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Elastic Scattering of Electrons by Helium and Hydrogen Atoms in Ground Quantum States

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The direct and exchange scattering amplitudes for helium $(1s)^2$ with antiparallel spins in a three-body approximation, and for hydrogen $1s$, are treated. The fundamental differential and integral equations are arrived at by using a simple atomic model given by Allis and Morse. Analytical formulas for differential elastic cross sections are derived for the collisions of an unpolarized electron wave with helium and hydrogen atoms in the above-mentioned quantum states. The second Born approximation is given, and distortion and exchange effects are taken into consideration. The exchange effect is calculated in the second Born approximation and the perturbed exchange integral is calculated analytically to a good degree of approximation.

The analytical formulas derived for higher scattering angles are in qualitative agreement with experimental results in the low-energy range.

I. INTRODUCTION

A PROBLEM of basic importance in the quantum theory is the theoretical explanation[1–3] of phenomena occurring in electron collisions with atoms in the low-energy range. Especially noticeable discrepancies between the theoretical and experimental data appear in atomic systems of light elements such as helium and hydrogen, in which a large number of effects occur for this energy range. A number of papers are in agreement that the Born approximation method appears suitable for higher energies of the incident electrons, though these papers possess differences in the number of summands included in the perturbed member of the Schrödinger equation, which is then solved with the help of different methods. However, the Born approximation neglects the indistinguishability of the electrons. The use of the first approximation in perturbation theory and the neglect of the indistinguishability of the electrons appear to be very substantial faults in calculations at lower electron energies (distortion and exchange effect).

One might therefore suppose that in the solution of the complex problem some progress may be achieved (1) through specialization of all expressions on the basis of broad energy intervals of a proved atomic model (Allis and Morse[4]), (2) through the inclusion of the distortion effect corresponding to a given number of summands in the perturbed member of the Schrödinger equation according to successive approximations (with regard to convergence in a closed analytical form), and (3) by including the exchange effect by the Oppenheimer method in lower energy ranges in corresponding analytical (if possible closed) expressions.

On this basis—besides deriving formulas for the individual effects—the aim of this paper is to find the corresponding extension of the validity of analytical relations for lower energy ranges.

II. FUNDAMENTAL EQUATIONS; DIRECT SCATTERING

The Schrödinger wave equation describing the incidence of an electron wave on a helium atom in the ground quantum state, assuming that the infinitely heavy[5] nucleus is at rest at the origin during the collision, may, by using the simplified atomic model, be written in the form

$$\left\{\sum_{i=1}^{3}\left[\left(\frac{\hbar^2}{2m}\right)\nabla_i^2+\frac{2\epsilon^2}{r_i}-\frac{\epsilon^2}{r_{ii'}}\right]+E\right\}\Psi=0, \tag{1}$$

where suffix 1 denotes the incident electron, suffixes 2 and 3 denote the orbital electrons, and i' denotes always the nearest higher suffix to i in a cyclic suffix permutation (1,2,3).

Let the total energy of the system E be given as the sum of the energy E_0 of the orbital electrons and the kinetic energy of the incident electron. Then the function Ψ may be expressed in the form

$$\Psi(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)=\left(\sum_n+\int\right)\psi_n(\mathbf{r}_2,\mathbf{r}_3)F_n(\mathbf{r}_1), \tag{2}$$

where the symbol $(\sum+\int)$ signifies summation over the wave functions of the discrete spectrum and integration over the wave functions of the continuous spectrum and ψ_n is a set of orthonormalized helium functions.

Multiplication of Eq. (1) by $\psi_n^*(\mathbf{r}_2,\mathbf{r}_3)$, with the form of Ψ given in (2), and integration over the space of the orbital electrons with the help of the orthonormality of helium wave functions, lead to the expression

$$\{\nabla_1^2+k_n^2\}F_n(\mathbf{r}_1)=V_{0n}F_0(\mathbf{r}_1), \tag{3}$$

where

$$k_n^2=(2m/\hbar^2)(E-E_n),$$

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[1] H. S. W. Massey and C. B. O. Mohr, Proc. Roy. Soc. (London) **A136**, 289 (1932); **139**, 187 (1932); **140**, 613 (1933).

[2] B. L. Moiseiwisch, Proc. Roy. Soc. (London) **A219**, 102 (1953).

[3] S. Borowitz, Phys. Rev. **96**, 1523 (1954); **101**, 1835 (1956).

[4] W. P. Allis and P. M. Morse, Z. Physik **70**, 567 (1931).

[5] The corrections for a nucleus of finite mass are not considered. For the corresponding transformation equation, see S. Borowitz and B. Friedman, Phys. Rev. **89**, 441 (1953); **93**, 251 (1954).

and

$$V_{0n}=\frac{2m}{\hbar^2}\int\int\left(\frac{\epsilon^2}{r_{12}}+\frac{\epsilon^2}{r_{13}}-\frac{2\epsilon^2}{r_1}\right)\times\psi_0(\mathbf{r}_2,\mathbf{r}_3)\psi_n{}^*(\mathbf{r}_2,\mathbf{r}_3)d\mathbf{r}_2d\mathbf{r}_3. \quad (4)$$

By including known approximate auxiliary conditions, according to which the asymptotic form of the function F_0 represents an incident (plane) wave and a scattered (spherical) one, whereas the function F_n ($n\neq0$) represents scattered waves only, we may, by determining the Green's function of the given problem, pass to the integral equation

$$F_n(\mathbf{r}_1)=\delta_{n0}\exp(i\mathbf{k}_n\cdot\mathbf{r}_1)-\int V_{0n}(\mathbf{r}_1')F_0(\mathbf{r}_1')\frac{\exp(ik_n|\mathbf{r}_1-\mathbf{r}_1'|)}{4\pi|\mathbf{r}_1-\mathbf{r}_1'|}d\mathbf{r}_1'. \quad (5)$$

From the asymptotic form of (5) ($r_1\gg r_1'$), it may immediately be seen that the amplitudes of the scattered waves are of the form

$$f_n(\theta,\varphi)=-\frac{1}{4\pi}\int V_{0n}(\mathbf{r}_1')F_0(\mathbf{r}_1')\exp(-i\mathbf{k}_n\cdot\mathbf{r}_1')d\mathbf{r}_1'. \quad (6)$$

An expression formally identical to (6) would have been obtained in the case of an electron wave incident hydrogen atom in the ground quantum state, with the difference that V_{0n} in (4) is now

$$V_{0n}'=\frac{2m}{\hbar^2}\int\left(\frac{\epsilon^2}{r_{12}}-\frac{\epsilon^2}{r_1}\right)\psi_0'(\mathbf{r}_2)\psi_n'^*(\mathbf{r}_2)d\mathbf{r}_2; \quad (4')$$

i.e., for hydrogen we denote the corresponding quantities in (4) with a prime. The functions ψ_n' here represent a set of orthonormal hydrogen functions which—unlike those of helium—may be obtained in exact analytical form.

