Screening Effects in Elastic Electron Scattering*

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(Received 16 July 1964)

In elastic electron scattering atomic screening is shown to affect the cross section both at very small and at very large angles. However, for energies above approximately 200 keV the large-angle screening effects are small, and the cross section may be written as a product of two factors, one depending on the screening effect only and the other on the spin and relativistic effects only. The cross section thus obtained is shown to be in good agreement with previous exact numerical calculations for all angles and all elements. Approximate expressions for large-angle scattering are obtained.

I. INTRODUCTION

THE effect of atomic screening on the elastic electron-scattering cross section has been considered previously by various authors,[1] in the first- and second-order Born approximation,[2] in the Molière approximation,[3] and more recently for electron energies in the range from 50 to 400 keV using phase-shift calculations.[4] The inclusion of the screening effect in the cross section is complicated by the presence of the spin and relativistic effects for the electron. The purpose of the present paper is to point out that spin and relativistic effects may be treated separately from the effect of atomic screening over a wide range of elements and atomic numbers. It is found that if the electron energy is larger than approximately 200 keV, then for any element and any scattering angle the cross section may be written as a product of two factors, one depending only on the atomic screening and the other only on the spin and relativistic effects. The evaluation of the first factor follows the method of Molière,[3] although the derivation given here is different. Since Molière was the first to apply the WKB method to scattering by screened nuclei we would like to call this approximation Molière approximation. For larger scattering angles two even simpler approximations can be applied, namely, a stationary phase approximation which is identical to a classical computation, and an expansion leading to integrals which can be performed analytically. The present treatment of the screening effects is much simpler than the exact phase-shift calculations and yet yields values which are sufficiently accurate.

* This work was supported in part by research contract, Project No. 3AO12501A818, from the Medical Research and Development Command, United States Army, Washington, D. C. 20315, and in part by Grant No. 259C from the American Cancer Society.

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[1] For a review on electron scattering, see J. W. Motz, H. Olsen, and H. W. Koch, Rev. Mod. Phys. **36**, 881 (1964).

[2] R. H. Dalitz, Proc. Roy. Soc. (London) **A206**, 509 (1951); V. G. Gorshkov, Zh. Eksperim. i Teor. Fiz. **41**, 977 (1961) [English transl.: Soviet Phys.—JETP **14**, 694 (1962)].

[3] G. Molière, Z. Naturforsch. **2a**, 133 (1947).

[4] Shin-R Lin, Phys. Rev. **133**, A965 (1964).

II. ESTIMATE OF SCREENING EFFECTS

In order to estimate the relative importance of the atomic screening and the spin, it is convenient to treat separately the case of small angles, for which the momentum transfer $q=2p\sin\theta/2\ll p$, and the case of large angles, for which $q\sim 2p$. Here p is the momentum of the electron and θ the scattering angle. Throughout this paper energies and momenta are measured in units of mc^2 and mc, and lengths are measured in units of the electron Compton wavelength.

a. Small Angles, $q\ll p$

Since for small angles $q\ll p$ the field in which the electron is scattered is weak, it is sufficient for an estimate to consider the first-order Born approximation cross section for a potential $V=-(Z/137r)e^{-\Lambda r}$ where the screening radius $1/\Lambda$ is of the order $137Z^{-1/3}$. With E as the total electron energy, the cross section becomes

$$\frac{d\sigma}{d\Omega}=4\left(\frac{Z}{137}\right)^2\frac{E^2}{(q^2+\Lambda^2)^2}(1-\beta^2\sin^2\theta/2). \tag{1}$$

The factor $(q^2+\Lambda^2)^{-2}$ accounts for the atomic screening and the factor $(1-\beta^2\sin^2\theta/2)$ describes the spin effect. Thus, the latter is unimportant when

$$\beta\sin\theta/2=q/2E\ll 1, \tag{2}$$

whereas screening effects are important when

$$q\lesssim\Lambda=Z^{1/3}/137. \tag{3}$$

It is possible then to treat spin and screening effects separately as long as both conditions (2) and (3) are maintained simultaneously. This requirement can be stated as

$$Z^{1/3}/137\times 2E\ll 1, \tag{4}$$

which is easily fulfilled for all elements and energies. Thus, in the region of small values of q, spin and screening effects may always be treated separately.

b. Large Angles, $q\sim 2p$

For large angles, $q\sim 2p$, the field in which the electron is scattered is no longer weak and the first-order Born approximation is not adequate for estimating the effects of spin and screening. From Dalitz's calculations performed in second-order Born approximation, we may obtain an estimate of these effects. The condition for small overlap of spin and screening effects for large angles is[5]

$$\xi=\frac{Z^{4/3}}{(137)^2}\frac{2}{\beta p}\ll 1. \tag{5}$$

In Table I, ξ is given for $Z=29$ and $Z=79$ for several electron energies. Since in the present treatment we do not try to incorporate the overlapping of the spin and screening effects, the values of ξ in Table I indicate the order of magnitude of the error to be expected. It then follows that for electron energies above 200 keV the errors are small for all elements and for all angles. For lower energies the overlapping of the spin and screening effects may be appreciable for heavy elements and large angles.

