the "adiabatic" potential is simply $V_0(R)$. The $V_2(R)P_2(\cos\theta)$ term affects the $j=0$ elastic scattering only by causing excitations to and from the $j=2$ rotator state.

[13]W. H. Miller (private communication).

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Low-Energy Electron Ejection of Atoms in Collisions with Relativistic Electrons

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Low-energy electron-ejection cross sections of atoms in collisions with relativistic electrons have been calculated. The calculations are similar to those of Weber *et al.* In the approximate integration of the differential cross section over certain angles, Weber *et al.* considered Z small and obtained a $(\alpha Z)^4$-dependent result. We have followed a different type of approximation, valid for $Z \gg 1$, and obtained the explicit $(\alpha Z)^5$-dependent result. The result shows a much stronger dominance of the distribution of ejected electrons over the "Parzen distribution" in the low-energy region than the results of Weber *et al.* when applied to atoms with $Z \gg 1$.

I. INTRODUCTION

Mullin and co-workers have pointed out[1,2] that the low-energy large-angle scattering of electrons from atomic bound electrons in collisions with relativistic electrons may be sufficient to mask the "Parzen peak" that exists in the low-energy region of scattered electrons which have lost energy in the bremsstrahlung production. For high-energy colliding electrons, the Parzen peak[3] is situated at an energy W of the scattered electrons for which $1 < W \lesssim 1.2\, mc^2$ (or in terms of momentum, $0 < p \lesssim \frac{2}{3} mc$). The "Parzen distribution" is, moreover, independent of the nuclear charge Z of the atoms.

Weber *et al.*, in Ref. 2, have given a relativistic treatment to the scattering of low-energy electrons by bound electrons. In that paper they have described the bound and ejected electrons with wave functions which are obtained by an expansion in the parameters αZ and $\alpha Z/\beta$, and which are correct to first relative orders in these expansion parameters. Consistent with the neglect of higher powers of $\alpha Z/\beta$ in the wave functions, Weber *et al.* have a cross section which is valid to the lowest order in $(\alpha Z)^5$ and the highest order in the energy W_i of the incident electron. In the approximate evaluation of certain integrals[4] I_{nm} occurring in the expression for the cross section, they considered

Z small. Hence, their final results are applicable only to atoms of small Z. In fact, their results have the correct $(\alpha Z)^4$ dependence in the limit $Z \to 0$ and $p \neq 0$ (p is the momentum of the ejected electron). But these approximations are not valid (an analysis of Sec. II B will justify this) for $Z \gg 1$. In that case, we must take recourse to a different type of approximation, like the one described in Sec. II C.

Apart from its connection with the Parzen peak, the problem of low-energy scattering of electrons from atoms by relativistic electrons is inherently a problem of considerable importance. The total cross section for ionization of atoms by relativistic electrons is dominated by the ejection of low-energy electrons only and for this a small momentum transfer is necessary. For incoming electron energy of the order of several MeV, the ejection of electrons with momentum greater than mc will have insignificant effects on the total ionization cross section. In our present reinvestigation of the problem of low-energy scattering, we need therefore only consider the ejection of electrons with momentum less than mc. The relativistic result[5] from which we start has been derived by the use of the Schrödinger representation, the many-particle theory, and Coulomb gauge, together with the quantized electromagnetic field. This result may not differ significantly from that referred to by Mullin and co-workers. The present form of this result also has the advantage of getting separate contributions from the pure-Coulomb interaction as well as from the transverse radiation field. This may help us in estimating the retardation effects. In our calculation, we use for the wave functions of the bound and ejected electrons the same Born approximations as were used by Weber *et al.*[2] We may note that the results obtained with these expressions may not be accurate for very low energies, in fact, the validity condition of the Born approximation for the ejected electrons is $p \gg \alpha Zmc$. For very low energies ($p \lesssim \alpha Zmc$), a proper approximation[6] for the wave function of the ejected electrons would be the Sommerfeld-Maue-type approximation.

Applying suitable approximations in integrating the differential cross section over angles of the scattered-electron momentum $\vec{p}_f$, we have a result that may be used to study the distribution of ejected electrons in the momentum interval $\alpha Zmc \ll p < mc$ (which contains the Parzen peak) for atoms with $Z \gg 1$.