III. EXCHANGE SCATTERING

If $E>E_n$, i.e., for small energies of the incident particles, there is always the possibility that in the nth quantum state the incident electron will be captured and the orbital electron ejected. Equation (1) will then be satisfied for parahelium by the functions $\Psi(\mathbf{r}_2,\mathbf{r}_3,\mathbf{r}_1)$ and $\Psi(\mathbf{r}_3,\mathbf{r}_1,\mathbf{r}_2)$. Analogously to the preceding part, with the difference that the asymptotic forms determining the boundary conditions are here in the form of scattered waves only, we get from the asymptotic form of the integral equation the amplitudes of the scattered waves:

$$\begin{aligned}{}^ig_n(\theta_i,\varphi_i)&=-\frac{1}{4\pi}\int\int Q_{0n}(\mathbf{r}_1',\mathbf{r}_i')F_0(\mathbf{r}_1')\times\exp(-i\mathbf{k}_n\cdot\mathbf{r}_1')d\mathbf{r}_1'd\mathbf{r}_i',\\ Q_{0n}(\mathbf{r}_1',\mathbf{r}_i')&=\frac{2m}{\hbar^2}\int\left(\frac{\epsilon^2}{r_{1j}'}+\frac{\epsilon^2}{r_{ij}'}-\frac{2\epsilon^2}{r_i'}\right)\psi_n{}^*(\mathbf{r}_1',\mathbf{r}_j')\times\psi_0(\mathbf{r}_i',\mathbf{r}_j')d\mathbf{r}_j';\quad i,j=2,3;\quad i\neq j\end{aligned} \quad (7)$$

for helium, whereas for hydrogen we have only

$$\begin{aligned}g'(\theta_2',\varphi_2')&=-\frac{1}{4\pi}\int\int Q_{0n}'(\mathbf{r}_1',\mathbf{r}_2')F_0(\mathbf{r}_1')\times\exp(-i\mathbf{k}_n\cdot\mathbf{r}_2')d\mathbf{r}_1'd\mathbf{r}_2',\\ Q_{0n}'(\mathbf{r}_1',\mathbf{r}_2')&=\frac{2m}{\hbar^2}\left(\frac{\epsilon^2}{r_{21}'}-\frac{\epsilon^2}{r_2'}\right)\psi_n{}^*(\mathbf{r}_1')\psi_0(\mathbf{r}_2').\end{aligned} \quad (7')$$

The exchange with incident electrons may, however, take place only in accordance with the Pauli principle which requires in Eq. (1) an antisymmetrical wave function. For parahelium this function must be an antisymmetrical wave function for each of the electron pairs. With the help of the spin functions it is possible to write such an antisymmetrical wave function which is in agreement with this formalism in the separate form

$$\Psi=\left(\sum_n+\int\right)\left[\psi_n(\mathbf{r}_2,\mathbf{r}_3)F_n(\mathbf{r}_1)\frac{(\alpha_2\beta_3-\alpha_3\beta_2)\alpha_1}{\sqrt{2}}+\psi_n(\mathbf{r}_3,\mathbf{r}_1)\,{}^2G_n(\mathbf{r}_2)\frac{(\alpha_3\beta_1-\alpha_1\beta_3)\alpha_2}{\sqrt{2}}+\psi_n(\mathbf{r}_1,\mathbf{r}_2)\,{}^3G_n(\mathbf{r}_3)\frac{(\alpha_1\beta_2-\alpha_2\beta_1)\alpha_3}{\sqrt{2}}\right], \quad (8)$$

where $2^{-\frac{1}{2}}(\alpha_2\beta_3-\alpha_3\beta_2)\alpha_1$ is an antisymmetrical spin function with regard to electrons 2 and 3, F_n is given by expression (5), and the functions ${}^2G_n$ and ${}^3G_n$ are analogous solutions of Eq. (3) with the asymptotic forms given in (7) for helium.

For hydrogen the antisymmetrical wave function is

$$\Psi'=\left(\Sigma+\int\right)\times[\psi_n'(\mathbf{r}_2)F_n(\mathbf{r}_1)\beta_2\alpha_1-\psi_n(\mathbf{r}_1)G_n(\mathbf{r}_2)\beta_1\alpha_2], \quad (8')$$

in which the G_n are solutions of Eq. (3) with the asymptotic forms (7′).

As we consider neither the emission nor the absorption of electrons, we have the scattering coefficient in the form

$$\sigma_{0n}=(k'/k_0)|(0,k_0|V|n,k')|^2, \quad (9)$$

where $(0,k_0|V|n,k')$ denotes the transformation matrix. For the incident electron beam, which is considered unpolarized, both polarization states must be admitted. Symmetrical spin functions are then obtained with threefold degeneracies ($s=1$), whereas the antisymmetrical spin functions correspond to singlets with lower energy states than triplets. The corresponding scattering coefficient[6] is

$$\sigma_{0n}=(k'/k_0)\{w_s|f_n+g_n|^2+w_a|f_n-g_n|^2\}, \qquad (10)$$

where the statistical weights related to spin states may be determined with the help of spin functions in (8) and (8′), respectively. We thus get $w_s=0$, $w_a=1$ for parahelium, and $w_s=\frac{3}{4}$, $w_a=\frac{1}{4}$ for hydrogen.

