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Infinite-Channel Close-Coupling Theory in the Second Born Approximation. I. Charge Polarization in the Elastic Electron Scattering from H and He† *

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One of the oldest methods suggested for treating the effect of charge polarization on elastic scattering is revived by the use of certain physically reasonable assumptions, and is shown to lead to results, in the limit of small scattering angles and high incident energies, which are in quantitative agreement with experimental and theoretical expectations. The theory is worked out in detail for one- and two-electron atoms, and the extension to more complex systems is also discussed. The effect of charge polarization on the elastic differential cross section for 500-eV incident electrons on He is calculated and compared with the experimental results of Bromberg and the theoretical results of LaBahn and Callaway. The agreement is good over the angular range $0° \leq \theta < 6°$ if exchange scattering contributions are included.

I. INTRODUCTION

Numerous treatments of charge polarization or charge distortion of the target on scattering by charged particles have been considered.[1] These methods can be put into two classifications. The first will consist of the so-called rigorous methods which are designed for use in the region of low incident energy of the bombarding charged particle. Such methods, in the case of electron scattering from atoms and molecules, become computationally messy at energies above 100 eV because of the proliferation of open excitation channels. The second class of methods, generally more empirical in nature, either simplify rigorous theory by the use of approximations or use parametrized models to represent the polarizing process.

One of the oldest methods of the second type, which is here called "the infinite-channel close-coupling theory in the second Born approximation," was first suggested by Massey and Mohr[2] and is the method to be dealt with in this paper. It simply consists of writing the coupled-channel differential equations, neglecting exchange and relativistic effects, in the form

$$\begin{aligned}
(\nabla^2 + k^2) f_0(\vec{r}) &= \sum_{l=0}^{\infty} U_{0l}(\vec{r}) f_l(\vec{r}) \ , \\
(\nabla^2 + k_1^2) f_1(\vec{r}) &= \sum_{l=0}^{\infty} U_{1l}(\vec{r}) f_l(\vec{r}) \ , \\
&\ \ \vdots \qquad\qquad \vdots \\
(\nabla^2 + k_n^2) f_n(\vec{r}) &= \sum_{l=0}^{\infty} U_{nl}(\vec{r}) f_l(\vec{r}) \ ,
\end{aligned} \tag{1}$$

where k^2 is the incident energy, $k_n^2 = k^2 - \Delta E_{0n}$ is the scattered energy after exciting the target to the state n, and $f_n(\vec{r})$ is the wave function for the scattering process where the scatterer is initially in its ground state and is left in its nth excited state. The interaction potential $U_{nl}(\vec{r})$ is given as

$$U_{nl}(\vec{r}) = \frac{2m}{m_0} \left\langle \psi_n(\vec{r}_1, \ldots, \vec{r}_N) \right| -\frac{z}{r} + \sum_{i=1}^{N} \frac{1}{|\vec{r} - \vec{r}_i|} \left| \psi_l(\vec{r}_1, \ldots, \vec{r}_N) \right\rangle \ , \tag{2}$$

where m/m_0 is the electron mass ratio $(1 - v^2/c^2)^{-1/2}$ introduced to provide the main relativistic effects on the scattered electron in the forward scattering direction with incident energies less than 50 keV.

Note, also, that the relativistic value of $k = 2\pi/\lambda$ for the incident electron is used throughout. The approximate method of treating relativistic effects is good to at least 2% or better for incident energies less than 50 keV. The interaction potential is given here for the case of atomic scattering and ψ_n and ψ_l are the stationary-state eigenfunctions for the nth and lth bound state of the scatterer, respectively. Equation (1) can be put into the form of an integral equation as

$$\begin{pmatrix} f^{(n)}(\vec{r}) \\ f_1^{(n)}(\vec{r}) \\ \vdots \\ f_N^{(n)}(\vec{r}) \\ \vdots \end{pmatrix} = \begin{pmatrix} e^{ikz} \\ 0 \\ \vdots \\ 0 \\ \vdots \end{pmatrix} + \begin{pmatrix} (\nabla^2+k^2)^{-1}U_{00}(\vec{r}), & (\nabla^2+k^2)^{-1}U_{01}(\vec{r})\cdots(\nabla^2+k^2)^{-1}U_{0N}(\vec{r})\cdots \\ (\nabla^2+k_1^2)^{-1}U_{10}(\vec{r}), & (\nabla^2+k_1^2)^{-1}U_{11}(\vec{r})\cdots(\nabla^2+k_1^2)^{-1}U_{1N}(\vec{r}) \\ \vdots & \vdots \\ (\nabla^2+k_N^2)^{-1}U_{N0}(\vec{r}), & (\nabla^2+k_N^2)^{-1}U_{N1}(\vec{r})\cdots(\nabla^2+k_N^2)^{-1}U_{NN}(\vec{r})\cdots \\ \vdots & \vdots \end{pmatrix} \begin{pmatrix} f_0^{(n-1)}(\vec{r}) \\ f_1^{(n-1)}(\vec{r}) \\ \vdots \\ f_N^{(n-1)}(\vec{r}) \\ \vdots \end{pmatrix}, \tag{3}$$

where e^{ikz} is an incident plane wave, the superscripts n and $n-1$ denote successive approximations to a particular wave function, and the integral operators are the usual Green's functions for an outgoing scattered wave. In order to obtain the first Born approximation, the column vector on the right-hand side of Eq. (3) is replaced by the column vector containing the incident plane wave for $f_0^{(0)}(\vec{r})$ and zero for the other elements. This zeroth-order guess produces, upon carrying out the indicated operations, the following familiar asymptotic results at large distances from the scatterer:

$$\begin{pmatrix} f_0^{(1)}(\vec{r}) \\ f_1^{(1)}(\vec{r}) \\ f_N^{(1)}(\vec{r}) \end{pmatrix} = \begin{pmatrix} \dfrac{e^{ikr}}{r}\left[-\dfrac{1}{4\pi}\displaystyle\int d\vec{r}\,' \, U_{00}(\vec{r})\, e^{i\vec{K}_{00}\cdot\vec{r}\,'}\right] \\ \dfrac{e^{ik_1 r}}{r}\left[-\dfrac{1}{4\pi}\displaystyle\int d\vec{r}\,' \, U_{10}(\vec{r}\,')\, e^{i\vec{K}_{10}\cdot\vec{r}\,'}\right] \\ \dfrac{e^{ik_N r}}{r}\left[-\dfrac{1}{4\pi}\displaystyle\int d\vec{r}\,' \, U_{N0}(\vec{r}\,')\, e^{i\vec{K}_{N0}\cdot\vec{r}\,'}\right] \end{pmatrix}_{\text{asymp}},$$

where the terms in square brackets in the column vector on the right-hand side are just the first Born scattering amplitudes. The second Born approximation is obtained by iteration from the nonasymptotic form of the first, and can be written for elastic scattering as

$$f_{00}^{(2)} = \sum_{l=0}^{M} \frac{1}{2\pi^2} \int \frac{d\vec{q} f_{l0}^{(1)}(\vec{k}_i - \vec{q}) f_{0l}^{(1)}(\vec{q} - \vec{k}_s)}{q^2 - k_l^2 - i\epsilon},$$

where the energy for the quantum state labeled M is k^2, $E_M = k^2$, and the double-subscript notation indicates that the f's are now asymptotic scattered amplitudes. The second Born approximation for the scattered amplitude thus depends only on a knowledge of the first-Born-approximation amplitudes

$$f_{0l}^{(1)}(\vec{k}_i - \vec{q}) = -(1/4\pi)\int d\vec{r}\,' \, U_{l0}(\vec{r}\,') e^{i(\vec{k}_i - \vec{q})\cdot\vec{r}\,'},$$

$$f_{l0}^{(1)}(\vec{q} - \vec{k}_s) = -(1/4\pi)\int d\vec{r}\,' \, U_{0l}(\vec{r}\,') e^{i(\vec{q} - \vec{k}_s)\cdot\vec{r}\,'}, \tag{4}$$

