Modified Born model for excitation of atoms by electrons

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A modification of the Born approximation is employed to compute the differential cross section for excitation of the $2s$ and $2p$ states of hydrogen by electrons at energies of 100, 200, 500, 1000, and 1500 eV. The modification consists of expanding the exact wave function of the total Hamiltonian in terms of Coulomb functions as opposed to plane waves in the normal Born approximation. The differential cross sections thus obtained are orders of magnitude larger at back angles and thus in much better agreement with experiment.

I. INTRODUCTION

Several methods exist for the computation of the differential cross section for the scattering by atoms of electrons at energies greater than about 100 eV.[1-4] While Born plane-wave-like models generally require small amounts of computer time, they yield differential cross sections which are orders of magnitude too low at large angles. More elaborate methods such as distorted-wave methods[5,6] yield much improved differential cross sections, but require considerable amounts of computer time. The Glauber approximation will be discussed in Sec. III.

A modification of the Born model can be made which retains the simplicity of the Born approaches yet better reproduces the experimental cross sections. Geltman and Hidalgo[7] suggested a distorted-wave-like model which will be shown to be a special case of the modified Born model. Since exchange is neglected in this paper, only electron energies above 100 eV will be considered.

In Sec. II we discuss the Born and two-potential (generalized[8] or distorted wave) Born models, and modifications of each. In Sec. III the various models are applied to the excitation of the $2s$ and $2p$ states of hydrogen by electrons. Finally, in Sec. IV the models are discussed, as well as applications to other phenomena. Atomic units are employed except where otherwise specified.

II. BORN AND MODIFIED BORN MODELS

Collisions between atoms and electrons can result in the atoms remaining in their initial state or undergoing a transition to some other state. The Hamiltonian for the total system is given by

$$H=\left[-\tfrac{1}{2}\nabla_0^2+\sum_i\left(-\tfrac{1}{2}\nabla_i^2-\frac{Z}{r_i}+\sum_{j\neq i}\frac{1}{r_{ij}}\right)\right]+\left[\frac{-Z}{r_0}+\sum_i\frac{1}{r_{i0}}\right]\equiv H^0+V\,, \tag{1}$$

where square brackets group the operators defined by H^0 and V. The index 0 refers to the scattered electron, the indices i and j refer to the atomic electrons, and Z is the nuclear charge. We will also define two potentials U and W such that

$$U+W=V\,. \tag{2}$$

If the atom is assumed to be initially in state a and finally in state w, the energy of the system is given by

$$E=\epsilon_a+k_I^2/2 \tag{3a}$$

$$=\epsilon_w+k_F^2/2\,, \tag{3b}$$

where ϵ_a and ϵ_w are the energies of the initial and final atomic states and k_I and k_F are the magnitudes of the initial and final propagation vectors. We also define functions Φ_β, χ_β, and Ψ_β which satisfy the equations

$$H^0\Phi_\beta=E\Phi_\beta\,, \tag{4a}$$

$$(H^0+U)\chi_\beta\equiv H^1\chi_\beta=E\chi_\beta\,, \tag{4b}$$

$$H\Psi_\beta=E\Psi_\beta\,. \tag{4c}$$

The label β defines the state of the atom and the incident or scattered electron, and the functions Φ_β, χ_β, and Ψ_β satisfy appropriate boundary conditions depending on the asymptotic limits of H^0, U, and V.

If $G_0^{(\pm)}$ and $G_1^{(\pm)}$ are the appropriate Green's functions for H^0 and H^1, respectively, $\Psi_\beta^{(\pm)}$ can be expanded in terms of Φ_β or $\chi_\beta^{(\pm)}$ as

$$\Psi_\beta^{(\pm)}=\left(1+\sum_{n=1}^{\infty}(G_0^{(\pm)}V)^n\right)\Phi_\beta \tag{5a}$$

and

$$\Psi_\beta^{(\pm)}=\left(1+\sum_{n=1}^{\infty}(G_1^{(\pm)}W)^n\right)\chi_\beta^{(\pm)}\,. \tag{5b}$$