IV. DISTORTION EFFECT

For the functions F_n we have derived the differential equation (3), the right-hand side of which is negligible for high velocities of the incident particles. The exact solution of the differential equation (3) with regard to the boundary conditions (5) is given formally with the help of Green's theorem in the form of the integral equation (6). When the right-hand side of Eq. (3) is negligibly small, the second term of this formal solution is also negligibly small. This represents a zero approximation for the function F_n in the solution of the integral equation (6) from the point of view of successive approximations. Thus,

$$F_0(\mathbf{r}_1)=\exp(i\mathbf{k}_n\cdot\mathbf{r}_1), \quad F_n=0, \quad (n\neq 0). \qquad (11)$$

Using (11) in (6), we get the first Born approximation. We may thus say that in this approximation we neglect the influence of scattered waves for all values of n. With regard to the fact that the probability of inelastic collisions relative to elastic collisions is negligibly small for all energy values except those which approach the resonance potential and correspond to atomic polarization by the electron wave, we may not, considering polarization, neglect the functions F_n even for $n\geq 1$. Likewise, the probabilities of the exchange effect are negligibly small[1] ($G_n\sim 0$) in elastic collisions. Thus it may be expected that the leading terms for higher approximations will involve only the function F_0. To solve the differential equation (3) for $n=0$, we express F_0 by zonal Legendre polynomials in the form

$$F_0(\mathbf{r}_1)=\frac{1}{r_1}\sum_{l=0}^{\infty} f_l(r_1)P_l(\cos\theta). \qquad (12)$$

By substituting (12) into (3), we get

$$\left[\frac{d^2}{dr_1^2}+k_0^2-V_{00}(r_1)-\frac{l(l+1)}{r_1^3}\right]f_l(r_1)=0, \qquad (13)$$

where, in the asymptotic form,

$$f_l(r_1)\sim C_l\sin(kr_1-\tfrac{1}{2}l\pi+\eta_l), \qquad (14)$$

η_l denoting a phase constant. The asymptotic solution of Eq. (3) for $n=0$ is thus given by the series (12), where the f_l are given by expression (14). We again substitute suffix l for n, since this will not lead to misunderstanding. If we include the boundary condition in the solution, we get, as is known from the quantum-mechanical problem on scattering, a relation between C_n and the phase constants η_n in the form

$$C_n=i^n(2n+1)e^{i\eta_n}. \qquad (15)$$

The phase constants in expression (15) for $n\geq 1$ assume, for energy values smaller than 200 ev, especially small values in comparison with η_0.[7] Therefore, if we compare F_0 in (12) with the known expansion of the plane wave,

$$e^{i\mathbf{k}\cdot\mathbf{r}}=(\pi/2kr)^{\frac{1}{2}}\sum i^n(2n+1)J_{n+\frac{1}{2}}(kr)P_n(\cos\theta), \qquad (16)$$

we may identify all the terms in the series (16) for $n\geq 1$ with terms in the series (12) for $n\geq 1$. Then

$$F_0(\mathbf{r}_1)=\exp(i\mathbf{k}\cdot\mathbf{r}_1)-\alpha'(kr_1)^{-1}\exp(ikr_1), \qquad (17)$$

where

$$-\alpha'=(1/2i)[\exp(2i\eta_0)-1]=\tfrac{1}{2}\sin(2\eta_0)+i\sin^2\eta_0. \qquad (18)$$

In the same manner, we may take into account even higher approximations in the series (12); however, as already mentioned, these will not be considered further. Let us define here the constant α, such that

$$\alpha'=i\alpha. \qquad (19)$$

Let us consider more closely the formal solution of Eq. (3) given in the form of the integral equation (5) for $n=0$. In the asymptotic form, it is possible to write this solution

$$F_0(\mathbf{r}_1)=\exp(i\mathbf{k}_0\cdot\mathbf{r}_1)-f_0(\vartheta_1,\varphi_1)r_1^{-1}\exp(ik_0r_1),$$

where f_0 is given by (6). Taking note of the remarks in the text preceding Eq. (12), substituting into (6) for F_0 only the leading term from the series (12) ($l=0$), and using in (4) the Hylleraas functions,[8] we see that in the first approximation (the term which is only a function of k) we obtain after the integrations exactly expression (17). In the sense of successive approximations, the expression (17) for F_0 represents the first approximation of such a rearranged integral equation (5).

The distortion effect appears considerably more strongly in an incident electron wave than in the scattered waves, and therefore in the future we shall assume only the incident electron wave to be in the form of a perturbed wave function.

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[6] N. F. Mott and H. S. W. Massey, *The Theory of Atomic Collisions* (Oxford University Press, London, 1949), second edition.

[7] I. MacDougal, Proc. Roy. Soc. (London) **A136**, 549 (1932).

[8] V. A. Fok, Izvest. Akad Nauk Ser. Fiz. S.S.S.R. **18**, 161 (1954).

V. SECOND BORN APPROXIMATION

For the calculation in the second Born approximation it is necessary to know only the function f_0. This function for helium, after substitutions using the perturbed wave function (17), is

$$f_0(\theta,\varphi)=c\int\int\int\left(\frac{1}{r_{12}}+\frac{1}{r_{13}}-\frac{2}{r_1}\right)\exp[-2b(r_2+r_3)]\times\exp(-i\mathbf{k}\cdot\mathbf{r}_1)\left[\exp(i\mathbf{k}_0\cdot\mathbf{r}_1)-\frac{\alpha'}{k_0r_1}\exp(ik_0r_1)\right]\times d\mathbf{r}_1d\mathbf{r}_2d\mathbf{r}_3, \quad (20)$$

where the constants c and b are given by

$$c=-m\epsilon^2 2^{-1}\pi^{-3}\hbar^{-2}b^6, \quad b=Z_{\text{eff.}}a_0^{-1}.$$

Dividing the potential term into two parts, integrating over $\mathbf{r}_3$ in the first part, over $\mathbf{r}_2$ in the second, and using the gamma function

$$\int_0^\infty t^{n-1}\exp(-\kappa t)dt=\kappa^{-n}\Gamma(n), \quad (21)$$

we get, after suffix change and addition of the two parts,

$$f_0(\theta,\varphi)=c\frac{2\pi}{b^3}\int\int\left(\frac{1}{r_{12}}-\frac{1}{r_1}\right)\exp(-2br_2)\exp(-i\mathbf{k}\cdot\mathbf{r}_1)\times\left[\exp(i\mathbf{k}_0\cdot\mathbf{r}_1)-\frac{\alpha'}{k_0r_1}\exp(ik_0r_1)\right]d\mathbf{r}_1d\mathbf{r}_2, \quad (20')$$