where k_i is the incident wave vector and k_s is the scattered wave vector and both have the same magnitude k. In order to obtain a simple approximation for the charge polarization, it will be assumed that the incident energy is sufficiently high so that closure can be approximately invoked ($E_M = k^2 \simeq \infty$). This is what is meant by infinite-channel close-coupling theory. Since the charge polarization depends only on the terms for which $l \neq 0$, the result for the polarization amplitude is

$$f_{\text{pol}}(\theta) = \frac{2m^2}{\pi^4 m_0^2} \int \frac{d\vec{q}}{q^2 - \hat{k}_l^2 - i\epsilon} \times \left(\left\langle \psi_0 \middle| \sum_{i=1}^{N} e^{i(\vec{k}_i - \vec{q})\cdot\vec{r}_i} \sum_{j=1}^{N} e^{i(\vec{q} - \vec{k}_s)\cdot\vec{r}_j} \middle| \psi_0 \right\rangle - \sum_{i=1}^{N}\sum_{j=1}^{N} \langle \psi_0 | e^{i(\vec{k}_i - \vec{q})\cdot\vec{r}_i} | \psi_0 \rangle \langle \psi_0 | e^{i(\vec{q} - \vec{k}_s)\cdot\vec{r}_j} | \psi_0 \rangle \right) \times |\vec{k}_i - \vec{q}|^{-2} \cdot |\vec{q} - \vec{k}_s|^{-2}, \tag{5}$$

where not only must a complete set of states be assumed to be available but $k_l^2 = k^2 - \Delta E_{0l}$ must be replaced by an average value independent of l denoted as $\hat{k}_l^2$.

The main reason why this approach has not been widely used previously is because of the ambiguity in the choice of $\hat{k}_l$ and, in part, because of the supposed numerical complexity of the resultant integrals.

Massey and Mohr[2] were able to show that the real part of f_{pol} given in Eq. (5) behaved as if it were determined by an effective potential which varied in the limit of large r as $-c/r^4$, as expected,

and they speculated that the imaginary part must be closely related to the inelastic scattering. Moiseweitsch[3] showed that if $\hat{k}_I$ were simply chosen as k then the resultant integrals would be singular at the origin. The author attempted to evaluate Eq. (5) including corrections for the inclusion of excited states not accessible to the incident energy by interpreting the infinity discussed by Moiseweitsch as a constant phase factor and choosing the constant so that the polarization amplitude vanished in the limit of large scattering angles.[4] This last work contains an error because of the retention of the nuclear interaction in the potential [see Eq. (5) for the correct form].

A further effort to utilize this approach in a meaningful way is dictated by the wealth of experimental data accumulated over the past few years,[5] which seems to indicate that the first Born amplitude provides an excellent description of the optically allowed inelastic processes which, for high incident energy, constitute the major contribution to the total inelastic scattering in the small-angle region. Note, that if $f_{0I}^{(1)}$ is in fact exact, then the Born series converges at this point and Eq. (5) provides the exact description of charge polarization except for corrections from the two approximations made in its derivation. Therefore, experimental results would seem to indicate strongly that the use of Eq. (5) is justified in the small-scattering-angle region at incident energies of 200 eV or more in the case of electron scattering.

It was recently pointed out by the author, that by use of the plane-wave approximation a simple form for the absorptive part (imaginary part) of Eq. (5) could be obtained if $\hat{k}_I$ was chosen to be given by $\hat{k}_I = (k^2 - \Delta E_{01})^{1/2}\cos\theta$.[6] The result was not only finite at the origin, but yielded an amplitude such that $(4\pi/k)f_{\text{pol}}(0)$ reduced to the expression for the total inelastic scattering

$$\sigma_{\text{tot}} = (4\pi/a^2k^2)\int_{K^2_{\text{min}}}^{4k^2} dK^2 S(K)/K^4 ,$$

where a is the relativistic Bohr radius $\hbar^2/me^2$, $S(K)$ is the Heisenberg (Thomas-Fermi) inelastic scattering factor, and $K^2_{\text{min}} = \Delta E^2_{01}/4k^2$ with ΔE_{01} the resonance energy of the atom. The reason for the choice was that $k\cos\theta$ gives the proper approximate angular dependence of the average energy loss on scattering,[7] with the added condition that all inelastic scattering vanishes at 90°. The addition of ΔE_{01} was needed to eliminate the singularity at $\theta = 0$ by limiting the momentum transfer to its minimum allowed value. The choice of $\hat{k}_I$ can be further improved by choosing an effective or mean excitation energy in place of ΔE_{01} as ΔE_m in such a way that the closure result for the total inelastic differential cross section has the exact asymptotic value in the limit as $\theta \to 0$ and $k \to \infty$.[8] This choice results in the expression

$$\Delta E_m = [\,\mathcal{S}(-1)/\mathcal{S}(-3)]^{1/2},$$

where $\mathcal{S}(-1)$ and $\mathcal{S}(-3)$ are the oscillator strength sums

$$\mathcal{S}(-1) = \sum_{n=0}^{\infty} \left\langle \psi_0 \middle| \sum_{i=1}^{N} z_i \middle| \psi_n \right\rangle \left\langle \psi_n \middle| \sum_{j=1}^{N} z_j \middle| \psi_0 \right\rangle = \left\langle \psi_0 \middle| \sum_{i=1}^{N}\sum_{j=1}^{N} z_i z_j \middle| \psi_0 \right\rangle ,$$

$$\mathcal{S}(-3) = \sum_{n\neq 0}^{\infty} \left\langle \psi_0 \middle| \sum_{i=1}^{N} z_i \middle| \psi_n \right\rangle \frac{1}{(\Delta E_{0n})^2} \left\langle \psi_n \middle| \sum_{j=1}^{N} z_j \middle| \psi_0 \right\rangle ,$$

where z_i is the projection of the position vector $\vec{r}_i$ of the ith electron on the z axis. Values for $\mathcal{S}(-1)$ and $\mathcal{S}(-3)$ can be obtained from the wavelength dependence of the refractive index or from theoretical calculation in the case of He. The value of ΔE_m for He is 28.0 eV and 11.6 eV for H. An even better choice may be to choose ΔE_m so that the total inelastic scattering cross section is given exactly in the first Born approximation up to order $1/k^4$, where k^2 is the incident electron energy. This choice leads to $\Delta E_m = e^{\mathcal{L}(-1)/\mathcal{S}(-1)}$,[9] which for He is 31.7 and 12.6 eV for H. These values are not significantly different in their effect on the polarization amplitude (± 5%) from the previously quoted values. The optical quantity $\mathcal{L}(-1)$ is given as

$$\mathcal{L}(-1) = \sum_{n\neq 0}^{\infty} \left\langle \psi_0 \middle| \sum_{i=1}^{N} z_i \middle| \psi_n \right\rangle \ln\Delta E_{0n} \left\langle \psi_n \middle| \sum_{j=1}^{N} z_j \middle| \psi_0 \right\rangle$$

and is discussed in Ref. 9.

With the encouraging result obtained for the absorptive part of the polarization amplitude, it seemed worth while to attempt a more detailed calculation of f_{pol}, including both real and imaginary parts using a Hartree-Fock description of the scattered field.

The most recent accurate theoretical treatment so far appears to be the extended polarization potential method of LaBahn and Callaway.[10] This method suffers from the fact that a large number of phase shifts are required, and extension to more complex systems appears to be somewhat more difficult. The results of this method appear to be in good qualitative agreement with the experiment of Bromberg.[11,12] Further references to earlier works along the same lines can be found in Ref. 10. The results of the two approaches are compared in Sec. IV.