III. THE CROSS SECTION

The estimates made in Sec. II show that screening and spin effects may be treated separately for all angles when condition (5) is fulfilled. The separate treatment suggests that the exact cross section may be written as a product of two factors, one of which takes into account screening effects but neglects spin, while the other takes into account spin effects but neglects screening. Thus the exact cross section is given by

$$\left[\frac{d\sigma}{d\Omega}\right]_{\rm ex}=R\times\left[\frac{d\sigma}{d\Omega}\right]_{\rm ex,\ no\ sc}, \tag{6}$$

where $[d\sigma/d\Omega]_{\rm ex,\ no\ sc}$ is the exact cross section for elastic scattering of an electron in an unscreened Coulomb field.[6] The factor R takes into account screening, but does not contain electron spin effects,

$$R=\left[\frac{d\sigma}{d\Omega}\right]_{\rm sc}\Big/\left[\frac{d\sigma}{d\Omega}\right]_{\rm no\ sc}, \tag{7}$$

[5] The Dalitz cross section of Ref. 2 is given by (see Ref. 1 for this particular form of the cross section)

$$\frac{d\sigma}{d\Omega}=4\left(\frac{Z}{137}\right)^2\frac{E^2}{q^4}\Big[(1-\beta^2\sin^2\theta/2)\left(\frac{q^2}{q^2+\Lambda^2}\right)^2+\frac{Z}{137}\left(\frac{q^2}{q^2+\Lambda^2}\right)\frac{q}{E}$$
$$\times\left\{\tan^{-1}\frac{q}{2\Lambda}-\sin\theta/2\,\tan^{-1}\frac{2p}{\Lambda}+\frac{1}{A}\left(\Lambda^2+4E^2-\frac{q^2}{2}\right)\tan^{-1}\frac{\Lambda q}{2A}\right\}\Big]$$

where $A=(p^2q^2+4p^2\Lambda^2+\Lambda^4)^{1/2}$ and $\Lambda\approx Z^{1/3}/137$. For $q\sim 2p\gg\Lambda$ the second-order Born term in the square bracket becomes

$$\frac{Z}{137}\frac{(2-\beta^2)\Lambda}{\beta p}\leqslant\frac{Z^{4/3}}{(137)^2}\frac{2}{\beta p}$$

which leads to the condition Eq. (5).

[6] Tables for the exact relativistic electron Coulomb scattering cross section are given by J. A. Doggett and L. V. Spencer, Phys. Rev. **103**, 1597 (1956); N. Sherman, *ibid.* **103**, 1601 (1956).

TABLE I. Values for $\xi=Z^{4/3}/(137)^2(2/\beta p)$.

T(keV)	50	100	200	400
$Z=29$	0.05	0.025	0.014	0.01
$Z=79$	0.19	0.10	0.05	0.03

where $[d\sigma/d\Omega]_{\rm sc}$ and $[d\sigma/d\Omega]_{\rm no\ sc}$ are the cross sections for scattering of a spinless electron in a screened and unscreened potential, respectively.

The ratio R may also be expressed in terms of the T matrices,

$$R=|T_{\rm sc}|^2/|T_{\rm no\ sc}|^2. \tag{8}$$

The T matrix for a spinless particle is

$$T=\int e^{-i\mathbf{p}_2\cdot\mathbf{r}}V(r)\psi_1(\mathbf{r})d^3x, \tag{9}$$

where ψ_1 is the scattering-state solution of

$$(\nabla^2+p^2-2EV+V^2)\psi_1(\mathbf{r})=0; \tag{10}$$

here the subscripts 1 and 2 refer to initial and final state, respectively.

In Eqs. (9) and (10) the pure Coulomb potential $V=-Z/137r$ is used for obtaining $T_{\rm no\ sc}$, while the appropriate screened potential is used for finding $T_{\rm sc}$.

If we introduce $\psi_1(\mathbf{r})=e^{i\mathbf{p}_1\cdot\mathbf{r}}F(\mathbf{r})$, the T matrix, Eq. (9), becomes

$$T=\int e^{i\mathbf{q}\cdot\mathbf{r}}VF(\mathbf{r})d^3x \tag{9a}$$

and the wave equation, Eq. (10), becomes

$$(\nabla^2+2i\mathbf{p}_1\cdot\nabla-2EV+V^2)F(\mathbf{r})=0. \tag{10a}$$

The T matrix for small values of q is obtained in the same manner as in a previous work[7] where the case of high energies was considered. From Eq. (9a) we observe that for the case of the first-order Born approximation, $F\equiv 1$, the most important region in the integral is $r\sim 1/q$. Since, as discussed in Sec. II, screening effects are only important for small values of q when the condition (5) is satisfied, the important region of r in the integral (9a) is $r\gg 1$. Moreover, since for these large values of r the field is weak, $F(\mathbf{r})$ is a slowly varying function. Therefore, the estimate based on the first-order Born approximation is valid. Thus the important region in the integral (9a) including $F(\mathbf{r})$ is $r\sim 1/q\gg 1$. In this region the terms ∇^2F and V^2F are of the relative order $q/2E$ and $Zq/137\times 2E$ as compared to the term $2EVF$, and may be neglected. We are therefore left with

$$(i\mathbf{p}_1\cdot\nabla-EV)F(\mathbf{r})=0,$$

[7] H. Olsen, L. C. Maximon, and H. Wergeland, Phys. Rev. **106**, 27 (1957). Note: Sec. 9.