which, apart from the factor $2\pi b^{-3}$, is exactly the same form as would have been obtained for hydrogen by the above substitutions with the corresponding constants c' and b':

$$c'=-m\epsilon^2 2^{-1}\pi^{-2}\hbar^{-2}b'^3, \quad b'=a_0^{-1}.$$

In order to carry out further integrations, let us choose the axis of the polar coordinates along the direction of the vector $\mathbf{k}_0$ and let the y axis lie in the plane of the vectors $\mathbf{k}_0$ and $\mathbf{k}'$. Then

$$\mathbf{k}_0\cdot\mathbf{r}_i=k_0r_i\cos\theta_i,$$
$$\mathbf{k}'\cdot\mathbf{r}_i=k'r_i(\cos\theta_i\cos\theta+\sin\theta_i\sin\theta\cos\varphi_i), \quad (22)$$

where θ is the angle formed by vectors $\mathbf{k}_0$ and $\mathbf{k}$ determining the angular distribution of the scattered electrons.

Integration of that part of (20′) involving the first term in the second bracket gives the first Born approximation:

$$dI_{1B}=-d(\pi^2/b^5)[2+z^2\sin^2(\theta/2)]/[1+z^2\sin^2(\theta/2)]^2,$$
$$z=k/b \text{ for helium}, \quad z=k/b' \text{ for hydrogen}, \quad (23)$$

where the constant d is equal to $2\pi cb^{-3}$ for helium and to c' for hydrogen. The square of the absolute value of expression (23) is the well-known Born formula.

For the calculation of the perturbed part in Eq. (20′) (deleting the constants before the integration sign), we have

$$I_{1D}=-\alpha'\int\int\left(\frac{1}{r_{12}}-\frac{1}{r_1}\right)\exp(-2br_2)\times\exp(-i\mathbf{k}'\cdot\mathbf{r}_1)\frac{\exp(ik_0r_1)}{k_0r_1}d\mathbf{r}_1d\mathbf{r}_2, \quad (24)$$

we use the expansion

$$\frac{1}{r_{12}}-\frac{Z}{r_1}=\sum_{\gamma=0}^{\infty}\sum_{p=-\gamma}^{\gamma}\delta_\gamma(r_1,r_2)P_\gamma{}^p(\cos\theta_1)\times P_\gamma{}^p(\cos\theta_2)\cos[p(\varphi_2-\varphi_1)], \quad (25)$$

where

$$\begin{aligned}\delta_0&=(1-Z)/r_1, \quad r_2<r_1\\&=1/r_2-Z/r_1, \quad r_2>r_1;\\ \delta_\gamma&=r_2{}^\gamma/r_1{}^{\gamma+1}, \quad r_2<r_1\\&=r_1{}^\gamma/r_2{}^{\gamma+1}, \quad r_2>r_1.\end{aligned} \quad (26)$$

where in our case $Z=1$. Substituting (25) into (24) and integrating over φ_2, we see that in the second summation sign only the term with $p=0$ is different from zero. By further integration over φ_1, using

$$\int_0^{2\pi}\exp(ik'r_1\sin\theta_1\cos\varphi_1\sin\theta)\exp(-im\varphi_1)d\varphi_1=2\pi i^mJ_m(k'r_1\sin\theta_1\sin\theta), \quad (27)$$

and over ϑ_2 using[9,10]

$$\int_0^{2\pi}\exp(i\varphi\cos\theta_1\cos\psi)\times J_{\gamma-\frac{1}{2}}(\varphi\sin\theta_1\sin\psi)C_r{}^\gamma(\cos\theta_1)\sin^{\gamma+\frac{1}{2}}\theta_1d\theta_1=(2\pi/\varphi)^{\frac{1}{2}}i^r\sin^{\gamma-\frac{1}{2}}\psi C_r{}^\gamma(\cos\psi)J_{\gamma+r}(\varphi), \quad (28)$$

we find that also all integrals for $\gamma\neq 0$ vanish. For the only nonzero term of the series, in which we again integrate over ϑ_1 with the help of (28), we get

$$-\alpha'(16\pi^2)\int_0^\infty\int_0^\infty\delta_0(r_1,r_2)\exp(-2br_2)\times\frac{\exp(ik_0r_1)}{k_0r_1}\frac{\sin(k'r_1)}{k'r_1}r_1{}^2dr_1r_2{}^2dr_2,$$

where δ_0 is given by (26). Through the influence of the potential terms this integral is not identically equal to zero if $r_2>r_1$, and we may therefore still rearrange it

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[9] G. N. Watson, *Theory of Bessel Functions* (Cambridge University Press, New York, 1944), p. 379, Eq. (1).

[10] E. T. Whittaker and G. N. Watson, *A Course of Modern Analysis* (Cambridge University Press, New York, 1952), fourth edition, p. 329.

to the form

$$-\alpha'\left(\frac{16\pi^2}{k_0k'}\right)\int_0^\infty \exp(-2br_2)r_2\int_0^{r_2}\left(\frac{r_1-r_2}{r_1}\right)$$
$$\times\exp(ik_0r_1)\sin(k'r_1)dr_1dr_2. \quad (29)$$

Considering the fact that we treat only elastic electron collisions, the law of conservation of energy ($k_0=k'=k$) must be satisfied. Let us introduce in (29) the substitutions $kr_1=x_1$ and $kr_2=x_2$; then we can find the integral over x_1 by elementary integrations:

$$\int_0^{x_2}\left(\frac{x_1-x_2}{x_1}\right)\exp(ix_1)\sin x_1dx_1=-\tfrac{1}{4}[\exp(2ix_2)-1]$$
$$-\tfrac{1}{2}ix_2[\mathrm{Ci}(2x_2)-\ln\delta 2x_2-i\,\mathrm{Si}(2x_2)-1], \quad (30)$$
$$\delta=\exp C,$$

where C is Euler's constant ($\delta=1.781072\cdots$). By substituting (30) into (29) using (21), by differentiations with respect to the parameter with the help of the expressions for the cosine integral and sine integral:

$$\left.\begin{aligned}\int_0^\infty \exp(-pt)\,\mathrm{Ci}(gt)dt&=-\frac{1}{p}\ln\left(1+\frac{p^2}{g^2}\right),\\ \int_0^\infty \exp(-pt)\,\mathrm{Si}(gt)dt&=-\frac{1}{p}\arctan\left(\frac{p}{g}\right),\end{aligned}\right\} \quad (31)$$

we get after integrations of the contributions of individual terms in (30) the perturbed integral in the closed form

$$I_{1D}=\frac{2\pi^2}{b^5}\frac{1}{z^2}\left\{\frac{1}{2(1+z^2)^2}\left[\frac{\alpha'}{z}(z^4-3z^2-2)+\alpha(1+z^4)\right]\right.$$
$$\left.-\alpha'\left[\arctan\left(\frac{1}{z}\right)-\frac{\pi}{2}\right]+\alpha\left[\ln\left(1+\frac{1}{z^2}\right)-\frac{1}{\delta^2}\right]\right\}, \quad (32)$$

where $z=k/b$.