The cross section for a collision in which an electron excites an atom from state α to state ω is given by

$$\left.\frac{d\sigma}{d\Omega}\right|_{\alpha\to\omega} = \frac{V_F}{4\pi^2 V_I} |\langle \Phi_\omega | T | \Phi_\alpha \rangle|^2 , \tag{6}$$

where V_I and V_F are the initial and final velocities of the scattered electron. For a partitioning of the Hamiltonian H into H^0 and V Eq. (6) becomes

$$\left.\frac{d\sigma}{d\Omega}\right|_{\alpha\to\omega} = \frac{V_F}{4\pi^2 V_I} |\langle \Phi_\omega | V | \Psi_\alpha^{(+)} \rangle|^2 , \tag{7}$$

whereas the partitioning of H into H^0, U_1, and W_1 yields

$$\left.\frac{d\sigma}{d\Omega}\right|_{\alpha\to\omega} = \frac{V_F}{4\pi V_I} |\langle \Phi_\omega | U_1 | \chi_{\alpha 1}^{(+)} \rangle + \langle \chi_{\omega 1}^{(-)} | W_1 | \Psi_\alpha^{(+)} \rangle|^2 . \tag{8}$$

For the exact Φ_β, χ_β, and Ψ_β, we also have

$$\left.\frac{d\sigma}{d\Omega}\right|_{\alpha\to\omega} = \frac{V_F}{4\pi V_I} |\langle \Psi_\omega^{(-)} | V | \Phi_\alpha \rangle|^2 \tag{9}$$

and

$$\left.\frac{d\sigma}{d\Omega}\right|_{\alpha\to\omega} = \frac{V_F}{4\pi V_I} |\langle \chi_{\omega 1}^{(-)} | U_1 | \Phi_\alpha \rangle + \langle \Psi_\omega^{(-)} | W_1 | \chi_{\alpha 1}^{(+)} \rangle|^2 . \tag{10}$$

In the Born (B) and two-potential Born (TPB) approximations one retains only the first term in the expansions (5a) and (5b), respectively, and neglects exchange. Then the respective T-matrix elements become

$$T^{\mathrm{B}}_{\alpha\to\omega} = \langle \Phi'_\omega | V | \Phi'_\alpha \rangle \tag{11a}$$

and

$$T^{\mathrm{TPB}}_{\alpha\to\omega} = \langle \Phi'_\omega | U_1 | \chi_{\alpha 1}^{(+)\prime} \rangle + \langle \chi_{\omega 1}^{(-)\prime} | W_1 | \chi_{\alpha 1}^{(+)\prime} \rangle . \tag{11b}$$

The prime implies the scattered electron is assumed distinct from the atomic electrons.

The Born differential cross sections for electrons inelastically scattered from hydrogen are orders of magnitude lower than experimental cross sections[9] for angles greater than 30° to 40°. This is also true when one compares the Born cross sections with those of the distorted-wave approximation. The Born approximation is an expansion of $\Psi_\beta^{(\pm)}$ such that the first term has the correct asymptotic form. On the other hand, the principal contributions to the T-matrix element of (7) are from the region where the operator is largest. The expansion of $\Psi_\beta^{(\pm)}$ need not be with respect to H^0, but need only satisfy

$$\Psi_\beta^{(\pm)} = \left(1 + \sum_n (G_2^{(\pm)} W_2)\right) \chi_{\beta 2}^{(\pm)} , \tag{12}$$

where

$$H \equiv H_2 + W_2 \tag{13a}$$

$$\equiv H_0 + U_2 + W_2 . \tag{13b}$$

Consider the partitioning of H such that

$$H_2 = H_0 - \delta/r_0 \tag{14a}$$

and

$$W_2 = -\frac{(Z-\delta)}{r_0} + \sum_i \frac{1}{r_{i0}} . \tag{14b}$$

Basically this corresponds to expanding $\Psi_\beta^{(\pm)}$ in a series about an effective nuclear charge of δ instead of zero. Neglecting exchange we have for the first term of the T-matrix element

$$T^{\mathrm{MB}}_{\alpha\to\omega} = \langle \Phi'_\omega | V | \chi_{\alpha 2}^{(+)\prime} \rangle , \tag{15}$$

where MB implies modified Born. A similar expansion could be performed for the TPB, resulting in

$$T^{\mathrm{MTPB}}_{\alpha\to\omega} = \langle \Phi'_\omega | U_1 | \chi_{\alpha 1}^{(+)\prime} \rangle + \langle \chi_{\omega 1}^{(-)\prime} | W_1 | \chi_{\alpha 2}^{(+)\prime} \rangle . \tag{16}$$

U_1 and W_1 can be defined in various ways so long as Eqs. (2) and (4b) are satisfied. The calculation of Geltman and Hidalgo corresponds to choosing $U_1 = -1/r_0$ and using Eq. (16) with δ equal zero or the normal Born expansion.