which has the solution

$$F(\rho,z)=\exp\left[-\frac{i}{\beta}\int_{-\infty}^{z}V(\rho,\zeta)d\zeta\right],$$

where the z axis is along $\mathbf{p}_1$. The T matrix Eq. (9a) then becomes, upon introducing cylindrical coordinates ρ,φ, and z,

$$T=\int e^{i\mathbf{q}_\perp\cdot\rho+q_z z}V(\rho,z)\exp\left[-\frac{i}{\beta}\int_{-\infty}^{z}V(\rho,\zeta)d\zeta\right]d\varphi\rho d\rho dz,$$

where $\mathbf{q}_z$ and $\mathbf{q}_\perp$ are the components of $\mathbf{q}$ parallel and perpendicular to $\mathbf{p}_1$, respectively. For small angles, $q_z\ll q$, $q-q_\perp\ll q$ and, since $z\sim 1/q$, the factor $e^{iq_z z}\approx 1+0(q_z/q)$. Neglecting small terms of the order q_z/q, the z integration may be performed, giving [8]

$$T=\frac{\beta}{i}\int e^{i\mathbf{q}\cdot\rho}\left\{\exp\left[-\frac{i}{\beta}\int_{-\infty}^{+\infty}V(\rho,\zeta)d\zeta\right]-1\right\}d\varphi\rho d\rho$$

$$=-2\pi i\beta\int_0^\infty J_0(q\rho)\times\left\{\exp\left[-\frac{i}{\beta}\int_{-\infty}^{+\infty}V(\rho,\zeta)d\zeta\right]-1\right\}\rho d\rho, \quad (11)$$

where $J_0(q\rho)$ is the Bessel function of zeroth order.

Equation (11) is the Moliére approximation[3] for the T matrix. The same formula has been derived by several authors[9] in different ways. The only application to atomic screening, however, is in Molière's paper.

For the case of an unscreened potential $V=-Z/137r$, $|T_{\text{no sc}}|$ equals the Born approximation expression[7]

$$|T_{\text{no sc}}|=4\pi(Z/137q^2).$$

Thus R [Eq. (8)] may be written in the form

$$R=\left(\frac{137}{Z}\right)^2\frac{q^4\beta^2}{4}\left|\int_0^\infty J_0(q\rho)\{\ \}\rho d\rho\right|^2, \quad (12)$$

where $V(r)=V(\rho,\zeta)$ is the appropriate screened potential.

The cross section is then given by Eq. (6) with R as given by Eq. (12). The quantity ξ in Eq. (5) and Table I represents the error to be expected in the expression for R Eq. (12).

Table II. Parameters in screened potential Eq. (13).

	a_1	a_2	a_3	b_1	b_2	b_3
$Z=29$	0.22	0.78	0	0.319	1.081	0
$Z=79$	0.19	0.56	0.25	0.257	0.779	3.16

Although we have assumed small scattering angles in deriving formula (12), *we shall henceforth assume this formula to be valid for all angles.* This assumption is justifiable on the grounds that for large angles screening is unimportant and the potential approaches the pure Coulomb potential $V=-Z/137r$. The ratio R as a function of q Eq. (12) approaches the value unity, which is the correct value for large angles in the absence of large-angle screening effects as discussed in Sec. IIb. The ultimate justification for extending the assumption to all angles will be the close agreement between the results of the approximated and the exact calculations.

IV. NUMERICAL INTEGRATION

To establish the accuracy of the present theory we have integrated Eq. (12) numerically for the values of Z and electron energies shown in Table I which are the same parameters as those used by Lin[4] in his exact phase-shift analysis thus making a direct comparison with his results possible. We also use the same Hartree-Byatt[10] potentials as does Lin.[4] These are of the form

$$V(r)=-(Z/137r)\sum_1^3 a_i e^{-b_i\Lambda r}, \quad (13)$$

where the constants a_i and b_i are given in Table II, and where $\Lambda=Z^{1/3}/0.885\times 137$.

The integral in the exponent in Eq. (11) then becomes

$$-(i/\beta)\int_{-\infty}^{+\infty}V(\rho,\zeta)d\zeta=2ia\sum_1^3 a_j K_0(b_j\rho\Lambda), \quad (14)$$

where $a=Z/137\beta$. For the numerical calculation it is convenient to perform a partial integration on the integral in Eq. (12); using $q\rho J_0(q\rho)=d/d\rho[\rho J_1(q\rho)]$ we obtain with $y=q/\Lambda$ and $x=\rho\Lambda$,

$$R=y^2\left|\sum_1^3 a_k b_k\int_0^\infty xdxJ_1(xy)K_1(b_k x)\times\exp\{2ia\sum a_j K_0(b_j x)\}\right|^2$$

$$=Q_1^2+Q_2^2, \quad (15)$$

[8] It might be shown that the phase-shift analysis at small angles leads to the same expression as Eq. (11); see Refs. 3 and 7.

