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PHYSICAL REVIEW A

VOLUME 3, NUMBER 6

JUNE 1971

Infinite-Channel Close-Coupling Approximation in the Second Born Approximation. II. Treatment of Charge Polarization in Elastic Scattering by Use of the T -Matrix Formalism*

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(Received 8 August 1970)

An operator expansion of the T matrix is shown to lead to an equation for describing charge polarization on elastic scattering similar to that reported previously by use of the infinite-channel close-coupling approximation in the second Born approximation. The resulting equations are used to calculate the charge-polarization corrections for elastic electron scattering from H and He at incident electron energies of 100 eV, 500 eV, and 40 keV over the angular range of 0° to 50° . The results agree well with those of Bromberg and LaBahn and Callaway for elastic scattering from He with an incident electron energy of 500 eV.

In the first paper in this series^{1,2} it was shown that an old approach to the problem of describing the effects of charge polarization on the elastic cross section was capable of yielding results in excellent agreement with experiment at incident energies as low as 500 eV, providing certain reasonable assumptions were made concerning the choice of the one adjustable parameter present in the theory. This approach called the infinite-channel close-coupling approximation in the second Born approximation (ICCCA) was also found to compare favorably with the results of the extended polarization potential method of LaBahn and Callaway.³ Other theoretical approaches, which in principle can be used to attack this same problem but where detailed calculations are not yet available for the case of He at 500 eV, are versions of the coupled-channel partial-wave theory,⁴ the method of equivalent potentials,⁵ and the phase-grating approximation.⁶ Recently two studies have appeared which apply the nuclear independent-particle model⁷ to the calculation of charge polarization in elastic electron scattering for the case of He at incident energies of 100 to 500 eV with excellent results. This last approach can in some sense be considered a variant of the approach outlined in Ref. 5.

The purpose of this paper is to investigate the use of the T -matrix formalism for the description of charge polarization. This approach depends only on an operator expansion and bypasses the necessity of using closure as an approximation.

I. T -MATRIX DESCRIPTION OF CHARGE POLARIZATION

In the nonrelativistic T -matrix formalism, the exact elastic scattering amplitude can be written as⁸

$$f(\theta) = f^{\text{Born}}(\theta) + \frac{1}{4\pi} \times \left\langle \psi_0 \left| e^{-i\vec{k}_s \cdot \vec{r}_0} V \bar{A} \frac{1}{H - E - i\epsilon} V e^{i\vec{k}_i \cdot \vec{r}_0} \right| \psi_0 \right\rangle, \quad (1)$$

where

$$f^{\text{Born}}(\theta) = (1/4\pi) \langle \psi_0 | e^{-i\vec{k}_s \cdot \vec{r}_0} V \bar{A} e^{i\vec{k}_i \cdot \vec{r}_0} | \psi_0 \rangle,$$

and ψ_0 is the ground-state wave function of the target; \vec{k}_i and \vec{k}_s are the wave vectors of the incident and scattered electron; V is the interaction potential between the incident electron and the target; and H is the complete Hamiltonian with E the total energy. The operator \bar{A} is an anti-symmetrizer acting to the left which permutes the coordinates of the incident electron \vec{r}_0 , with those of the target electron in such a way that the overall matrix element is antisymmetric with respect to electron exchange.⁹ The procedure to be followed here¹⁰ is to express V in the Fourier form

$$V = \frac{1}{\pi^2} \int \frac{d\vec{q}}{q^2} e^{i\vec{q} \cdot \vec{r}_0} \times \left(\sum_{n=1}^M Z_n e^{-i\vec{q} \cdot \vec{R}_n} - \sum_{\nu=1}^N e^{-i\vec{q} \cdot \vec{r}_\nu} \right), \quad (2)$$

where atomic units (1 a. u. = 13.6 eV) have been employed and it has been assumed that the target is a molecule with M nuclei and N electrons. Note that \vec{R}_n and \vec{r}_ν are nuclear and electron coordi-

nates, respectively, and Z_n is the n th nuclear charge. The inverse operator can be commuted through the product $V e^{i\vec{k}_i \cdot \vec{r}_0}$ with the result¹⁰

$$\frac{1}{H-E-i\epsilon} V e^{i\vec{k}_i \cdot \vec{r}_0} = \frac{e^{i\vec{k}_i \cdot \vec{r}_0}}{\pi^2} \int \frac{d\vec{q}}{q^2} e^{i\vec{q} \cdot \vec{r}_0} \times \left[\sum_{n=1}^M Z_n e^{-i\vec{q} \cdot \vec{R}_n} \left(\frac{1}{H_0 + V - \epsilon_0 + q^2(1+m_n) + 2i\vec{q} \cdot m_n \vec{\nabla}_n - 2i\vec{q} \cdot \vec{\nabla}_0 + 2\vec{q} \cdot \vec{k}_i} \right) - \sum_{\nu=1}^N e^{-i\vec{q} \cdot \vec{r}_\nu} \left(\frac{1}{H_0 + V - \epsilon_0 + 2q^2 + 2i\vec{q} \cdot \vec{\nabla}_\nu - 2i\vec{q} \cdot \vec{\nabla}_0 + 2\vec{q} \cdot \vec{k}_i} \right) \right], \quad (3)$$

where ϵ_0 is the ground-state energy of the target and M_n is the ratio of the electron mass to the nuclear mass and will be neglected in this work.

To proceed further it is convenient to neglect exchange effects. Since the matrix element under evaluation represents contributions from the second and all higher Born approximations, the neglect of exchange at this stage should be a second-order effect at high incident energies. Exchange corrections to the non-charge-polarization part of the scattered amplitude should be obtained, where possible, by making use of partial-wave amplitudes describing elastic electron scattering including exchange.¹¹

Next, the inverse operators can be expanded in powers of

$$H_0 + V - \epsilon_0 + 2i\vec{q} \cdot m_n \vec{\nabla}_n - 2i\vec{q} \cdot \vec{\nabla}_0$$

or

$$H_0 + V - \epsilon_0 + 2i\vec{q} \cdot \vec{\nabla}_\nu - 2i\vec{q} \cdot \vec{\nabla}_0.$$

The first term in this expansion will correspond roughly to the second Born approximation. The convergence of such an expansion will not be considered here. The justification for this particular choice will rest instead on the physical reasonableness of the final result and its connection with previous results.