II. APPLICATION OF THEORY TO ONE- AND TWO-ELECTRON SYSTEMS

In this section, Eq. (5) is applied to scattering of electrons by He and H atoms initially in their

ground state. To do this, the Hartree-Fock wave function for He is chosen in the form

$$\psi_0(1,2)=\tfrac{1}{2}\sqrt{2}\phi_{1s}^{\mathrm{He}}(1)\,\phi_{1s}^{\mathrm{He}}(2)[\alpha(1)\beta(2)-\beta(1)\alpha(2)]\ ,$$

and for hydrogen the exact ground-state wave function is taken as

$$\psi_0(1)=\phi_{1s}^{\mathrm{H}}(1)[\alpha(1)\text{ or }\beta(1)]\ .$$

Equation (5) can then be written as

$$f_{\mathrm{pol}}(\theta)=\frac{2Nm^2}{\pi^2 m_0^2}\int\frac{d\vec{q}[f(K)-f(\vec{k}_i-\vec{q})f(\vec{q}-\vec{k}_s)]}{(q^2-\hat{k}^2-i\epsilon)|\vec{k}_i-\vec{q}|^2|\vec{q}-\vec{k}_s|}\ , \tag{6}$$

where N is the number of electrons and is 1 and 2 for H and He, respectively, $\vec{K}=\vec{k}_i-\vec{k}_s$ is proportional to the elastic momentum transfer, and

$$f(\vec{k}_i-\vec{q})=\frac{1}{4\pi}\int d\vec{r}\,|\phi_{1s}^{\mathrm{H,He}}(\vec{r})|^2 e^{i(\vec{k}_i-\vec{q})\cdot\vec{r}}\ .$$

Since, for the two cases considered here, $|\phi_{1s}^{\mathrm{H,He}}(\vec{r})|^2$ is the one-electron density divided by the number of electrons in the atom, it is unnecessary to use the explicit analytical forms for $\phi_{1s}(\vec{r})$ since very accurate and simple analytical expressions for the electron density in terms of Yukawa functions are available.[13] These expressions are of the form

$$\frac{\rho(r)}{N}=\sum_{i=1}^{M}\gamma_i\lambda_i^2 e^{-\lambda_i r}/r\ ,$$

with

$$\sum_{i=1}^{M}\gamma_i=1\ , \tag{7}$$

where $M=3$ for H and 5 for He. The parameters given in Ref. 13 give values for $\rho(r)$ for H and He with an average error of about 0.1%. In terms of these density expressions, Eq. (6) can be reduced to the form

$$f_{\mathrm{pol}}(\theta)=\frac{2Nm^2}{\pi^2 m_0^2}\int\frac{d\vec{q}}{q^2-\hat{k}_i^2-i\epsilon}\times\Bigg(\frac{[f(K)-1]}{|\vec{k}_i-\vec{q}|^2|\vec{q}-\vec{k}_s|^2}+\sum_{j=1}^{M}\frac{\gamma_j}{|\vec{k}_i-\vec{q}|^2(\lambda_j^2+|\vec{q}-\vec{k}_s|^2)}+\sum_{j=1}^{M}\frac{\gamma_j}{|\vec{q}-\vec{k}_s|^2(\lambda_j^2+|\vec{k}_i-\vec{q}|^2)}-\sum_{i=1}^{M}\sum_{j=1}^{M}\frac{\gamma_i\gamma_j}{(\lambda_i^2+|\vec{k}_i-\vec{q}|^2)(\lambda_j^2+|\vec{q}-\vec{k}_i|^2)}\Bigg), \tag{8}$$

where

$$f(K)=\sum_{i=1}^{M}\frac{\gamma_i\lambda_i^2}{K^2+\lambda_i^2}$$

All integrals in Eq. (8) are expressible in terms of the general integral

$$A(\alpha,\beta)=\frac{1}{2\pi^2}\int\frac{d\vec{q}}{(q^2-\hat{k}_i^2-i\epsilon)(\alpha^2+|\vec{k}_i-\vec{q}|^2)(\beta^2+|\vec{q}-\vec{k}_s|^2)}\ , \tag{9}$$

since

$$f_{\mathrm{pol}}(\theta)=\frac{4Nm^2}{m_0^2}\sum_{i=1}^{M}\sum_{j=1}^{M}\gamma_i\gamma_j\{A(0,0)[f(K)-1]+A(0,\lambda_j)+A(\lambda_i,0)-A(\lambda_i,\lambda_j)\}\ . \tag{10}$$

The integral $A(\alpha,\beta)$ can be obtained in closed analytical form by use of standard techniques. A Feynman identity is first used to rewrite the reciprocal of the product $(\alpha^2+|\vec{k}_i-\vec{q}|^2)(\beta^2+|\vec{q}-\vec{k}_s|^2)$ as

$$\frac{1}{(\alpha^2+|\vec{k}_i-\vec{q}|^2)(\beta^2+|\vec{q}-\vec{k}_s|^2)}=\frac{1}{2}\int_{-1}^{1}\frac{dz}{(q^2-2pqx+p^2+\tau^2)^2}\ , \tag{11}$$

where

$$\vec{p}=\tfrac{1}{2}\vec{k}_i(1+z)+\tfrac{1}{2}\vec{k}_s(1-z)$$

is chosen as the z direction for the integration over $\vec{q}$ with x the cosine of the angle between $\vec{p}$ and $\vec{q}$, and τ^2 is given as

$$\tau^2=\tfrac{1}{2}(\alpha^2+\beta^2)+\tfrac{1}{2}(\alpha^2-\beta^2)z+\tfrac{1}{4}K^2(1-z^2)\ .$$

The integration over q can then be carried out in the upper-half complex q plane after changing the limits of integration from $0\to\infty$ to $-\infty\to\infty$. The term $-i\epsilon$ designates the choice of contour which corresponds to an outgoing scattered wave, and the two poles contained in the contour are at $q_1=\hat{k}_i+i\epsilon/2\hat{k}_i+0(\epsilon^2)$ and $q_2=px+i[\tau^2+p^2(1-x^2)]^{1/2}$. By application of the Cauchy residue theorem and integrating over the angular coordinates of $\vec{q}$, Eq. (10) can be reduced to the single integration over z of a real (Re) and imaginary (Im) part as

$$\mathrm{Re}\,A(\alpha,\beta)=A_R(\alpha,\beta)=\frac{1}{4}\int_{-1}^{1}\frac{dz\,(p^2+\tau^2-\hat{k}_i^2)}{[(\hat{k}_i^2+p^2+\tau^2)^2-4\hat{k}_i^2p^2]\tau}\ , \tag{12}$$

$$\mathrm{Im}\,A(\alpha,\beta)=A_I(\alpha,\beta)=\tfrac{1}{2}\hat{k}_i\int_{-1}^{1}\frac{dz}{[(\hat{k}_i^2+p^2+\tau^2)^2-4\hat{k}_i^2p^2]}\ . \tag{13}$$

The remaining integrations, although messy, can be carried out in closed form by noting that all

terms in square roots or brackets are at most quadratic functions of z. The final results are given in Appendix A.

Before proceeding to a discussion of the numerical results obtained from Eqs. (12) and (13), it is of interest to consider the limit of Eq. (13) as $\theta \to 0$. The result for $\lim(4\pi/k)\,\mathrm{Im}f_{\mathrm{pol}}(\theta)$ as $\theta \to 0$ for He can be written as

$$\lim_{\theta\to 0}\frac{4\pi}{k}\,\mathrm{Im}f_{\mathrm{pol}}(\theta)$$

$$=\frac{16\pi}{a^2k^2}\left(\sum_{i=1}^{M}\frac{\gamma_i}{\lambda_i^2}\ln\left|\frac{1+\lambda_i^2/(k-\hat{k}_1)^2}{1+\lambda_i^2/(k+\hat{k}_1)^2}\right| - 2k\hat{k}_1\sum_{i=1}^{M}\gamma_i^2/\{[\lambda_i^2+(k-\hat{k}_1)^2][\lambda_i^2+(k+\hat{k}_1)^2]\}\right.$$

$$\left.-\frac{1}{2}\sum_{i\neq j=1}^{M}\sum^{M}\frac{\gamma_i\gamma_j}{\lambda_i^2-\lambda_j^2}\ln\left|\frac{[1+\lambda_i^2/(k-\hat{k}_1)^2][1+\lambda_j^2/(k+\hat{k}_1)^2]}{[1+\lambda_i^2/(k+\hat{k}_1)^2][1+\lambda_j^2/(k-\hat{k}_1)^2]}\right|\right), \tag{14}$$

which can be compared with the estimate of the total inelastic scattering factor obtained from the Morse expression $S(K)=N-F(K)^2/N$ for He as

$$\sigma_{\mathrm{tot}}^{\mathrm{inel}}=\frac{4\pi}{a^2k^2}\int_{k_{\mathrm{min}}^2}^{k^2}dK\,\frac{2S(K)}{K^4}=\frac{16\pi}{a^2k^2}\left[\sum_{i=1}^{M}\frac{\gamma_i}{\lambda_i^2}\ln\left(\frac{1+\lambda_i^2/(k-\hat{k}_1)^2}{1+\lambda_i^2/k^2}\right)\right.$$

$$\left.-\left(1-\frac{\hat{k}_1}{2k}\right)k\hat{k}_1\sum_{i=1}^{M}\gamma_i^2/\{[\lambda_i^2+k^2][\lambda_i^2+(k-\hat{k}_1)^2]\}-\frac{1}{2}\sum_{i\neq j=1}^{M}\sum^{M}\frac{\gamma_i\gamma_j}{\lambda_i^2-\lambda_j^2}\ln\left|\frac{1+\lambda_i^2/(k-\hat{k}_1)^2}{1+\lambda_i^2/k^2}\,\frac{1+\lambda_j^2/k^2}{1+\lambda_j^2/(k-\hat{k}_1)^2}\right|\right]. \tag{15}$$