II. DISCUSSION OF THEORY

A. Differential Cross Section

The differential cross section for the ejection of electrons from the ground-state atoms in collisions with electrons of extreme relativistic energy in the lowest-order Born approximation can be shown[5] to have the following form:

$$d\sigma^I = \frac{W_i^2 p W(p) dW(p) d\Omega_p d\Omega_{p_f} (4\pi\alpha)^2}{(2\pi)^5} \times \left(\frac{1}{t^4} \left| M_1 \right|^2 + \frac{1}{(t^2 - E^2_{\alpha'\alpha})^2} \left| M_2 \right|^2 \right) , \quad (1)$$

where

$$M_1 = \chi^{(2)*}(\vec{p}_f)\, \chi^{(2)}(\vec{p}_i) \int d\vec{r}_1\, U_{\alpha'}^{(1)*}(\vec{r}_1)\, e^{i\vec{t}\cdot\vec{r}_1}\, U_\alpha^{(1)}(\vec{r}_1) ,$$

$$M_2 = \sum_{\vec{\epsilon}} \chi^{(2)*}(\vec{p}_f)\, (\vec{\alpha}^{(2)} \cdot \vec{\epsilon})\, \chi^{(2)}(\vec{p}_i) \int d\vec{r}_1\, U_{\alpha'}^{(1)*}(\vec{r}_1) \times (\vec{\alpha}^{(1)} \cdot \vec{\epsilon})\, e^{i\vec{t}\cdot\vec{r}}\, U_\alpha^{(1)}(\vec{r}_1) , \quad (2)$$

$$W_i + E_\alpha = W_f + E_{\alpha'} .$$

Here the superscript 1 refers to the atomic electron and 2 to the colliding electron. $\chi(\vec{q})$ refers to the free Dirac spinor with momentum $\vec{q}$ in momentum space, $U_\alpha^{(1)}(\vec{r}_1)$ to the ground-state atomic wave function in coordinate space, and $U_{\alpha'}^{(1)}(\vec{r}_1)$ to that of the ejected electron with momentum $\vec{p}$ also in the coordinate space. $\vec{p}_i$ and $\vec{p}_f$ are the momenta of the colliding electron before and after interaction. $E_\alpha = (1-\lambda^2)^{1/2}$, $E_{\alpha'} = (1+p^2)^{1/2}$ are, respectively, the energies of the states $U_\alpha^{(1)}(\vec{r}_1)$ and $U_{\alpha'}^{(1)}(\vec{r}_1)$. $\vec{t} = (\vec{p}_i - \vec{p}_f)$ is the momentum transfer vector and $\vec{\epsilon}$ is the polarization vector of the exchanged photon and $E_{\alpha'\alpha} = E_{\alpha'} - E_\alpha$. (We shall use a natural system of units unless otherwise stated.)

Because of the absence of an energy term in the denominator of the first term in Eq. (1), it is natural that one may suspect that retardation effects have not been included. But this is not true. The second term alone represents the full retardation effect and the first term represents the Coulomb effect. It may be mentioned here that the above cross section is exact to the first order in α^2 to the extent of the omission of the spin-orbit interaction of the atomic electron.

Now we take for $U_\alpha^{(1)}(\vec{r}_1)$ and $U_{\alpha'}^{(1)}(\vec{r}_1)$ the following expressions, which are correct[7] to the first order in $\lambda = (\alpha Z)$:

$$U_\alpha^{(1)}(\vec{r}_1) = \int d\vec{q}\, V_\alpha(\vec{q})\, e^{i\vec{q}\cdot\vec{r}_1} , \qquad U_{\alpha'}^{(1)}(\vec{r}_1) = \int d\vec{q}\,'\, V_{\alpha'}(\vec{q}\,')\, e^{i\vec{q}\,'\cdot\vec{r}_1} , \quad (3)$$

where

$$V_\alpha(\vec{q}) = \frac{N\lambda}{2\pi^2} \frac{2 + \vec{\alpha}^{(1)}\cdot\vec{q}}{(q^2+\lambda^2)^2}\, \chi^{(1)}(0) ,$$