If the remaining potential term in Eq. (1) is also cast into Fourier form, the final result for the matrix element can be written as

$$\frac{1}{4\pi} \langle \psi_0 | e^{-i\vec{k}_s \cdot \vec{r}_0} V \frac{1}{H-E-i\epsilon} V e^{i\vec{k}_i \cdot \vec{r}_0} | \psi_0 \rangle \approx \frac{2}{\pi^2} \langle \psi_0 | \int \frac{d\vec{q}}{q^2 |\vec{K} + \vec{q}|^2} \left(\sum_{i=1}^M \sum_{n=1}^M Z_i Z_n \frac{e^{i\vec{K} \cdot \vec{R}_i} e^{i\vec{q} \cdot \vec{R}_{in}}}{q^2 + 2\vec{q} \cdot \vec{k}_i - i\epsilon} - \sum_{i=1}^M \sum_{\nu=1}^N \frac{Z_i e^{i\vec{K} \cdot \vec{R}_i} e^{i\vec{q} \cdot (\vec{R}_i - \vec{r}_\nu)}}{2q^2 + 2\vec{q} \cdot \vec{k}_i - i\epsilon} - \sum_{n=1}^M \sum_{\mu=1}^N \frac{Z_n e^{-i\vec{K} \cdot \vec{r}_\mu} e^{i\vec{q} \cdot (\vec{r}_\mu - \vec{R}_n)}}{q^2 + 2\vec{q} \cdot \vec{k}_i - i\epsilon} + \sum_{\nu=1}^N \sum_{\mu=1}^N \frac{e^{i\vec{K} \cdot \vec{r}_\mu} e^{i\vec{q} \cdot \vec{r}_{\mu\nu}}}{2q^2 + 2\vec{q} \cdot \vec{k}_i - i\epsilon} \right) | \psi_0 \rangle, \quad (4)$$

where \vec{K} is the elastic momentum transfer $\vec{k}_i - \vec{k}_s$. Equation (4) does not look very familiar as it stands, but if the new variable $\vec{m} = \vec{k}_i + \vec{q}$ is used, then the leading term on the right-hand side of the result

$$\frac{1}{4\pi} \langle \psi_0 | e^{-i\vec{k}_s \cdot \vec{r}_0} V \frac{1}{H-E-i\epsilon} V e^{i\vec{k}_i \cdot \vec{r}_0} | \psi_0 \rangle = \frac{2}{\pi^2} \langle \psi_0 | \int \frac{d\vec{m}}{|\vec{k}_i - \vec{m}|^2 |\vec{m} - \vec{k}_s|^2} \left(\sum_{i=1}^M \sum_{n=1}^M \frac{Z_i Z_n e^{i[(\vec{k}_i - \vec{m}) \cdot \vec{R}_n + (\vec{m} - \vec{k}_s) \cdot \vec{R}_i]}}{m^2 - k^2 - i\epsilon} - \sum_{i=1}^M \sum_{\nu=1}^N \frac{Z_i e^{i[(\vec{m} - \vec{k}_s) \cdot \vec{R}_i + (\vec{k}_i - \vec{m}) \cdot \vec{r}_\nu]}}{2m^2 - 2\vec{m} \cdot \vec{k}_i - i\epsilon} - \sum_{n=1}^M \sum_{\mu=1}^N \frac{Z_n e^{i[(\vec{k}_i - \vec{m}) \cdot \vec{R}_n + (\vec{m} - \vec{k}_s) \cdot \vec{r}_\mu]}}{m^2 - k^2 - i\epsilon} + \sum_{\nu=1}^N \sum_{\mu=1}^N \frac{e^{i[(\vec{k}_i - \vec{m}) \cdot \vec{r}_\nu + (\vec{m} - \vec{k}_s) \cdot \vec{r}_{\mu\nu}]}{2m^2 - 2\vec{m} \cdot \vec{k}_i - i\epsilon} \right) | \psi_0 \rangle \quad (5)$$

can be easily identified as part of the second Born approximation for elastic scattering. In fact if all energy denominators were of the form $m^2 - k^2 - i\epsilon$, Eq. (5) would be identical to the ICCCA result. The physical meaning of the new energy denominator $2m^2 - 2\vec{m}\cdot\vec{k}_i - i\epsilon$ can be understood in terms of a binary collision model. For electron-electron scattering, the momentum- and energy-conservation conditions for a binary collision are

$$\vec{k}_i + \vec{P}_0 = \vec{m} + \vec{P}'_0, \quad k_i^2 + P_0^2 = m^2 + P_0'^2, \quad (6)$$

where \vec{m} is the momentum of the incident electron after the first of its two collisions within the target where the usual double-scattering interpretation of the second Born approximation is employed. The quantities \vec{P}_0 and \vec{P}'_0 represent the initial and final momenta of the first target electron encountered. There are two more such conditions for the second collision, but they are not needed in the present argument except to take care of energy conservation for the over-all process. It can be shown from Eq. (6) that if the incident energy k_i^2 is much greater than the binding energy of the target electron P_0^2 , then $2m^2 - 2\vec{m}\cdot\vec{k}_i \approx 0$.¹² Since the largest contribution from the energy denominator comes exactly when this condition is fulfilled, the energy denominator approximately imposes the conditions for conservation of energy and momentum in a binary-electron collision. The energy denominator encountered in the ICCCA method and in the nuclear terms in the T -matrix approach imposes energy- and momentum-conservation conditions for the collision of an electron with an infinitely massive particle.

While it can be expected that the new energy denominator should lead to an improved description of the scattering at larger scattering angles, the results will be singular at $\theta = 0^\circ$ as in the ICCCA case with $\hat{k}_i = k$. In order to avoid this difficulty the energy denominator can be written in the form $2|\vec{m} - \frac{1}{2}\vec{k}_i|^2 - \frac{1}{2}k_i^2$ and the final term $\frac{1}{2}k_i^2$ can be replaced by $\frac{1}{2}k_i^2 = \frac{1}{2}(k_i^2 - \Delta E_{\text{eff}})$, where ΔE_{eff} is an effective energy loss. The physical justification for such a procedure is that $2(m^2 - \vec{m}\cdot\vec{k}_i)$ is not exactly zero but, according to conservation of energy and momentum, is equal to $2\vec{P}'_0 \cdot (\vec{P}'_0 - \vec{P}_0)$, which it is assumed can be replaced by its average value. In this approximation, the effective energy ΔE_{eff} should be approximately given by 4 times the average of $\vec{P}'_0 \cdot (\vec{P}'_0 - \vec{P}_0)$. The evaluation of this average will not be attempted here; rather, the effective energy ΔE_{eff} will be employed as an adjustable parameter subject to the constraints that

$$\frac{4\pi}{k} \text{Im}f_{\text{pol}}(0) \quad \text{and} \quad -\frac{1}{4}\pi \lim_{k \rightarrow 0} \frac{\partial \text{Re}f_{\text{pol}}(\theta)}{\partial k}$$

must simultaneously yield reasonable values for the total inelastic scattering cross section and the

static polarizability with the correct dependence on the incident energy.²

If the missing electron-electron terms in Eq. (5) needed to produce the usual expression for the elastic second Born amplitudes, but with energy denominators for electron-electron collisions, in the absence of exchange and polarization, are added to and subtracted from Eq. (5), the charge-polarization amplitude may be written as

$$f_{\text{pol}}^{(2)}(\theta) = \frac{2}{\pi^2} \int \frac{d\vec{m}}{[2|\vec{m} - \frac{1}{2}\vec{k}_i|^2 - \frac{1}{2}k_i^2 - i\epsilon]|\vec{k}_i - \vec{m}|^2|\vec{m} - \vec{k}_s|^2} \\ \times \sum_{\nu=1}^N \sum_{\mu=1}^N (\langle \psi_0 | e^{i[(\vec{k}_i - \vec{m}) \cdot \vec{r}_\nu + (\vec{m} - \vec{k}_s) \cdot \vec{r}_\mu]} | \psi_0 \rangle \\ - \langle \psi_0 | e^{i(\vec{k}_i - \vec{m}) \cdot \vec{r}_\nu} | \psi_0 \rangle \langle \psi_0 | e^{i(\vec{m} - \vec{k}_s) \cdot \vec{r}_\mu} | \psi_0 \rangle), \quad (7)$$

