High-energy forward elastic scattering of electrons: Born amplitudes for a pseudostate model of atomic hydrogen

S. Geltman
Joint Institute for Laboratory Astrophysics, National Bureau of Standards and University of Colorado, Boulder, Colorado 80309

R. K. Nesbet
IBM Research Laboratory, San Jose, California 95193
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Exact second-Born-approximation elastic scattering amplitudes are computed for a dipole excitation pseudostate model of electron scattering by ground-state atomic hydrogen. Calculations at 15, 25, and 35 keV incident energy show a forward peak in the differential elastic cross section. The optical theorem is exactly satisfied by these calculations, and the magnitude of the forward peak is determined primarily by physical values of the atomic static polarizability and oscillator strength. In the energy range considered, the computed peak is smaller by a large factor than the magnitude required to interpret recently observed experimental data in terms of single elastic collisions of electrons with ground-state atoms.

I. INTRODUCTION

A strong forward peak and rapid angular variation, essentially a Fraunhofer diffraction pattern, have been observed in extreme forward elastic scattering of 15—25-keV electrons by rare-gas atoms.[1] Geiger and Móron-León interpret their data as a diffraction pattern due to shadow scattering. The removal of forward electron flux, due to inelastic scattering, which dominates elastic scattering by a factor $k^2a_0^2$ in the forward direction, may affect the elastic cross section analogously to the optical scattering effect of a black disk, whose shadow is described by a Fraunhofer diffraction pattern.

As shown by Joachain,[2] a strongly absorptive potential (complex square well) with a finite radius produces a Fraunhofer diffraction pattern. The purpose of the present work is to see if such a result can emerge from a detailed study of electron scattering by an atom. To simplify the theory, the hydrogen atom is considered here in a pseudostate model, in which electric dipole excitation from the ground state is described by transitions to a single pseudostate. This pseudostate, constructed to give the exact static dipole polarizability, is known explicitly for hydrogen.[3] Using this pseudostate, the second Born scattering amplitude has been computed exactly for the coupled elastic and inelastic scattering channels, in the energy range 15—35 keV.

Details of the model and derivations of formulas used for computation are given in Sec. II, and results of the calculations are given in Sec. III. These results are discussed in relation to experiment and prior theory in Sec. IV.

Because the present results apparently disagree both with prior theory in the keV energy range and with experiment, the authors consider it essential to publish enough detail so that the calculations could easily be duplicated if necessary and verified without any uncertainty. Prior literature contains many second Born calculations of $e^-+\mathrm{H}$ or e^-+rare-gas scattering, generally at much lower collision energies than those considered here. This field was reviewed in 1976 by Walters,[4] and several relevant papers have been published since.[5—7] At relatively low energy (30 eV) Ermolaev and Walters[5] computed the exact second Born elastic scattering amplitude for $e^-+\mathrm{H}$, summing over all intermediate-bound and continuum states. In the range 50—500 eV, Byron and Joachain[6,7] summed second Born elastic amplitudes over $2s$, $2p$, and the pseudostate $3\bar{p}$ explicitly, approximating the residual sum by closure, with an average excitation energy parameter. The eikonal-Born series was used to construct a third-order optical potential. An important qualitative point made by Byron and Joachain[6,8] is that $\mathrm{Re}\bar{f}_{\mathrm{B}2}$ dominates forward angular structure in elastic scattering at high energies, through interference with $f_{\mathrm{B}1}$. The latter amplitude is slowly varying at small angles because it represents the effect of a short-range potential. The present work concentrates on obtained $\mathrm{Re}\bar{f}_{\mathrm{B}2}$ with high numerical accuracy for a well-defined model, at much higher energies than considered earlier.

An important question is whether, for high-energy forward elastic scattering, the second Born sum over intermediate states is adequately modeled by a single pseudostate. This is best examined by partial-wave analysis, considered in a separate publication. Formal analysis leads to an exact asymptotic expansion of the complex optical potential for high-energy elastic scattering.[9] Crucially, the leading terms due to all intermediate dipole-coupled states are of the same form. For a single pseudostate at excitation energy ΔE_p, the optical potential in every partial-wave channel is

$$V^{\mathrm{opt}}(r)=-\tfrac{1}{2}\alpha\left[r^{-4}-\frac{2ik}{\Delta E_p}r^{-5}+O(r^{-6})\right].$$

Since α is a physical constant and total oscillator strength is fixed by a sum rule, the effect of subdividing oscillator strength among a series of intermediate states can be approximated by adjusting ΔE_p to some empirical mean value, as is done in typical second Born calculations. Clearly, the use of a single pseudostate with correct α cannot introduce a large qualitative error.

