Elastic Electron Scattering by Screened Nuclei*

SHIN-R LIN

Physics Department, Yale University, New Haven, Connecticut (Received 16 September 1963)

The differential cross section and the asymmetry function of the elastic scattering of electrons from screened nuclei were computed at 10-deg intervals from 10° to 170°. We report here the results of the calculation for (1) gold, with electron energies of 400, 200, 188, 120, 100, and 50 keV; (2) copper, with electron energies of 400, 200, 100, and 50 keV; and (3) mercury, with electron energy of 204 keV. The screening potentials used were a three-terms exponential potential for gold, a two-terms exponential potential for copper, and the Hartree potential for mercury. The modified method of the summation of the phase shifts series leads to improved accuracy. The error in the calculated cross section and the asymmetry function is estimated to be not greater than one percent. All results together with the corresponding calculations for Coulomb field are given in tabulated form.

I. INTRODUCTION

N connection with the electron scattering experi- \blacksquare ments carried out at the Bureau of Standards¹ and performed at Yale,² it is desirable to calculate the differential cross section and the asymmetry function for elastic scattering of electrons from screened nuclei for different targets and electron energies from those previously calculated.³

In this paper, the results of the calculations for (1)gold, with electron energies of 400, 200, 188, 120, 100, and 50 keV, (2) copper, with electron energies of 400, 200, 100, and 50 keV, and (3) mercury, with electron energy of 204 keV, are reported.

The method of calculation is the same as that previously reported except for an important modification on the summation of the phase shift series. This modification leads to improved accuracy; we estimate that the error in the cross section and the asymmetry function is not greater than 1%.

In the following section, we discuss the modified method of summation of the phase shift series. In Sec. III, we discuss the potentials used and tabulate the results. In the same section we also discuss our results in connection with the various measurements of the cross section and the asymmetry function.

II. METHOD OF CALCULATION

The scattering cross section and the asymmetry function are defined as⁴

$$d\sigma(\theta)/d\Omega = |f(\theta)|^2 + |g(\theta)|^2, \qquad (1)$$

$$S\frac{d\sigma}{d\Omega} = i(fg^* - gf^*), \qquad (2)$$

* Supported in part by the National Science Foundation and the U. S. Atomic Energy Commission. ¹ J. W. Motz, R. C. Placious, and C. E. Dick, Phys. Rev. 132,

⁴ N. F. Mott and H. S. W. Massey, The Theory of Atomic Collisions (Oxford University Press, Oxford, 1949), 2nd ed., p. 75. where f and g are expressed in terms of phase shifts δ_l, δ_{l-1} as

$$2ikf = \sum \{(l+1)[\exp(2i\delta_l) - 1] + l[\exp(2i\delta_{-l-1}) - 1]\}P_l(\cos\theta), \quad (3)$$

$$2ikg = \sum \left[\exp(2i\delta_{-l-1}) - \exp(2i\delta_l) \right] P_l^1(\cos\theta).$$
(4)

The phase shifts are all obtained by numerical integration of the equation derived from the Dirac equation as in the previous paper.³ The phase shift series for f and g, (3) and (4), are now summed first by applying the "reduced series" method of Yennie, Ravenhall, and Wilson⁵ to improve the convergence. This transformation can be applied to any series containing the Legendre polynomials. If

$$f(\cos\theta) = \sum_{l} a_{l} P_{l}(\cos\theta)$$
,

then from the recursion relation for $P_l(\cos\theta)$, this series can be transformed into

$$(1 - \cos\theta)^m f(\cos\theta) = \sum_l a_l^m P_l(\cos\theta), \qquad (5)$$

where

$$a_{l}(m+1) = a_{l}(m) - \frac{l+1}{2l+3} a_{l+1}^{(m)} - \frac{l}{2l-1} a_{l-1}^{(m)}.$$
 (6)

For large *l*,

$$a_{l}^{(m+1)} = O(a_{l}^{m}/l^{2}),$$

so that the reduced series converges considerably faster than the original series.⁶

The series (3) and (4) are reduced in this manner with m=2 and m=1, respectively. Even with these reduced series, the convergence is rather slow especially at large angles $(>90^\circ)$ where the series almost become alternating. We decided to apply the second transformation to (3) and (4), which is useful for alternating

^{2558 (1963).}

² D. M. Lazarus, J. S. Greenberg, and R. L. Gluckstern (private communication).

⁸S. R. Lin, N. Sherman, and J. K. Percus, Nucl. Phys. 45, 492 (1963).

⁵D. R. Yennie, D. G. Ravenhall, and R. W. Wilson, Phys. Rev. 95, 500 (1954).

⁶ It should be pointed out, however, that owing to the round off and truncation error in summing the series, there is an optimum $m = m_0$ such that further application of this transformation will not improve, but rather worsen, the convergence of the series.

series. This is the well-known Euler transformation⁷:

$$\sum_{n=0}^{\infty} (-)^{n} f_{n} = \frac{1}{2} \sum_{k=0}^{m} \frac{(-)^{k}}{2k} \Delta^{k} f_{0} + \frac{(-)^{m+1}}{2^{m+1}} \sum_{k} (-)^{k} \Delta^{m+1} f_{k}.$$
 (7)

With this transformation, the reduced series for f and g converge rapidly.⁸ The number of terms necessary to achieve the accuracy of 1% or better in $d\sigma/d\Omega$ and S never exceeds fifty terms.⁹ We recall here that in the previous calculation,³ even with the use of more than two hundred terms we only attained an accuracy of not better than 3% in $d\sigma/d\Omega$ and S.

We also tried the summation method first used by Bartlett and Welton,¹⁰ and afterwards by others.¹¹ We

TABLE I. Cross section for gold at 400 and 200 keV.