which is identical to the ICCCA result except for the new energy denominator. The superscript 2 denotes the fact that this is a kind of second Born correction in the sense that it is a matrix element of order V^2 in the interaction potential. The second Born approximation for ordinary potential scattering can be combined with the first Born nonexchange amplitude, and the two terms can be replaced by the partial-wave amplitude for the static potential. The resultant total amplitude can be written as

$$f(\theta) = f^{\text{PW}}(\theta) + f^{\text{EX}}(\theta) + f_{\text{pol}}(\theta), \quad (8)$$

where $f^{\text{PW}}(\theta)$ is the elastic partial-wave amplitude which is available for Hartree-Fock atomic wave functions for most atoms in the Periodic Table over a large range of energies.¹³ The exchange amplitude $f^{\text{EX}}(\theta)$ can be approximated by its first Born value. In some cases the partial-wave amplitude including exchange has been obtained,¹¹ and if available it should be used in place of the sum $f^{\text{PW}}(\theta) + f^{\text{EX}}(\theta)$. Here the small-angle approximation¹⁴ to $f^{\text{EX}}(\theta)$ is given as

$$f^{\text{EX}}(\theta) = -2N_{\text{ex}}F(K)/k_i^2, \quad (9)$$

where $F(K)$ is the x-ray coherent scattering factor and N_{ex} is a constant determined from an approximate treatment of the initial spin state of the target. (Note that this treatment is exact for H and He.) For singlet states $N_{\text{ex}} = 2$, for doublet states $N_{\text{ex}} = 1$, and for triplet states $N_{\text{ex}} = 2$. Note that only the term

$$2 \text{Re}f^{\text{EX}}(\theta)f^{\text{PW}}(\theta) = 2|f^{\text{PW}}(\theta)| \cos \eta(\theta) f^{\text{EX}}(\theta)$$

in the cross section, where $\eta(\theta)$ is the phase of $f^{\text{PW}}(\theta)$, should involve the constant N_{ex} . The terms involving $f^{\text{EX}}(\theta)^2$, if included, should be multiplied by 1, 1, and 3, respectively, for the spin states mentioned above. The expression for the differential cross section can be written as

$$\frac{d\sigma}{d\mathbf{r}} = |f^{\text{PW}}(\theta)|^2 + 2|f^{\text{PW}}(\theta)| \cos \eta(\theta) [\text{Re}f_{\text{po1}}^{(2)}(\theta) + f^{\text{E}\mathbf{x}}(\theta)] \\ + 2|f^{\text{PW}}(\theta)| \sin \eta(\theta) \text{Im}f_{\text{po1}}^{(2)}(\theta) \\ + f^{\text{E}\mathbf{x}}(\theta)^2 + \text{Re}f_{\text{po1}}^{(2)}(\theta)^2 + \text{Im}f_{\text{po1}}^{(2)}(\theta)^2, \quad (10)$$

where it is not clear whether it is justifiable to retain the last three terms. In previous work the term $f^{\text{E}\mathbf{x}}(\theta)^2$ did not make an appreciable contribution to the final result and can probably be discarded. If higher Born terms are thought to give appreciable corrections, then the terms $\propto f_{\text{po1}}^{(2)}(\theta)^2$ should of course be neglected. Again, as in the previous study of the ICCCA method this term did not make an important correction, although its omission did lead to a slightly improved comparison with experiment at small angles. In this work both the perturbation expression [nonsquare terms in Eq. (10)] and Eq. (10) will be employed in comparisons with experiment.

II. INTEGRAL EVALUATION

For the case of a one-electron target system or a Hartree-Fock description of a two-electron target system in a ground singlet state, Eq. (7) can be written as²

$$f_{\text{po1}}^{(2)}(\theta) = \frac{2N}{\pi^2} \\ \times \int \frac{d\vec{m} [f(\vec{K}) - f(\vec{k}_i - \vec{m})f(\vec{m} - \vec{k}_s)]}{[2|\vec{m} - \frac{1}{2}\vec{k}_i|^2 - \frac{1}{2}k_i^2 - i\epsilon] |\vec{k}_i - \vec{m}|^2 |\vec{m} - \vec{k}_s|^2}, \quad (11)$$

where N is the number of electrons in the target and

$$f(\vec{x}) = \int d\vec{r} \rho(\vec{r}) e^{i\vec{x}\cdot\vec{r}}$$

is a one-electron x-ray coherent scattering factor, where $\rho(\vec{r})$ is the one-electron density. As in Ref. 2, the density can be expanded in a series of Yukawa functions¹³ to high accuracy ($\pm 0.1\%$) so that, for instance,

$$f(\vec{k}_i - \vec{m}) = \sum_{i=1}^L \gamma_i \lambda_i^2 / [\lambda_i^2 + |\vec{k}_i - \vec{m}|^2], \\ f_{\text{po1}}^{(2)}(\theta) = 4N \sum_{i=1}^L \gamma_i \sum_{j=1}^L \gamma_j \{ [f(K) - 1] A(0, 0) + A(\lambda_i, 0) \\ + A(0, \lambda_j) - A(\lambda_i, \lambda_j) \}, \quad (12)$$

where the basic integral to be evaluated is

$$A(\alpha, \beta) = \frac{1}{2\pi^2} \int \frac{d\vec{m}}{(2|\vec{m} - \frac{1}{2}\vec{k}_i|^2 - \frac{1}{2}k_i^2 - i\epsilon)(\alpha^2 + |\vec{k}_i - \vec{m}|^2)(\beta^2 + |\vec{m} - \vec{k}_s|^2)}. \quad (13)$$

The analysis is quite identical to that of the first paper in this series except for the different energy denominator. That is,² we have

$$A(\alpha, \beta) = \frac{1}{8\pi^2} \int_{-1}^1 dz \\ \times \int \frac{d\vec{m}}{(|\vec{m} - \frac{1}{2}\vec{k}_i|^2 - \frac{1}{4}k_i^2 - i\epsilon)(|\vec{m} - \vec{p}|^2 + \tau^2)^2}, \quad (14)$$

where

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

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

Just as in Ref. 2, Eq. (14) can be rewritten in the same form as used there by letting $\vec{q} = \vec{m} - \frac{1}{2}\vec{k}_i$, so that

$$A(\alpha, \beta) = \frac{1}{8\pi^2} \int_{-1}^1 dz \\ \times \int \frac{d\vec{q}}{(q^2 - \frac{1}{4}k_i^2 - i\epsilon)(|\vec{q} - \vec{p}'|^2 + \tau^2)^2}, \quad (15)$$

where $\vec{p}' = \vec{p} - \frac{1}{2}\vec{k}_i$. By use of the results obtained in Ref. 2, the real and imaginary parts of $A(\alpha, \beta)$

are found to be expressible as

$$\text{Re}A(\alpha, \beta) = A_R(\alpha, \beta) = \frac{1}{8} \int \frac{dz (p'^2 + \tau^2 - \frac{1}{4}k_i^2)}{\pi [(\frac{1}{4}k_i^2 + p'^2 + \tau^2)^2 - k_i^2 p'^2]}, \quad (16)$$

$$\text{Im}A(\alpha, \beta) = A_I(\alpha, \beta)$$

$$= \frac{k_i}{8} \int_{-1}^1 \frac{dz}{[(\frac{1}{4}k_i^2 + p'^2 + \tau^2)^2 - k_i^2 p'^2]}. \quad (17)$$

The final remaining integrations over z can be carried out analytically in a straightforward way; the results are presented in the Appendix. Extension of this type of approach to Hartree-Fock wave functions or configuration-interaction wave functions with Slater orbital analytic basis sets is described in Appendix B of Ref. 2.