Earlier theoretical studies of the elastic optical potential due to intermediate dipole excitation are relevant. In particular, Huo[10] showed that the αr^{-4} static polarization potential is corrected by a complex term varying asymptotically as r^{-5}. Valone *et al.*[11] derive an absorption potential proportional to r^{-5}. Byron and Joachain[7] express third-order eikonal-Born theory in terms of a complex optical potential. Kohl *et al.*[12] derive a complex optical potential that varies as r^{-2} and r^{-3} in an intermediate range of r.

II. H MODEL: BORN SCATTERING AMPLITUDES

Neglecting electron exchange, the Schrödinger equation for electron scattering by a one-electron atom is

$$\left[-\tfrac{1}{2}\vec{\nabla}^2+H_a(\vec{r}\,')-\frac{1}{r}+\frac{1}{|\vec{r}-\vec{r}\,'|}-E\right]\Psi(\vec{r},\vec{r}\,')=0\ , \quad (1)$$

where H_a is the Hamiltonian operator of the neutral atom, and $\vec{r}$ is the coordinate of the scattered electron. The simplest dynamical model of electric dipole polarization and excitation effects is obtained by representing the wave function Ψ in terms of two target states: ground state $\psi_0(\vec{r})$ and a dipole pseudostate $\psi_{pm}(\vec{r})$, constructed to give the exact static polarizability. For the hydrogen atom

$$\psi_0=2e^{-r}Y_{00}(\hat{r})\ , \quad (2)$$

and the pseudostate wave function[3] is

$$\psi_{pm}=(\tfrac{32}{129})^{1/2}(r+\tfrac{1}{2}r^2)e^{-r}Y_{1m}(\hat{r})\ . \quad (3)$$

The model scattering wave function is

$$\Psi(\vec{r},\vec{r}\,')=\psi_0(\vec{r}\,')F_0(\vec{r})+\sum_{m=-1}^{+1}\psi_{pm}(\vec{r}\,')F_{pm}(\vec{r})\ . \quad (4)$$

Substitution of this function into the Schrödinger equation gives the close-coupling equations (without exchange) for F_0 and F_{pm}. The potentials in these equations, in Hartree atomic units, are

$$V_{00}(\vec{r})=-e^{-2r}\left[1+\frac{1}{r}\right]\ , \quad (5)$$

$$V_{p0}^{(m)}(\vec{r})=[V_{0p}^{(m)}(\vec{r})]^*$$
$$=9\left[\frac{2\pi}{129}\right]^{1/2}v_{p0}(r)Y_{1m}^*(\hat{r})\ , \quad (6)$$

where

$$v_{p0}(r)=\frac{1}{r^2}-e^{-2r}\left[\frac{2}{9}r^2+\frac{10}{9}r+2+\frac{2}{r}+\frac{1}{r^2}\right] \quad (7)$$

and $V_{pp}^{(mm')}(\vec{r})$, which is not used in the present work. In atomic units the ground-state energy E_0 is $-\frac{1}{2}$ and the pseudostate energy E_p is $-\frac{7}{86}$, so that the pseudostate excitation energy ΔE_p is $\frac{18}{43}$ a.u. By construction,[3] the present coupled equations give the full static electric dipole polarizability of the hydrogen ground state,

$$\alpha=\tfrac{9}{2}\ \text{a.u.}\ , \quad (8)$$

corresponding to oscillator strength

$$f=\tfrac{1458}{1849}=0.788\,534 \quad (9)$$

for excitation to the pseudostate. For comparison with model calculations, the reduced transition moment is

$$\mu=-(u_p\,|\,r\,|\,u_0)=-(\tfrac{243}{86})^{1/2}\ , \quad (10)$$

where $u_p(r)$ and $u_0(r)$ are the radial factors of ψ_{pm} and ψ_0, respectively.

The ground-state channel wave function is the formal solution of a Lippmann-Schwinger equation, for an incident plane wave in this channel,

$$F_0(\vec{r})=e^{i\vec{k}\cdot\vec{r}}-\frac{1}{2\pi}\int d^3\vec{r}\,'\frac{e^{ik|\vec{r}-\vec{r}\,'|}}{|r-r'|}\left[V_{00}(\vec{r}\,')F_0(\vec{r}\,')+\sum_m V_{0p}^{(m)}(\vec{r}\,')F_{pm}(\vec{r}\,')\right]\ . \quad (11)$$

The corresponding integral equation for the pseudostate channel wave function is

$$F_{pm}(\vec{r})=-\frac{1}{2\pi}\int d^3\vec{r}\,'\frac{e^{ik_p|\vec{r}-\vec{r}\,'|}}{|\vec{r}-\vec{r}\,'|}\left[V_{p0}^{(m)}(\vec{r}\,')F_0(\vec{r}\,')+\sum_{m'} V_{pp}^{(mm')}(\vec{r}\,')F_{pm'}(r')\right]\ . \quad (12)$$