Z = 79 400 keV			200 keV			
θ	$d\sigma/d\Omega_{\rm sc^a}$	$d\sigma/d\Omega_{\rm c}{}^{\rm b}$	R°	$d\sigma/d\Omega_{ m sc}$	$d\sigma/d\Omega_{c}$	R
10 20	1.158×10 ⁶ 9.213×10 ⁴	1.501×10 ⁶ 1.020×10 ⁵	0.7714 0.9032	3.100×10 ⁶ 2.600×10 ⁵	4.870×10 ⁶ 3.203×10 ⁵	0.6364 0.8116
30 40	2.143 ×104 8.131 ×103	2.293 ×104 8.448 ×103	0.9345 0.9625	6.236×104 2.389×104	6.996×104 2.535×104	0.8915 0.9420
50 60	3.997×10 ³ 2.231×10 ³	4.034×10 ³ 2.243×10 ³	0.9909 0.9947	1.170×104 6.653×103	1.206×104 6.738×103	0.9701 0.9874
70 80	1.369×10^{3} 8.930×10^{2}	1.373×10^{3} 8.948×10^{2}	0.9971 0.9980	4.146×10^{3} 2.778 × 10 ³	4.174×10^{3} 2.774 × 10 ³	0.9933
100	4.280×10^{2} 4.003×10^{2}	4.278×10^{2} 4.278×10^{2}	0.9972 1.000	$1.905 \times 10^{\circ}$ 1.439×10^{3} 1.000×10^{3}	$1.940 \times 10^{\circ}$ 1.411 × 10 ⁸ 1.062 × 10 ³	1.013
120	2.272×10^{2} 1.700 × 10 ²	2.252×10^{2} 1.680 × 10 ²	1.009	8.504×10^{2} 6.836 × 10 ²	8.241×10^{2} 6.590×10^{2}	1.032
140 150 160	1.309×10^{2} 1.030×10^{2} 8.481×10 7.477×10	1.280×10^{2} 1.006×10^{2} 8.270×10 7.260×10	1.023 1.024 1.026	5.686×10^{2} 4.886×10^{2} 4.361×10^{2} 4.073×10^{2}	5.441×10^{2} 4.653×10^{2} 4.142×10^{2} 4.952×10^{2}	1.046 1.050 1.053

 $d\sigma/d\Omega_{sC}$, $d\sigma/d\Omega_{C}$ denote the cross section for the screened field and the Coulomb field, respectively.

^b The cross section is given in barns/steradian. • R is the ratio $(d\sigma/d\Omega_{sc})/(d\sigma/d\Omega_{o})$.

TABLE II. Cross section for gold at 188 and 120 keV.

Z = 7	9	188 keV			120 keV	
θ	$d\sigma/d\Omega_{ m so}$	$d\sigma/d\Omega_{\rm o}$	R	$d\sigma/d\Omega_{ m sc}$	$d\sigma/d\Omega_{c}$	R
10	3.378×106	5.427×106	0.6224	6.225×10 ⁶	1.211 ×107	0.5140
20	2.859 ×10 ⁵	3.558×105	0.8035	5.538 ×10⁵	7.765 ×105	0.7132
30	6.873 ×104	7.744 ×104	0.8875	1.360×105	1.643 ×10 ⁵	0.8278
40	2.628×10^{4}	2.800 ×104	0.9386	5.193×104	5.822 ×104	0.8920
50	1.289 ×104	1.331 ×104	0.9684	2.569×10^{4}	2.740 ×104	0.9376
ĞÕ	7.332 × 108	7.438 × 10 ³	0.9857	1.485 ×104	1.531 ×104	0.9700
70	4.574 × 10 ³	4.613 × 10 ⁸	0.9915	9.447 ×10 ³	9.560 ×108	0.9882
80	3.077 ×10 ³	3.071 × 10 ³	1.002	6.469 ×10 ³	6.444 ×10 ³	1.004
90	2.186×10^{3}	2.153×10^{3}	1.015	4.680 ×10 ³	4.600 × 10 ³	1.017
100	1.606 ×10 ³	1.572×10^{3}	1.022	3.546 ×10 ³	3.438 ×108	1.031
110	1.221 ×103	1.188 ×10 ³	1.028	2.793 ×10 ³	2.674 ×10 ⁸	1.045
120	9.580×10^{2}	9.259 ×102	1.035	2.275 ×10 ³	2.155×10^{3}	1.056
130	7.750×10^{2}	7.445×10^{2}	1.041	1.915 ×103	1.797×10^{3}	1.066
140	6.496 × 10 ²	6.183 ×10 ²	1.051	1.675×10^{3}	1.549×10^{3}	1.081
150	5.599×10^{2}	5.319×10^{2}	1.053	1.502×10^{3}	1.380×10 ³	1.088
160	5.015 ×10 ²	4.757×10^{2}	1.054	1.385×10^{3}	1.271 × 10 ⁸	1.090
170	4.682 ×102	4.441×10^{2}	1.054	1.330×108	1.209 ×10 ⁸	1.100

⁷ F. B. Hilderbrand, Introduction to Numerical Analysis (McGraw-Hill Book Company, Inc., New York, 1956), p. 158. ⁸ These two transformations, the reduced series method and Euler transformation, were used by Sherman in his calculation of Mott scattering [N. Sherman, Phys. Rev. 103, 1601 (1956)]. ⁹ The summation of series was performed using double precision arithmetic.

¹⁰ J. H. Bartlett and T. A. Welton, Phys. Rev. 59, 281 (1941).
 ¹¹ C. B. O. Mohr and L. J. Tassie, Proc. Phys. Soc. (London)
 A67, 711 (1954); E. B. Gunnersen, Austral. J. Sci. Res. A5, 259 (1952).

found, however, that this method does not accelerate the convergence of the series for f and g fast enough, especially for large angles, and to achieve the same accuracy, we still need more than two hundred terms in the series.

III. RESULTS AND DISCUSSION

In this section, we first discuss the potentials used in the calculation and then present the results of the calculation in tabulated form. We then comment on the accuracy of the calculation and discuss our results

TABLE III. Cross section for gold at 100 and 50 keV.