III. APPLICATION TO HYDROGEN

For electrons scattered from hydrogen atoms, application of the Born approximation is straightforward. We have chosen $U_1 = -1/r_0$ as in the calculation of Geltman and Hidalgo. The δ required in the modified Born approximation may be defined in many ways. It could be considered to be a function of the scattering angle and related to an impact-parameter or impulse approximation. Since, as stated above, we wish to construct a model which not only yields accurate differential cross sections, but does so with a minimum of computation time, the determination of δ should not require a large amount of time. We have used the following definition of δ. Let r_0 be the value of r for which

$$r_0^2 \int_0^{2\pi}\int_0^{\pi}\int_0^{\infty} \phi_{nlm}^*(\vec{r}_1)\frac{1}{r_{10}}\phi_{100}(\vec{r}_1) \times r_1^2 \sin\theta_1 \, dr_1 \, d\theta_1 \, d\phi_1 \tag{17}$$

is a maximum, that is, the region of r_0 space which should contribute most to the scattering amplitude. If several maxima occur r_0 can be taken as any one of the maxima, the value of r at the largest maximum, or some average. δ is then defined according to the equation

$$\delta = Z - \int_0^{2\pi}\int_0^{\pi}\int_0^{r_0} \phi_{nlm}^* \phi_{nlm} r^2 \sin\theta \, dr \, d\theta \, d\phi . \tag{18}$$

TABLE I. Values of δ.

Model	$\delta(2s)$	$\delta(2p)$	Model	$\delta(2s)$	$\delta(2p)$
B	0.000	0.000	TPBG	0.000	0.000
BI	0.346	0.852	TPBI	0.346	0.852
BF	0.946	0.943	TPBF	0.946	0.943
			TPB	1.000	1.000

That is, δ is the total nuclear charge reduced by the electron charge within a sphere of radius r_0. $\phi(nlm)$ in Eq. (18) is $\phi(100)$ for Eqs. (15) and (16) and $\phi(200)$ or $\phi(2lm)$ for Eqs. (9) and (10) after exchange is neglected. The value of δ employed in the various formalisms is given in Table I.

In Tables II and III the differential cross sections for excitation of the $2s$ and $2p$ states of hydrogen are presented for several models (for details of the computation see the Appendix). BI represents the cross section obtained by (15) where α implies the initial state. BF represents the cross section obtained from (9) after neglecting exchange. Here ω labels the final state, $2s$ or $2p$. TPBG, TPBI, TPBF, and TPB represent cross sections obtained from two-potential formalisms based on the expansion of $\Psi_\beta^{(\pm)'}$ in terms of a plane wave, a Coulomb wave with δ defined with respect to the initial state, a Coulomb wave with δ defined with respect to the final state, and a Coulomb wave with δ equal to 1, respectively.

These results are compared in Figs. 1 and 2 with the experimental cross sections of Williams[9] at 100 and 200 eV; all curves have been normalized to the TPB at 21° for the sake of comparison.

TABLE II. $2s$ differential cross sections (a.u.). The notation $A \pm n$ means $A \times 10^{\pm n}$.