Thus, if the exchange effect is not considered, the scattering intensity in the second Born approximation is given by

$$I(\vartheta)=d^2|I_{1B}+I_{1D}|^2, \quad (33)$$

where $d_{\mathrm{He}}=2\pi c/b^3$ and $d_{\mathrm{H}}=c'$ and where I_{1B} is given by Eq. (23), I_{1D} by Eq. (32). We have thus included in the calculation the distortion effect in the second Born approximation; its influence in exchange scattering will be shown in the next section.

VI. DISTORTION EFFECT IN EXCHANGE SCATTERING

The amplitudes of the scattered waves in exchange scattering ${}^ig_0$ are, as has been shown for helium, equivalent for both superscripts i, so we may limit ourselves to the calculation of the integral

$${}^2g_0(\theta_2,\varphi_2)=c\int\int\int\left(\frac{1}{r_{12}}+\frac{1}{r_{13}}-\frac{2}{r_1}\right)$$
$$\times\exp[-b(r_1+r_2+2r_3)]\exp(-i\mathbf{k}'\cdot\mathbf{r}_1)$$
$$\times\left[\exp(i\mathbf{k}_0\cdot\mathbf{r}_2)-\alpha'\frac{\exp(ik_0r_2)}{k_0r_2}\right]d\mathbf{r}_1d\mathbf{r}_2d\mathbf{r}_3. \quad (34)$$

By dividing the potential term in the first parentheses into two parts and by integrating the first part over $\mathbf{r}_3$, we get two integrals

$$g_0(\vartheta,\varphi)=\tfrac{1}{2}d(I_{21}+I_{22}). \quad (35)$$

The first of these,

$$I_{21}=\int\int\left(\frac{1}{r_{12}}-\frac{1}{r_1}\right)\exp[-b(r_1+r_2)]\exp(-i\mathbf{k}'\cdot\mathbf{r}_1)$$
$$\times\left[\exp(i\mathbf{k}_0\cdot\mathbf{r}_2)-\alpha'\frac{\exp(ik_0r_2)}{k_0r_2}\right]d\mathbf{r}_1d\mathbf{r}_2 \quad (34')$$

is identical with the expression which would have been obtained for hydrogen. The corresponding constant for hydrogen ($d=c'$) is given by Eq. (20). The second integral is equal to the product of two independent integrals,

$$I_{22}=\frac{b^3}{\pi}\int\exp(-br_2)\left[\exp(i\mathbf{k}_0\cdot\mathbf{r}_2)-\alpha'\frac{\exp(ikr_2)}{kr_2}\right]d\mathbf{r}_2$$
$$\times\int\int\left(\frac{1}{r_{13}}-\frac{1}{r_1}\right)\exp[-b(r_1+2r_3)]$$
$$\times\exp(-i\mathbf{k}'\cdot\mathbf{r}_1)d\mathbf{r}_1d\mathbf{r}_3, \quad (36)$$

and need be taken into consideration only for helium.

First we shall show the method for calculating the exchange integral I_{21}, which we again divide into two parts: the part originating from the unperturbed wave function in F_0, which will further be denoted $I_{21}{}^N$, and the part giving the distortion of this wave function, which will be called $I_{21}{}^D$.

For reasons to be indicated later, we shall first deal with the second part of the exchange integral, $I_{21}{}^D$. The orientation of the axes will be chosen identical to that in the preceding part of the calculation of the Born second approximation. Substituting into $I_{21}{}^D$ for the potential term the expansion (25), we find by integration over φ_1 that $p=0$. By integration over θ_1 we see that γ must also be equal to zero in order to obtain a term of the series which is not identically equal to zero. If, after the thus executed rearrangements, we use Eq. (27) for the integration over φ_2, and Gegenbauer's integral, Eq. (28), for the integration over θ_2, we get

$$I_{21}{}^{D}=-\frac{16\pi^2\alpha'}{k_0k'}\int_0^\infty\int_0^\infty\delta_0(r_1,r_2)\exp[-b(r_1+r_2)]\times\exp(ik_0r_1)\sin(k'r_2)r_1dr_1r_2dr_2,$$

where δ_0 is again given by Eq. (26) for $Z=1$. Therefore, after the substitutions $x'=kr_2$, $x=kr_1$, and having satisfied the law of conservation of energy $(k_0=k'=k)$, the nonzero part of the integral $I_{21}{}^{D}$ is

$$I_{21}{}^{D}=-\frac{16\pi^2\alpha'}{k^3}\int_0^\infty\exp(-\kappa x)\exp(ix)\left(\frac{1}{k^2}\right)\int_0^x(x'-x)\times\exp(-\kappa x')\sin x'dx'dx, \quad (37)$$

where $\kappa=b/k=1/z$. By differentiation with respect to the parameter κ in the second integral, we get the result that the second integral in x' is, with the exception of the factor k^{-2}, expressed by elementary integrations in the form

$$\left(x+\frac{\partial}{\partial\kappa}\right)\left[\frac{\exp(-\kappa x)}{\kappa^2+1}(\kappa\sin x+\cos x)-\frac{1}{\kappa^2+1}\right]. \quad (38)$$