Z = 7	'9	100 keV			50 keV	
θ	$d\sigma/d\Omega_{\rm SO}$	$d\sigma/d\Omega_{0}$	R	$d\sigma/d\Omega_{ m sc}$	$d\sigma/d\Omega_0$	R
10	7.937×106	1.692 × 107	0.4689	1.912 ×107	6.235×107	0.3067
20	7.246 ×105	1.077 ×106	0.6727	1.954×106	3.950 ×106	0.4947
30	1.787 ×10 ⁵	2.250 × 105	0.7941	4.992 ×10 ⁵	7.912 ×10 ⁵	0.6309
40	6.854×10^{4}	7.887×10^{4}	0.8690	1.930 ×105	2.633 ×105	0.7329
50	3.391 ×104	3.690 × 104	0.9190	9.593 ×104	1.184 ×10 ⁵	0.8102
60	1.970 × 104	2.059×10^{4}	0.9568	5.633 ×104	6.474 ×104	0.8701
70	1.264 × 104	1.288 × 104	0.9814	3.723 ×104	4.035×10^{4}	0.9227
80	8.746 × 108	8.719 ×10 ³	1.003	2.669 ×104	2.760×10^{4}	0.9670
90	6.381 ×10 ³	6.267 ×103	1.018	2.035 ×104	2.027 ×104	1.004
100	4.902 ×108	4.727×10^{3}	1.037	1.647×10^{4}	1.577×10^{4}	1.044
110	3.910 × 10 ³	3.716 × 10 ³	1.052	1.398×10^{4}	1.287 ×104	1.086
120	3.236 × 10 ³	3.032×10^{3}	1.067	1.218 ×104	1.095 ×104	1.112
130	2.758×10^{3}	2.562×10^{3}	1.076	1.102×10^{4}	9.654 ×10 ³	1.142
140	2.450×10^{3}	2.237 ×10 ³	1.095	1.030 ×104	8.775 ×10 ³	1.174
150	2.227 × 10 ³	2.016 × 10 ³	1.105	9.752 × 10 ³	8.187 ×10 ³	1.191
160	2.073 × 108	1.873 × 10 ³	1.107	9.388 × 10 ³	7.813 × 10 ³	1.202
170	2.006×10 ⁸	1.793×10 ³	1.119	9.250×10 ³	7.604×10 ³	1.217
						· · · · · · · · · · · · · · · · · · ·

TABLE IV. Cross section for copper at 400 and 200 keV.

Z = 2	9	400 keV			200 keV	
θ	$d\sigma/d\Omega_{ m sc}$	$d\sigma/d\Omega_{c}$	R	$d\sigma/d\Omega_{ m sc}$	$d\sigma/d\Omega_{c}$	R
10	1.988×10 ⁵	2.016×10 ⁵	0.9865	6.210×10 ⁵	6.605×105	0.9387
20	1.340 ×104	1.318×10^{4}	1.017	4.285×10^{4}	4.311 ×104	0.9941
30	2.780 ×103	2.711×10^{3}	1.025	8.899 ×10 ³	8.888 ×103	1.001
40	8.949×10^{2}	8.881 ×10 ²	1.0075	2.962 ×10 ⁸	2.929 ×10 ³	1.011
50	3.703×10^{2}	3.743 ×102	0.9893	1.249×10^{3}	1.247×10^{3}	1.002
60	1.810×10^{2}	1.846×10^{2}	0.9805	6.267×10^{2}	6.238 × 10 ²	1.005
70	9.960 × 10	1.014×10^{2}	0.9822	3.511 ×10 ²	3.489 ×10 ²	1,006
80	5.891 ×10	6.017 ×10	0.9791	2.125×10^{2}	2.119×10^{2}	1.003
90	3.728 ×10	3.787 ×10	0.9844	1.372 ×10 ²	1.373×10^{2}	0.9993
100	2.488×10	2.497×10	0.9964	9.369 ×10	9.383×10	0.9985
110	1.705 ×10	1.712×10	0.9959	6.678 ×10	6.711 × 10	0.9951
120	1.210 × 10	1.215×10	0.9959	5.038×10	5.004×10	1.007
130	8.969	8.922	1.005	3.902 ×10	3.885×10	1.005
140	6.926	6.794	1.019	3.159 ×10	3.142×10	1.005
150	5.582	5.400	1.034	2.680×10	2.650×10	1.011
160	4.770	4.524	1.054	2.425×10	2.340×10	1.036
170	4 342	4 041	1.075	2.188 × 10	2.168 × 10	1.009

TABLE V. Cross section for copper at 100 and 50 keV.

Z = 2	9	100 keV			50 keV	
θ	$d\sigma/d\Omega_{ m sc}$	$d\sigma/d\Omega_{c}$	R	$d\sigma/d\Omega_{ m sc}$	$d\sigma/d\Omega_{ m c}$	R
10	1.994×10 ⁶	2.295×106	0.8691	6.147×10 ⁶	8.399×106	0.7318
20	1.442×10^{5}	1.492 ×106	0.9661	4.947 ×10 ⁵	5.434×105	0.9102
30	3.038 ×104	3.080 ×104	0.9862	1.083×105	1.121 ×10 ⁵	0.9664
40	1.026×10^{4}	1.020×104	1.005	3.708×10^{4}	3.723×104	0.9957
50	4.430 × 10 ³	4.382×103	1.011	1.633×10^{3}	1.608×10^{3}	1.016
60	2.248×10^{3}	2.219×10^{3}	1.013	8.403 ×10 ³	8.218×10 ³	1.023
70	1.276×10 ³	1.261 × 10 ³	1.012	4.864 ×10 ³	4.724 ×10 ³	1.030
80	7.930 ×10 ²	7.814×10^{2}	1.015	3.064×10^{3}	2.967×10^{3}	1.033
90	5.295×10^{2}	5.183×10^{2}	1.022	2.072×10^{3}	$2,000 \times 10^{3}$	1.036
100	3.705×10^{2}	3.638×10^{2}	1.018	1.487×10^{3}	1.429×10^{3}	1.041
110	2.702×10^{2}	2.682×10^{2}	1.008	1.119×10^{3}	1.074×10^{3}	1.042
120	2.153×10^{2}	2.067×10^{2}	1.042	8.827×10^{2}	8,444 × 10 ²	1.045
130	1.696 × 10 ²	1.660×10^{2}	1.022	7.227×10^{2}	6.918 × 10 ²	1.045
140	1.405×10^{2}	1.388×10^{2}	1.012	6.167 ×10 ²	5.891 ×10 ²	1.047
150	1.220×10^{2}	1.208×10^{2}	1.010	5.470×10^{2}	5.208×10^{2}	1.050
160	1.190×10^{2}	1.093×10^{2}	1.089	5.026 ×10 ²	4.771×10^{2}	1.053
170	1.030×10^{2}	1.029×10^{2}	1.001	4.730 ×10 ²	4.528×10^{2}	1.045