[9] L. D. Landau and E. M. Lifshitz, *Quantum Mechanics* (Ogiz, Moscow, 1948), (in Russian), Part I, pp. 184–203, 470–473 [(English transl.: Pergamon Press, Inc., New York, 1958)]; G. Parzen, Phys. Rev. **81**, 808 (1951); R. J. Glauber, Phys. Rev. **91**, 459 (1953); E. W. Montroll and J. M. Greenberg, Proc. Symp. Appl. Math. **5**, 103 (1954); B. J. Malenka, Phys. Rev. **95**, 522 (1954); I. I. Gol'dman and A. B. Migdal, Zh. Eksperim. i Teor. Fiz. **28**, 394 (1954) [(English transl.: Soviet Phys.—JETP **1**, 304 (1955)]; L. I. Schiff, Phys. Rev. **103**, 443 (1956); D. S. Saxon and L. I. Schiff, Nuovo Cimento **6**, 614 (1957).

[10] W. J. Byatt, Phys. Rev. **104**, 1298 (1956).

where

$$Q_1=y\sum_1^3 a_kb_k\int_0^\infty xdxJ_1(xy)K_1(b_kx)\times\cos\{2a\sum a_jK_0(b_jx)\},$$
$$Q_2=-y\sum_1^3 a_kb_k\int_0^\infty xdxJ_1(xy)K_1(b_kx)\times\sin\{2a\sum a_jK_0(b_jx)\}. \quad (16)$$

The partial integration thus produced the factor $K_1(b_kx)$ in the integrands of Q_1 and Q_2. The integrals are then rapidly converging for large values of x by virtue of the exponentially decaying $K_1(b_kx)$. Moreover, the infinite oscillations of the integrand due to the logarithmic divergence of $K_0(b_jx)$ for small x are suppressed by the vanishing Bessel function $J_1(xy)$.

The computations were programmed in Fortran and run on an IBM-7090 computer. Subroutines for the Bessel functions $J_1(x)$ with accuracy better than 0.08% were available. A program for the Hankel functions $K_0(x)$ and $K_1(x)$ was developed, with an accuracy better than 0.1%. The results of the integration are given in Table III. It is seen that the magnitude of the maximum error in R is very close to the errors given by the values of ξ in Table I as was anticipated in Sec. II.

From Table III it is seen that errors of the ratio R given by the present theory are of the order of 5% or less for all angles and for energies above 50 keV in the case of the light elements, and for energies above 200 keV in the case of the heavy elements. The errors for small angles $\theta\leqslant 10°$ where screening is most important are much smaller, of the order 1% or less for all elements.

The present method of calculation, which is much simpler than the exact phase-shift analysis thus provides values of the cross section sufficiently accurate for most experimental applications for all elements and all angles in a wide range of energies.

V. STATIONARY-PHASE APPROXIMATION

Although the expression Eq. (15) gives R in a form which readily may be used for numerical integration, it might be of interest to derive approximate expressions for R valid in restricted ranges of $y=q/\Lambda$. One way of doing this is to use the method of stationary phase.[11]

In our case the magnitude of $2a=2(Z/137\beta)$, which is crucial for the application of the stationary-phase approximation, does not seem large enough to give accurate values for R. Since, however, the method gives an expression for R which in the case of moderately small angles is identical to the classically derived expression as we shall see, the procedure should be reliable as long as the effect of screening is not too strong. In other words the stationary-phase approximation should be accurate for large values $y=q/\Lambda$. Here we use the same arguments in extending the small-angle results to large angles as at the end of Sec. III.

[11] See also G. Molière, Ref. 3, Sec. 5.

We write Eq. (11) in the form

$$T=(\beta/i)\int e^{i[\mathbf{q}\cdot\boldsymbol{\rho}-\phi(\rho)]}d\varphi\rho d\rho, \quad (17)$$

where

$$\phi=(1/\beta)\int_{-\infty}^{+\infty}V(\rho,\zeta)d\zeta.$$

The second term in Eq. (11) which is equal to $-(\beta/i)\times(2\pi)^2\delta(\mathbf{q})$ is zero for finite angles and has been left out. The point of stationary phase (φ_0,ρ_0) is given by $\nabla_\rho[\mathbf{q}\cdot\boldsymbol{\rho}-\phi(\rho)]=0$, or $\varphi_0=0$, and

$$q(\rho_0)=|\partial\phi(\rho_0)/\partial\rho_0|. \quad (18)$$

Then the scattering matrix is

$$T=2\pi\beta\left[\frac{1}{\rho_0}\frac{\partial\phi(\rho_0)}{\partial\rho_0}\frac{\partial^2\phi(\rho_0)}{\partial^2\rho_0}\right]^{-1/2}. \quad (19)$$