The two expressions are not exactly equivalent, because in Eq. (15) the large-angle Bethe behavior $|\vec{k}_s|=k\cos\theta$ has been used and the integration was carried out between $0\le\theta\le\frac{1}{2}\pi$. Still, at energies where $k^2\gg\lambda^2$ the two results will be essentially identical. At 500 eV for He, Eq. (14) yields a value of 0.355 Å^2 and Eq. (15) the value 0.351 Å^2, for a difference of about 1%. A more accurate value including estimates for electron correlation is 0.324 Å^2.[9] The imaginary or absorptive part of the polarization amplitude overestimates the actual value, but the error is probably less than 15%. It is also pleasing to note that the pole at $q=\hat{k}_1$ produces the absorptive part of the polarization amplitude and depends in a sensitive manner on the choice of $\hat{k}_1$.

The real part of $f_{\mathrm{pol}}(\theta)$, on the other hand, should depend more strongly on the choice of the inverse range parameters λ_i and, therefore, the shape of the electron density. Rather than attempt an analytical analysis of the complicated formula of the real part to determine the asymptotic form at large r for the polarization potential, a numerical procedure discussed in Sec. III will be employed.

III. NUMERICAL RESULTS FOR H AND HE

The main results presented in this paper have been computed for an incident energy of 500 eV, for He in order to compare with the most definitive experimental results so far available, obtained by Bromberg.[11] These data consist of absolute measurements of the elastic differential cross section, to an accuracy of 4% or better, over the angular range $2^\circ\le\theta\le 60^\circ$ with an extrapolated estimate for the value at $\theta=0^\circ$. In order to compare theory with experiment, the difference between the differential partial-wave elastic scattering cross section for the Hartree-Fock static potential field for He and the experimental result is calculated. This difference should be given by the expression

$$\left(\frac{d\sigma}{d\Omega}\right)_{\mathrm{expt}}-\left(\frac{d\sigma}{d\Omega}\right)_{\mathrm{p.w.,theory}}$$

$$=2|f|\left[\cos\eta(\mathrm{Re}f_{\mathrm{ex}}+\mathrm{Re}f_{\mathrm{pol}})+\sin\eta(\mathrm{Im}f_{\mathrm{ex}}+\mathrm{Im}f_{\mathrm{pol}})\right]$$

$$+\mathrm{Re}f_{\mathrm{ex}}^2+2\mathrm{Re}f_{\mathrm{ex}}\mathrm{Re}f_{\mathrm{pol}}+\mathrm{Re}f_{\mathrm{pol}}^2$$

$$+\mathrm{Im}f_{\mathrm{ex}}^2+2\,\mathrm{Im}f_{\mathrm{ex}}\mathrm{Im}f_{\mathrm{pol}}+\mathrm{Im}f_{\mathrm{pol}}^2, \tag{16}$$

where $\mathrm{Re}f_{\mathrm{ex}}$, $\mathrm{Im}f_{\mathrm{ex}}$ are the real and imaginary parts of the exchange amplitude, $\mathrm{Re}f_{\mathrm{pol}}$ and $\mathrm{Im}f_{\mathrm{pol}}$ are the real and imaginary parts of the polarization

amplitude, and $|f|$ and η are the magnitude and phase of the partial-wave amplitude ($|f|e^{i\eta}$).[14] Note that the use of square terms in the theoretical expression is usually not justified for a perturbation-type calculation because there are neglected higher-order terms of the same order (i.e., the cross term between the real part of the third Born amplitude and the real part of the first may be of the same order of magnitude as the square of the real part of the second Born amplitude). Nonetheless, these square terms are employed here in the expectation that the Born series is rapidly convergent. This point is discussed in more detail in a later paragraph. The assumption has been made that the effects of exchange on the polarization amplitude and *vice versa* are negligible. Two comparisons will be made. In the first, the exchange amplitude will be set equal to zero in order to see more easily what fraction of the total correction is due to polarization. In the second comparison, the exchange amplitude will be replaced by its approximate Born value[15] $f_{ex} \simeq 2mF(K)/m_0k^2$ which, since it is real, means that $\mathrm{Im}f_{ex}$ will be zero.

In Table I, the calculated values of $\mathrm{Re}f_{pol}$ and $\mathrm{Im}f_{pol}$ at 100 and 500 eV, and 40 keV are given for both H and He. The 40-keV values are given here mainly as a check on the energy dependence of the scattered amplitude. In Fig. 1, the angular dependence of the real and imaginary contributions are shown for incident energies of 100 and 500 eV for the case of He. The inset of Fig. 1 contains a plot of the logarithm of the $\mathrm{Re}f_{pol}(\theta)$ at 100 and 500 eV against K. The linear behavior exhibited in this plot is suggestive of the behavior of a $1/r^4$ polarization potential. That is if, after Bromberg,[16] it is assumed that the polarization potential for the real part is of the form

$$U(r) = -\alpha/(r^2+r_0^2)^2 \tag{17}$$

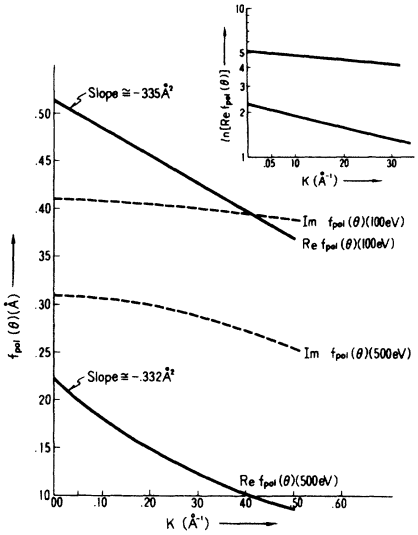

FIG. 1. Plot of the real and imaginary parts of $f_{pol}(\theta)$ in Å as a function of K in Å^{-1} in the small-angle region for He at incident electron energies of 100 and 500 eV. The inset is a plot of the logarithm of the real part of the polarization amplitude against K showing linear behavior in the small-angle region. The limiting slopes $\partial R_p f_{pol}(\theta)/\partial K$ in Å^2 as $\theta \to 0$ are given in the figure.

TABLE I. Imaginary and real parts of the polarization amplitude in Å for H and He at incident electron energies of 100, 500, and 40 000 eV.