Z = 79	400	keV	200	keV	188	keV
θ	S_{sc}^{a}	S _c ^a	S_{sc}	So	S_{sc}	S.
10	2.790×10 ⁻³	1.422×10 ⁻³	2.151×10 ⁻³	1.295×10 ⁻³	1.740×10^{-3}	1.246×10 ⁻³
20	6.717×10 ^{−3}	5.346×10 ⁻³	8.567×10 ⁻³	7.443×10 ^{−3}	8.978×10 ^{−3}	7.563×10⁻³
30	4.479×10 [−] ³	4.337×10 ³	1.197×10^{-2}	1.071×10^{-2}	1.254×10^{-2}	1.141×10^{-2}
40	-1.233×10^{-2}	-7.980×10^{-3}	3.697×10 ^{−3}	2.343×10 ⁻⁴	4.190×10 ^{−3}	1.423×10^{-3}
50	-2.240×10^{-2}	-3.306×10^{-2}	-2.457×10^{-2}	-2.807×10^{-2}	-2.747×10^{-2}	2.686×10^{-2}
60	-5.758×10^{-2}	-6.962×10^{-2}	-7.092×10^{-2}	-7.258×10^{-2}	-7.038×10^{-2}	-7.186×10^{-2}
70	-1.203×10^{-1}	-1.157×10^{-1}	-1.303×10^{-1}	-1.294×10^{-1}	-1.299×10^{-1}	-1.295×10^{-1}
80	-1.720×10^{-1}	-1.693×10^{-1}	-1.950×10^{-1}	-1.942×10^{-1}	-1.966×10^{-1}	-1.951×10^{-1}
90	-2.314×10^{-1}	-2.286×10^{-1}	-2.635×10^{-1}	-2.622×10^{-1}	-2.632×10^{-1}	-2.637×10^{-1}
100	-2.942×10^{-1}	-2.914×10^{-1}	-3.277×10^{-1}	-3.282×10^{-1}	-3.303×10^{-1}	-3.296×10^{-1}
110	-3.549×10^{-1}	-3.547×10^{-1}	-3.870×10^{-1}	-3.859×10^{-1}	-3.878×10^{-1}	-3.866×10^{-1}
120	-4.136×10^{-1}	-4.134×10^{-1}	-4.267×10^{-1}	-4.279×10^{-1}	-4.241×10^{-1}	-4.270×10^{-1}
130	-4.602×10^{-1}	-4.592×10^{-1}	-4.400×10^{-1}	-4.459×10^{-1}	-4.373×10^{-1}	-4.427×10^{-1}
140	-4.722×10^{-1}	-4.792×10^{-1}	-4.255×10^{-1}	-4.311×10^{-1}	-4.196×10^{-1}	-4.257×10^{-1}
150	-4.497×10^{-1}	-4.551×10^{-1}	-3.716×10^{-1}	-3.770×10^{-1}	-3.633×10^{-1}	-3.702×10^{-1}
160	-3.627×10^{-1}	-3.675×10^{-1}	-2.730×10^{-1}	-2.817×10^{-1}	-2.671×10^{-1}	-2.753×10^{-1}
170	-2.040×10^{-1}	-2.088×10^{-1}	-1.465×10^{-1}	-1.511×10 ⁻¹	-1.384×10^{-1}	-1.472×10^{-1}

TABLE VI. Asymmetry function for gold at 400, 200, and 188 keV.

 ${}^{\rm a}$ $S_{\rm sc},$ $S_{\rm c}$ denote the asymmetry function for the screened field and the Coulomb field, respectively.

TABLE VII. Asymmetry function for gold at 120, 100, and 50 keV.