Substituting the integration result (38) into (37), we see that for integrations over x we get special cases of integrals of the Lipschitz-Hankel type, i.e., the integral

$$\int_0^\infty\exp(-at)J_\gamma(b't)t^\gamma dt=\frac{(2b')^\gamma\Gamma(\gamma+\frac{1}{2})}{(a^2+b^2)^{\gamma+\frac{1}{2}}\sqrt{\pi}}, \quad (39)$$

and the integral

$$\int_0^\infty\exp(-\kappa x)J_\gamma(\delta x)dx=\frac{1}{\pi(\beta\delta)^{\frac{1}{2}}}Q_{\gamma-\frac{1}{2}}\left(\frac{\kappa^2+\beta^2+\delta^2}{2\beta\delta}\right). \quad (40)$$

For $\gamma=\frac{1}{2}$, the Legendre polynomial of the second order on the right side of (40) is equal to

$$Q_0(\mu)=\tfrac{1}{2}\ln(\mu+1)/(\mu+1).$$

For values $\kappa>\epsilon$, $\epsilon>0$ $(z<2/\epsilon)$ in which we are particularly interested in dealing with the slow collision of electrons with atoms, the convergence of this integral presents no difficulties. With the help of the special case of the Lipschitz-Hankel integral (30) and (40), after rearrangement, we get

$$I_{21}{}^{D}=-\frac{4\pi^2}{b^5}\frac{1}{(1+z^2)^3}\left[\alpha''(3-z^2)+\frac{2\alpha'}{z}\right], \quad (41)$$

which is the required evaluation of the integral belonging to the perturbed wave function. The constant α'' is here equal to α.

The calculation of the unperturbed exchange integral $I_{21}{}^{N}$ is very tedious and difficult. An approximate solution of this integral was obtained by Massey and Mohr,[11] by making an infinite series expansion, neglecting the contributions from the minima in the individual terms of the integrand, and considering that the expressions in the integrand replace the approximate terms. Massey and Mohr give a very detailed analysis of the contributions of the individual terms of the series and show in this connection, for slow electrons, the method of calculation of four terms of the thus-formed series. According to the analysis, two terms of the series for slow electrons already give a quite close approximation. Further, we are going to calculate these two substantial terms more accurately.

As shown in the Appendix, it is suitable to include in the integral $I_{21}{}^{D}$ the first term of the series [see (A2)]. Let us therefore introduce in the exchange integral I_{21} a division into parts,

$$I_{21}=I_{21}{}^{D'}+I_{21}{}^{N'}, \quad (42)$$

where $I_{21}{}^{D'}$ is the integral $I_{21}{}^{D}$ including the first term of series (A2) and $I_{21}{}^{N'}$ is the integral $I_{21}{}^{N}$ without this term. Then, as derived in the Appendix, the first part of the integral I_{21} is obtained in the form (41), where the constant α'' is

$$\alpha''=\alpha+1. \quad (43)$$

For the second part of the integral I_{21}, only an approximate solution may be given. Neglecting the influence of the terms of series (A2) in which $\gamma\geq 2$, we get the part $I_{21}{}^{N'}$ expressed in the form of an infinite series. The first terms of this series are then given as

$$I_{21}{}^{N'}=16\pi^2b^{-5}P_1(\cos\theta)(1+z^2)^{-3}\times(0.625-0.3z+1.539z^2-1.906z^3+0.377z^4-\cdots), \quad (44)$$

where the first two terms are given exactly and the others with accuracy 10^{-3}.

Now let us introduce the method of calculation of the integral I_{22} given by form (36). The first of the independent integrals, containing also the perturbed term, may be expressed by elementary integrations, using in the integration over r_2 differentiation by the parameter b. If we include in this integral the factor b^3/π, then we get the result of the integration for the unperturbed term in a simple form,

$$8/(1+z^2)^2,$$

where z is again k/b. Also the integration of the perturbed term may be performed by elementary integrations and with the help of differentiation with respect to the parameter b, so that we get

$$\frac{8}{(1+z^2)^2}\left[\alpha-\frac{\alpha'}{2z}(1-z^2)\right].$$

It remains, therefore, to evaluate the second inde-

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[11] H. S. W. Massey and C. B. O. Mohr, Proc. Roy. Soc. (London) **A132**, 605 (1931).

pendent integral containing the potential term. For this purpose we use again the expansion (25), first substituting in the integral the index 2 for index 3. After substituting the expansion (25), by an integration over φ_2 we see that $p=0$; by integration over φ_1 with the help of (27) and over ϑ_2 with the help of (28), we find also the $\gamma=0$. Using again Gegenbauer's integral (28) for the integration over ϑ_1, we then get, by the same rearrangement as for integral (24), the part of the integral which is not identically equal to zero for $r_2<r_1$ $(k_0=k'=k)$,

$$\frac{16\pi^2}{k}\int_0^\infty \exp(-2br_2)r_2\int_0^{r_2}(r_1-r_2) \times\exp(-br_1)\sin(kr_1)dr_1dr_2.$$

Let us introduce the notation $x_2=kr_2$, $x_1=kr_1$; then we may write

$$\frac{16\pi^2}{k^3}\int_0^\infty \exp(-2\kappa x_2)x_2\left(\frac{1}{k^2}\right)\int_0^{x_2}(x_1-x_2) \times\exp(-\kappa x_1)\sin x_1dx_1dx_2, \quad (45)$$

where $\kappa=b/k=1/z$. The integral over x_1 is therefore identical with the integral given in (37). The result of this integration is given by Eq. (38). By substituting (38) into (45), we get by elementary integration and with the help of (21),

$$-\frac{4\pi^2}{b^5}\left[\frac{1}{z(9+z^2)}\right].$$

We have therefore the result for the integral I_{22} in the closed form

$$I_{22}=-16\pi^2b^{-5}z^{-1}[2(1+\alpha)-\alpha'(1-z^2)z^{-1}] \times(1+z^2)^{-2}(9+z^2)^{-1}. \quad (46)$$

With the given integration results (41), (44), and (46), we have thus obtained all the terms necessary for the expression of the amplitudes of scattered waves for exchange scattering, and thus the required formulas describing all effects which need be taken into consideration for collisions of unpolarized electrons with helium and hydrogen atoms. Let us state that with the exception of the higher terms $(\gamma\geq 1)$ of the series (A2) for the unperturbed exchange integral, in which the terms $\geq z$, as already mentioned,[11] are negligibly small in comparison with the other terms, we have expressed all the given integrations in a closed form. The convergence of the terms of the series $\gamma=1$ in the exchange integral, which we have in turn expressed by a series, will be better for small values of z, i.e., for small energies of the incident electrons.