$$V_{\alpha'}(\vec{q}\,') = \left(\delta(\vec{q}\,' - \vec{p}) + \frac{\lambda}{2\pi^2} \frac{\vec{\alpha}^{(1)}\cdot\vec{q}\,' + \beta^{(1)} + W(\vec{q}\,')}{(\vec{q}\,' - \vec{p})^2 [q'^2 - p^2 - i\delta]} \right) \chi^{(1)}(\vec{p}) ,$$

and the normalization constant

$$N=\left(\frac{[1+(1-\lambda^2)^{1/2}](2\lambda)^{2(1-\lambda^2)^{1/2}+1}}{8\pi\Gamma[2(1-\lambda^2)^{1/2}+1]}\right)^{1/2}$$

$$\simeq(\lambda^3/\pi)^{1/2}\,.$$

Now the matrix element M_1 may be written as

$$M_1=(4\pi N\lambda)\chi^{(2)*}(\vec{p}_f)\chi^{(2)}(\vec{p}_i)\int d\vec{q}\,\chi^{(1)*}(\vec{p})\left[\left(\delta(\vec{q}-\vec{p})\right.\right.$$

$$\left.\left.+\frac{\lambda}{2\pi^2}\,\frac{\vec{\alpha}^{(1)}\cdot\vec{q}+\beta^{(1)}+W(\vec{q})}{(\vec{p}-\vec{q})^2(q^2-p^2+i\delta)}\right)\left(\frac{2+\vec{\alpha}^{(1)}\cdot(\vec{t}-\vec{q})}{[(\vec{t}-\vec{q})^2+\lambda^2]^2}\right)\right]\chi^{(1)}(0)\,. \tag{4}$$

One can very easily integrate[8] the expressions correct to the lowest order in λ using Feynmann integrals. The result to the lowest order in λ is

$$M_1=(4\pi N\lambda)\chi^{(2)*}(\vec{p}_f)\chi^{(2)}(\vec{p}_i)\chi^{(1)*}(\vec{p})\left(\frac{2+\vec{\alpha}^{(1)}(\vec{t}-\vec{p})}{[(\vec{t}-\vec{p})^2+\lambda^2]^2}\right.$$

$$\left.+\frac{\vec{\alpha}^{(1)}\cdot\vec{t}+\beta^{(1)}+W(t)}{(\vec{t}-\vec{p})^2[t^2-p^2-2p\lambda i]}\right)\chi^{(1)}(0)\,. \tag{5}$$

Summing over polarization directions and integrating over coordinate space, the matrix element M_2 may be similarly expressed to the lowest order in λ as

$$M_2=4\pi N\lambda\left[\sum_{j=1}^{3}\chi^{(2)*}(\vec{p}_f)\alpha_j^{(2)}\chi^{(2)}(\vec{p}_i)\chi^{(1)*}(\vec{p})\right.$$

$$\times\left(\frac{2\alpha_j^{(1)}}{[(\vec{t}-\vec{p})^2+\lambda^2]^2}+\frac{\vec{\alpha}^{(1)}\cdot\vec{t}+\beta^{(1)}+W(t)}{(\vec{t}-\vec{p})^2[\vec{t}^2-\vec{p}^2-2p\lambda i]}\;\alpha_j^{(1)}\right)\chi^{(1)}(0)$$

$$-\frac{1}{t^2}\chi^{(2)*}(\vec{p}_f)(\vec{\alpha}^{(1)}\cdot\vec{t})\chi^{(2)}(\vec{p}_i)\chi^{(1)*}(\vec{p})\left(\frac{2(\vec{\alpha}^{(1)}\cdot\vec{t})}{[(t-\vec{p})^2+\lambda^2]^2}\right.$$

$$\left.\left.+\frac{\vec{\alpha}^{(1)}\cdot\vec{t}+\beta^{(1)}+W(t)}{(\vec{t}-\vec{p})^2[t^2-p^2-2p\lambda i]}\;(\vec{\alpha}^{(1)}\cdot\vec{t})\right)\chi^{(1)}(0)\right]. \tag{6}$$