III. NUMERICAL RESULTS

The real and imaginary parts of the polarization amplitude were evaluated for incident energies of 100 eV, 500 eV, and 40 keV as a function of the effective energy ΔE_{eff} for both H and He using the potential-field parameters given in Ref. 13. In the

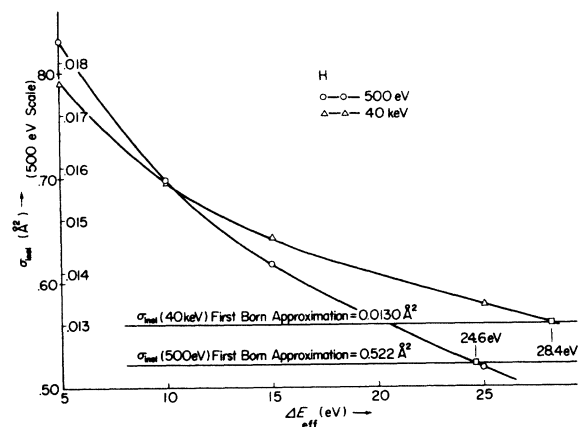


FIG. 1. Variation of σ_{inel} with changes in the effective energy ΔE_{eff} for the H atom as a function of the incident energy.

case of H the field is essentially exact (accurate to better than $\pm 0.1\%$ for the electron density), and for He it is an excellent approximation to the Hartree-Fock field (again $\pm 0.1\%$ accuracy in describing the electron density).

Figures 1-4 show that if ΔE_{eff} is chosen to yield accurate values of the total inelastic scattering factor from the relation²

$$\sigma_{inel} = (4\pi/k_i) \text{Im} f_{p01}^{(2)}(0), \quad (18)$$

reasonable values of the polarizability given by

$$\alpha = -\left(\frac{4}{\pi}\right) \lim_{K \rightarrow 0} \frac{\partial \text{Re} f_{p01}(\theta)}{\partial K} \quad (19)$$

are obtained and vice versa. In the limit as $K \rightarrow 0$, α is independent of the incident energy as shown in the Appendix. The small differences between Figs. 2 and 4 were caused by rounding errors in the nu-

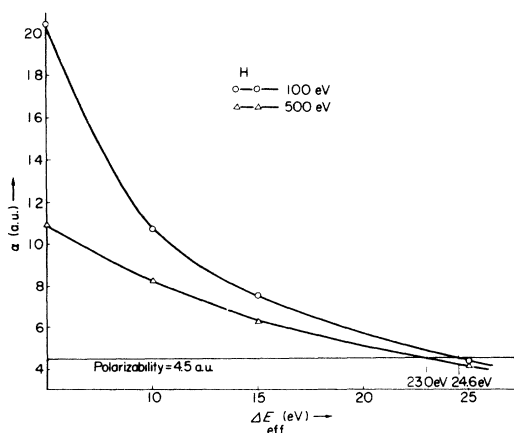


FIG. 2. Variation of the static polarizability α with changes in the effective energy ΔE_{eff} for the H atom as a function of the incident energy.

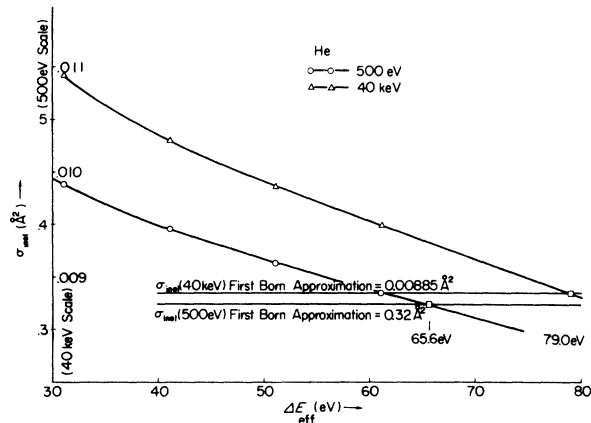


FIG. 3. Variation of σ_{inel} with changes in the effective energy ΔE_{eff} for the He atom as a function of the incident energy.

merical estimation of the limiting slope. The purpose of the numerical estimates was to determine the angular range over which the cross section exhibited a first Born behavior for a potential of the form $\alpha/(r^2 + r_0^2)^2$. Further, the energies ΔE_{eff} for which the exact polarizabilities are given turn out to be fairly close approximations to one-half the value of the mean excitation energy [see Eq. (A8)]. The mean excitation energy which gives the proper value for the Bethe asymptotic inelastic cross section is $\exp[L(-1)/M_{tot}^2]$,^{15, 16} and is given by 12.64 eV for H and 31.77 eV for He¹⁶; twice these values, 25.3 and 63.5 eV, correspond rather well to values of ΔE_{eff} yielding reasonable estimates of σ_{inel} and α for all incident energies studied so far. In this paper the compromise values of $\Delta E_{eff} = 25$ eV for H and $\Delta E_{eff} = 61.1$ eV for He were employed for all the calculations.

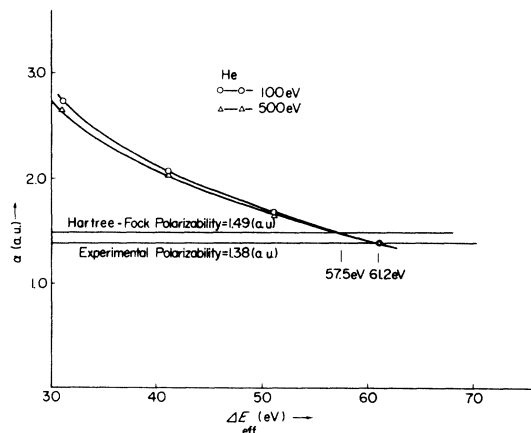


FIG. 4. Variation of the static polarizability α with changes in the effective energy ΔE_{eff} for the He atom as a function of the incident energy.