VII. SUMMARY AND DISCUSSION OF RESULTS

For the intensity $I(\vartheta)$ of electrons scattered by helium and hydrogen in ground quantum states, we have derived the formulas

$$I(\theta)=|f-g|^2,\quad f=d(I_{1B}+I_{1D}),\quad g=\tfrac{1}{2}d(I_{21}+I_{22}) \quad (47)$$

for helium;

$$I(\theta)=\tfrac{1}{4}|f'-g'|^2+\tfrac{3}{4}|f'+g'|^2,\quad f'=c'(I_{1B}+I_{1D}),\quad g'=\tfrac{1}{2}c'I_{21} \quad (47')$$

for hydrogen. The constants d $(=2\pi cb^{-3})$ and c' were given for Eqs. (20) and (20′) respectively. The Born approximation, I_{1B}, and the influence of distortion effects, I_{1D} and I_{22}, were developed in a closed form by analytical expressions (23), (32), and (46). The exchange integral I_{21}, which we divided in (42) into parts $I_{21}{}^{D'}$ and $I_{21}{}^{N'}$, was determined by Eq. (41) in which α'' is equal to $\alpha+1$, and the approximate part $I_{21}{}^{N'}$ was given by Eq. (44).

For Eqs. (47) and (47′) to become complete formulas for intensities of scattered electrons, it remains to determine the parameter α', including the first approximation in the zero quantum state, which we had hitherto considered as known. The accurate values of this parameter are given by the absolute terms in expression (6).

In the first approximation we have determined α' by Eq. (18), in which the phase factor η_0 had been considered as known. This phase factor, as is known, is in the required approximation given by the Mott formula

$$\eta_0=-\frac{\pi m}{\hbar^2}\int_0^\infty V(r)J_{\frac{1}{2}}{}^2(kr)rdr,$$

which for our case, in which we use the above atomic model, acquires the form

$$\eta_0=m\epsilon^2(2\hbar^2)^{-1}b^{-1}[z^{-1}\ln(1+z^2)+z/(1+z^2)]. \quad (48)$$

The intensities of the electrons scattered by helium and hydrogen in the ground quantum states are then, in the approximation considered, given by formulas (47) and (47′) and the expressions for the parameter by (18) and (48), valid for greater scattering angles ($\gtrsim 45°$).

In special cases the derived analytical formulas may be considerably simplified. For high energies of incident electrons (above 200 ev), this simplification lies in the neglect of the exchange amplitudes g or g' in (47) or in (47′). The small contribution of the distortion effect is here then introduced by the part I_{1D}. If we do not neglect the exchange amplitudes, it is necessary to determine a greater number of terms for extremely high energies, with respect to the convergence of the series in (44). A good approximation for the parameter α' may be obtained, in cases in which α' assumes extremely small values, by the expression

$$-\alpha'=\eta_0, \quad (49)$$

where η_0 is given in (48).

A comparison with the experimental results, which

TABLE I. Differential cross section$\times 10^{18}$ (theoretical) (units cm^2).

25 ev		700 ev		50 ev		75 ev	
65°	7.87	60°	0.234	67°	5.81	67°	4.69
90°	5.96	90°	0.086	90°	3.61	90°	3.39
125°	5.73	120°	0.052	127°	1.97	127°	2.78
		135°	0.018				

includes also inelastic collisions, for the angular distribution of scattered electrons, will be carried out for helium in the ground quantum state. Experimental results for the energy interval 25–700 ev have been reported by Hughes, McMillen, and Webb[12] and for incident electron energies 25 and 50 ev by Bullard and Massey. These results have been obtained by normalizing on the basis of Mott's theoretical curve for 700 ev. For the analysis of the obtained results for greater scattering angles ($\gtrsim 45°$) we list in Table I the values of the differential cross sections, determined by Eq. (47), for 25 and 700 ev. The values for 700 ev, which were partly used for the normalization, were obtained here without the inclusion of the exchange effect and are marked in the left half of Fig. 1 by crosses.

The stronger continuous line in this figure represents the experimental curves obtained by Hughes *et al.*

With regard to the fact that we have not considered the polarization of the electrons and with regard to the extent of the energy interval, it is possible to consider the analytical results obtained in this way, which are equivalent to the numberical results of Massey and Mohr, to be satisfactory.

The possibility of using Eq. (47) with the first two terms of the series of the unperturbed exchange integral (nonclosed analytical form), with the influence of the exchange effect thus taken into account, is investigated for incident electron energies of 50 and 75 ev. For these energies the condition $z<1$ introduced in the Appendix in the calculation of the terms of the series of the unperturbed exchange integral is not satisfied. Nevertheless, the influence of the exchange effect for these energies drops considerably. The values for the differential cross sections obtained in this way are also included in Table I and are compared with the experimental data in the right half of Fig. 1. From the figure it is evident that for 75-ev maximum with a corresponding difference this method is acceptable. For energies of incident electrons, for which $z>1$, it is therefore better to use the unperturbed exchange integral in another approximation, cited in the literature, e.g., in reference 11.

The results (not including the polarization effect) which were obtained for the atoms in the ground quantum states may also be used for molecular hydrogen. Likewise the total effective cross sections cited in the experimental works of Ramsauer and Kollath are determined through our results in a broad energy interval.

APPENDIX. CALCULATION OF THE INTEGRAL $I_{21}{}^N$

For the calculation of the integral $I_{21}{}^N$ we use again the development (25). Then by integration over φ_2 we get $p=0$; the integration over φ_1 may then be carried out with the help of (27). If we use further the special case of the Gegenbauer-Poisson integral,

$$J_{n+\frac{1}{2}}(x)=(-i)^n\left(\frac{x}{2\pi}\right)^{\frac{1}{2}}\int_0^\pi \exp(ix\cos\theta)\times P_n(\cos\theta)\sin\theta d\theta, \quad \text{(A1)}$$

for the integration over ϑ_2, and the Gegenbauer integral (28) for the integration over ϑ_1, we get

$$I_{21}{}^N=16\pi^2\sum_{\gamma=0}^{\infty}C_\gamma{}^{\frac{1}{2}}(\cos\theta)\int\int\delta_\gamma(r_1,r_2)\times\exp[-b(r_1+r_2)]j_\gamma(k'r_1)j_\gamma(k_0r_2)r_1{}^2r_2{}^2dr_1dr_2, \quad \text{(A2)}$$

where

$$j_\gamma(x)=(\pi/2x)^{\frac{1}{2}}J_{\gamma+\frac{1}{2}}(x) \quad \text{(A3)}$$

and δ_γ is given by Eqs. (26) for $Z=1$. We can easily check that the first term of series (A2) is, for $\gamma=0$, apart from the constant $-i\alpha'(=\alpha)$, identical with the imaginary part of $I_{21}{}^D$; and this means that in the result for the integral $I_{21}{}^D$ one may simply write $\alpha+1$ instead of α'' in Eq. (41). We have thus included the first term of the expression $I_{21}{}^D$. This arrangement of terms in the integral I_{21} will be denoted in the individual summands from now on with a prime on the upper right of the symbol.