Energy (eV)	Model	0°	10°	21°	40°	60°	80°	100°	120°	140°	160°	180°
100	B	8.86−1	5.19−1	1.14−1	4.24−3	1.95−4	1.77−5	2.91−6	7.85−7	3.22−7	1.92−7	1.62−7
	BI	8.51−1	4.94−1	1.05−1	3.54−3	1.83−4	3.79−5	1.78−5	1.12−5	8.19−6	6.86−6	6.47−6
	BF	9.17−1	5.28−1	1.10−1	4.76−3	7.43−4	2.90−4	1.50−4	9.37−5	6.79−5	5.64−5	5.30−5
	TPBG	9.10−1	5.23−1	1.09−1	4.79−3	8.00−4	3.18−4	1.66−4	1.03−4	7.50−5	6.23−5	5.87−5
	TPBI	9.01−1	5.23−1	1.16−1	7.80−3	1.60−3	5.91−4	2.87−4	1.71−4	1.20−4	9.83−5	9.20−5
	TPBF	7.94−1	4.65−1	1.12−1	1.21−2	3.09−3	1.16−3	5.60−4	3.31−4	2.32−4	1.89−4	1.77−4
	TPB	7.91−1	4.65−1	1.13−1	1.27−2	3.27−3	1.23−3	5.95−4	3.52−4	2.47−4	2.01−4	1.88−4
200	B	9.36−1	3.25−1	2.40−2	2.41−4	6.00−6	4.10−7	5.85−8	1.46−8	5.73−9	3.34−9	2.80−9
	BI	9.18−1	3.16−1	2.25−2	2.27−4	1.44−5	4.57−6	2.27−6	1.40−6	1.01−6	8.40−7	7.90−7
	BF	9.52−1	3.25−1	2.34−2	5.12−4	9.71−5	3.61−5	1.79−5	1.09−5	7.85−6	6.49−6	6.10−6
	TPBG	9.48−1	3.23−1	2.32−2	5.42−4	1.07−4	4.01−5	1.99−5	1.21−5	8.71−6	7.20−6	6.77−6
	TPBI	9.43−1	3.26−1	2.60−2	1.00−3	2.02−4	7.08−5	3.38−5	2.01−5	1.42−5	1.17−5	1.09−5
	TPBF	8.84−1	3.09−1	2.89−2	1.89−3	4.10−4	1.43−4	6.81−5	4.04−5	2.86−5	2.34−5	2.20−5
	TPB	8.82−1	3.09−1	2.94−2	2.00−3	4.34−4	1.52−4	7.22−5	4.29−5	3.03−5	2.48−5	2.33−5
500	B	9.66−1	8.82−2	1.00−3	2.47−6	3.81−8	2.15−9	2.80−10	6.64−11	2.54−11	1.46−11	1.22−11
	BI	9.59−1	8.66−2	9.61−4	5.20−6	8.02−7	2.89−7	1.43−7	8.71−8	6.27−8	5.19−8	4.88−8
	BF	9.73−1	8.74−2	1.13−3	2.88−5	6.11−6	2.21−6	1.08−6	6.58−7	4.72−7	3.91−7	3.68−7
	TPBG	9.71−1	8.72−2	1.14−3	3.19−5	6.80−6	2.46−6	1.21−6	7.34−7	5.27−7	4.36−7	4.10−7
	TPBI	9.69−1	8.87−2	1.48−3	5.99−5	1.22−5	4.29−6	2.07−6	1.25−6	8.93−7	7.36−7	6.91−7
	TPBF	9.44−1	8.86−2	2.12−3	1.24−4	2.52−5	8.86−6	4.28−6	2.58−6	1.84−6	1.52−6	1.43−6
	TPB	9.43−1	8.88−2	2.10−3	1.31−4	2.67−5	9.37−6	4.53−6	2.73−6	1.95−6	1.61−6	1.51−6
1000	B	9.76−1	1.59−2	4.34−5	5.41−8	6.94−10	3.66−11	4.60−12	1.07−12	4.07−13	2.33−13	1.94−13
	BI	9.73−1	1.57−2	4.48−5	4.83−7	9.81−8	3.56−8	1.75−8	1.07−8	7.70−9	6.38−9	6.00−9
	BF	9.80−1	1.58−2	7.68−5	3.48−6	7.42−7	2.68−7	1.32−7	8.03−8	5.78−8	4.78−8	4.50−8
	TPBG	9.79−1	1.58−2	8.07−5	3.88−6	8.27−7	2.99−7	1.47−7	8.96−8	6.45−8	5.34−8	5.02−8
	TPBI	9.78−1	1.63−2	1.27−4	7.10−6	1.47−6	5.26−7	2.57−7	1.56−7	1.12−7	9.24−8	8.68−8
	TPBF	9.65−1	1.69−2	2.28−4	1.48−5	3.06−6	1.09−6	5.34−7	3.24−7	2.33−7	1.93−7	1.81−7
	TPB	9.65−1	1.70−2	2.38−4	1.56−5	3.24−6	1.16−6	5.65−7	3.43−7	2.46−7	2.04−7	1.91−7
1500	B	9.80−1	4.18−3	5.58−6	5.34−9	6.42−11	3.30−12	4.11−13	9.54−14	3.61−14	2.06−14	1.72−14
	BI	9.77−1	4.13−3	6.65−6	1.36−7	2.88−8	1.05−8	5.16−9	3.15−9	2.27−9	1.88−9	1.77−9
	BF	9.81−1	4.21−3	1.71−5	1.01−6	2.17−7	7.84−8	3.86−8	2.36−8	1.70−8	1.41−8	1.32−8
	TPBG	9.81−1	4.21−3	1.85−5	1.13−6	2.42−7	8.75−8	4.31−8	2.63−8	1.90−8	1.57−8	1.48−8
	TPBI	9.81−1	4.42−3	3.18−5	2.05−6	4.31−7	1.55−7	7.59−8	4.62−8	3.32−8	2.75−8	2.58−8
	TPBF	9.72−1	4.76−3	6.21−5	4.28−6	8.98−7	3.22−7	1.58−7	9.65−8	6.94−8	5.74−8	5.40−8
	TPB	9.72−1	4.80−3	6.52−5	4.52−6	9.49−7	3.41−7	1.68−7	1.02−7	7.33−8	6.07−8	5.71−8

Although the models with the most distortion agree better with experiment, one must be careful of drawing conclusions about the several models which yield similar cross sections since distortions of the atomic wave function as well as exchange have been neglected. At these energies these effects could be important.