The cross section is

$$d\sigma/d\Omega=|T|^2E^2/(2\pi)^2. \quad (20)$$

When T Eq. (19) is substituted into Eq. (20) and the relations $\partial\phi/\partial\rho_0=q$, $\partial^2\phi/\partial^2\rho_0{}^2=\partial q/\partial\rho_0$ from Eq. (18) are used, we find

$$d\sigma=2\pi\frac{p^2\rho_0\sin\theta d\theta}{qdq/d\rho_0}=2\pi\rho_0d\rho_0. \quad (21)$$

Equation (21) is identical to the classical expression for the scattering cross section in terms of the impact parameter ρ_0. Equation (18) giving the impact parameter in terms of the momentum transfer is identical to the classical small-angle relation between the scattering angle and the potential.[12] Since the classical cross section for an unscreened potential (the Rutherford cross section) is exact, we conclude that the stationary-phase method is reliable as long as the screening is not too strong, i.e., for large values of $y_0=q(\rho_0)/\Lambda$.

Written in terms of y_0 and $x_0=\rho_0\Lambda$, the stationary-phase approximation for R, which is identical to the classically computed R_{class}, is

$$R_{\text{class}}=x_0{}^2(y_0/2a)^3[(y_0/2a)+x_0\sum a_ib_i{}^2K_0(b_ix_0)]^{-1}, \quad (22)$$

where we have used the potential given in Eq. (13) and Table II. The quantity x_0 in terms of y_0 follows from Eq. (18)

$$y_0/2a=\sum a_ib_iK_1(b_ix_0). \quad (23)$$

Values for R_{class} calculated numerically from Eqs. (22) and (23) given in Table III are seen to be close to

[12] The classical action function $S(\mathbf{r})$ satisfying $(\nabla S)^2+2EV-V^2+m^2=E$ is for large impact parameters $S=p_1z-(1/\beta)\times\int_{-\infty}^{z}V(\rho,\zeta)d\zeta$, where the z-axis is along $\mathbf{p}_1$. The transverse momentum at $Z\to\infty$ which is equal to $\mathbf{q}_\perp$ is

$$q_\perp=\left|\frac{\partial S}{\partial\rho}\right|=\left|\frac{\partial}{\partial\rho}\frac{1}{\beta}\int_{-\infty}^{+\infty}V(\rho,\zeta)d\zeta\right|$$

and thus equal to Eq. (18) for small angles.

TABLE III. Values for the exact cross-section ratio R_{ex}; the Molière approximation R, Eqs. (15) and (16); the classical approximation R_{class}, Eqs. (22) and (23); the large-angle approximation $R_{L.A.}$, Eqs. (25) and (26); and the first-order Born approximation R_{Born}, $\epsilon=(R-R_{ex})/R_{ex}$.