	H					
	100 eV		500 eV		40 keV	
θ	$\mathrm{Im}f_{pol}(\theta)$	$\mathrm{Re}f_{pol}(\theta)$	$\mathrm{Im}f_{pol}(\theta)$	$\mathrm{Re}f_{pol}(\theta)$	$\mathrm{Im}f_{pol}(\theta)$	$\mathrm{Re}f_{pol}(\theta)$
0.0	0.731	0.640	0.475	0.281	0.110	0.035
1.0	0.724	0.556	0.410	0.124	0.0065	6.5×10^{-5}
2.0	0.703	0.475	0.313	0.055	8.8×10^{-4}	3.5×10^{-5}
4.0	0.632	0.336	0.183	0.018	8.1×10^{-5}	5.0×10^{-6}
8.0	0.452	0.163	0.068	0.006	3.5×10^{-6}	1.5×10^{-7}
16.0	0.195	0.049	0.010	0.003	-2.5×10^{-7}	4.4×10^{-10}
32.0	0.031	0.015	0.001	0.001	-1.3×10^{-7}	-5.5×10^{-10}
			He			
0.0	0.412	0.515	0.309	0.223	0.079	0.027
1.0	0.411	0.488	0.299	0.165	0.011	1.0×10^{-4}
2.0	0.409	0.461	0.273	0.116	0.0031	8.8×10^{-5}
4.0	0.399	0.408	0.208	0.058	4.2×10^{-4}	3.1×10^{-5}
8.0	0.363	0.309	0.112	0.019	4.1×10^{-5}	3.1×10^{-6}
16.0	0.260	0.164	0.033	0.006	1.8×10^{-6}	9.4×10^{-8}
32.0	0.096	0.048	0.004	0.003	2.0×10^{-8}	1.4×10^{-9}

in rydberg energy units, where α is the static polarizability of the atom and r_0 is the range of the potential, then the scattered amplitude in the first Born approximation will have the form

$$f_{\mathrm{pol}}^{(1)}(\theta) = (\alpha\pi/4r_0)\, e^{-Kr_0} \ . \qquad (18)$$

From the slope of the plot of $\mathrm{Re}f_{\mathrm{pol}}(\theta)$ versus K in Fig. 1, α was found to be 1.52 and 1.51 at 500 and 100 eV, respectively, in Ry compared to the Hartree-Fock (HF) value[17] of 1.49 and exact value[18] of 1.38. The range at 500 eV turned out to be ~ 0.90 Å, which means that $-\alpha/r^4$ represents the potential of Eq. (17) to an accuracy of better than 10% for $r > 3$ Å.

This result suggests that the expression for $\mathrm{Re}f_{\mathrm{pol}}(\theta)$ be expanded in a power series in K of the form

$$\ln \mathrm{Re}f_{\mathrm{pol}}(\theta) = \ln \mathrm{Re}f_{\mathrm{pol}}(0) + \frac{K}{\mathrm{Re}f_{\mathrm{pol}}(0)} \left.\frac{\mathrm{Re}\partial f_{\mathrm{pol}}(0)}{\partial K}\right|_{\theta=0} + \cdots \ , \qquad (19)$$

and the coefficients compared with the result given in Eq. (18). The polarizability is found in this way to be given by the formula

$$\alpha = \frac{-4}{\pi} \left.\frac{\mathrm{Re}\partial f_{\mathrm{pol}}}{\partial K}\right|_{K=0} = \frac{16}{\Delta E_m} \sum_{i=1}^{m} \frac{\gamma_i}{\lambda_i^2} = \frac{8}{3\Delta E_m} \langle r^2 \rangle = 1.52 \ , \qquad (20)$$

in Ry, which is quite close to the HF value of 1.49. The possibility of using a different effective energy for the real and imaginary parts suggests itself. That is, for the real part an effective energy, given by $\Delta E_m = \mathcal{S}(-1)/\mathcal{S}(-2)$, would guarantee that the limiting slope would be equal to the exact value of the polarizability, since $\frac{2}{3}\langle r^2 \rangle$ is just the HF estimate of $\mathcal{S}(-1)$ for the case of He so that α is $\times \exp[-L(-1)/\mathcal{S}(-1)]$ depending on the choice of ΔE_m.

It is very encouraging that the model investigated here not only has the proper asymptotic behavior as $\theta \to 0$, as pointed out previously by Massey and Mohr,[2] but, in fact, yields quantitative estimates of the total inelastic scattering cross section and the atomic polarizability in the process. Since accurate values of α and $\sigma_{\mathrm{tot}}^{\mathrm{inel}}$ are available, it is possible to estimate that the real and imaginary parts are in error by at most 10%, assuming that the choice of the range parameter r_0 is exact. It may be that r_0 is sensitive to electron correlation within the target system, so that the magnitude of the real part at small angles must be considered to be uncertain.

Besides electron correlation, this leaves only the failure of the Born series as a source of error in the theory. Since the Born series generally converges much faster at small scattering angles than at large, the small-angle results can be regarded as being the most accurate in the present calculation.

The sensitivity of the results to the choice of the atomic field was investigated. The inverse-range-potential parameters (λ_i's) were systematically varied over a range of 2% of their original values. It was found that the sensitivity of $\mathrm{Re}f_{\mathrm{pol}}(\theta)$ to variation in the λ_i's was the same as that of the variation (2%), and hence cannot account for any large deviations between the present theory and experiment at small scattering angles.

In Table II, the intensity difference function for He at 500 eV and defined by Eq. (16) is tabulated along with the contributions from the real and imaginary parts of the polarization amplitude and the Born exchange amplitude. The agreement between experiment and theory for angles less than 6° is qualitatively pleasing. It is also interesting to note that the experimental values fall below the theoretical values, since the theoretical estimates at $\theta = 0°$ are probably too high.

It can also be concluded, assuming that the description of exchange scattering employed in this paper is valid, that the inclusion of square terms in the theoretical correction is probably justified for angles less than 6° in the present case. The behavior of the amplitudes for H and He appeared to be quite reasonable for all the angles and energies studied. In addition to the values reported here,

TABLE II. Comparison of the difference between the absolute experimental elastic differential cross section for He at 500 eV in Å^2 and the partial-wave results for a Hartree-Fock atomic field with first Born exchange and infinite-channel close-coupling charge-polarization corrections in the second Born approximation.

θ^0	$\frac{\Delta d\delta}{d\Omega}$ (expt) [a] Å^2	Exchange	Polarization	Polarization[b] + exchange
0	0.354 ± 0.030[c]	0.051	0.378	0.455
2	0.245 ± 0.013	0.050	0.226	0.299
4	0.137 ± 0.009	0.048	0.124	0.178
6	0.087 ± 0.007	0.044	0.072	0.119
8	0.055 ± 0.005	0.040	0.044	0.086
10	0.036 ± 0.004	0.035	0.028	0.064
14	0.019 ± 0.003	0.025	0.014	0.039
20	0.006 ± 0.002	0.014	0.005	0.019
30	0.001 ± 0.0007	0.005	0.001	0.006

[a] Difference between the data of Bromberg (Ref. 11) and the partial-wave differential cross section (Ref. 14).

[b] This column includes the cross term arising between the exchange and polarization, $2\mathrm{Re}f_{\mathrm{pol}}(\theta)f_{ex}(\theta)$, which is important only for $\theta < 6°$.

[c] Author's own estimate of the uncertainty in the extrapolated experimental value. The remaining uncertainties are those given by Bromberg.

the polarization amplitude was calculated for both H and He at values just above the mean excitation energy.

As the incident energy is lowered the real part of the polarization becomes greater than the imaginary part, while at high energy the situation is reversed. (See Fig. 1 for an example.) Despite the fact that the imaginary part is dominant at high energy, the contribution to the cross section is generally smaller than that for the real part, since the phase $\eta(\theta)$ in the main contributing term $2|f(\theta)|\ \sin\eta(\theta)\ \mathrm{Im}f_{\mathrm{pol}}(\theta)$ is generally a very small number in the limits of high incident energy and small scattering angle. The extension of the present treatment to more complex cases is straightforward and only involves the computation of the needed integrals. These can be related to the integrals given in this study, and the methods for doing so are discussed in Appendix B.

IV. COMPARISON WITH PREVIOUS CALCULATIONS

The calculations of LaBahn and Callaway for the differential cross section have been compared with the recent results of Bromberg and are 10% too high in the angular region $\theta < 10^\circ$ discussed here. A rough comparison of these results with those of the present study are given in Table III. In general, the results of this work are closer to those given in Ref. 12 despite the use of a more approximate treatment of exchange in the present study. While not presented here, the results of the present study are also in good agreement with the results of the extended polarization potential model[10] at lower energies. It is interesting to note that both theories seem to predict an appreciably higher intensity at zero scattering angle than observed in Bromberg's[11] experiment. It should be noted, as pointed out in Sec. III, that further improvements in the present theory are likely to lead to smaller results in the small-angle region so that better agreement might be expected (i.e., the total inelastic cross section and static polarizability are both too large in the present work).