The Glauber approximation also results in differential cross sections similar to those of Figs. 1 and 2. Hambro *et al.* have shown, on the other hand, that the approximation of replacing the total momentum transfer in the system by only its transverse component results in the neglect of a dampening factor which would decrease the scattering amplitude particularly at large angles.[4] Although this would tend to increase the differences between the Glauber and experiment, the magnitude of this dampening has not been investigated.

A crude estimate of the importance of exchange can be obtained by using the Born-Oppenheimer approximation to compute the exchange amplitude $g(\theta)$ for hydrogen,[10] and then combining $g(\theta)$ with the direct amplitude, obtained for each model above. The results of such a calculation for the TPBI, TPBF, and TPB approximations along with the results of Williams are illustrated in Figs. 3 and 4. The exchange cross section for the 100-eV collision is so large it should be properly incorporated into the calculation. At 200 eV the exchange cross section is small and tends to increase the cross section at back angles as required, while the effect of exchange is negligible for collision energies of 500 eV and higher.

TABLE III. $2p$ differential cross sections (a.u.). The notation $A \pm n$ means $A \times 10^{\pm n}$.

Energy (eV)	Model	0°	10°	21°	40°	60°	80°	100°	120°	140°	160°	180°
100	B	9.88+1	5.04+0	2.71−1	2.91−3	6.30−5	3.45−6	4.00−7	8.44−8	2.94−8	1.60−8	1.31−8
	BI	7.74+1	4.37+0	2.27−1	3.78−3	5.18−4	1.76−4	8.39−5	5.01−5	3.56−5	2.93−5	2.75−5
	BF	9.65+1	5.87+0	3.24−1	7.97−3	1.40−3	5.08−4	2.50−4	1.52−4	1.09−4	9.04−5	8.49−5
	TPBG	9.56+1	5.94+0	3.30−1	8.73−3	1.57−3	5.69−4	2.80−4	1.70−4	1.22−4	1.01−4	9.49−5
	TPBI	7.60+1	5.61+0	3.23−1	8.68−3	1.59−3	7.02−4	4.36−4	3.23−4	2.67−4	2.40−4	2.32−4
	TPBF	7.09+1	5.59+0	3.36−1	1.10−2	1.98−3	7.65−4	4.22−4	2.87−4	2.24−4	1.95−4	1.87−4
	TPB	7.03+1	5.61+0	3.41−1	1.11−2	2.00−3	8.01−4	4.60−4	3.22−4	2.58−4	2.27−4	2.19−4
200	B	2.15+2	1.65+0	2.82−2	8.08−5	9.42−7	3.90−8	3.91−9	7.63−10	2.55−10	1.35−10	1.10−10
	BI	1.89+2	1.54+0	2.69−2	4.36−4	8.55−5	3.05−5	1.49−5	9.02−6	6.47−6	5.35−6	5.03−6
	BF	2.10+2	1.79+0	3.48−2	8.38−4	1.73−4	6.26−5	3.07−5	1.87−5	1.34−5	1.11−5	1.05−5
	TPBG	2.10+2	1.80+0	3.58−2	9.41−4	1.95−4	7.04−5	3.45−5	2.10−5	1.51−5	1.25−5	1.17−5
	TPBI	1.86+2	1.74+0	3.43−2	7.62−4	1.86−4	9.09−5	5.87−5	4.42−5	3.68−5	3.32−5	3.21−5
	TPBF	1.79+2	1.74+0	3.68−2	9.92−4	2.24−4	9.85−5	5.89−5	4.21−5	3.40−5	3.01−5	2.90−5
	TPB	1.78+2	1.75+0	3.72−2	9.93−4	2.28−4	1.04−4	6.38−5	4.64−5	3.79−5	3.39−5	3.27−5
500	B	5.62+2	1.79−1	4.66−4	3.27−7	2.36−9	8.05−11	7.37−12	1.37−12	4.44−13	2.33−13	1.88−13
	BI	5.33+2	1.74−1	7.73−4	3.30−5	7.04−6	2.54−6	1.25−6	7.64−7	5.50−7	4.55−7	4.28−7
	BF	5.57+2	1.87−1	1.04−3	5.20−5	1.11−5	4.03−6	1.99−6	1.21−6	8.73−7	7.22−7	6.80−7
	TPBG	5.56+2	1.88−1	1.13−3	5.87−5	1.25−5	4.54−6	2.24−6	1.36−6	9.82−7	8.13−7	7.65−7
	TPBI	5.28+2	1.83−1	8.57−4	3.64−5	1.15−5	6.12−6	4.11−6	3.14−6	2.64−6	2.39−6	2.32−6
	TPBF	5.20+2	1.83−1	9.90−4	4.59−5	1.33−5	6.66−6	4.29−6	3.20−6	2.64−6	2.38−6	2.30−6
	TPB	5.19+2	1.85−1	9.63−4	4.62−5	1.37−5	7.03−6	4.60−6	3.47−6	2.88−6	2.60−6	2.51−6
1000	B	1.14+3	1.61−2	1.00−5	3.56−9	2.14−11	6.81−13	6.03−14	1.10−14	3.55−15	1.85−15	1.49−15
	BI	1.11+3	1.62−2	6.58−5	4.59−6	9.88−7	3.59−7	1.77−7	1.08−7	7.81−8	6.47−8	6.09−8
	BF	1.13+3	1.72−2	9.17−5	6.55−6	1.41−6	5.12−7	2.53−7	1.55−7	1.11−7	9.23−8	8.69−8
	TPBG	1.13+3	1.74−2	1.03−4	7.37−6	1.58−6	5.77−7	2.85−7	1.74−7	1.25−7	1.04−7	9.77−8
	TPBI	1.10+3	1.66−2	5.08−5	3.97−6	1.42−6	7.94−7	5.43−7	4.19−7	3.53−7	3.20−7	3.10−7
	TPBF	1.10+3	1.67−2	6.17−5	4.82−6	1.61−6	8.66−7	5.77−7	4.39−7	3.67−7	3.32−7	3.21−7
	TPB	1.09+3	1.73−2	6.24−5	4.88−6	1.68−6	9.15−7	6.16−7	4.22−7	3.96−7	3.58−7	3.47−7
1500	B	1.72+3	2.82−3	8.60−7	2.34−10	1.31−12	4.09−14	3.59−15	6.51−16	2.09−16	1.09−16	8.78−17
	BI	1.69+3	2.99−3	1.88−5	1.42−6	3.08−7	1.12−7	5.54−8	3.39−8	2.44−8	2.02−8	1.90−8
	BF	1.71+3	3.20−3	2.56−5	1.95−6	4.22−7	1.54−7	7.60−8	4.64−8	3.35−8	2.77−8	2.60−8
	TPBG	1.71+3	3.26−3	2.88−5	2.20−6	4.75−7	1.73−7	8.55−8	5.23−8	3.77−8	3.12−8	2.94−8
	TPBI	1.68+3	3.01−3	1.11−5	1.11−6	4.22−7	2.40−7	1.65−7	1.28−7	1.08−7	9.81−8	9.50−8
	TPBF	1.67+3	3.04−3	1.35−5	1.32−6	4.74−7	2.62−7	1.77−7	1.35−7	1.14−7	1.03−7	9.99−8
	TPB	1.67+3	3.34−3	1.37−5	1.34−6	4.94−7	2.77−7	1.89−7	1.45−7	1.22−7	1.11−7	1.07−7