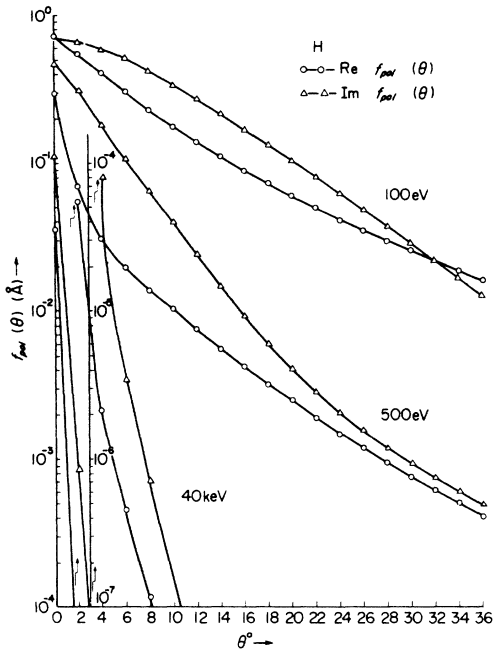


FIG. 5. Variation of the real and imaginary parts of the polarization amplitude as a function of the scattering angle for the H atom at incident energies of 100 eV, 500 eV, and 40 keV.

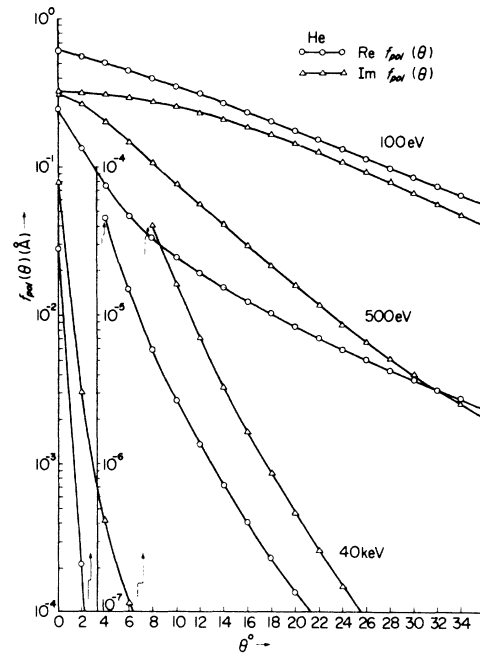


FIG. 6. Variation of the real and imaginary parts of the polarization amplitude as a function of the scattering angle for the He atom at incident energies of 100 eV, 500 eV, and 40 keV.

In Figs. 5 and 6, the dependence of the real and imaginary parts of the polarization amplitude on the incident energy as a function of scattering angle is displayed. In Table I a breakdown of the various correction values for scattering from He at an incident energy of 500 eV is given. Comparison with experiment¹⁷ and the results of a calculation by the extended-polarization potential (EP) method are given in Fig. 7. The agreement is rather good and might even be better if exchange were included in the partial-wave method. The results of Walker¹¹ show that the exchange correction at angles slightly larger than zero will tend to lie below the Born exchange value. Note that the major source of discrepancy between the present results and those of Bromberg¹⁷ for $\theta > 10^\circ$ is the exchange correction and not the polarization correction. It would of course be expected that at lower energies, where the second Born approximation fails, the results at larger angles will generally contain greater corrections from higher Born terms than the small-angle results.

In Table II the results for the present approach are compared with those obtained earlier by the ICCCA method for incident electron energies of 100 and 500 eV. The comparison for 40 keV is not given since the differences between the results of the two methods was less than 2% for all values in the angular range where the polarization correction was sig-

nificant ($>0.1\%$ of the total intensity). The imaginary part of $f_{\text{pol}}(\theta)$ in the T -matrix approach at $\theta = 0$ is generally lower, which means that it yields more reasonable estimates of σ_{ine1} . Comparison of the results for the two methods with experiment (see Table III), indicates that the ICCCA result may be better at small scattering angles. Until a more realistic treatment of exchange is employed, it will not be clear which method is best at larger angles although in theory the T -matrix approach should be superior.

TABLE I. Amplitude and phase of the elastic partial-wave electron scattering factor, the real and imaginary parts of the polarization amplitude, and the first Born exchange amplitude for He with an incident energy of 500 eV.

θ°	$ f^{\text{PW}}(\theta) $	$\eta(\theta)$	$\text{Re}f_{\text{pol}}^{(2)}(\theta)$	$\text{Im}f_{\text{pol}}^{(2)}(\theta)$	$f^{\text{Ex}}(\theta)$
0	0.4192	0.185	0.2432	0.3053	0.0577
2	0.4161	0.186	0.1345	0.2683	0.0572
4	0.4072	0.189	0.0749	0.2028	0.0557
6	0.3931	0.195	0.0472	0.1476	0.0534
8	0.3749	0.203	0.0331	0.1068	0.0504
10	0.3538	0.212	0.0248	0.0772	0.0469
14	0.3074	0.238	0.0154	0.0405	0.0395
20	0.2402	0.288	0.0085	0.0158	0.0288
30	0.1563	0.393	0.0036	0.0040	0.0163
40	0.1057	0.509	0.0018	0.0014	0.0094
50	0.0754	0.622	0.0010	0.0007	0.0056

TABLE II. Comparison of polarization amplitudes calculated by the ICCCA and T -matrix approaches for H and He at 100 and 500 eV.

θ°	100 eV				500 eV			
	$\text{Re}f_{\text{pol}}(\theta)$ (\AA)		$\text{Im}f_{\text{pol}}(\theta)$ (\AA)		$\text{Im}f_{\text{pol}}(\theta)$ (\AA)		$\text{Im}f_{\text{pol}}(\theta)$ (\AA)	
	ICCCA ^a	T^b	ICCCA	T	ICCCA	T	ICCCA	T
H								
0	0.640	0.721	0.731	0.697	0.281	0.297	0.475	0.473
5	0.280	0.354	0.588	0.554	0.0122	0.0240	0.142	0.139
10	0.116	0.176	0.371	0.339	0.00471	0.0102	0.0415	0.0395
20	0.0318	0.0600	0.124	0.103	0.00200	0.00245	0.00468	0.00401
30	0.0167	0.0251	0.0389	0.0282	0.000584	0.000760	0.00119	0.000927
50	0.00796	0.00665	0.00540	0.00191	0.000097	0.000119	0.000206	0.000137
He								
0	0.515	0.616	0.412	0.324	0.223	0.243	0.309	0.305
5	0.382	0.477	0.392	0.305	0.0420	0.0585	0.179	0.173
10	0.266	0.350	0.339	0.258	0.0129	0.0248	0.0823	0.0772
20	0.118	0.174	0.209	0.145	0.00494	0.00849	0.0184	0.0158
30	0.0550	0.0853	0.110	0.0673	0.00297	0.00365	0.00537	0.00399
50	0.0210	0.0228	0.0254	0.00910	0.000974	0.000957	0.00118	0.000666

^aEffective energies used in the ICCCA calculation were $\Delta E_{\text{eff}} = 12.6$ eV for H and $\Delta E_{\text{eff}} = 31.18$ eV for He.

^bEffective energies used in the T -matrix calculation were $\Delta E_{\text{eff}} = 25$ eV for H and $\Delta E_{\text{eff}} = 61.1$ eV for He.