TABLE III. Comparison of the Results of LaBahn and Callaway with the present results and Bromberg's experiment for $d\sigma/d\Omega\,(a_0^2)$.

ϑ°	Bromberg[a]	EP[b]	Present results
0	1.89	2.45	2.25
2	1.49	1.87	1.69
4	1.08	1.33	1.23
6	0.863	1.08	0.976
8	0.700	0.82	0.817
10	0.576	0.65	0.675
14	0.405	0.39	0.478

[a]Values taken from Ref. 11 and are in units of a_0^2.
[b]Extended polarization potential model (EP) values were estimated from Fig. 1 in Ref. 12.

The principal advantages of the present approach, besides the somewhat better agreement with experiment shown in Table III, lie in the simplicity of the calculation and ability to easily extend the theory to more complex systems. This approach, excepting relativistic corrections, should also furnish an increasingly accurate description of the polarization correction in the high-energy limit where all the assumptions involved in its derivation become more valid.

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APPENDIX A: INTEGRALS $A_I(\alpha,\beta)$ AND $A_R(\alpha,\beta)$

The final forms of the integral $A_I(\alpha, \beta)$ can be written as

$$A_I(\alpha,\beta)=\frac{1}{4k(u)^{1/2}}\ \ln\left|\frac{(k^2+\hat{k}_i^2+\alpha^2)(k^2+\hat{k}_i^2+\beta^2)-4k^2\hat{k}_i^2\cos\theta+2k\hat{k}_i(u)^{1/2}}{(k^2+\hat{k}_i^2+\alpha^2)(k^2+\hat{k}_i^2+\beta^2)-4k^2\hat{k}_i^2\cos\theta-2k\hat{k}_i(u)^{1/2}}\right|, \tag{A1}$$

with

$$u=(k^2+\hat{k}_i^2+\alpha^2)^2+(k^2+\hat{k}_i^2+\beta^2)^2-2\cos\theta(k^2+\hat{k}_i^2+\alpha^2)(k^2+\hat{k}_i^2+\beta^2)-4k^2\hat{k}_i^2\sin^2\theta\ . \tag{A2}$$

The special cases $A_I(0, 0)$ and $A_I(\alpha, \alpha)$ can be written as

$$A_I(0,0)=\frac{1}{2K[(k^2-\hat{k}_i^2)^2+\hat{k}_i^2K^2]^{1/2}}\ln\left|\frac{\hat{k}_iK+[(k^2-\hat{k}_i^2)^2+\hat{k}_i^2K^2]^{1/2}}{\hat{k}_iK-[(k^2-\hat{k}_i^2)^2+\hat{k}_i^2K^2]^{1/2}}\right|, \tag{A3}$$

$$A_I(\alpha,\alpha)=\frac{1}{2K[(k^2-\hat{k}_i^2)^2+2\alpha^2(k^2+\hat{k}_i^2)+\alpha^4+\hat{k}_i^2K^2]^{1/2}}\ln\left|\frac{\hat{k}_iK+[(k^2-\hat{k}_i^2)^2+2\alpha^2(k^2+\hat{k}_i^2)+\alpha^4+\hat{k}_i^2K^2]^{1/2}}{\hat{k}_iK-[(k^2-\hat{k}_i^2)^2+2\alpha^2(k^2+\hat{k}_i^2)+\alpha^4+\hat{k}_i^2K^2]^{1/2}}\right| . \quad \text{(A4)}$$

Finally, the values at zero angle can be written as

$$\lim_{\theta\to 0}A_I(\alpha,\beta)=\frac{1}{4k(\alpha^2-\beta^2)}\ln\left|\frac{(k^2-\hat{k}_i^2)^2+\alpha^2(k+\hat{k}_i)^2+\beta^2(k-\hat{k}_i)^2+\alpha^2\beta^2}{(k^2-\hat{k}_i^2)^2+\alpha^2(k-\hat{k}_i)^2+\beta^2(k+\hat{k}_i)^2+\alpha^2\beta^2}\right| , \quad (\alpha\neq\beta) \quad \text{(A5)}$$

$$\lim_{\theta\to 0}A_I(\alpha,\alpha)=\frac{\hat{k}_i}{(k^2-\hat{k}_i^2)^2+2\alpha^2(k^2+\hat{k}_i^2)+\alpha^4} , \quad \text{(A6)}$$

$$\lim_{\theta\to 0}A_I(0,0)=\hat{k}_i/(k^2-\hat{k}_i^2)^2 . \quad \text{(A7)}$$

The terms $A_I(\alpha,0)$ or $A_I(0,\beta)$ for $\theta\neq 0$ and $\theta=0$, which are equivalent if $\alpha=\beta$, follow trivially from Eqs. (A1) and (A5), and hence are not shown here. In some applications it is of interest to know (A5) and (A6) at zero incident energy. These results are

$$\lim_{k\to 0}A_I(\alpha,\beta)=\lim_{k\to 0}\frac{k_i}{\alpha^2\beta^2}=\frac{i(\Delta E_m)^{1/2}}{\alpha^2\beta^2} , \quad \text{(A8)}$$

$$\lim_{k\to 0}A_I(\alpha,\alpha)=\lim_{k\to 0}\frac{k_i}{\alpha^4}=\frac{i(\Delta E_m)^{1/2}}{\alpha^4} , \quad \text{(A9)}$$

$$\lim_{k\to 0}A_I(\alpha,0)=\lim_{k\to 0}\frac{1}{\hat{k}_i(1+\alpha^2)}=\frac{-i}{(\Delta E_m)^{1/2}(1+\alpha^2)} , \quad \text{(A10)}$$

$$\lim_{k\to 0}A_I(0,0)=i/\Delta E_m^{3/2} . \quad \text{(A11)}$$

We have saved the real part for last because it is the more difficult of the two results and requires special handling in carrying out its numerical evaluation in the two cases $A_R(\alpha,\beta)$, and $A_R(\alpha,0)$ or $A_R(0,\beta)$. The general result can be obtained by rewriting the integral over z, which is of the basic form

$$A_R(\alpha,\beta)=\frac{1}{4}\int_{-1}^{1}\frac{dz(A+Bz+k^2-\hat{k}_i^2)}{[A+Bz+\frac{1}{4}K^2(1-z^2)]^{1/2}[(k^2-\hat{k}_i^2)^2+2(k^2+\hat{k}_i^2)(A+Bz)+(A+Bz)^2+\hat{k}_i^2K^2(1-z^2)]} , \quad \text{(A12)}$$

where

$$A=\tfrac{1}{2}(\alpha^2+\beta^2) \quad \text{and} \quad B=\tfrac{1}{2}(\alpha^2-\beta^2) ,$$

as

$$A_R(\alpha,\beta)=\frac{1}{8k\hat{k}_i(u)^{1/2}}\left((A+Bz_1+k^2-\hat{k}_i^2)\int_{-1}^{1}\frac{dz}{[A+Bz+\frac{1}{4}K^2(1-z^2)]^{1/2}(z-z_1)}\right.$$
$$\left.-(A+Bz_2+k^2-\hat{k}_i^2)\int_{-1}^{1}\frac{dz}{[A+Bz+\frac{1}{4}K^2(1-z^2)]^{1/2}(z-z_2)}\right) , \quad \text{(A13)}$$

where u is given in Eq. (A2) and z_1 and z_2 are the roots of the quadratic form in z in the square brackets on the right-hand side of the denominator of Eq. (A12), and can be written as

$$z_1=\frac{-\frac{1}{2}(\alpha^2-\beta^2)[k^2+\hat{k}_i^2+\frac{1}{2}(\alpha^2+\beta^2)]+k\hat{k}_i(u)^{1/2}}{\frac{1}{4}(\alpha^2-\beta^2)^2-\hat{k}_i^2K^2} , \quad \text{(A14)}$$

$$z_2=\frac{-\frac{1}{2}(\alpha^2-\beta^2)[k^2+\hat{k}_i^2+\frac{1}{2}(\alpha^2+\beta^2)]-k\hat{k}_i(u)^{1/2}}{\frac{1}{4}(\alpha^2-\beta^2)^2-\hat{k}_i^2K^2} . \quad \text{(A15)}$$

Note that these roots are real but that the sign may change as a function of increasing K and will be singular when $K^2=(\alpha^2-\beta^2)^2/4\hat{k}_i^2$. The over-all result will remain finite, however, since both numerator and denominator contain the same largest power of z_1 or z_2. The sign of the term depending on Z_2 will change when this happens, although the sign of the Z_1 term will not.