With the above expressions for M_1 and M_2, the differential cross section in the extreme relativistic limit is

$$d\sigma^I=\frac{1}{\pi}4\alpha^2N^2\lambda^2W_i^2\,p\,dW(p)\,d\Omega_p\,d\Omega_{p_f}\left\{\left[\frac{4[W(p)+1]+4(\vec{p}\cdot\vec{t})-4p^2}{t^4[(\vec{t}-\vec{p})^2+\lambda^2]^4}+\frac{[W(p)W(t)+W(p)+W(t)+1][W(t)+1]+(\vec{p}\cdot\vec{t})}{t^4(\vec{t}-\vec{p})^4[(t^2-p^2)^2+4p^2\lambda^2]}\right.\right.$$

$$\left.+\frac{2(t^2-p^2)[4W(p)\,W(t)+4(\vec{p}\cdot\vec{t})-2p^2]}{t^4(\vec{t}-\vec{p})^2[(t^2-p^2)^2+4p^2\lambda^2][(\vec{t}-\vec{p})^2+\lambda^2]^2}\right]+\left[\frac{2[p_i^2-(\vec{p}_i\cdot\vec{t})(\vec{p}_f\cdot\vec{t})/t^2]}{W_i^2[t^2-E_{\alpha',\alpha}^2]^2}\right.$$

$$\left.\left.\times\left(\frac{p^2}{[(\vec{t}-\vec{p})^2+\lambda^2]^4}+\frac{t^2}{(\vec{t}-\vec{p})^4[(t^2-p^2)^2+4p^2\lambda^2]}+\frac{2(t^2-p^2)(\vec{p}\cdot\vec{t})}{(\vec{t}-\vec{p})^2[(\vec{t}-\vec{p})^2+\lambda^2]^2[(t^2-p^2)^2+4p\lambda^2]}\right)\right]\right\}. \tag{7}$$

The terms in the first large square brackets correspond to the contribution from a pure-Coulomb interaction, while those in the second large square brackets arise from the interaction with the transverse radiation field. Again, the first term in the large square brackets corresponds to the plane-wave part of the ejected electron, the second term arises from the Coulomb distortion and is due to the second part of $V_{\alpha'}(\vec{q}\,')$, and the third term arises from interference of these two parts. We now integrate over angles of $\vec{p}_f$. The exact evaluation of these integrals would be difficult even if we use Feynmann techniques. This may be avoided if we note that the denominators of the different terms have factors like t^4 and $(\vec{t}-\vec{p})^4$ which make the terms having sharp peaks along certain directions, particularly for large p_i. This makes it easy to calculate the integrals by taking into account contributions from these peaks separately. To justify the procedure we next give a quantitative estimate of these peaks.

B. Quantitative Analysis of Peaks of the Differential Cross Section

The differential cross section given by Eq. (7) contains some strongly varying functions of angles of $\vec{p}_f$ and these give rise to certain peaks. For example,

$$J=1/\{t^4(\vec{t}-\vec{p})^4[(t^2-p^2)^2+4p^2\lambda^2]\}$$

is such a function. If we consider $p<1$ then $W\simeq 1+\frac{1}{2}p^2$ and the minimum value of t^2 may be shown to be

$$(t^2)_{\min}=(p_i-p_f)^2\simeq[(1+p^2)^{1/2}-(1-\lambda^2)^{1/2}]^2$$

$$\simeq[\tfrac{1}{2}(p^2+\lambda^2)]^2\ll 1.$$

Now the function J has certain peaks, particularly for large p_i, and these peaks correspond to the following directions:

(i) $\theta_f=0$ (for min of t^4, i.e., for $\vec{p}_f\parallel\vec{p}_i$),

$$J\sim 1/\{[\tfrac{1}{2}(p^2+\lambda^2)]^2+p_i^2\Delta\theta_f^2\}$$

$$\times\{[\tfrac{1}{2}(p^2+\lambda^2)]^2+p^2-p(p^2+\lambda^2)\cos\theta_f\}^2$$

$$\times\{[(\tfrac{1}{2}(p^2+\lambda^2))^2-p^2]^2+4p^2\lambda^2\};$$

(ii) $\theta_f \simeq p\sin\theta_p/p_i$, $\varphi_f=0$ [for min of $(\vec{t}-\vec{p})^4$, i.e., for $\vec{p}_f \parallel (\vec{p}_i-\vec{p})$],

$$J\sim 1/\{[\tfrac{1}{2}(p^2+\lambda^2)]^2+p^2\sin\theta_p\}^2 \times\{[\tfrac{1}{2}(p^2+\lambda^2)-p\cos\theta_p]^2+p_i^2\Delta\theta_f^2\}^2 \times\{[(\tfrac{1}{2}(p^2+\lambda^2))^2-p\cos^2\theta_p]^2+4p^2\lambda^2\}\,;$$