Here, for total energy E,

$$k^2=2(E-E_0)=2E_i\ , \quad (13)$$

$$k_p^2=2(E-E_p)=2(E_i-\Delta E_p)\ , \quad (14)$$

where E_i is the energy of the incident electron. From the asymptotic forms $(r\to\infty)$ of these equations the scattering amplitudes in the coupled channels for outgoing momenta $\vec{k}\,'$ and $\vec{k}_p$ are

$$f_0=-\frac{1}{2\pi}\int d^3\vec{r}\,e^{-i\vec{k}\,'\cdot r}\left[V_{00}(\vec{r})F_0(\vec{r})+\sum_m V_{0p}^{(m)}(\vec{r})F_{pm}(\vec{r})\right]\ , \quad (15)$$

$$f_{pm}=-\frac{1}{2\pi}\int d^3\vec{r}\,e^{-i\vec{k}_p\cdot\vec{r}}\left[V_{p0}^{(m)}(\vec{r})F_0(\vec{r})+\sum_{m'}V_{pp}^{(mm')}(\vec{r})F_{pm'}(\vec{r})\right]. \tag{16}$$

The Born series is generated by iteration of Eqs. (11) and (12), starting with

$$F_0^{(0)}(\vec{r})=e^{i\vec{k}\cdot\vec{r}},$$
$$F_{pm}^{(0)}(\vec{r})=0\,. \tag{17}$$

The first Born elastic scattering amplitude is

$$f_0^{(\mathrm{B1})}(K_0)=\frac{1}{2}\left[\frac{1}{1+K_0^2/4}+\frac{1}{(1+K_0^2/4)^2}\right], \tag{18}$$

where $\vec{K}_0=\vec{k}-\vec{k}'$, with magnitude

$$K_0=2k\sin(\tfrac{1}{2}\theta)\,, \tag{19}$$

the elastic momentum transfer for scattering angle θ. The differential elastic cross section is

$$d\sigma_{00}^{(\mathrm{B1})}/d\Omega=|f_0^{(\mathrm{B1})}|^2\,. \tag{20}$$

The first Born inelastic scattering amplitude is

$$f_{pm}^{(\mathrm{B1})}(\vec{K})=\frac{18}{i}\left[\frac{2\pi}{129}\right]^{1/2}Y_{1m}^*(\hat{K})\int_0^\infty r^2dr j_1(Kr)v_{p0}(r)\,, \tag{21}$$

where K is the magnitude of the inelastic momentum transfer

$$\vec{K}=\vec{k}-\vec{k}_p\,. \tag{22}$$

With $v_{p0}(r)$ given by Eq. (7), the integral in Eq. (21) can be evaluated either directly or more easily by substituting the Fourier transform

$$\int d^3\vec{r}\frac{e^{i\vec{K}\cdot\vec{r}}}{|\vec{r}-\vec{r}'|}=\frac{4\pi}{K^2}e^{i\vec{K}\cdot\vec{r}'} \tag{23}$$

into the defining equation

$$f_{pm}^{(\mathrm{B1})}=-\frac{1}{2\pi}\int d^3\vec{r}e^{i\vec{K}\cdot\vec{r}}\int d^3r'\psi_{pm}^*(\vec{r}')\times\left[\frac{1}{|\vec{r}-\vec{r}'|}-\frac{1}{r}\right]\psi_0(\vec{r}')\,. \tag{24}$$

This gives

$$f_{pm}^{(\mathrm{B1})}=\frac{1}{iK^2}\left[\frac{2048\pi}{129}\right]^{1/2}I_p(K)Y_{1m}^*(\hat{K})\,, \tag{25}$$

where

$$I_p(K)=\int_0^\infty r^2dr(r+\tfrac{1}{2}r^2)e^{-2r}j_1(Kr) \tag{26}$$
$$=12K(12+K^2)/(4+K^2)^4\,. \tag{27}$$

From Eq. (21) the differential inelastic cross section is

$$d\sigma_{0p}^{(\mathrm{B1})}/d\Omega=\frac{k_p}{k_n}\sum|f_{pm}^{(\mathrm{B1})}|^2=\frac{512}{43}\frac{k_p}{k}I_p^2(K)/K^4\,, \tag{28}$$

and the total inelastic cross section is

$$\sigma_{0p}^{(\mathrm{B1})}=\frac{2\pi}{k^2}\sum_m\int|f_{pm}^{(\mathrm{B1})}(K)|^2KdK \tag{29}$$
$$=\frac{1024}{43}\frac{\pi}{k^2}\int_{k-k_p}^{k+k_p}dK\frac{I_p^2(K)}{K^3}\,. \tag{30}$$

In the limit of forward scattering, $K=k-k_p$. Comparing Eq. (20) for $K_0=0$ and Eq. (28) for $K=k-k_p$, at keV energies, the forward inelastic cross section is many orders of magnitude greater than the forward elastic cross section. The factor is 2.4×10^4 at 15 keV for the present model. Because of this large ratio it is important to evaluate the induced effect of the inelastic process on forward elastic scattering, even though the direct second-order term, of order V_{00}^2, may be negligible.