By use of the substitutions $y=1/(z-z_1)$ and $y'=1/(z-z_2)$, the integrals in (A11) can be transformed to the forms

$$\int_{-1}^{1}\frac{dz}{[A+Bz+\frac{1}{4}K^2(1-z^2)]^{1/2}(z-z_1)}=\int_{(z_1+1)^{-1}}^{(z_1-1)^{-1}}\frac{dy}{(ay^2-by+c)^{1/2}} ,$$

$$\int_{-1}^{1} \frac{dz}{[A+Bz+\frac{1}{4}K^2(1-z^2)]^{1/2}(z-z_2)}$$

$$= \int_{(z_2+1)^{-1}}^{(z_2-1)^{-1}} \frac{dy'}{(a'y'^2 - b'y' + c')^{1/2}} , \qquad \text{(A17)}$$

with

$$a = A + \tfrac{1}{4}K^2 + Bz_1 - \tfrac{1}{4}K^2 z_1^2 ,$$

$$a' = A + \tfrac{1}{4}K^2 + Bz_2 - \tfrac{1}{4}K^2 z_2^2 ,$$

$$b = B - \tfrac{1}{2}k^2 z_1 , \qquad b' = B - \tfrac{1}{2}k^2 z_2$$

and

$$c = c' = -\tfrac{1}{4}K^2 .$$

Note that

$$b^2 - 4ac = b'^2 - 4a'c' = \tfrac{1}{4}(\alpha^2 - \beta^2)^2 + \tfrac{1}{2}K^2(\alpha^2 + \beta^2) + \tfrac{1}{4}K^4 ,$$

which is always ≥ 0. Since the special cases $A_R(0, 0)$ and $A_R(\alpha, \alpha)$ can be treated in a simpler manner, only the case where $b^2 - 4ac > 0$ need be considered here (i.e., $\alpha \neq \beta \neq 0$). The results are

$$\int_{(z_{1,2}+1)^{-1}}^{(z_{1,2}-1)^{-1}} \frac{dy}{(ay^2 - by + c)^{1/2}} \begin{cases} = \dfrac{1}{(a)^{1/2}} \ln \left| \dfrac{(z_{1,2}+1)[(3\alpha^2+\beta^2+K^2)+(\alpha^2-\beta^2-K^2)z_{1,2}+4\alpha(a)^{1/2}]}{(z_{1,2}-1)[(\alpha^2+3\beta^2+K^2)+(\alpha^2-\beta^2+K^2)z_{1,2}+4\beta(a)^{1/2}]} \right| & \text{for } a>0 \\ = + \dfrac{1}{(|a|)^{1/2}} \arctan\left(\dfrac{(3\alpha^2+\beta^2+K^2)+(\alpha^2-\beta^2-K^2)z_{1,2}}{4\alpha(|a|)^{1/2}} \right) & \\ \quad - \dfrac{1}{(|a|)^{1/2}} \arctan\left(\dfrac{(\alpha^2+3\beta^2+K^2)+(\alpha^2-\beta^2+K^2)z_{1,2}}{4\beta(|a|)^{1/2}} \right) & \text{for } a<0 . \end{cases} \qquad \text{(A18)}$$

In the limit as $\theta \to 0$ and $k \to 0$ Eq. (A13) can be combined with the results of Eq. (A18), with the results that

$$\lim_{\theta \to 0} A_R(\alpha, \beta) = \frac{1}{2k(\alpha^2 - \beta^2)} \times \left[\arctan\left(\frac{\alpha}{k - \hat{k}_l}\right) + \arctan\left(\frac{\alpha}{k + \hat{k}_l}\right) - \arctan\left(\frac{\beta}{k - \hat{k}_l}\right) - \arctan\left(\frac{\beta}{k + \hat{k}_l}\right) \right], \qquad \text{(A19)}$$

$$\lim_{\substack{\theta \to 0 \\ k \to 0}} A_R(\alpha, \beta) = \frac{\alpha}{\alpha^2 - \beta^2} \left(\frac{1}{\Delta E_m - \alpha^2} \right) - \frac{\beta}{\alpha^2 - \beta^2} \left(\frac{1}{\Delta E_m - \beta^2} \right) .$$

The case where $\alpha \neq 0$, $\beta = 0$ can also be obtained in a similar fashion as

$$A_R(\alpha, 0) = \frac{1}{8k\hat{k}_l(u)^{1/2}} \left\{ \frac{A + Bz_1 + k^2 - \hat{k}_l^2}{(|a|)^{1/2}} \times \left[\arctan\left(\frac{(\alpha^2 - K^2)z_1 + 3\alpha^2 + K^2}{4\alpha(|a|)^{1/2}} \right) + \tfrac{1}{2}\pi \operatorname{sign}(z_1 + 1) \right] - \frac{A + Bz_2 + k^2 - \hat{k}_l^2}{(|a'|)^{1/2}} \times \left[\arctan\left(\frac{(\alpha^2 - K^2)z_2 + 3\alpha^2 + K^2}{4\alpha(|a'|)^{1/2}} \right) - \tfrac{1}{2}\pi \operatorname{sign}(z_2 + 1) \right] \right\}, \qquad \text{(A20)}$$

where only the arctan form was found to be necessary and where $\operatorname{sign}(z_1 + 1)$ was -1 and $\operatorname{sign}(z_2 + 1)$ was $+1$ in all the calculations made so far. In the limit as θ and $k \to 0$, Eq. (A20) reduces to

$$\lim_{\theta \to 0} \alpha_R(\omega, 0) = \frac{1}{2k\alpha^2} \arctan\left(\frac{\alpha}{k - \hat{k}_l}\right) + \frac{1}{2k\alpha^2} \arctan\left(\frac{\alpha}{k + \hat{k}_l}\right) , \qquad \text{(A21)}$$

$$\lim_{\theta \to 0, k \to 0} A_R(\alpha, 0) = 1/\alpha(\Delta E_m - \alpha^2) . \qquad \text{(A22)}$$

When $\alpha = \beta \neq 0$ the real part can be expressed in the relatively simple form

$$A_R(\alpha, \alpha) = K^{-1}[(k^2 - \hat{k}_l^2)^2 + 2\alpha^2(k^2 + \hat{k}_l^2) + \alpha^4 + \hat{k}_l^2 K^2]^{-1/2} \times \arctan \frac{K(k^2 - \hat{k}_l^2 + \alpha^2)}{2\alpha[(k^2 - \hat{k}_l^2)^2 + 2\alpha^2(k^2 + \hat{k}_l^2) + \alpha^4 + \hat{k}_l^2 K^2]^{1/2}} , \qquad \text{(A23)}$$

which reduces to

$$\lim_{\theta \to 0} A_R(\alpha, \alpha) = \frac{k^2 - \hat{k}_l^2 + \alpha^2}{2\alpha[(k^2 - \hat{k}_l^2)^2 + 2\alpha^2(k^2 + \hat{k}_l^2) + \alpha^4]} \qquad \text{(A24)}$$

in the limit of zero angle, and

$$\lim_{k\to 0} A_R(\alpha,\alpha) = (\Delta E_m + \alpha^2)/2\alpha(\Delta E_m^2 - 2\alpha^2\Delta E_m + \alpha^4) \tag{A25}$$

in the limit of zero incident energy. Finally, the case of $A_R(0,0)$ can be shown to be expressible as

$$A_R(0,0) = \pi/2K[(k^2 - \hat{k}_i^2)^2 + \hat{k}_i^2 K^2]^{1/2} . \tag{A26}$$

In the foregoing it should be noted that cases (A18) and (A20) have multiple forms depending on the choice of parameters. Since these forms may be ambiguous within an additive factor of π to the argument of the arctan function, it is essential to test the continuity of the results for $A_R(\alpha,\beta)$ and $A_R(\alpha,0)$ to determine if an additive factor is needed. The limit as $K\to 0$ is unambiguous in all cases, and the demand that A_R be continuous from $\theta = 0$ to larger values of θ is sufficient to determine if any additive factors of π are needed. A check showed that in all the calculations reported here only the arctan forms were used. All computations were carried out on the University of Tokyo Hitac 5020 computer using both 32- and 64-bit word lengths.