(iii) $\theta_f\simeq p/p_i$ {for min of $[(t^2-p^2)^2+4p^2\lambda^2]$, i.e., for $t^2=p^2$},

$$J\sim 1/\{[\tfrac{1}{2}(p^2+\lambda^2)]^2+p^2\}^2\{[\tfrac{1}{2}(p^2+\lambda^2)]^2+2p^2(1-\cos\theta_p)\}^2 \times[4p^2p_i^2\Delta\theta_f^2+4p^2\lambda^2]\,.$$

For $\theta_p\neq 0$ or $\pi/2$ these peaks are well separated.

Now we consider the following two cases.

Case (a) $p\sim\lambda$. For $\theta_f=0$, the three factors in J are of the orders λ^{-8}, λ^{-4}, λ^{-4}, so that J is of the order λ^{-16}. For $\theta_f\simeq p\sin\theta_p/p_i$, $\varphi_f=0$, the corresponding three factors and the function J are of the orders λ^{-4}, λ^{-4}, λ^{-4}, and λ^{-12}, respectively. Finally, for $\theta_f=p/p_i$, the factors in J and the function J are of the orders λ^{-4}, λ^{-4}, λ^{-4}, and λ^{-12}. This shows that the forward peak is large compared to other peaks for such order of momentum. If we consider the third factor in particular, we find it to vary smoothly over a wide region covering the forward peak. Its value at $\theta_f=0$ is approximately equal to $\frac{1}{5}\lambda^{-4}$, but at $\theta_f=p/p_i$ it is approximately $\frac{1}{4}\lambda^{-4}$ (maximum value). The forward peak is very narrow because the dominating factor t^{-4} falls off from its maximum value to one-fourth of it only at an angle $\theta_f\simeq\lambda^2/p_i$ (which is considerably closer to $\theta_f=0$ than the positions of other peaks). Thus for the function in question and for $p\sim\lambda$, the most significant peak is the forward peak and not the one which corresponds to $t^2=p^2$.

Case (b) $\lambda\ll p<1$. To have an idea of the magnitude of the peaks in this case, we consider the particular point $p=\frac{2}{3}$ of the position of the Parzen peak for $W_i=60$. Here we compare only the forward peak with that corresponding to $t^2=p^2$ and we see their relative importance. For $Z=20(\lambda\sim\frac{1}{7})$, the forward peak has a magnitude of the order $J\sim 400\times 2\times 5=4000$ while at the peak corresponding to $t^2=p^2$, $J\sim 5\times\frac{1}{2}\times 30=75$. For $Z=10(\lambda\sim\frac{1}{4})$, corresponding orders of magnitude of the two peaks are 4000 and 300, respectively. The location of the third peak is at $\theta_f\simeq p/p_i=2/(3p_i)$ while the factor t^{-4} falls to one-fourth its maximum value at $\theta_f\simeq 2/(9p_i)$.

Now, compiling the results of the above two cases, we may safely say that for $0<p<1$ and $Z\gg 1$, the peak corresponding to $t^2=p^2$ is insignificant compared to the other peaks so far as integration of J over angles of $\vec{p}_f$ is concerned. For some other parts of $d\sigma^I$, the peaks corresponding to $\vec{p}_f \parallel (\vec{p}_i-\hat{p})$ are most significant, and in no case are the $t^2=p^2$ peaks important. Thus considering all strongly varying functions of $d\sigma^I$ in Eq. (7), one may state that the peaks corresponding to $\theta_f=0$ and $\theta_f\simeq p\sin\theta_p/p_i$, $\phi_f=0$ are the most significant ones where integration is concerned. However for $Z\sim 1$, the peak corresponding to $t^2=p^2$ gives the dominant contribution.