In order to analyze the possible sources of error in the T -matrix and ICCCA approaches it is helpful to recapitulate the underlying assumptions. It was assumed in the ICCCA method that the bound-state optically allowed transitions dominated the inelastic scattering and that the differential cross section for these transitions is given accurately by the first Born approximation. These assumptions, neglecting relativistic effects which introduce errors probably not greater than 10–20% for incident energies less than 50 keV,¹⁶ should become increasingly better with increasing energy. These same assumptions are implicitly contained in the T -matrix method as developed here because of the way in which the inverse operator was expanded. It was also assumed that the form of the optical theorem

$$\sigma_{\text{tot}} = \sigma_{\text{elastic}} + \sigma_{\text{inel}} = (4\pi/k) \text{Im}f_{(0)}^{\text{PW}} + (4\pi/k) \text{Im}f_{\text{pol}}^{(2)}(0) \quad (20)$$

was valid. This seems very reasonable since $(4\pi/k) \text{Im}f_{(0)}^{\text{PW}}$ for He at 500 eV is 0.085 \AA^2 and Bromberg's experimental value¹⁷ is 0.095 \AA^2 . The σ_{inel} values obtained from $\text{Im}f_{\text{pol}}^{(2)}(0)$ seem to be reasonable values¹⁸ and Eq. (17) can certainly be expected to improve with increasing energy. Thus it would seem that the limiting magnitude of $\text{Im}f_{\text{pol}}(0)$ is determined by the total inelastic cross section.

The proper behavior of the real part of the polarization amplitude at small angles is more difficult to ascertain. It seems likely that the large r dependence of the scattering potential must have the limiting form $1/r^4$.¹⁸ Because of this, the procedure of fitting the $\text{Re}f_{\text{pol}}(0)$ in the limit as $\theta \rightarrow 0$ to the

first Born amplitude for the potential $\alpha/(r_0^2 + r^2)^2$ seems reasonable, although by no means rigorous. The fact that

$$-\frac{4}{\pi} \lim_{k \rightarrow 0} \frac{\partial \text{Re}f_{\text{pol}}^{(2)}(\theta)}{\partial K}$$

yields an excellent estimate of the polarizability, lends some credence to this approach. The effective-range parameter r_0 in the potential is given in Table IV as a function of the incident energy for H and He. Insofar as it does not appear that a high-energy form of the effective-range theory, predicting the effective range as a function of energy, has yet

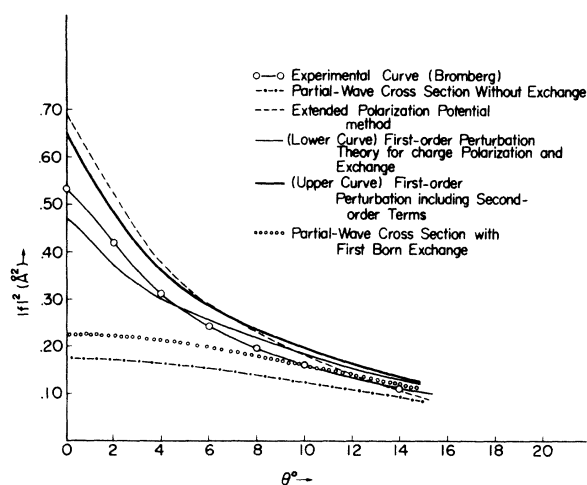


FIG. 7. Comparison of the experimental results for the absolute differential cross section for He at 500 eV with the results of various theoretical calculations.

TABLE III. Comparison of results for the elastic differential cross section, including exchange and polarization, given by the ICCA and T -matrix methods, with experiment.

θ°	$ f $ ICCA (\AA^2)	$ f ^2 T$ (\AA^2)	$ f ^2 \text{expt}^a$ (\AA^2)
0	0.630	0.653	0.530
2	0.472	0.480	0.418
4	0.344	0.360	0.303
6	0.273	0.287	0.242
8	0.226	0.237	0.196
10	0.189	0.197	0.161
14	0.134	0.137	0.114
20	0.077	0.079	0.064
30	0.030	0.031	0.026
40	0.012	0.013	0.011
50	0.0064	0.0066	0.0057

^aData of Bromberg (see Ref. 17).

been developed, little can be said about the quantitative behavior of the r_0 values reported in Table IV. Qualitatively, it seems reasonable that the effective range should increase with increasing incident energy as the $1/r^4$ interaction is made less important out to larger distances from the nucleus at high incident energies.

The analysis of the charge polarization given in Ref. 7 indicated that r_0 for He varied as the square root of the incident energy as $r_0^2(\text{a. u.}) = \frac{1}{200}E + 0.4$ and $r_0^2(\text{a. u.}) = \frac{1}{200}E$, respectively, where E was the incident energy in eV. A similar analysis of the data in Table IV yielded the results $r_0^2(\text{a. u.}) = (E/13.5) - 0.9$ for H and $r_0^2(\text{a. u.}) = \frac{1}{70}E - 0.14$ for He. The dependence of r_0^2 on E was approximately linear between 100 and 50 keV. This can be regarded as an independent confirmation of the ideas presented in Ref. 7. It should be noted that the use of the smaller values of r_0 (i. e., $\frac{1}{200}E$) will worsen the agreement between the results presented here and the experimental results. The differences cannot be considered significant though, since the methods in Ref. 7 differ significantly in other ways from the method described here.

Variation of the potential-field parameters (λ_i 's) by 2% indicated similar percentage changes in r_0 , α , and σ_{tot} . Thus, the only possibilities for changes within the present theoretical framework would seem to lie in the use of correlated wave functions to describe the target system or corrections from higher-order Born terms. The latter seems unlikely however in the keV range of incident energies.

The foregoing discussion brings up one last comparison between the results of this paper and previous theoretical results for H given in the work of Mohr⁴ for an incident energy of 34 keV. The results of the comparison are summarized in Table

V. Since the method of this paper agrees with experiment and the calculations of the EP method³ for He at an incident energy of 500 eV and since the formalism should be even more exact at higher energy, the strong peaking of the elastic cross section at 34 keV found in the work of Mohr⁴ is indeed puzzling.

The results of the T -matrix method for H at the other two energies, 50 and 19.5 eV, for which results were reported by Mohr⁴ showed a stronger peaking in the forward direction with decreasing energy. At 54 eV the intensity at $\theta = 0$ was 4 times the Born value and about 16 times the Born value at 19.5 eV. While the validity of the T -matrix approach must surely be questionable at these lower energies, the qualitative behavior of the result does seem to be reasonable. The results of Mohr⁴ at 19.5 and 54 eV show the same qualitative behavior (intensity at $\theta = 0$ for 19.5 eV is approximately twice as large as in the case of 54 eV). Why the polarization correction, which is decreasing with increasing incident energy between 19.5 and 54 eV, should start to increase again at a higher energy seems to be an additional anomaly in the results presented by Mohr.⁴

The calculations in this paper were carried out on the Hokkaido University FACOM 23060 computer in double-precision arithmetic. Comparison with single-precision results indicated that no rounding errors of any consequence were present in the calculation. Calculation of the real and imaginary parts of the polarization amplitude for 100 different values of the scattering angle at each of three different energies required 50 sec in double-precision arithmetic. Judging from the comments in the lit-

TABLE IV. Variation of r_0 in the limiting potential $\alpha/(\gamma_0^2 + r^2)^2$ with incident energy for H and He obtained from the $\text{Ref}_{\text{pol}}(\theta)$ in the small-angle limit.