						$Z=29$						
			50 keV						100 keV			
θ (degrees)	R_{ex}	R	ϵ (%)	R_{class}	$R_{L.A.}$	R_{Born}	R_{ex}	R	ϵ (%)	R_{class}	$R_{L.A.}$	R_{Born}
2		0.118		0.248		0.137		0.240		0.445		0.267
4		0.352		0.459		0.426		0.552		0.681		0.620
6		0.527		0.609		0.638		0.714		0.766		0.792
8		0.638		0.689		0.763		0.799		0.844		0.872
10	0.732	0.711	−2.83	0.758	0.696	0.835	0.869	0.853	−1.82	0.895	0.849	0.915
20	0.910	0.878	−3.55	0.900	0.883	0.953	0.966	0.949	−1.78	0.963	0.951	0.977
30	0.966	0.933	−3.47	0.945	0.937	0.979	0.986	0.974	−1.28	0.981	0.976	0.990
40	0.996	0.957	−3.88	0.964	0.960	0.988	1.005	0.985	−1.91	0.988	0.985	0.994
50	1.016	0.970	−4.58	0.975	0.972	0.992	1.011	0.989	−2.20	0.991	0.990	0.996
60	1.023	0.976	−4.56	0.981	0.979	0.994	1.013	0.992	−2.09	0.994	0.992	0.997
70	1.030	0.981	−4.72	0.985	0.983	0.996	1.012	0.994	−1.75	0.995	0.994	0.998
80	1.033	0.984	−4.75	0.987	0.986	0.996	1.015	0.996	−1.84	0.996	0.995	0.998
90	1.036	0.987	−4.74	0.989	0.988	0.997	1.022	0.997	−2.43	0.996	0.996	0.999
100	1.041	0.988	−5.04	0.991	0.990	0.997	1.018	0.998	−1.95	0.997	0.996	0.999
110	1.042	0.989	−5.10	0.992	0.991	0.998	1.008	0.999	−0.93	0.997	0.997	0.999
120	1.045	0.990	−5.26	0.992	0.992	0.998	1.042	0.999	−4.09	0.997	0.997	0.999
130	1.045	0.991	−5.17	0.993	0.992	0.998	1.022	1.000	−2.18	0.998	0.997	0.999
140	1.047	0.991	−5.32	0.993	0.993	0.998	1.012	1.000	−1.15	0.998	0.997	0.999
150	1.050	0.992	−5.41	0.994	0.993	0.998	1.010	1.000	−0.96	0.998	0.998	0.999
160	1.053	0.992	−5.82	0.994	0.993	0.998	1.089	1.001	−8.06	0.998	0.998	0.999
170	1.045	0.992	−5.09	0.994	0.994	0.998	1.001	1.001	−0.05	0.998	0.998	0.999
						$Z=29$						
			200 keV						400 keV			
2		0.427		0.660		0.465		0.643		0.825		0.677
4		0.735		0.845		0.786		0.866		0.933		0.897
6		0.849		0.919		0.894		0.931		0.963		0.952
8		0.904		0.939		0.938		0.958		0.979		0.972
10	0.939	0.931	−0.77	0.959	0.934	0.959	0.986	0.971	−1.60	0.984	0.972	0.982
20	0.994	0.979	−1.53	0.987	0.980	0.989	1.017	0.993	−2.39	0.995	0.992	0.995
30	1.001	0.990	−1.06	0.993	0.990	0.995	1.025	0.997	−2.71	0.998	0.996	0.997
40	1.011	0.995	−1.57	0.996	0.994	0.997	1.007	0.999	−0.82	0.998	0.998	0.999
50	1.002	0.997	−0.47	0.997	0.996	0.998	0.989	1.001	1.17	0.999	0.998	0.999
60	1.005	0.999	−0.62	0.998	0.997	0.999	0.980	1.002	2.22	0.999	0.999	0.999
70	1.006	1.000	−0.62	0.998	0.998	0.999	0.982	1.004	2.26	0.999	0.999	1.000
80	1.003	1.001	−0.21	0.999	0.998	0.999	0.979	1.005	2.68	0.999	0.999	1.000
90	0.999	1.002	0.30	0.999	0.998	0.999	0.984	1.007	2.29	0.999	0.999	1.000
100	0.998	1.003	0.46	0.999	0.999	0.999	0.996	1.008	1.16	0.999	0.999	1.000
110	0.995	1.004	0.85	0.999	0.999	0.999	0.996	1.009	1.32	0.998	1.000	1.000
120	1.007	1.005	−0.82	0.999	0.999	1.000	0.996	1.010	1.45	0.999	1.000	1.000
130	1.005	1.006	0.05	0.999	0.999	1.000	1.005	1.011	0.61	0.999	1.000	1.000
140	1.005	1.006	0.09	0.999	0.999	1.000	1.019	1.012	−0.65	0.998	1.000	1.000
150	1.011	1.006	−0.43	0.999	0.999	1.000	1.034	1.013	−2.01	0.997	1.000	1.000
160	1.036	1.007	−2.82	0.999	0.999	1.000	1.054	1.013	−3.86	0.997	1.000	1.000
170	1.009	1.007	−0.19	0.999	0.999	1.000	1.075	1.014	−5.50	0.997	1.000	1.000
						$Z=79$						
			50 keV						100 keV			
2		0.049		0.054		0.082		0.109		0.131		0.162
4		0.133		0.136		0.263		0.240		0.249		0.397
6		0.200		0.201		0.410		0.330		0.340		0.544
8		0.254		0.257		0.515		0.400		0.404		0.643
10	0.307	0.298	−2.83	0.299	22.06	0.594	0.469	0.464	−2 35	0 464	1.996	0.715
20	0.495	0.470	−4.84	0.474	1.874	0.808	0.673	0.661	−2.66	0.661	0.629	0.889
30	0.631	0.586	−7.04	0.588	0.825	0.895	0.794	0.756	−4.77	0.765	0.699	0.944
40	0.733	0.663	−9.58	0.668	0.691	0.934	0.869	0.817	−5.93	0.827	0.776	0.967
50	0.810	0.720	−11.2	0.725	0.696	0.955	0.919	0.860	−6.42	0.866	0.829	0.978
60	0.870	0.759	−12.8	0.767	0.727	0.967	0.957	0.890	−7.01	0.892	0.864	0.984
70	0.923	0.786	−14.8	0.798	0.758	0.975	0.981	0.909	−7.34	0.910	0.888	0.988
80	0.967	0.811	−16.1	0.822	0.785	0.980	1.003	0.921	−8.17	0.923	0.905	0.990
90	1.004	0.833	−17.0	0.841	0.807	0.983	1.018	0.933	−8.32	0.933	0.918	0.992
100	1.044	0.851	−18.4	0.856	0.825	0.986	1.037	0.944	−8.97	0.940	0.927	0.993
110	1.086	0.861	−20.7	0.867	0.839	0.987	1.052	0.947	−10.0	0.946	0.935	0.994
120	1.112	0.868	−21.9	0.876	0.850	0.989	1.067	0.949	−11.0	0.950	0.940	0.994
130	1.142	0.876	−23.3	0.883	0.859	0.990	1.076	0.953	−11.4	0.953	0.944	0.995
140	1.174	0.882	−24.9	0.888	0.866	0.990	1.095	0.957	−12.6	0.956	0.947	0.995
150	1.191	0.885	−25.7	0.892	0.870	0.991	1.105	0.958	−13.4	0.957	0.949	0.996
160	1.202	0.889	−26.0	0.895	0.874	0.991	1.107	0.961	−13.2	0.959	0.951	0.996
170	1.217	0.892	−26.7	0.897	0.876	0.991	1.119	0.962	−14.0	0.959	0.952	0.996