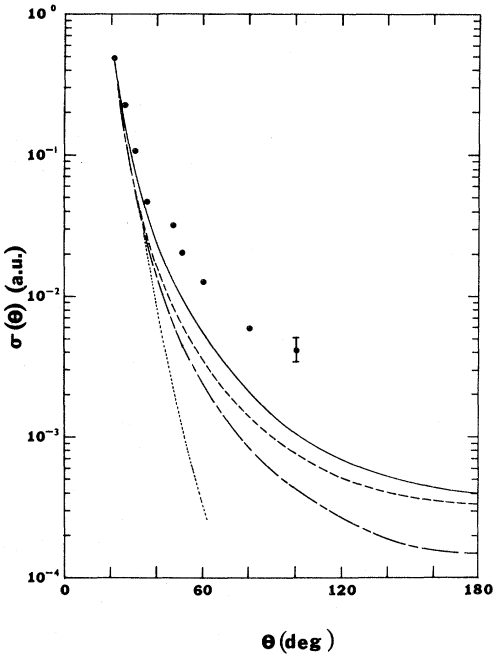

FIG. 1. Sum of differential cross sections for exciting $2s$ and $2p$ states without exchange for 100-eV electrons. ●, experiment; solid line, TPB; long-dashed line, TPBI; long-short-dashed line, BF; short-dashed line, B.