Element	Incident energy (eV)	α (Ry a. u.)	r_0 (\AA)
H	50	4.3	0.9
	100		1.3
	250		2.2
	500		3.2
	1 000		4.5
	5 000		10
	10 000		15
50 000	29		
He	100	1.53	0.6
	250		0.9
	500		1.4
	1 000		2.0
	5 000		4.7
	10 000		6.6
	50 000		13

TABLE V. Comparison of the total elastic differential cross section for H at an incident electron energy of 34 keV.

θ°	$ f ^2$ partial wave (\AA^2)	Polarization correction (\AA^2)	$ f ^2$ total ^a (\AA)	$ f ^2$ total (\AA)
0.000	0.318	0.063	0.381	2×10^4
0.025	0.315	0.014	0.329	3
0.050	0.312	0.009	0.321	1.5
0.075	0.309	0.006	0.315	1.2
0.100	0.306	0.005	0.311	0.9

^aSee Ref. 5.

erature concerning computing difficulties (see Ref. 3 and Mohr in Ref. 4) in other methods, it appears that the present scheme is simpler than previously proposed methods, although the potential user should not lose sight of the fact that it is essentially a high-energy approximation.

Another advantage of the ICCCA or T -matrix approaches is the fact that their success or failure can

be predicted in advance if experimental data on the angular dependence of the differential cross sections for the most prominent inelastic events are available. If the first Born approximation describes the angular dependence of the differential cross section of the main inelastic transitions (i. e., those transitions accounting for 90% or so of the total inelastic scattering) correctly, then the method described here and in Ref. 2 must give a good description of the polarization process. On the other hand, if there are serious discrepancies between first Born theory and experimental results for major contributing excitation processes, then a failure of these approaches can be anticipated.

ACKNOWLEDGMENTS

The author wishes to thank Professor M. Kimura and Professor T. Iijima for their kind hospitality during the course of his visit. Thanks are also due Mrs. K. Kashiwagi for her help in typing the manuscript and the Hokkaido University Computing Center for the use of their facilities.

APPENDIX: EXPLICIT FORMULAS FOR THE CALCULATION OF $A_I(\alpha, \beta)$ AND $A_R(\alpha, \beta)$

As in the ICCCA method, the results for the imaginary part will be given first, since they are the simplest to obtain. Only two formulas are needed to calculate the imaginary part:

$$A_I(\alpha, \beta) = \frac{k_i}{8(b^2 - 4ac)^{1/2}} \ln \left| \frac{c - a + (b^2 - 4ac)^{1/2}}{c - a - (b^2 - 4ac)^{1/2}} \right|, \quad (\text{A1})$$

$$A_I(\alpha, \alpha)_{(\theta=0)} = \frac{k_i}{4[\alpha^4 + \frac{1}{2}\alpha^2(k_i^2 + k_i^2) + \frac{1}{16}(k_i^2 - k_i^2)^2]}, \quad (\text{A2})$$

where

$$a = A^2 + \frac{1}{2}A(k_i^2 + k_i^2 + K^2) + a_0, \quad b = 2AB + \frac{1}{2}B(k_i^2 + k_i^2 + K^2) + b_0, \quad c = B^2 - \frac{1}{2}BK^2 + c_0,$$

with

$$A = \frac{1}{2}(\alpha^2 + \beta^2), \quad B = \frac{1}{2}(\alpha^2 - \beta^2), \quad a_0 = \frac{1}{8}K^2(k_i^2 + k_i^2 + \frac{1}{2}K^2) + \frac{1}{16}(k_i^2 - k_i^2)^2, \quad b_0 = \frac{1}{8}K^2(k_i^2 - k_i^2 + K^2), \quad c_0 = \frac{1}{4}K^2(k_i^2 - \frac{1}{4}K^2).$$

Note that Eq. (A1) can be used for the nonequivalent cases $A_I(\alpha, 0)$ and $A_I(0, \beta)$ as well as $A_I(\alpha, \alpha)$ when $\theta \neq 0$. Also Eq. (A1) for the three cases $A_I(\alpha, \beta)$, $A_I(\alpha, 0)$, and $A_I(0, \beta)$ will remain finite at zero angle with the result

$$A_I(\alpha, \beta)_{(\theta=0)} = \frac{1}{4k_i(\alpha^2 - \beta^2)} \ln \left| \frac{\alpha^2\beta^2 + \frac{1}{4}\alpha^2(k_i + k_i)^2 + \frac{1}{4}\beta^2(k - k_i)^2 + \frac{1}{16}(k_i^2 - k_i^2)^2}{\alpha^2\beta^2 + \frac{1}{4}\alpha^2(k_i - k_i)^2 + \frac{1}{4}\beta^2(k_i + k_i)^2 + \frac{1}{16}(k_i^2 - k_i^2)^2} \right|. \quad (\text{A3})$$

Equation (A2) is needed for the cases where $\alpha = \beta \neq 0$, $\theta = 0$ and $\alpha = \beta = 0$, $\theta = 0$. Note that Eq. (A1) will also suffice for the case $\alpha = \beta = 0$ but $\theta \neq 0$.

Again, as in the ICCCA case, the real part of $A(\alpha, \beta)$ is more complex, and the integral for the general case can be written as

$$A_R(\alpha, \beta) = \frac{1}{8(b^2 - 4ac)^{1/2}} \left((A_0 + B_0 z_1) \int_{-1}^1 \frac{dz}{(\alpha + \beta z + \gamma z^2)^{1/2}(z - z_1)} - (A_0 + B_0 z_2) \int_{-1}^1 \frac{dz}{(\alpha + \beta z + \gamma z^2)^{1/2}(z - z_2)} \right), \quad (\text{A4})$$

where

$$\alpha = \frac{1}{2}(\alpha^2 + \beta^2) + \frac{1}{4}K^2 = A + \frac{1}{4}K^2, \quad \beta = \frac{1}{2}(\alpha^2 - \beta^2) = B, \quad \gamma = -\frac{1}{4}K^2,$$

$$A_0 = A + \frac{1}{4}(k_i^2 - k_i^2 + K^2), \quad B_0 = B - \frac{1}{4}K^2, \quad z_{1,2} = [-b \pm (b^2 - 4ac)^{1/2}]/2c,$$

with a , b , and c given as in Eq. (A2). The result of the integration in Eq. (A4) is

$$A_R(\alpha, \beta) = \frac{1}{8(b^2 - 4ac)^{1/2}} \left\langle \frac{(A_0 + B_0 z_1)}{(|a_1|)^{1/2}} \left[\arctan \left(\frac{(\alpha^2 - \beta^2 - K^2)z_1 + 3\alpha^2 + \beta^2 + K^2}{4\alpha(|a_1|)^{1/2}} \right) \right. \right. \\ \left. \left. - \arctan \left(\frac{(\alpha^2 - \beta^2 + K^2)z_1 + \alpha^2 + 3\beta^2 + K^2}{4\beta(|a_1|)^{1/2}} \right) \right] - \frac{(A_0 + B_0 z_2)}{(|a_2|)^{1/2}} \left[\arctan \left(\frac{(\alpha^2 - \beta^2 - K^2)z_2 + 3\alpha^2 + \beta^2 + K^2}{4\alpha(|a_2|)^{1/2}} \right) \right. \right. \\ \left. \left. - \arctan \left(\frac{(\alpha^2 - \beta^2 + K^2)z_2 + \alpha^2 + 3\beta^2 + K^2}{4\beta(|a_2|)^{1/2}} \right) \right] \right\rangle, \quad (\text{A5})$$

where $\alpha_{1,2} = \gamma z_{1,2}^2 + \beta z_{1,2} + \alpha$. Strictly speaking Eq. (A5) is valid only if $\alpha_{1,2} < 0$. Since this was the case for the corresponding term in the ICCCA method, only the arctan form is displayed here. Individual $\alpha_{1,2}$ terms were tested in the computer program to make sure that $\alpha_{1,2}$ was always negative.