The direct second Born scattering amplitude is

$$f_0^{(\mathrm{B2})}=\frac{1}{(2\pi)^2}\int d^3\vec{r}\int d^3\vec{r}'e^{i(\vec{k}\cdot\vec{r}'-\vec{k}'\cdot\vec{r}+k|\vec{r}-\vec{r}'|)}\times|\vec{r}-\vec{r}'|^{-1}V_{00}(\vec{r})V_{00}(\vec{r}')\,. \tag{31}$$

By Fourier transformation with

$$\vec{t}=\vec{k}-\vec{q},\quad \vec{t}'=\vec{k}'-\vec{q}\,, \tag{32}$$

this becomes

$$f_0^{(\mathrm{B2})}=\frac{1}{2\pi^2}\int\frac{d^3\vec{q}}{q^2-k^2-i\epsilon}[f_0^{(\mathrm{B1})}(\vec{t}')]^*f_0^{(\mathrm{B1})}(\vec{t})\,. \tag{33}$$

Here $f_0^{(\mathrm{B1})}(\vec{t})$ is given by Eq. (18), so Eq. (33) reduces to the integral

$$f_0^{(\mathrm{B2})}=\frac{2}{\pi^2}\int\frac{d^3\vec{q}}{q^2-k^2-i\epsilon}\frac{(8+t^2)(8+t'^2)}{(4+t^2)^2(4+t'^2)^2}\,. \tag{34}$$

This can be evaluated by the method of Feynman and Dalitz.[13] Details are given in the Appendix.

The indirect second Born scattering amplitude is of the same form as Eq. (31), except that k multiplying $|\vec{r}-\vec{r}'|$ in the exponent is replaced by k_p, and $V_{00}V_{00}$ is replaced by the indirect second-order term

$$\sum_m V_{0p}^{(m)}(\vec{r})V_{p0}^{(m)}(\vec{r}')\,. \tag{35}$$

As before, by Fourier transformation, the scattering amplitude can be expressed in the form

$$f_p^{(\mathrm{B2})}=\frac{1}{2\pi^2}\int\frac{d^3\vec{q}}{q^2-k_p^2-i\epsilon}\sum_m[f_{pm}^{(\mathrm{B1})}(\vec{t}')]^*f_{pm}^{(\mathrm{B1})}(\vec{t})\,. \tag{36}$$

Using

$$\sum_m Y_{1m}^*(\hat{t}')Y_{1m}(\hat{t})=\frac{3}{4\pi}\frac{\vec{t}\cdot\vec{t}'}{tt'} \tag{37}$$

and Eq. (25), this becomes

$$f_p^{(\mathrm{B2})}=\frac{256}{43\pi^2}\int d^3\vec{q}\,\frac{1}{q^2-k_p^2-i\epsilon}\,\frac{\vec{t}\cdot\vec{t}\,'I_p(t)I_p(t')}{t^3t'^3}\ . \tag{38}$$

From Eq. (27) and using

$$\vec{t}\cdot\vec{t}\,'=\tfrac{1}{2}(t^2+t'^2-K_0^2)\ , \tag{39}$$

the explicit integral is

$$f_p^{(\mathrm{B2})}=\frac{18\,432}{43\pi^2}\times\int d^3\vec{q}\,\frac{1}{q^2-k_p^2-i\epsilon}\times\frac{(t^2+t'^2-K_0^2)(12+t^2)(12+t'^2)}{t^2t'^2(4+t^2)^4(4+t'^2)^4}\ , \tag{40}$$

which can be evaluated by the method of the Appendix.

III. RESULTS OF CALCULATIONS

Equations (18), (34), and (40) were evaluated at incident electron energies 15, 25, and 35 keV. Summing the computed B1 and B2 amplitudes gives the full second Born amplitude $f^{(\mathrm{B2})}$, whose squared magnitude is shown as the elastic differential cross section in Fig. 1, for angles up to 10 mrad. The first Born elastic differential cross section $|f^{(\mathrm{B1})}|^2$ is also shown in Fig. 1. Typical numerical values of the separate contributions to $f^{(\mathrm{B2})}$ are listed in Table I, for 15-keV incident energy.