C. Integration of Differential Cross Section over Angles of $\vec{p}_f$

The analysis of Sec. II B now indicates a way[9] for carrying out integration of $d\sigma^I$ over angles of $\vec{p}_f$. Thus to integrate the terms containing

$$1/\{t^4(\vec{t}-\vec{p})^4[(t^2-p^2)^2+4p^2\lambda^2]\}\,,$$

we make the following approximation:

$$1/\{t^4(\vec{t}-\vec{p})^4[(t^2-p^2)^2+4p^2\lambda^2]\} \simeq\frac{1}{t^4}\left(\frac{1}{(\vec{t}-\vec{p})^4[(t^2-p^2)^2+4p^2\lambda^2]}\right)_{\vec{p}_f\parallel\vec{p}_i} +\frac{1}{(\vec{t}-\vec{p})^4}\left(\frac{1}{t^4[(t^2-p^2)^2+4p^2\lambda^2]}\right)_{\vec{p}_f\parallel(\vec{p}_i-\vec{p})}\,.$$

The two parts may now be separately integrated and then added to find the total contribution. In our present calculation we shall further put $\vec{p}=\vec{t}=0$ in the numerators of the terms of Eq. (7) other than those in the second square bracket where appropriate values are substituted. Integrating in this way we get the following result:

$$d\sigma^I=\frac{4\alpha^2\lambda^5 p\,dW(p)\,d\Omega_p}{\pi}\left\{\left[\frac{32}{(p^2+\lambda^2)^6[1-p\cos\theta_p+\frac{1}{4}(p^2+\lambda^2)]^4}\right.\right.$$
$$+\frac{8}{3[(\frac{1}{2}(p^2+\lambda^2)-p\cos\theta_p)^2+\lambda^2]^3\,[(\frac{1}{2}(p^2+\lambda^2))^2+p^2\sin^2\theta_p]^2}$$
$$+\frac{32}{(p^2+\lambda^2)^2[(\frac{1}{2}(p^2+\lambda^2))^2-p\cos\theta_p(p^2+\lambda^2)+p^2]^2\{[(\frac{1}{2}(p^2+\lambda^2))^2-p^2]^2+4p^2\lambda^2\}}$$
$$+\frac{8}{[\frac{1}{2}(p^2+\lambda^2)-p\cos\theta_p]^2[(\frac{1}{2}(p^2+\lambda^2))^2+p^2\sin^2\theta_p]^2\{[(\frac{1}{2}(p^2+\lambda^2))^2-p^2\cos^2\theta_p]^2+4p^2\lambda^2\}}$$

$$
\begin{aligned}
&-\frac{32[p^2-(\frac{1}{2}(p^2+\lambda^2))^2]}{(p^2+\lambda^2)^4[1-p\cos\theta_p+\frac{1}{4}(p^2+\lambda^2)]^2\,[(\frac{1}{2}(p^2+\lambda^2))^2-p\cos\theta_p(p^2+\lambda^2)+p^2]\{[(\frac{1}{2}(p^2+\lambda^2))^2-p^2]^2+4p^2\lambda^2\}} \\
&+\frac{8[(\frac{1}{2}(p^2+\lambda^2))^2-p^2\cos^2\theta_p]}{\lambda^2[(\frac{1}{2}(p^2+\lambda^2))^2+p^2\sin^2\theta_p]^2\,\{[(\frac{1}{2}(p^2+\lambda^2))^2-p^2\cos^2\theta_p]^2+4p^2\lambda^2\}} \\
&\times\left(\frac{1}{\lambda^2}\ln\frac{[\frac{1}{2}(p^2+\lambda^2)-p\cos\theta_p]^2+\lambda^2}{[\frac{1}{2}(p^2+\lambda^2)-p\cos\theta_p]^2}-\frac{1}{[\frac{1}{2}(p^2+\lambda^2)-p\cos\theta_p]^2+\lambda^2}\right)\Bigg] \\
&+2\,[\ln W_i^2-1]\Bigg[\frac{4p^2}{(p^2+\lambda^2)^6[1-p\cos\theta_p+\frac{1}{4}(p^2+\lambda^2)]^4} \\
&+\frac{1}{[(\frac{1}{2}(p^2+\lambda^2))^2-p\cos\theta_p(p^2+\lambda^2)+p^2]^2\,\{[(\frac{1}{2}(p^2+\lambda^2))^2-p^2]^2+4p^2\lambda^2\}} \\
&-\frac{4p\cos\theta_p[p^2-(\frac{1}{2}(p^2+\lambda^2))^2]}{(p^2+\lambda^2)^3\,[(\frac{1}{2}(p^2+\lambda^2))^2-p\cos\theta_p(p^2+\lambda^2)+p^2]^2\,[1-p\cos\theta_p+\frac{1}{4}(p^2+\lambda^2)]^2\,\{[(\frac{1}{2}(p^2+\lambda^2))^2-p^2]^2+4p^2\lambda^2\}}\Bigg]\Bigg\}\;.
\end{aligned}
\tag{8}
$$