Taking into account the fact that the contributions of the other terms of the series for $\gamma>1$ are negligibly small even for small electron energies, we shall give only an approximate expression for $I_{21}{}^N$, namely,

$$I_{21}{}^{N'}=\frac{16\pi^2}{k^5}P_1(\cos\theta)\left\{\int_0^\infty\exp(-\kappa x_1)j_1(x_1)\times\int_0^{x_1}\exp(-\kappa x_2)j_1(x_2)x_2{}^3dx_2dx_1+\int_0^\infty\exp(-\kappa x_1)\times j_1(x_1)x_1{}^3\int_{x_1}^\infty\exp(-\kappa x_2)j_1(x_2)dx_2dx_1\right\}, \quad \text{(A4)}$$

where $\kappa=b/k_0$ $(k=k_0=k')$, $x_1=kr_1$, $x_2=kr_2$. By elementary integrations in the first integral over x_2 and by using repeated differentiations with respect to the parameter to obtain derivatives of higher order, we may

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[12] Hughes, McMillen, and Webb, Phys. Rev. **41**, 155 (1932).

transform this integral into the form

$$\int_0^{x_1} (3x_2-\kappa x_2^2)\exp(-\kappa x_2)\sin x_2 dx_2$$

$$=\frac{\partial}{\partial\kappa}\left\{\frac{\exp(-\kappa x_1)}{(\kappa^2+1)^2}\{[(2-\kappa x_1)(\kappa^2+1)+2]\kappa\sin x_1\right.$$

$$\left.+(1-\kappa x_1)(\kappa^2+1)\cos x_1\}-\frac{\kappa^2+3}{(\kappa^2+1)^2}\right\}. \quad \text{(A5)}$$

We carry out the integration over x_2 in the second integral by decomposing the integrand into an infinite series, in which we may change the order of summation and integration, so that we have

$$\sum_{\gamma=0}^{\infty}\frac{(-1)^\gamma}{(2\gamma+1)!}\int_{x_1}^{\infty}\exp(-\kappa x_2)x_2^{2\gamma}dx_2$$

$$=\sum_{\gamma=0}^{\infty}\frac{(-1)^\gamma}{(2\gamma+1)!}\kappa^{-2\gamma-1}\exp(-\kappa x_1)[(\kappa x_1)^{2\gamma}+2\gamma(\kappa x_1)^{2\gamma-1}$$

$$+2\gamma(2\gamma-1)(\kappa x_1)^{2\gamma-2}+\cdots+(2\gamma)!], \quad \text{(A6)}$$

which is a very well convergent series for each value of x_1.

Now we introduce the approximate expansions

$$j_1(x)\sin x=x^2\left(\frac{1}{3}-\frac{4}{45}x^2+\frac{1}{80}x^4-\frac{7}{7200}x^6+\cdots\right), \quad \text{(A7)}$$

$$j_1(x)\cos x$$

$$=x\left(\frac{1}{3}-\frac{1}{5}x^3+\frac{1}{720}x^4-\frac{1}{288}x^6+\frac{1}{5760}x^8+\cdots\right), \quad \text{(A8)}$$

which we have obtained by multiplying the series for both factors and which again are very quickly convergent series. If we then substitute (A5) into the first integral (A4) and if we use for the term containing $\sin x_1$ in integral (A4) the expansion (A7) and for the term containing $\cos x_1$ the expansion (A8), then, after performing the differentiation in (A5) and rearranging, we integrate term by term by using (21).

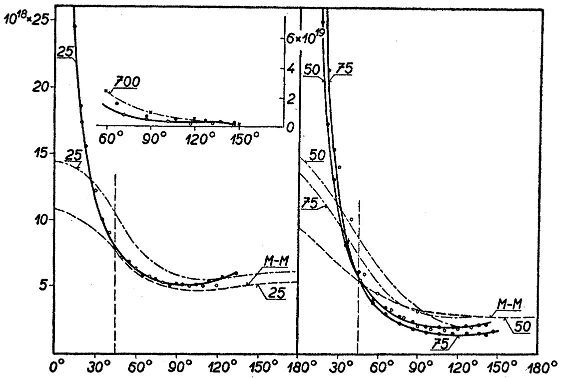

FIG. 1. Scattering of electrons by helium atoms. Angular distributions for 700, 25, 50, and 75 ev. Heavier full curve and full circles: experimental data by Bullard and Massey (for 25 and 50 ev only). Curve dash-and-dot: theoretical curves given by Eq. (47) with the first two terms of the series in the exchange integral. Broken curve: theoretical curves derived numerically by Massey and Mohr (for 25 and 50 ev only). 700 ev: full and empty circles respectively: experimental points by Hughes *et al.* without recalculating (and with recalculating respectively) to the normal. Crosses and dash-and-dot curve: theoretical values according to (47) neglecting the exchange effect.

To obtain the second integral from (A4), we make use of the expansion

$$j_1(x)=\tfrac{1}{2}x(\tfrac{2}{3}-x^2/15+x^4/420-\cdots). \quad \text{(A9)}$$

By substituting the latter into the second integral (A4) and using (A6), we may evaluate the integral by term-by-term integration, again with the help of the gamma function. By adding the terms of equal power, and rearranging, we get the second term of the series (A2) ($\gamma=1$), given by Eq. (44). In the same manner we could obtain the term $\gamma=2$ in the series (A2) which, however, is negligible for all values of $z<1$, in relation to the contributions of the other integrals; the same is valid for the other terms $x>2$ of the series.