Results at $\theta=0$ are computed by taking the limits of the relevant formulas. Both $f_0^{(\mathrm{B2})}$ and $f_p^{(\mathrm{B2})}(0)$ reduce to explicit sums of Dalitz integrals, eliminating integration over the auxiliary variable u in Eq. (A2). This serves as a check on calculations for nonzero θ. The computed $f^{(\mathrm{B2})}(\theta)$ amplitudes extrapolate smoothly to the limit $\theta=0$. Because $\mathrm{Re}f_p^{(\mathrm{B2})}(\theta)$ varies linearly with θ in this limit, while $\mathrm{Im}f_p^{(\mathrm{B2})}(\theta)$ varies quadratically, the forward peak in the differential cross sections varies linearly with θ for very small angles.

As is evident in Fig. 1, the second Born terms are significant only at very small angles, where they superimpose a forward peak on the first Born cross section. From the numbers shown in Table I, this peak is entirely due to the indirect scattering amplitude $f_p^{(\mathrm{B2})}$. As incident energy increases, this forward peak becomes smaller and is concentrated at smaller angles. At $\theta=0$ the largest contribution to this peak is the cross term between $f^{(\mathrm{B1})}$ and $\mathrm{Re}f_p^{(\mathrm{B2})}$. A diffraction pattern occurs in this cross term, because $\mathrm{Re}f_p^{(\mathrm{B2})}$ changes sign at small angles but the effect is too small to be visible on the scale of Fig. 1. $\mathrm{Im}f_p^{(\mathrm{B2})}$ decreases monotonically from its peak value at $\theta=0$.

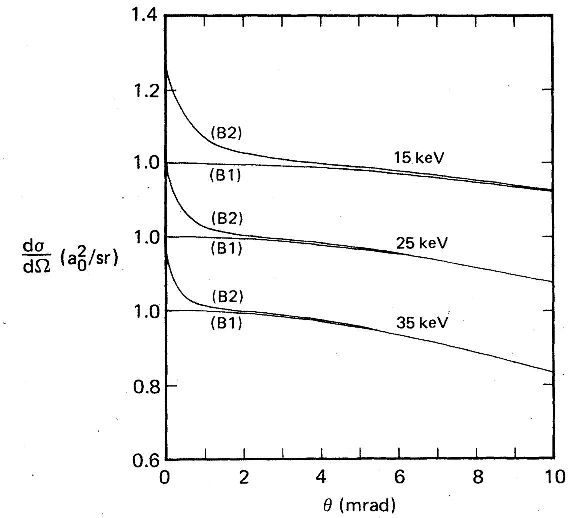

FIG. 1. H-atom model: differential elastic cross section in the forward direction.

For exact solutions of the scattering equations, the forward value of $\mathrm{Im}f(\theta)$ is determined by the optical theorem,

$$\mathrm{Im}f(0)=\frac{k}{4\pi}\sigma_{\mathrm{tot}}\ , \tag{41}$$

where the total cross section σ_{tot} includes all elastic and inelastic processes. Because of the structure of Eqs. (33) and (36) for the $f^{(\mathrm{B2})}$ amplitudes, specialized versions of the optical theorem can be obtained by computing $\mathrm{Im}f^{(\mathrm{B2})}(\theta)$ in the limit $\theta=0$. This gives two independent formulas

TABLE I. Elastic born amplitudes at 15 keV.

θ (mrad)	$f^{(\mathrm{B1})}$	$\mathrm{Re}f_0^{(\mathrm{B2})}$	$\mathrm{Im}f_0^{(\mathrm{B2})}$	$\mathrm{Re}f_p^{(\mathrm{B2})}$	$\mathrm{Im}f_p^{(\mathrm{B2})}$	$d\sigma/d\Omega$ (a_0^2/sr)
0	1.000 00	0.000 37	0.017 56	0.088 42	0.216 66	1.240 31
2	0.998 34	0.000 37	0.017 56	0.005 08	0.126 89	1.028 48
4	0.993 42	0.000 37	0.017 54	0.000 85	0.085 61	0.999 95
6	0.985 31	0.000 37	0.017 51	0.000 01	0.062 64	0.978 00
8	0.974 15	0.000 37	0.017 47	−0.000 28	0.047 16	0.953 32
10	0.960 12	0.000 36	0.017 42	−0.000 39	0.035 82	0.924 62
12	0.943 47	0.000 36	0.017 35	−0.000 43	0.027 16	0.891 97
14	0.924 43	0.000 36	0.017 28	−0.000 44	0.020 39	0.855 84
16	0.903 31	0.000 36	0.017 20	−0.000 43	0.015 04	0.816 86
18	0.880 39	0.000 35	0.017 10	−0.000 41	0.010 90	0.775 76
20	0.855 98	0.000 35	0.017 00	−0.000 38	0.007 42	0.733 23