Z = 7	9 120	keV	100	keV	50 1	keV
θ	Ssc	Sc	SBC	S.	$S_{ m sc}$	S_{c}
10 20 30 40 50 60 70 80 90 100 110 120 130	$\begin{array}{c} 1.518 \times 10^{-3} \\ 9.611 \times 10^{-3} \\ 1.900 \times 10^{-2} \\ 1.456 \times 10^{-2} \\ -1.008 \times 10^{-2} \\ -5.711 \times 10^{-2} \\ -5.711 \times 10^{-2} \\ -1.217 \times 10^{-1} \\ -2.648 \times 10^{-1} \\ -3.306 \times 10^{-1} \\ -3.811 \times 10^{-1} \\ -4.072 \times 10^{-1} \\ -4.067 \times 10^{-1} \end{array}$	$\begin{array}{c} 7.125 \times 10^{-4} \\ 7.628 \times 10^{-3} \\ 1.631 \times 10^{-2} \\ 1.205 \times 10^{-2} \\ -1.382 \times 10^{-2} \\ -6.077 \times 10^{-2} \\ -1.233 \times 10^{-1} \\ -1.944 \times 10^{-1} \\ -2.665 \times 10^{-1} \\ -3.320 \times 10^{-1} \\ -3.832 \times 10^{-1} \\ -4.129 \times 10^{-1} \\ -4.151 \times 10^{-1} \end{array}$	$\begin{array}{c} 1.287 \times 10^{-3} \\ 9.173 \times 10^{-3} \\ 2.106 \times 10^{-2} \\ 2.112 \times 10^{-2} \\ -7.547 \times 10^{-4} \\ -4.841 \times 10^{-2} \\ -1.140 \times 10^{-1} \\ -1.892 \times 10^{-1} \\ -2.623 \times 10^{-1} \\ -3.270 \times 10^{-1} \\ -3.752 \times 10^{-1} \\ -3.978 \times 10^{-1} \\ -3.934 \times 10^{-1} \end{array}$	$\begin{array}{r} 4.356 \times 10^{-4} \\ 7.104 \times 10^{-3} \\ 1.787 \times 10^{-2} \\ 1.706 \times 10^{-2} \\ -6.431 \times 10^{-3} \\ -5.316 \times 10^{-2} \\ -1.172 \times 10^{-1} \\ -1.904 \times 10^{-1} \\ -2.639 \times 10^{-1} \\ -3.294 \times 10^{-1} \\ -3.786 \times 10^{-1} \\ -4.047 \times 10^{-1} \\ -4.027 \times 10^{-1} \end{array}$	$\begin{array}{c} -1.411\times10^{-4}\\ 3.907\times10^{-3}\\ 2.182\times10^{-2}\\ 4.179\times10^{-2}\\ 4.066\times10^{-2}\\ 5.951\times10^{-3}\\ -6.165\times10^{-2}\\ -1.454\times10^{-1}\\ -2.292\times10^{-1}\\ -2.984\times10^{-1}\\ -3.409\times10^{-1}\\ -3.562\times10^{-1}\\ -3.411\times10^{-1}\end{array}$	$\begin{array}{c} -1.846 \times 10^{-4} \\ 1.837 \times 10^{-3} \\ 1.661 \times 10^{-2} \\ 3.307 \times 10^{-2} \\ 2.878 \times 10^{-2} \\ -7.909 \times 10^{-3} \\ -7.307 \times 10^{-2} \\ -1.540 \times 10^{-1} \\ -2.356 \times 10^{-1} \\ -3.044 \times 10^{-1} \\ -3.503 \times 10^{-1} \\ -3.559 \times 10^{-1} \end{array}$
140 150 160 170	$\begin{array}{r} -3.755 \times 10^{-1} \\ -3.141 \times 10^{-1} \\ -2.268 \times 10^{-1} \\ -1.188 \times 10^{-1} \end{array}$	$\begin{array}{r} -3.860 \times 10^{-1} \\ -3.249 \times 10^{-1} \\ -2.351 \times 10^{-1} \\ -1.234 \times 10^{-1} \end{array}$	$\begin{array}{r} -3.583 \times 10^{-1} \\ -2.968 \times 10^{-1} \\ -2.123 \times 10^{-1} \\ -1.103 \times 10^{-1} \end{array}$	$\begin{array}{r} -3.704 \times 10^{-1} \\ -3.086 \times 10^{-1} \\ -2.214 \times 10^{-1} \\ -1.156 \times 10^{-1} \end{array}$	$\begin{array}{r} -2.994 \times 10^{-1} \\ -2.405 \times 10^{-1} \\ -1.677 \times 10^{-1} \\ -8.540 \times 10^{-2} \end{array}$	$\begin{array}{c} -3.174 \times 10^{-1} \\ -2.568 \times 10^{-1} \\ -1.800 \times 10^{-1} \\ -9.258 \times 10^{-2} \end{array}$

TABLE VIII. Asymmetry function for copper at 200, 100, and 50 keV.

Z = 29	200	keV	100	keV	50 1	xeV
θ	Ssc	So	Ssc	So	$S_{ m sc}$	$S_{\mathfrak{o}}$
10 20 30 40 50 60 70 80 90 100 110 120 130 140	$\begin{array}{c} 6.338 \times 10^{-4} \\ 5.656 \times 10^{-4} \\ -5.115 \times 10^{-4} \\ -1.254 \times 10^{-2} \\ -2.625 \times 10^{-2} \\ -2.970 \times 10^{-2} \\ -4.002 \times 10^{-2} \\ -5.724 \times 10^{-2} \\ -5.724 \times 10^{-2} \\ -7.457 \times 10^{-2} \\ -8.598 \times 10^{-2} \\ -9.090 \times 10^{-2} \\ -1.054 \times 10^{-1} \\ -1.002 \times 10^{-1} \\ -9.343 \times 10^{-1} \\ -9.343 \times 10^{-1} \\ -9.343 \times 10^{-1} \\ \end{array}$	$\begin{array}{c} -6.415 \times 10^{-5} \\ -1.263 \times 10^{-3} \\ -5.010 \times 10^{-3} \\ -5.010 \times 10^{-3} \\ -2.043 \times 10^{-2} \\ -2.043 \times 10^{-2} \\ -3.152 \times 10^{-2} \\ -3.152 \times 10^{-2} \\ -4.417 \times 10^{-2} \\ -5.768 \times 10^{-2} \\ -7.119 \times 10^{-2} \\ -8.365 \times 10^{-2} \\ -9.380 \times 10^{-2} \\ -1.002 \times 10^{-1} \\ -1.012 \times 10^{-1} \\ -9.531 \times 10^{-2} \\ -9.531$	$\begin{array}{r} 8.258 \times 10^{-4} \\ 9.927 \times 10^{-5} \\ -3.939 \times 10^{-3} \\ -9.618 \times 10^{-3} \\ -2.196 \times 10^{-2} \\ -3.112 \times 10^{-2} \\ -4.117 \times 10^{-2} \\ -5.554 \times 10^{-2} \\ -6.728 \times 10^{-2} \\ -7.646 \times 10^{-2} \\ -8.202 \times 10^{-2} \\ -8.202 \times 10^{-2} \\ -8.472 \times 10^{-2} \\ -7.385 \times$	$\begin{array}{c} 1.538 \times 10^{-4} \\ -8.353 \times 10^{-4} \\ -4.314 \times 10^{-3} \\ -1.953 \times 10^{-2} \\ -3.047 \times 10^{-2} \\ -4.265 \times 10^{-2} \\ -5.517 \times 10^{-2} \\ -6.700 \times 10^{-2} \\ -7.702 \times 10^{-2} \\ -8.410 \times 10^{-2} \\ -8.523 \times 10^{-2} \\ -7.776 $	$\begin{array}{r} 5.238 \times 10^{-4} \\ 2.071 \times 10^{-4} \\ -2.382 \times 10^{-3} \\ -7.607 \times 10^{-3} \\ -1.638 \times 10^{-2} \\ -2.634 \times 10^{-2} \\ -3.754 \times 10^{-2} \\ -4.888 \times 10^{-2} \\ -5.924 \times 10^{-2} \\ -6.753 \times 10^{-2} \\ -7.290 \times 10^{-2} \\ -7.416 \times 10^{-2} \\ -7.094 \times 10^{-2} \\ -6.339 \times$	$\begin{array}{c} 2.766 \times 10^{-4} \\ -1.501 \times 10^{-4} \\ -2.877 \times 10^{-3} \\ -8.452 \times 10^{-3} \\ -1.667 \times 10^{-2} \\ -2.688 \times 10^{-2} \\ -3.820 \times 10^{-2} \\ -4.957 \times 10^{-2} \\ -4.957 \times 10^{-2} \\ -5.994 \times 10^{-2} \\ -7.350 \times 10^{-2} \\ -7.208 \times 10^{-2} \\ -7.208 \times 10^{-2} \\ -6.469 $
160 170	-6.124×10^{-3} -3.138×10^{-2}	-6.001×10^{-2} -3.187×10^{-2}	-4.854×10^{-2} -2.886×10^{-2}	-4.641×10^{-2} -2.427×10^{-2}	-3.190×10^{-2} -3.698×10^{-2} -1.944×10^{-2}	-3.299×10^{-2} -3.760×10^{-2} -1.952×10^{-2}

TABLE IX. Cross section and asymmetry function for mercury at 204 keV.