TABLE III (*continued*)

	$Z=79$											
	200 keV						400 keV					
θ (degrees)	R_{ex}	R	ϵ (%)	R_{class}	$R_{L.A.}$	R_{Born}	R_{ex}	R	ϵ (%)	R_{class}	$R_{L.A.}$	R_{Born}
2		0.204		0.237		0.285		0.336		0.363		0.440
4		0.377		0.387		0.538		0.528		0.552		0.682
6		0.484		0.497		0.677		0.646		0.668		0.803
8		0.569		0.579		0.766		0.726		0.744		0.870
10	0.636	0.630	−1.03	0.643	0.582	0.826	0.771	0.779	1.02	0.797	0.700	0.910
20	0.812	0.802	−1.19	0.816	0.747	0.943	0.903	0.903	−0.00	0.913	0.883	0.974
30	0.891	0.879	−1.45	0.887	0.851	0.973	0.934	0.943	0.12	0.950	0.937	0.988
40	0.942	0.916	−2.73	0.922	0.901	0.984	0.962	0.961	−0.15	0.968	0.960	0.993
50	0.970	0.936	−3.35	0.943	0.928	0.989	0.991	0.969	−2.18	0.977	0.972	0.995
60	0.987	0.950	−3.76	0.955	0.945	0.992	0.995	0.973	−2.22	0.982	0.979	0.997
70	0.993	0.957	−3.63	0.964	0.956	0.994	0.997	0.977	−2.06	0.986	0.983	0.997
80	1.001	0.962	−3.80	0.970	0.963	0.995	0.998	0.980	−1.81	0.988	0.986	0.998
90	1.013	0.964	−4.79	0.974	0.968	0.996	0.997	0.980	−1.82	0.990	0.988	0.998
100	1.020	0.965	−5.41	0.977	0.973	0.997	1.000	0.982	−1.79	0.991	0.990	0.999
110	1.026	0.968	−5.64	0.979	0.976	0.997	1.006	0.982	−2.36	0.992	0.991	0.999
120	1.032	0.969	−6.14	0.981	0.978	0.997	1.009	0.986	−2.32	0.993	0.992	0.999
130	1.037	0.967	−6.77	0.982	0.979	0.998	1.012	0.986	−2.54	0.993	0.992	0.999
140	1.046	0.966	−7.67	0.983	0.980	0.998	1.023	0.986	−3.62	0.994	0.993	0.999
150	1.050	0.967	−7.88	0.984	0.981	0.998	1.024	0.987	−3.45	0.994	0.993	0.999
160	1.053	0.968	−8.04	0.985	0.982	0.998	1.026	0.989	−3.55	0.994	0.993	0.999
170	1.057	0.968	−8.43	0.985	0.982	0.998	1.030	0.990	−3.92	0.994	0.994	0.999

the values obtained by the numerical integration in Sec. IV for $\theta \gtrsim 10°$, i.e., for values of y somewhat larger than one. Note that $y \gtrsim 3.1$ when $T \gtrsim 50$ keV and $\theta > 10°$ for $Z=29$, and under the same conditions $y \gtrsim 2.2$ for $Z=79$.

The incorrectness of Eq. (22) for small angles may be seen explicitely if the error in the stationary-phase expression is computed. This is found to be of the order $(Zy_0/137)^{-2}$ for small values of y_0, and thus becomes very large for small y_0. It should also be pointed out that the cross section Eq. (20) with T given by Eq. (19) gives an infinite total cross section even for an exponentially screened potential. The classically computed cross section is thus infinite for any continuous potential; it is only finite for a (discontinuous) potential which is *identically* zero outside a given distance from the scatterer.

From Eqs. (22) and (23) it follows that R_{class} depends on the scattering angle and energy through the variable $y_0/2a = q\beta 137/2Z\Lambda$. Thus for a given element R_{class} is constant for $q\beta = 2\beta^2 E \sin\theta/2 = \text{const}$. Note that the Born approximation which is less accurate for low velocities predicts $R = \text{const}$ for $q = 2\beta E \sin\theta/2 = \text{const}$.

VI. LARGE-ANGLE APPROXIMATION

Another approximate formula for R for large values of y may be obtained by observing that for large values of q in Eq. (11) only small values of ρ are important.[11] Expanding the exponent in Eq. (12) we find introducing as before $y=q/\Lambda$ and $x=\rho\Lambda$

$$R=\frac{y^2}{4a^2}\left|\int_0^\infty dx x^{1-2ia} J_0(xy)\exp[2iax^2(\phi_1-\phi_2\ln x)]\right|^2, \tag{24}$$

where as in Sec. V we have left out the term proportional to $\delta(\mathbf{q})$ and where

$$\phi_1=\sum_1^3 a_i b_i(\ln(2/\gamma b_i)+1),$$

$$\phi_2=\sum_1^3 a_i b_i^2,$$

with $\gamma=1.7807$ (Euler's constant).