$$\mathrm{Im} f_0^{(\mathrm{B2})}(0) = \frac{k}{4\pi}\sigma_{00}^{(\mathrm{B1})} \tag{42}$$

and

$$\mathrm{Im} f_p^{(\mathrm{B2})}(0) = \frac{k}{4\pi}\sigma_{0p}^{(\mathrm{B1})} , \tag{43}$$

which can be used to check the numerical accuracy of the present calculations. In particular, $\sigma_{00}^{(\mathrm{B1})}$ can be evaluated from Eqs. (18) and (20) to give

$$\mathrm{Im} f_0^{(\mathrm{B2})}(0) = \frac{k}{4\pi}\sigma_{00}^{(\mathrm{B1})} = \frac{12k+18k^3+7k^5}{12(1+k^2)^3} , \tag{44}$$

in agreement with the value listed in Table I. Equation (30) for $\sigma_{0p}^{(\mathrm{B1})}$ has been evaluated and agrees with the computed values of $\mathrm{Im} f_p^{(\mathrm{B2})}(0)$.

TABLE II. Comparison of $f^{(\mathrm{B2})}(0)$ with exact values.[a]

k (a_0^{-1})	$[f_0^{(\mathrm{B2})}(0)+f_p^{(\mathrm{B2})}(0)]$ Re	Im	$f_{\mathrm{exact}}^{(\mathrm{B2})}(0)$ Re	Im
4.0	0.716	0.942	0.878	1.264
5.0	0.577	0.840	0.698	1.111
7.0	0.415	0.691	0.481	0.896

[a]Holt, Ref. 16.

IV. DISCUSSION AND CONCLUSIONS

The essential conclusion from the present work is that it is not possible to interpret the experimental data of Geiger and Morón-León as the result of single elastic collisions between electrons and ground-state atoms. Experimental data[14] for elastic scattering of 25-keV electrons by He show an incremental forward peak 10 times as large as the first Born forward cross section. This is at least an order of magnitude larger than the present result for atomic hydrogen. The experimental peak height increases with incident energy, in contrast to the decrease shown in Fig. 1.

Although the forward scattering peak found in the present work agrees in qualitative features (angular range, linear dependence on momentum transfer) with the published experimental data, the magnitude is much too small compared with the first Born cross section. While the atomic radius, polarizability, and oscillator strength of heavier atoms are larger than for hydrogen or helium, no reasonable increase of these parameters in the range appropriate to ground-state atoms can account for the discrepancy.

The internal consistency of the present calculations is evident. The optical theorem is exactly satisfied as a relationship between the first Born total cross section and the imaginary part of $f^{(\mathrm{B2})}$ in the forward direction. The incremental terms $f_0^{(\mathrm{B2})}$ and $f_p^{(\mathrm{B2})}$ are small compared with $f^{(\mathrm{B1})}$ at all angles considered here, although not negligible in the extreme forward direction. Magnitudes of the real and imaginary parts of $f^{(\mathrm{B2})}$ are related since they are derived from the same formalism. Both depend on the magnitude of the effective transition moment μ, which is determined by atomic polarizability. The only reasonable way to increase the relative magnitude of the forward elastic peak substantially is to increase μ by a large factor. This would occur for an excited atom, in a Rydberg state, for which the effective radius varies as the square of the principal quantum number, but not for an atomic ground state.

The present results disagree by several orders of magnitude with the partial wave calculations of Mohr,[15] who computes a forward elastic scattering peak more than three orders of magnitude larger than first Born for atomic hydrogen at 34-keV incident electron energy. The angular range of this peak, despite the large discrepancy in magnitude, is very similar to that shown in Fig. 1, at 35 keV. While the present results indicate that a peak of such large magnitude is incompatible with the oscillator strength and polarizability of atomic hydrogen, the reason for this discrepancy has not been identified.

The present second Born calculations for a single pseudostate can be compared with exact calculations of $f^{(\mathrm{B2})}(0)$ for atomic hydrogen by Holt,[16] who extended earlier simplified second Born calculations[17] by explicitly summing the forward amplitude over discrete states and integrating over the continuum. Results are compared in Table II, for the largest k values considered by Holt. Results are of similar magnitude and become closer as k increases. This indicates that the present restriction to a single pseudostate does not introduce a large qualitative error.

Partial wave calculations based on a pseudostate model have been undertaken as part of the present project. In general, they confirm the results of the present work, while ensuring unitarity of the scattering matrix at all energies. Details will be published separately.