Z ≈ 8	30	204 keV			
0	$d\sigma/d\Omega_{10}$	$d\sigma/d\Omega_{\rm o}$	R	S	S.
10	3.031×10 ⁶	4.8241 ×10 ⁶	0.6283	2.219×10-8	1.2782×10-
20	2.516×105	3.1688 ×10 ⁵	0.7940	9.476 ×10-3	7.6390 ×10-8
30	5.993 ×104	6.9196 ×104	0.8661	1.317 × 10-2	1.1443 × 10 ⁻²
40	2.311 ×104	2.5123 ×104	0.9199	-1.708 ×10 ⁻²	1.3342 ×10-8
50	1.135 ×104	1.1983 ×104	0.9472	-2.981 ×10-2	-2.7087 ×10-2
60	6.501 ×10 ³	6.7191 ×10 ³	0.9675	-6.925 ×10-2	-7.2206 ×10-2
70	4.068 ×103	4.1756 ×10 ³	0.9742	-1.333×10^{-1}	-1.3003 ×10 ⁻¹
80	2.741 ×10 ⁸	2.7824 ×10 ⁸	0.9851	-1.960 ×10 ⁻¹	-1.9604 ×10 ⁻¹
90	1.943 ×108	1.9500 ×10 ³	0.9964	-2.685 ×10 ⁻¹	-2.6548 ×10-1
100	1.429 ×10 ³	1.4213 ×10 ³	1.005	-3.330×10^{-1}	-3.3301 ×10-1
110	1.086 ×10 ³	1.0705 ×103	1.015	-3.904 ×10 ⁻¹	-3.9235 ×10 ⁻¹
120	8.488 ×10 ²	8.3083 ×10 ²	1.022	-4.340 ×10 ⁻¹	-4.3594 ×10-1
130	6.814 ×10 ²	6.6423 ×10 ²	1.026	-4.497 ×10-1	-4.5510 ×10 ⁻¹
140	5.700 × 10 ²	5.4804 ×10 ²	1.040	-4.320 ×10 ⁻¹	-4.4090×10^{-1}
150	4.903 × 10 ²	4.6833×10^{2}	1.047	-3.751 ×10 ⁻¹	-3.8628 ×10 ⁻¹
160	4.395 ×10 ²	4.1646 × 10 ²	1.055	-2.780×10^{-1}	-2.8908 ×10-1
170	4.105 × 10 ²	3.8720 ×10 ²	1.060	-1.525 ×10 ⁻¹	-1.5527 ×10-1

in connection with the various measurements of $d\sigma/d\Omega$ and S.

The potentials used in these calculations are: (1) Gold:

$$V = -\frac{Ze^2}{r} [0.19 \exp(-0.257\chi) + 0.56 \exp(-0.779\chi) + 0.25 \exp(-3.16\chi)],$$

where $\chi = 1.13Z^{1/3}r/a_B$ and a_B is the Bohr radius. This potential was originally fitted to the Hartree potential for mercury by Byatt¹² with Z=80, but we used the same expression with Z = 79 for gold.

(2) Copper:

$$V = -\frac{Ze^2}{r} [0.22 \exp(-0.319\chi) + 0.78 \exp(-1.081\chi)],$$

where $\chi = 1.13 Z^{1/3} r/a_B$. This potential was originally

fitted to the Hartree potential for zinc also by Byatt¹² with Z=30, but we used the same expression with Z=29 for copper.

(3) Mercury: Hartree potential given in a numerical form by Cohen.13

In Tables I-IX, we tabulate our results together with the corresponding values for Coulomb field.¹⁴

As remarked in Sec. II, we estimate the error in $d\sigma/d\Omega$ and S of our calculation to be not greater than 1%. This estimate is based on the following observation: In the present calculation, the summation was carried out with double precision arithmetic. This includes the generation of necessary Legendre polynomials. For each case, the behaviors of Re f, Im f, Re g, and Im g were studied carefully and the errors in S and $d\sigma/d\Omega$ were estimated. The error estimate given above is the largest of all error estimates. In Table X, we give representative samples of convergence tests for $d\sigma/d\Omega$ and S.

It is of interest to compare our results with previous calculations of Bartlett and Welton¹⁰ and of Mohr and Tassie.11,15 The comparison is given in Tables XI and XII.

As can be seen from the tables given (Tables VI-IX), the deviation of S_{screened} from S_{Coulomb} at angles larger than 90 deg where the measurement on S is usually carried out, does not exceed 8%-10%. The experiment on S, however, gave considerably lower values¹⁶ $(S_{exp}/S_{Coulomb})^{17}$ is as low as 0.6). This large deviation is usually attributed mainly to the depolarization effects of plural and multiple scatterings of electrons in target (and source if a polarized electron beam is used). Even the latest experiment of Apalin et al.,¹⁶ which took the depolarization effect of multiple scatterings in target into account, shows $S_{exp}/S_{Coulomb}$ at

TABLE X. Sample convergence tests for $d\sigma/d\Omega$, S.