The above result is in conformity with the observation of Fano,[10] since the terms in the first square bracket, which corresponds to the Coulomb contribution, are independent of the incoming electron energy, while the terms in the second square bracket, whose origin is the interaction with the transverse radiation field, have a logarithmic dependence on the incoming electron energy. In our numerical evaluation of the result, it was observed that for $p \ll 1$ the radiative part gives only an insignificant contribution, while for $p\sim 1$ this part gives the dominant contribution. In fact for $p=\frac{2}{3}$, the radiative part contributes approximately two-thirds of the total cross section.

III. RESULT AND CONCLUDING REMARKS

We first observe that the results of the present calculation are most suitable for application to the cross section for ejection of electrons in the momentum range $\lambda mc \ll p < mc$ and $Z \gg 1$; this is the region in which the Parzen peak is situated. In this region the scattering cross section has an explicit $(\alpha Z)^5$ dependence in contrast to the $(\alpha Z)^4$ dependence obtained by Weber *et al.*

For a comparison of the present calculation with that of Weber *et al.* we have presented the numerical results in Fig. 1. The results of Parzen *et al.* for the bremsstrahlung electrons are shown in the same graph. In this figure the dimensionless quantity $\Sigma = 4\pi m_e d\sigma^I/Z^2 r_0^2 dW(p)d\Omega_p$ has been plotted against p for $0\le p\le 100\alpha mc$ in the case of the calcium atom ($Z=20$) for incoming electron energy $W_i = 60mc^2$, and for the particular ejection angle $\theta_f = 120°$. In this graph we have shown the results of Weber *et al.* for the momentum interval $\lambda mc \le p \le 100\alpha mc$ and the Parzen distribution in the interval $60\alpha mc \le p \le 100\alpha mc$. We may note that the interval $60\alpha mc\le p\le 100\alpha mc$ is a good region for the validity of our result in the case of the calcium atom and is the region in which the Parzen peak lies. From the graph it is clear that the Parzen distribution is insignificant compared to the distribution of electrons scattered by bound electrons. In some parts of the region the result of the present calculation is as large as eight times the result of Weber *et al.*

We have used a first Born approximation for the wave function of the ejected electron. This is much better than the plane-wave approximation, but may still not give accurate results for very small mo-

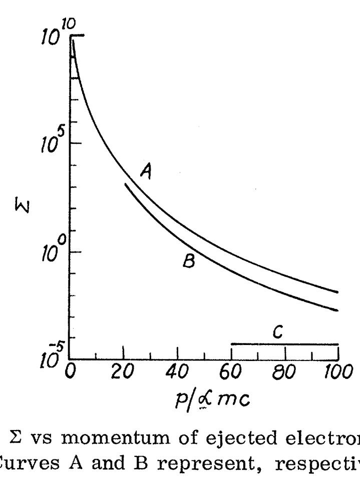

FIG. 1. Σ vs momentum of ejected electrons in units of αmc. Curves A and B represent, respectively, the dimensionless quantity Σ, as calculated from Eq. (8) of the present paper and Eq. (25) of Ref. 2 for $Z=20$, $\theta_p = 120°$, $W_i = 60mc^2$. Curve C represents the corresponding Parzen distribution (the graph fails to reveal the Parzen peak that exists at about $p\simeq 90\alpha mc$).

mentum, viz., $p \lesssim \alpha Zmc$ since the Born approximations are valid for $p \gg \alpha Zmc$. However the results for $p \lesssim \alpha Zmc$ may be used for a qualitative discussion and for a future comparison with an exact calculation. It may be mentioned in this connection that the transverse radiation field contribution is important only at higher energies. Thus for $p = 40\alpha mc$ it is about 8%, while for $p = 100\alpha mc$ the transverse field contribution is about 72%.