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APPENDIX: EVALUATION OF THE SECOND BORN INTEGRALS

The integral expressions for $f^{(\mathrm{B2})}$ are evaluated by reduction to Dalitz integrals,[13] as described by Joachain.[2] The integrand in Eq. (34) or (40) is first decomposed into partial fractions, giving a linear combination of integrals of the form

TABLE III. Dalitz integrals $Q_I = \sum CD^a\lambda^b f$.

I	a	b	f	C
2	-1	-1	$N-2p^2$	1
	-1	0	ip	2
3	-2	-1	$N(N-2p^2)$	1
	-1	-3	$N-2p^2$	$\frac{1}{4}$
	-1	-1	1	$-\frac{1}{2}$
	-2	0	iNp	2
4	-3	-1	$N^2(N-2p^2)$	$\frac{4}{3}$
	-2	-3	$N(N-2p^2)$	$\frac{1}{3}$
	-2	-1	$3N-2p^2$	$-\frac{1}{3}$
	-1	-5	$N-2p^2$	$\frac{1}{8}$
	-1	-3	1	$-\frac{1}{6}$
	-3	0	iN^2p	$\frac{8}{3}$
	-2	0	ip	$-\frac{2}{3}$
5	-4	-1	$N^3(N-2p^2)$	2
	-3	-3	$N^2(N-2p^2)$	$\frac{1}{2}$
	-3	-1	$N(N-p^2)$	-2
	-2	-5	$N(N-2p^2)$	$\frac{3}{16}$
	-2	-3	$3N-2p^2$	$-\frac{1}{8}$
	-2	-1	1	$\frac{1}{4}$
	-1	-7	$N-2p^2$	$\frac{5}{64}$
	-1	-5	1	$-\frac{3}{32}$
	-4	0	iN^3p	4
	-3	0	iNp	-2
6	-5	-1	$N^4(N-2p^2)$	$\frac{16}{5}$
	-4	-3	$N^3(N-2p^2)$	$\frac{4}{5}$
	-4	-1	$N^2(5N-6p^2)$	$-\frac{4}{5}$
	-3	-5	$N^2(N-2p^2)$	$\frac{3}{10}$
	-3	-3	$N(N-p^2)$	$-\frac{4}{5}$
	-3	-1	$5N-2p^2$	$\frac{1}{5}$
	-2	-7	$N(N-2p^2)$	$\frac{1}{8}$
	-2	-5	$3N-2p^2$	$-\frac{3}{40}$
	-2	-3	1	$\frac{1}{10}$
	-1	-9	$N-2p^2$	$\frac{7}{128}$
	-1	-7	1	$-\frac{1}{16}$
	-5	0	iN^4p	$\frac{32}{5}$
	-4	0	iN^2p	$-\frac{24}{5}$
	-3	0	ip	$\frac{2}{5}$
7	-6	-1	$N^5(N-2p^2)$	$\frac{16}{3}$
	-5	-3	$N^4(N-2p^2)$	$\frac{4}{3}$
	-5	-1	$N^3(3N-4p^2)$	$-\frac{8}{3}$
	-4	-5	$N^3(N-2p^2)$	$\frac{1}{2}$
	-4	-3	$N^2(5N-6p^2)$	$-\frac{1}{3}$
	-4	-1	$N(3N-2p^2)$	1
	-3	-7	$N^2(N-2p^2)$	$\frac{5}{24}$
	-3	-5	$N(N-p^2)$	$-\frac{1}{2}$
	-3	-3	$5N-2p^2$	$\frac{1}{12}$
	-3	-1	1	$-\frac{1}{6}$
	-2	-9	$N(N-2p^2)$	$\frac{35}{384}$
	-2	-7	$3N-2p^2$	$-\frac{5}{96}$
	-2	-5	1	$\frac{1}{16}$
	-1	-11	$N-2p^2$	$\frac{21}{512}$
	-1	-9	1	$-\frac{35}{768}$
	-6	0	iN^5p	$\frac{32}{3}$
	-5	0	iN^3p	$-\frac{32}{3}$
	-4	0	iNp	2
8	-7	-1	$N^6(N-2p^2)$	$\frac{64}{7}$
	-6	-3	$N^5(N-2p^2)$	$\frac{16}{7}$
	-6	-1	$N^4(7N-10p^2)$	$-\frac{16}{7}$
	-5	-5	$N^4(N-2p^2)$	$\frac{6}{7}$
	-5	-3	$N^3(3N-4p^2)$	$-\frac{8}{7}$
	-5	-1	$N^2(7N-6p^2)$	$\frac{8}{7}$
	-4	-7	$N^3(N-2p^2)$	$\frac{5}{14}$
	-4	-5	$N^2(5N-6p^2)$	$-\frac{3}{14}$
	-4	-3	$N(3N-2p^2)$	$\frac{3}{7}$
	-4	-1	$7N-2p^2$	$-\frac{1}{7}$
	-3	-9	$N^2(N-2p^2)$	$\frac{5}{32}$
	-3	-7	$N(N-p^2)$	$-\frac{5}{14}$
	-3	-5	$5N-2p^2$	$\frac{3}{56}$
	-3	-3	1	$-\frac{1}{14}$
	-2	-11	$N(N-2p^2)$	$\frac{9}{128}$
	-2	-9	$3N-2p^2$	$-\frac{5}{128}$
	-2	-7	1	$\frac{5}{112}$
	-1	-13	$N-2p^2$	$\frac{33}{1024}$
	-1	-11	1	$-\frac{9}{256}$
	-7	0	iN^6p	$\frac{128}{7}$
	-6	0	iN^4p	$-\frac{160}{7}$
	-5	0	iN^2p	$\frac{48}{7}$
	-4	0	ip	$-\frac{2}{7}$