APPENDIX B: INTEGRALS INVOLVED IN EXTENSION OF PRESENT TREATMENT OF POLARIZATION TO MORE COMPLEX ATOMS

It is convenient with little, if any, loss in generality to write the Hartree-Fock atomic orbitals for more complex atoms as linear combinations of analytic Slater-type orbitals (STO's) of the form

$$\varphi_{1s}^{\mathrm{STO}}(r) = (\alpha_1^3/\pi)^{1/2} e^{-\alpha_1 r} , \tag{B1}$$

$$\varphi_{2s}^{\mathrm{STO}}(r) = (\alpha_2^5/3\pi)^{1/2} r e^{-\alpha_2 r_2} , \tag{B2}$$

$$\varphi_{2p_z}^{\mathrm{STO}}(r) = (\alpha_3^5/\pi)^{1/2} r e^{-\alpha_3 r} , \tag{B3}$$

for normalized $1s$-, $2s$-, and $2p_z$-type STO's, respectively.

For the case of s-type orbitals, the integrals for the first Born matrix elements are

$$\langle \varphi_{1s}^{\mathrm{STO}}(r) | e^{i\vec{L}\cdot\vec{r}} | \varphi_{1s}^{\mathrm{STO}}(r)\rangle = 4\alpha_1^3 \left(-\frac{d}{d\beta}\right)\left(\frac{1}{\beta^2 + L^2}\right) , \tag{B4}$$

$$\langle \varphi_{1s}^{\mathrm{STO}}(r) | e^{i\vec{L}\cdot\vec{r}} | \varphi_{2s}^{\mathrm{STO}}(r)\rangle = \tfrac{4}{3}(\alpha_1^3\alpha_2^5)^{1/2} \left(-\frac{d}{d\beta}\right)^2\left(\frac{1}{\beta^2 + L^2}\right) , \tag{B5}$$

$$\langle \varphi_{2s}^{\mathrm{STO}}(r) | e^{i\vec{L}\cdot\vec{r}} | \varphi_{2s}^{\mathrm{STO}}(r)\rangle = \tfrac{4}{3}\alpha_2^5 \left(-\frac{d}{d\beta}\right)^3\left(\frac{1}{\beta^2 + L^2}\right) , \tag{B6}$$

where $\vec{L}$ is a generalized momentum transfer variable which, in this case, can take on the values $\vec{k}_i - \vec{q}$, $\vec{q} - \vec{k}_s$, and $\vec{k}_i - \vec{k}_s$. The constant β is $2\alpha_1$, $\alpha_1 + \alpha_2$, and $2\alpha_2$, respectively, for the three cases given above. It is clear from Eqs. (B4)–(B6) that all terms in the integrals involved in computing the polarization amplitude will reduce to parametric differentiation of the terms $A_R(\alpha,\beta)$ and $A_I(\alpha,\beta)$ given in Appendix A. This means that the present treatment can be extended at the Hartree-Fock level to the cases of atomic Li and Be, where only s orbitals are involved.

In the case of a p_z orbital, we can always select an arbitrary coordinate axis with center on the nucleus for the integration over $\vec{q}$ and note that

$$(r\cos\theta)^n e^{i\vec{k}_i\cdot\vec{r}} = (-id/dk_z)^n e^{i\vec{k}_i\cdot\vec{r}} , \tag{B7}$$

$$(r\cos\theta)^n e^{-i\vec{k}_i\cdot\vec{r}} = (id/dk_{sz})^n e^{-i\vec{k}_s\cdot\vec{r}} , \tag{B8}$$

where k_z is the z component of $\vec{k}_i$ and k_{sz} is the z component of $\vec{k}_s$ with respect to the coordinate axis on the atom. Other components can be used in the same way to eliminate the angular factors from $2p_x$ and $2p_z$ orbitals. Similar tricks involving higher derivatives with respect to the Cartesian coordinates of $\vec{k}_i$ and $\vec{k}_s$ can be used to reduce orbitals of even higher symmetry to $1s$ orbital form. The results for all combinations with the $2p_z$ orbital are

$$\langle \varphi_{1s}^{\mathrm{STO}}(r) | e^{i(\vec{k}_i - \vec{q})\cdot\vec{r}} | \varphi_{2p_z}^{\mathrm{STO}}(r)\rangle = -\frac{id}{dk_z} 4(\alpha_1^3\alpha_3^5)^{1/2} \left(-\frac{d}{d\beta}\right)\left(\frac{1}{\beta^2 + |\vec{k}_i - \vec{q}|^2}\right) , \tag{B9}$$

$$\langle \varphi_{2s}^{\mathrm{STO}}(r) | e^{i(\vec{k}_i - \vec{q})\cdot\vec{r}} | \varphi_{2p_z}^{\mathrm{STO}}(r)\rangle = -\frac{id}{dk_z} 4(\tfrac{1}{3}\alpha_2^5\alpha_3^5)^{1/2} \left(-\frac{d}{d\beta}\right)^2\left(\frac{1}{\beta^2 + |\vec{k}_i - \vec{q}|^2}\right), \tag{B10}$$

$$\langle \varphi_{2p_z}^{\mathrm{STO}}(r) | e^{i(\vec{k}_i - \vec{q})\cdot\vec{r}} | \varphi_{2p_z}^{\mathrm{STO}}(r)\rangle = -\left(\frac{d}{dk_z}\right)^2 4\alpha_3^5 \left(-\frac{d}{d\beta}\right)^2\left(\frac{1}{\beta^2 + |\vec{k}_i - \vec{q}|^2}\right) , \tag{B11}$$

where β is $\alpha_1 + \alpha_3$, $\alpha_2 + \alpha_3$, and $2\alpha_3$, respectively. Similar results can be obtained for the terms depending on $\vec{q} - \vec{k}_s$ by differentiation with respect to k_{sz}, and the extension to $2p_x$, $2p_y$, and higher symmetry cases is trivial. It should be noted, however, that the results for the amplitude will depend on the various orientation angles of $\vec{k}_i$ and $\vec{k}_s$ to the coordinate axis on the atom. After the differential cross section is computed utilizing all the terms, then it must be averaged over all angles of orientation of the atomic coordinate axis system with respect to the fixed plane determined by $\vec{k}_i$ and $\vec{k}_s$. Any convenient coordinate system can be chosen for this integration as, for example, letting the fixed-z axis be parallel to $\vec{k}_i$ with either the fixed-x or fixed-y axis in the $\vec{k}_i\,\vec{k}_s$ plane.

Since Eqs. (B9)–(B11) are in the same form as Eqs. (B4)–(B6), all polarization contributions will

again be expressible as parametric derivatives of the results for $A_R(\alpha,\beta)$ and $A_I(\alpha,\beta)$. Thus it is possible to extend the present analysis, obviously not without some bookkeeping problems, to any atom for which the analytic Hartree-Fock wave function has been given in terms of STO's.[19]

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[1]A fairly up-to-date bibliography can be found in N. F. Mott and H. S. W. Massey, *The Theory of Atomic Collisions* (Clarendon, Oxford, 1965), 3rd ed. Unfortunately, the important comments and speculations concerning the method discussed in this paper, which have by and large turned out to be correct, have been omitted from this edition but can be found in the first edition.

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$$\sigma_{tot} = \frac{4\pi}{a^2k^2}\int_{\Delta E^2/4k^2}^{4k^2} \frac{dK^2\,S(K)}{K^4}$$

$$= (4\pi/k^2)\,[M_{tot}^2 \ln 4k^2 - 2M_{tot}^2 \ln \Delta E + I_1 - I_2 + 0(1/k^2)\,].$$

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$$F^0(\vec{r}) = \frac{2e^{i\vec{k}_0\vec{r}}}{r}\,\frac{Z - F_x(s)\,(1 - s^2/k_0^2)}{s^2}\ .$$

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