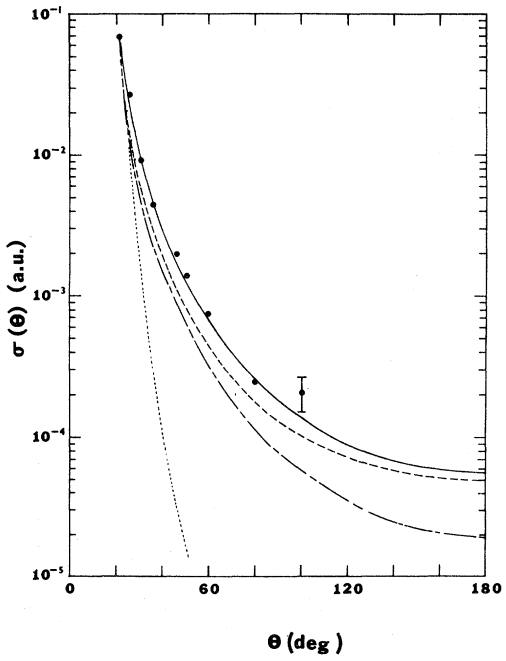

FIG. 2. Sum of differential cross sections for exciting $2s$ and $2p$ states without exchange for 200-eV electrons. ●, experiment; solid line, TPB; long-dashed line, TPBI; long-short-dashed line, BF; short-dashed line, B.

Shelton *et al.*[6] have performed distorted-wave calculations employing a static potential to determine the cross section for excitation of the $2s$ state of hydrogen at 13.6, 54.4, 136, and 680.3 eV. In Figs. 5 and 6 we compare the results for the above models at 136.0 and 680.3 eV. The curves, which are the actual values obtained from each model, indicate that the modified Born models represent a considerable improvement over the normal Born models.

The total cross sections are tabulated in Tables IV and V. Apart from the cross section for excitation of the $2p$ state with 100-eV electrons, the various models yield approximately the same total cross section. The basic reason, of course, is that the principal contributions to the total cross section are from relatively small angles where all of the models agree fairly well.

IV. CONCLUSION

The expansion of $\Psi_\beta^{(\pm)}$ in terms of the solutions of the operator defined by (14a) retains the simplicity of the plane-wave Born model while allowing for a certain amount of distortion. In particular, the "distorted waves" chosen offer the advantages that (i) the eigenfunctions of H_2 are known, (ii) a closed-form expression (A9) exist for the basic integral in the T-matrix element, and (iii) the decomposition of H into H_2 and W_2 contains a cer-

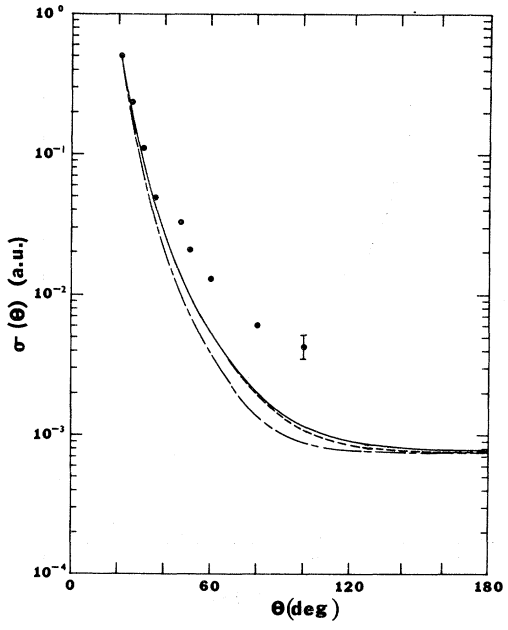

FIG. 3. Sum of differential cross sections for exciting $2s$ and $2p$ states with exchange estimated for 100-eV electrons. ●, experiment; solid line, TPB; long-dashed line, TPBF; long-short-dashed line, TPBI.

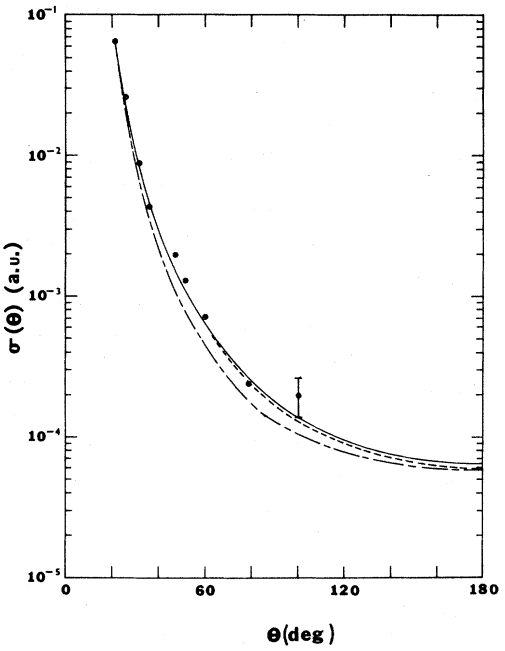

FIG. 4. Sum of differential cross sections for exciting $2s$ and $2p$ states with exchange estimated for 200-eV electrons. ●, experiment; solid line, TPB; long-dashed line, TPBF; long-short-dashed line, TBI.