$$I_{m,n}(\alpha,\beta;\vec{k},\vec{k}\,';p)=\frac{1}{\pi^2}\int d^3\vec{q}\,\frac{1}{(q^2-p^2-i\epsilon)}\,\frac{1}{[(\vec{q}-\vec{k})^2+\alpha^2]^m[(\vec{q}-\vec{k}\,')^2+\beta^2]^n}\ . \tag{A1}$$

In the present cases only terms with $m>0$ and $n>0$ have nonvanishing coefficients. The denominator in Eq. (A1) is simplified by using the integral representation of Feynman.[18] Then

$$I_{m,n}(\alpha,\beta;\vec{k},\vec{k}\,';p)=\frac{(m+n-1)!}{(m-1)!(n-1)!}\int_0^1 du\, u^{m-1}(1-u)^{n-1}Q_{m+n}(p,\lambda,\vec{\kappa})\ , \tag{A2}$$

in terms of Dalitz integrals

$$Q_I(p,\lambda,\vec{\kappa})=\frac{1}{\pi^2}\int d^3\vec{q}\,\frac{1}{(q^2-p^2-i\epsilon)}\,\frac{1}{[(\vec{q}-\vec{\kappa})^2+\lambda^2]^I}\ , \tag{A3}$$

where

$$\vec{\kappa}=\vec{k}u+\vec{k}\,'(1-u)\ ,$$
$$\lambda^2=\alpha^2u+\beta^2(1-u)+K_0^2u(1-u)\ . \tag{A4}$$

Here K_0 is the magnitude of the momentum transfer $\vec{k}-\vec{k}\,'$.

By contour integration

$$Q_1(p,\lambda,\vec{\kappa})=\frac{i}{\kappa}\ln\left[\frac{p+\kappa+i\lambda}{p-\kappa+i\lambda}\right]\ . \tag{A5}$$

For higher indices

$$Q_I=-\frac{1}{2(I-1)\lambda}\frac{\partial Q_{I-1}}{\partial\lambda},\quad I>1\ . \tag{A6}$$

In particular,

$$Q_2(p,\lambda,\vec{\kappa})=\frac{1}{\lambda(\kappa^2+\lambda^2-p^2-2p\lambda i)}\ . \tag{A7}$$

For $I\geq 2$ the Dalitz integrals are complex rational functions of p, λ, and κ. Those used in the present work ($I=2,\ldots,8$) are defined in Table III as sums of rational monomials in powers of λ and of

$$D=(\kappa^2+\lambda^2-p^2)^2+4p^2\lambda^2\ , \tag{A8}$$

multiplied by polynomials in p and

$$N=\frac{1}{4\lambda}\frac{\partial D}{\partial\lambda}=\kappa^2+\lambda^2+p^2\ . \tag{A9}$$

To evaluate $f^{(B2)}$ the required sum over Dalitz integrals is carried out for given variable u, and the integral over u from Eq. (A2) is done numerically. Because inverse square-root singularities occur at both end points, integration is facilitated by expressing the integral over u in the form

$$\int_0^1 du\,F(u)=\int_0^{1/2}du[F(u)+F(1-u)] \tag{A10}$$
$$=\int_0^1 dx\,x[F(\tfrac{1}{2}x^2)+f(1-\tfrac{1}{2}x^2)]\ . \tag{A11}$$

Since $xF[(\frac{1}{2})x^2]$ remains finite at $x=0$, this is suitable for numerical quadrature, especially with open-interval formulas that avoid a limiting process at the end point. For calculations reported here, subdivision into five subintervals with 48-point Gauss quadrature in each give indicated accuracy of eight decimal digits or better. For the elastic scattering amplitudes considered here, $F(u)$ and $F(1-u)$ are equal.

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