					-		
Z	Т	θ	20 terms	30 terms	40 terms	50 terms	
79	200 keV	30° $d\sigma/d\Omega$	6.2369×104	6.2364×10 ⁴	6.2366×10 ⁴	6.2362×10 ⁴	-
		150° 30°	4.8858×10^{2} 1.1833×10^{-2}	4.8885×10^{2} 1.2006×10^{-2}	4.8793×10 ² 1.1968×10 ⁻²	4.8856×10^{2} 1.1973×10^{-2}	
20	50 koV	150°	-0.37059	-0.37114	-0.37182	-0.37163	
29	JUKEV	$d\sigma/d\Omega$	1.0300×10 ²	1.1004×10°	1.0844 \ 103	1.0833×10 ³	
		30°	-2.3836×10^{-3}	-2.3857×10 ⁻³	-2.3831×10^{-3}	-2.3822×10^{-3}	
		150° S	−5.1883×10 ⁻²	-5.1909×10 ⁻²	-5.1893×10 ⁻²	-5.1903×10 ⁻²	

¹² W. J. Byatt, Phys. Rev. 104, 1298 (1956).

13 S. Cohen, The Rand Corporation, Report No. RM-2272-AEC, 1958 (unpublished).

¹⁴ The values of $d\sigma/d\Omega$ and S for Coulomb field were also obtained numerically using an IBM-7090 computer with double pre-cision arithmetic. The necessary formulas are to be found in Sherman (see footnote 8). The reduced series method with m=2 for F and m=3 for G was used. Our values of $d\sigma/d\Omega$ and S agree very well (<0.5%) with Sherman's calculation for Z=80 at T=204 keV and 46 keV. The necessary code was written in collaboration with Professor R. L. Gluckstern.

 ¹⁶ We should remark here that since these authors did not give any error estimate, the accuracy of their calculation is not known.
 ¹⁶ See V. A. Apalin, L. Yekutikov, I. I. Lukashevich, L. A. Mikaelyan, G. V. Smirou, and P. Ye. Spivak, Nucl. Phys. 31, 657 (1962). All measurements were summarized and the references to the experiments are given in this paper. ¹⁷ Here S_{exp} is the abbreviation for $S_{experiment}$.

TABLE XI. Comparison of S as obtained by Mohr and Tassie and the present calculation.

Z	θ (deg)	<i>S</i> м.т. ^а	S
79	80 90 100 110 120 130 140	$T = 121 \text{ keV} \\ -0.204 \\ -0.277 \\ -0.342 \\ -0.386 \\ -0.409 \\ -0.411 \\ -0.389$	T = 120 keV -0.195 -0.265 -0.330 -0.381 -0.407 -0.407 -0.376

 $^{*}S_{M.T.}$ represents the results obtained by Mohr and Tassie (Ref. 11). Since they did not give numbers, the values given here were estimated from their figure. S denotes the results obtained by the present calculation.

120° to be 0.79 at 45 keV and 0.92 at 170 keV. Bienlein et al.18 also measured S using Co⁶⁰ as a polarized electron beam source.19 They also took the effects of plural and multiple scattering in source and target into account. Their results show $S_{exp}/S_{Coulomb}$ at 120° to be 0.84 at 120 keV, 0.95 at 155 keV, and 1 at 209

TABLE XII. Comparison of S and $d\sigma/d\Omega$ as obtained by Bartlett and Welton and the present calculation.

Т	θ (deg)	$R_{\rm B.W.^{a}}$ Z=80	R = 79	$\begin{array}{c}S_{\mathrm{B.W.}^{\mathbf{a}}}\\Z=80\end{array}$	Z = 79
100 keV	30 60 90 120 150	0.774 1.02 0.976 1.21 1.19	0.794 0.957 1.02 1.07 1.11	-0.219 -0.336 -0.293	0.262 0.398 0.297

 $^{\rm a}$ S_{B.W.}, R_{B.W.} represent the results obtained by Bartlett and Welton (Ref. 10). S, R are those by the present author.

keV. Our calculation shows that the large deviation at 45 and 120 keV given by above authors cannot be attributed to the screening effects alone. The source of discrepancy may still lie in incomplete treatment of the plural and multiple scattering effects.

As for the cross section, it is interesting to note the

following behavior of R, the ratio of $d\sigma/d\Omega_{\rm screened}$ to $d\sigma/d\Omega_{\rm Coulomb}$. R is less than 1 for small angles as expected, but becomes larger than 1 at large angles. This behavior of R seems to be present in the cross section measurement made by Motz et al.¹ at the Bureau of Standards. They measured $d\sigma/d\Omega$ for unpolarized electron beam incident on thin gold, tin, and copper foils at electron energies of 400, 200, 100, and 50 keV. However, the experimental error does not allow us to confirm this behavior of R conclusively. In general, our results agree well with their measurements within the experimental error.¹ The only exception is the case of copper at the electron energy of 50 keV. The reason for such a big disagreement is not clear.

A969

Motz et al.¹ calculated R by using the Molière²⁰ approximation and found that there is considerable difference between values of R given by the present calculation and those by Molière's approximation. This difference is considerably smaller for copper than for gold.

In Tables XIII and XIV, we compare our results with those obtained from Dalitz' formula for the screened field.²¹ The screening parameter here is λ $=(Z)^{1/3}/(0.885a_B)$. It is seen from these tables that Dalitz' formula gives the cross section for copper to within 10% of our results. However, for gold, the disagreement between our results and those given by Dalitz' formula is very large at all angles. This suggests the fact that for such a high-Z material, the contribution from higher Born terms is not negligible.

Finally, let us comment on the sensitivity of $d\sigma/d\Omega$ and S to the choice of a potential. By comparing our result for gold at the electron energy of 120 keV (v/c=0.58) with the previous calculation³ where a one-term exponential potential was used, and also recalling the previous calculation for mercury at v/c=0.4 and 0.5, where a one-term exponential potential as well as a Hartree potential was used, it seems quite certain that the choice of a potential in the calculation of $d\sigma/d\Omega$ and S is important only in the small angle region (<60°). For large angles (90°-140°), $d\sigma/d\Omega$ and

TABLE XIII. Comparison of $d\sigma/d\Omega$ as obtained by using Dalitz' formula, and by the present calculation for the screened as well as the unscreened fields of copper.