We may further note that the differential cross section given by Eq. (8) cannot be simply integrated to get the total cross section. This is due to the presence of the term

$$\{[\tfrac{1}{2}(p^2+\lambda^2)]^2 - p\cos\theta_p\}^2 \simeq (p^2/2 - p\cos\theta_p)^2$$

for $\lambda \ll p$ in the denominator of $d\sigma^I$ which vanishes at certain small angles. Cutoff in angle is therefore necessary to find the total cross section, as it is in the Rutherford cross section. If we compare this with the result of Weber *et al.*, we find in its place their result contains a term

$$(W - 1 - p\cos\theta_p)^3 \simeq (\tfrac{1}{2}p^2 - p\cos_p)^3 ,$$

which makes their result for cross section even more divergent. Moreover, because of the third power, the term changes sign about its zero giving an unrealistic negative value to their calculated cross section for certain small angles. However, since they considered $\theta_p > 90°$, their result was positive definite. It may be mentioned in this connection that the divergence of our result is not due to the technique we used in evaluating the integrals, but is inherent in the approximate form of the wave function [Eq. (3)] used.

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[1]G. W. Ford and C. J. Mullin, Phys. Rev. 110, 520 (1958).

[2]T. A. Weber, R. T. Deck, and C. J. Mullin, Phys. Rev. 130, 660 (1963).

[3]D. G. Keiffer and G. Parzen, Phys. Rev. 110, 1244 (1956).

[4]See Eq. (21) of Ref. 2.

[5]This may be compared with Eq. (2) in the article by U. Fano, Phys. Rev. 102, 385 (1956).

[6]This point was recently brought to the attention of the author, and in the author's opinion it is essential for getting accurate results for extremely low energies.

[7]The above expressions were given by M. Gavrila in his paper [Phys. Rev. 113, 514 (1959)] on photo-ionization. Weber *et al.* used the same approximate wave functions in their calculation (Ref. 2).

[8]Various integrals of these types were evaluated and discussed by Gavrila in his paper (Ref. 7).

[9]For further justification of our procedure, we may note that R. H. Dalitz has used a similar technique in evaluating some integrals similar to those of ours in his paper [Proc. Roy. Soc. (London) A206, 509 (1951)].

[10]See discussion after Eq. (3) of Ref. 5.

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Nonadiabatic Effects in Slow Atomic Collisions. I. $He^+ + He$[†]

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In the collision $He^+ + He \rightarrow He^+ + He^*$, excitation at low incident ion energies ($\lesssim 1$ keV) proceeds via a pseudocrossing of the elastic ${}^2\Sigma_g$ diabatic potential with excited-state ${}^2\Sigma_g$ potentials. As previously reported, this excitation mechanism fails to explain diverse experimental data concerning total excitation cross sections. A new physical mechanism is hypothesized, its existence verified, and it is shown to provide good qualitative and semiquantitative interpretation of the observations. Nonadiabatic couplings among some excited states occur at pseudocrossings of the respective inelastic-channel molecular potentials at large internuclear separations, resulting in coherent phase interference in the inelastic-scattering amplitudes. A linear-combination-of-atomic-orbitals (LCAO) calculation of 18 excited-state ${}^2\Sigma_g$ potentials of the intermediate $(He_2^+)^*$ system verifies the presence of these outer pseudocrossings. Such a mechanism is shown to be likely in many ion-atom collisions.

I. INTRODUCTION

Over the past decade, high-resolution experiments involving low-velocity ($\lesssim 0.1$ a.u.) ion-atom collisions have led to an increased awareness of the important role played by the molecular potentials of the intermediate (molecular ion) collision complex. In elastic charge-exchange collisions between homonuclear ion-atom systems (e.g., $p + H$, $He^+ + He$), the differential cross sections exhibit an