Expanding the exponential function in Eq. (24) and keeping terms of order x^2 all integrals can be performed, and the final result is

$$R_{L.A.}=(Q_1^2+Q_2^2)_{L.A.}, \tag{25}$$

with

$$\begin{aligned} Q_1&=1-[\phi_1+\phi_2(\ln(y/2)-P)]\frac{4a^2}{y^2}+\phi_2\frac{3a^2-1}{y^2},\\ Q_2&=-[\phi_1+\phi_2(\ln(y/2)-P)]\frac{2a(1-a^2)}{y^2}+\phi_2\frac{4a}{y^2}, \end{aligned} \tag{26}$$

where

$$P=\mathrm{Re}[\psi(ia)].$$

For the values of a_i and b_i of Molière,[3] Eqs. (26) reduce to Molière's Eq. (8.4)[3] when terms of the order a^3 and a^4 are omitted.

Values for the large-angle approximation $R_{L.A.}$ are given in Table III. The accuracy is of the same order as for the classical result R_{class}, but the errors are always somewhat larger particularly for heavy elements.

VII. CONCLUSIONS

Four approximations for the ratio R of the scattering cross section of a screened potential to that of an un-

screened potential were calculated and compared with the result of exact phase-shift calculations, R_{ex}. Table III lists these results in detail and permits the recognition of the following:

(1) The Molière approximation renders R by Eqs. (15) and (16) with an error of the order ξ [Eq. (5) and Table I].

(2) The classical approximation renders R_{class} by Eqs. (22) and (23) with an error which is comparable to that of R for scattering angles larger than 10°.

(3) The large-angle approximation renders $R_{L.A.}$ by Eqs. (25) and (26) with errors generally larger than of R_{class}.

(4) The first-order Born approximation gives values, R_{Born}, the errors of which exceed those of all the other approximations. Even for the light element $Z=29$ and for small angles the errors are larger than 10%.

ACKNOWLEDGMENTS

We are indebted to J. W. Motz for numerous discussions and for pointing out to us the need for rather simple and yet sufficiently accurate calculations of the elastic electron-scattering cross section.

We would also like to acknowledge the valuable assistance of R. L. Scott in preparing the program and performing the computations.

PHYSICAL REVIEW VOLUME 136, NUMBER 6A 14 DECEMBER 1964

Analytical Relativistic Self-Consistent Field Theory*

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(Received 25 March 1964)

The analytical self-consistent field (SCF) theory, based on the relativistic Breit equation generalized for many particles, was developed for closed-shell systems. The relativistic SCF equations, both of the absolute and of the expansion method type, were derived in the four-component spinor representation. The Breit operator was considered in the first-order perturbation theory. The formulas for the relativistic atomic integrals were derived in terms of simple functions.

INTRODUCTION

IN this work the relativistic Breit equation[1] is considered generalized for many-particle systems. Then the relativistic self-consistent field (SCF) theory for closed-shell systems is developed, partially using an analogy with the expansion method[2,3] of the nonrelativistic theory. The applications[4] of the expansion method encourage such an attempt at a relativistic extension.

While this work was outlined,[5] an approach related to the numerical SCF method appeared in the literature.[6] Recently, another approach was made.[7]

GENERAL CONSIDERATIONS

The validity of the Breit equation for two electrons has been proved both theoretically[1] and by practical applications.[8] It is quite plausible to assume that even in a many-electron system mutual interactions between electrons can be approximated by interactions within all possible pairs of electrons where in every pair only the two-electron Breit interaction is considered. Similar although simpler consideration was performed already by Swirles[9] in an atomic case, by going from the Dirac equation to the approximate many-electron relativistic equation (while omitting the Breit operator). In the molecular case the influence of nuclei can be approximated as an external field.[10]

Hence we introduce the generalized Breit equation for a system of N electrons (and M nuclei) as follows:

$$\left(E-\sum_{\mu=1}^{N} H^{\mu}-\tfrac{1}{2}e^2\sum_{\substack{\mu,\nu=1;\\ \mu\neq\nu}}^{N}\frac{1}{r^{\mu\nu}}\right)U$$

$$=-\tfrac{1}{4}e^2\sum_{\substack{\mu,\nu=1;\\ \mu\neq\nu}}^{N}\frac{1}{r^{\mu\nu}}\left[\boldsymbol{\alpha}^{\mu}\cdot\boldsymbol{\alpha}^{\nu}+\frac{(\boldsymbol{\alpha}^{\mu}\cdot\mathbf{r}^{\mu\nu})(\boldsymbol{\alpha}^{\nu}\cdot\mathbf{r}^{\mu\nu})}{(r^{\mu\nu})^2}\right]U, \quad (1)$$

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* The work was originated at the University of Chicago, Chicago, Illinois.

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