	Z=29 $T=100 keV$							
θ (deg)	$d\sigma/d\Omega_{ m DS^a}$	$d\sigma/d\Omega_{\rm S^a}$	$d\sigma/d\Omega_{ m C}$	$d\sigma/d\Omega_{ m DS}$	$d\sigma/d\Omega_{\rm B}$	$d\sigma/d\Omega_{ m C}$		
30 60 90 120 150	8.705×10^{3} 5.910×10^{2} 1.271×10^{2} 4.582×10 2.424×10	8.899×10 ³ 6.267×10 ² 1.372×10 ² 5.038×10 2.680×10	8.888×10^{3} 6.238×10^{2} 1.373×10^{2} 5.004×10 2.650×10	3.049×10^{4} 2.137 × 10 ³ 4.883 × 10 ² 1.922 × 10 ² 1.116 × 10 ²	3.038×10^{4} 2.248×10^{8} 5.295×10^{2} 2.153×10^{2} 1.220×10^{2}	3.080×10^{4} 2.219×10^{3} 5.183×10^{2} 2.067×10^{2} 1.208×10^{2}		

 $\Delta d\sigma/d\Omega_{DS}$, $d\sigma/d\Omega_S$, $d\sigma/d\Omega_C$ denote the cross section for the screened field given by Dalitz' formula, by the present calculation, and that for the Coulomb field, respectively. Cross section is given in barns/steradian.

¹⁸ H. Bienlein, G. Fielsner, R. Fleishmann, K. Guthner, H. V. Issendorf, and G. Wegener, Z. Physik 154, 376 (1959); 155, 327 (1960). ¹⁹ They assumed the polarization of electron from Co⁶⁰ to be exactly -v/c.

²⁰ G. Molière, Z. Naturforsch. 2a, 133 (1947).
 ²¹ R. H. Dalitz, Proc. Phys. Soc. (London) A206, 509 (1951).

θ (deg)	$d\sigma/d\Omega_{ m DS}$	$T = 200 \text{ keV} \ d\sigma/d\Omega_{ m S}$	$Z = 79$ $d\sigma/d\Omega_{\rm C}$	$d\sigma/d\Omega_{ m DS}$	$T = 100 \text{ keV} \\ \frac{d\sigma}{d\Omega_{\rm S}}$	$d\sigma/d\Omega_{ m C}$
30	7.493×104	6.236×104	6.996×104	2.611×10 ⁵	1.787×10 ⁵	2.250×10 ⁵
60	5.351×10^{3}	6.653×10^{3}	6.738×10^{3}	1.910×10^{4}	1.970×10^{4}	2.059×10^{4}
90	1.148×10^{3}	1.965×10^{3}	1.940×10^{3}	4.339×10^{3}	6.381×10^{3}	6.267×10 ³
120	3.961×10^{2}	8.504×10^{2}	8.241×10^{2}	1.649×10^{3}	3.236×19 ³	3.032×10^{3}
150	1.953×10^{2}	4.886×10^{2}	4.653×10^{2}	9.144×10^{2}	2.227×10^{3}	2.016×10^{3}

TABLE XIV. Same as caption for Table XIII except copper is replaced by gold.

S would not change more than 10% even if we changed the potential from the one-term exponential to the three-term exponential potential or to the Hartree potential.

ACKNOWLEDGMENTS

It is a pleasure to thank Dr. J. W. Motz for informing the author of the experimental results performed at the Bureau of Standards. This experiment encouraged the author to carry out most of the calculations reported in the paper. The author is grateful to Dr. J. K. Percus who showed his continuous interest in the calculation and provided the necessary IBM-7090 computer time at NYU computing center. The author wishes to thank Professor N. Sherman and Professor G. Rawitcher for several illuminating discussions. The author is most indebted to Professor R. L. Gluckstern for his collaboration in preparing the necessary code for calculation of Mott scattering and his detailed criticism on the previous calculation and the manuscript.

PHYSICAL REVIEW

VOLUME 133, NUMBER 4A

17 FEBRUARY 1964

2s and 2p Electron Impact Excitation in Atomic Hydrogen

KAZEM OMIDVAR

National Aeronautics and Space Administration, Goddard Space Flight Center, Greenbelt, Maryland (Received 17 April 1963; revised manuscript received 23 October 1963)

A numerical calculation has been carried out to evaluate the 3×3 cross-section matrix involved in the electron impact excitation of the ground state of H atom to the 2s and 2p levels. The method of solution is that of atomic eigenstates expansion. In this paper, instead of the iterative technique used by other authors, the definite integral terms in the coupled radial differential equations are eliminated through some linear transformation of the radial functions, thus avoiding iteration of these equations. The accuracy of the numerical integration is tested by satisfying the equation of reciprocity and the equation of continuity of currents with an error-to-value ratio less than 1 per 1000 on the average; and the maximum of this ratio, except for a few cases, has been kept below 5%. The results are in agreement with the results of an iterative technique. To evaluate the effect of the long range and the centrifugal potential, a simple perturbation theory is developed. The six cross sections $1s \rightarrow 2s$, $1s \rightarrow 2p$, $1s \rightarrow 1s$, $2s \rightarrow 2p$, and $2p \rightarrow 2p$ are tabulated elsewhere, only the $2s \rightarrow 2p$ and the $2p \rightarrow 2p$ cross sections are reported here. The $2p \rightarrow 2p$ cross section requires the solution of the sets of differential equations with different parities. Assuming the validity of the eigenstates expansion, it is found by comparison with the eigenstates expansion calculation that the Born approximation, despite its simplicity, gives meaningful results for low and close-to-the-threshold energies of the bombarding electrons. The effect of the $1s \rightarrow 2s$ excitation cross section above threshold is found.

I. INTRODUCTION

CALCULATION of the excitation cross sections in atomic hydrogen by electron impact corresponds to the solution of the problem of three interacting bodies: one proton and two electrons. By taking the position of the proton as the center of mass, the problem will reduce to the task of finding the nonseparable wave function of the system of the two electrons with an attractive center of force. Such solution has not been found. However, if this wave function is expanded in terms of the eigenstates of the hydrogen atom, the coefficients of the expansion, which are functions of the position vector of the free electron, can be found through numerical integration. When an infinite number of terms are included in the expansion, the solution to the problem is exact. Furthermore, the expansion has the advantage that the asymptotic form of its coefficients are automatically the asymptotic form of the free-electron wave function scattered from different atomic states, which are simply related to the excitation cross sections.

In this paper atomic states 1s, 2s, 2p are included in