For the special cases at zero angle where (A5) breaks down, the formulas

$$A_R(\alpha, \alpha) = [\alpha^2 + \frac{1}{4}(k_i^2 - k_i^2)]/4\alpha[\alpha^4 + \frac{1}{2}\alpha^2(k_i^2 + k_i^2) + \frac{1}{16}(k_i^2 - k_i^2)^2], \quad (\text{A6})$$

$$A_R(0, 0) = \frac{\pi}{4K(b_0^2 - 4a_0c_0)^{1/2}} \left(\pm \frac{A'_0 - B'_0 z_1}{(z_1^2 - 1)^{1/2}} \pm \frac{A'_0 - B'_0 z_2}{(z_2^2 - 1)^{1/2}} \right) \quad (\text{A7})$$

can be used with

$$A'_0 = \frac{1}{4}(k_i^2 - k_i^2 + K^2), \quad B'_0 = \frac{1}{4}K^2.$$

The signs depend on whether or not $z_{1,2}$ is negative or positive. Since in the cases investigated here $z_1 < -1$ and $z_2 > 1$, the plus sign can be used for both terms. The limiting value of the slope of $\text{Re}f_{\text{pol}}(\theta)$ as $K \rightarrow 0$ yields the polarizability as in Ref. 2 according to

$$\alpha = -\frac{4}{\pi} \lim_{K \rightarrow 0} \frac{\partial \text{Re}f_{\text{pol}}(\theta)}{\partial K} = \frac{16}{\frac{1}{2} \Delta E_{\text{eff}}} \sum_{i=1}^L \frac{\gamma_i}{\lambda_i^2}, \quad (\text{A8})$$

which is identical to the previous result if the effective energy ΔE_{eff} is taken as twice the mean excitation energy discussed in Ref. 2.

Two further cases which bear some mentioning are the integrals $A_R(\alpha, 0)$ and $A_R(0, \beta)$, which are not equivalent in this treatment, and are given as

$$A_R(\alpha, 0) = \frac{1}{8(b^2 - 4ac)^{1/2}} \left\langle \frac{A_0 + B_0 z_1}{(|a_1|)^{1/2}} \left[\arctan \left(\frac{(\alpha^2 - K^2)z_1 + 3\alpha^2 + K^2}{4\alpha(|a_1|)^{1/2}} \right) - \frac{1}{2}\pi \text{sgn}(z_1 + 1) \right] \right. \\ \left. - \frac{A_0 + B_0 z_2}{(|a_2|)^{1/2}} \left[\arctan \left(\frac{(\alpha^2 - K^2)z_2 + 3\alpha^2 + K^2}{4\alpha(|a_2|)^{1/2}} \right) - \frac{1}{2}\pi \text{sgn}(z_2 + 1) \right] \right\rangle, \quad (\text{A9})$$

$$A_R(0, \beta) = \frac{1}{8(b^2 - 4ac)^{1/2}} \left\langle \frac{(A_0 + B_0 z_1)}{(|a_1|)^{1/2}} \left[-\arctan \left(\frac{(K^2 - \beta^2)z_1 + 3\beta^2 + K^2}{4\beta(|a_1|)^{1/2}} \right) + \frac{1}{2}\pi \text{sgn}(1 - z_1) \right] \right. \\ \left. - \frac{(A_0 + B_0 z_2)}{(|a_2|)^{1/2}} \left[-\arctan \left(\frac{(K^2 - \beta^2)z_2 + 3\beta^2 + K^2}{4\beta(|a_2|)^{1/2}} \right) + \frac{1}{2}\pi \text{sgn}(1 - z_2) \right] \right\rangle, \quad (\text{A10})$$

with the signs giving $+\frac{1}{2}\pi$, $-\frac{1}{2}\pi$, $+\frac{1}{2}\pi$, and $-\frac{1}{2}\pi$, respectively, for the cases investigated so far. The constants are defined as before by setting either β or α equal to zero.

*Contribution No. 1885 from the Chemical Laboratories of Indiana University. The author gratefully acknowledges financial support from the National Science Foundation, under Grant No. GF 328.

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Vibrational Excitation and Compound States in NO[†]

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(Received 22 December 1970)

The cross section for elastic scattering by electron impact on NO shows resonances in the energy range 0–2 eV. These resonances, with a spacing of about 0.16 eV ($\omega_e=0.17$ eV), are associated with vibrational levels of NO⁺, and there is a near-coincidence in energy between the 4th vibrational state of NO and the 6th vibrational state of NO⁺. The width of these resonances increases monotonically from 0.02 to 0.10 eV as the vibrational quantum number of NO⁺ goes from 1 to 6. The energy dependence of the vibrational cross sections exhibits peaks at the positions of these resonances, and the magnitude of these peaks is measured. The vibrational states of NO⁺ can decay by the emission of an electron into various vibrational levels of NO. The branching ratio for a few of these decays is measured. A potential energy diagram of NO⁺ is drawn, using the experimental evidence.

I. INTRODUCTION

This paper presents the results of measurements of elastic and inelastic processes occurring in nitric oxide at incident electron energies below about 2.0 eV. This work is an extension of previous work¹ of a similar nature in O₂. It is now well known that vibrational excitation can occur by "direct" excitation of the vibration, and by excitation of a compound state with subsequent decay into a free electron plus a vibrationally excited molecule. The latter process seems to be the dominant mode of vibrational excitation in diatomic molecules such as N₂, CO, O₂, and H₂.^{1–3} The "direct" process is larger in those molecules which have a permanent dipole moment.²

Nitric oxide forms a stable parent negative ion (as does O₂), and it has a permanent dipole moment. Thus one may expect not only excitation via the compound state formed by the traversal of the NO⁻ potential curve in the Franck-Condon region

of the NO molecule, but also a significant contribution from direct dipole interaction. Previous work in NO appears to have been confined to a study of resonances in the elastic scattering cross section at low electron energy. These resonances have been observed both in transmission⁴ and in pure elastic scattering.⁵

We show in this paper that the vibrational excitation cross section for NO consists of a series of spikes superimposed on a monotonically increasing background. The spacing of these spikes is about 160 mV, equal to the spacing of resonances in the elastic cross section. In contrast to O₂^{-*}, which has a lifetime against autoionization of about 10⁻¹⁰ sec, the lifetime of NO^{-*} is considerably shorter, leading to broader spikes in the elastic and the vibrational cross sections. Further, we find that these spikes become broader at higher energies. We find, as in the case of oxygen, that the compound states prefer to decay into the lower vibrational states of the molecule, though the branching