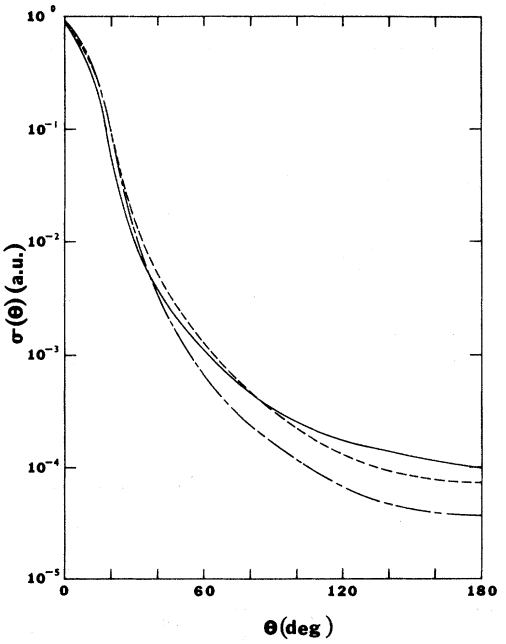

FIG. 5. Comparison of distorted-wave cross sections and modified Born cross sections for excitation of $2s$ state of hydrogen by 136.0-eV electrons. Solid line, distorted wave; long-dashed line, TPBF; long-short-dashed line, TPBI.

tain amount of physical significance. Despite the simplicity of the models, their predicted differential cross sections for the excitation of the $2s$ and $2p$ states of hydrogen by electrons are orders of magnitude larger at back angles than those from the Born plane-wave approximation. The cross sections are thus in much better agreement with the experimental cross sections[9] as indicated in Figs. 1 and 2 and with the distorted-wave calculations[6] as indicated in Figs. 5 and 6.

Comparing the Born differential cross sections at large angles with those of the other models, one observes that, although the absolute difference between them decreases as the energy increases, the relative error, i.e., the ratio of the cross sections for the various models to that of the Born model, increases. This result could have been anticipated, since in a "classical sense" large-angle scattering requires large momentum transfer and "deep" penetration of the atom or ion by the scattered electron. Thus the potential by which these electrons are scattered is not small even as the energy increases. Consequently, one need not expect the Born cross sections to converge to the experimental results even at high incident energies.

Another method for selecting δ which is suggested by the above discussion is to relate r_0 of Eq. (18) to the scattering angle through an impact-parameter-type procedure. δ would then increase from zero at forward angles to some value less

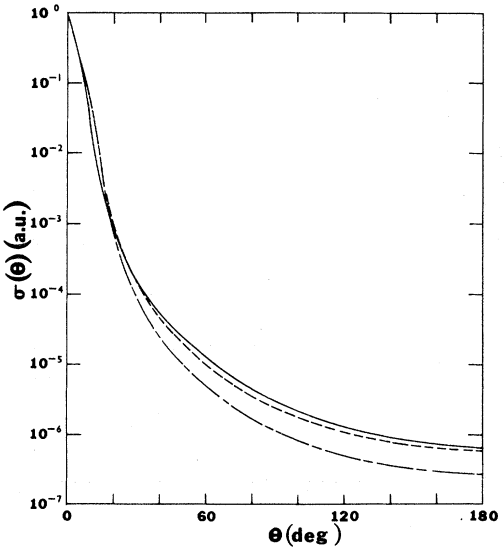

FIG. 6. Comparison of distorted-wave cross sections and modified Born cross sections for excitation of $2s$ state of hydrogen by 680.3-eV electrons. Solid line, distorted wave; long-dashed line, TPBF; long-short-dashed line, TPBI.

than Z at back angles. The TPBG, TPBI, and TPB models in Tables II and III indicate, in this case, there would probably be a slight improvement in the comparison with the experimental cross sections. On the other hand, as stated in Sec. III, the errors due to the neglect of exchange, particularly at the lower energies, and distortion of the atomic wave functions are probably the source of the main discrepancy and, in fact, Figs. 1–4 indicate that inclusion of exchange would raise the back-angle part of the cross section relative to the forward-angle part of the cross section.

These models could be applied to other atomic procedures such as elastic scattering of electrons by atoms, ionization of atoms by electrons, and charge-transfer reactions. It should be noted that this procedure is just as readily applicable to ions as to atoms with no major changes. Some of these phenomena will be investigated in later work.

ACKNOWLEDGMENT

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APPENDIX

The wave functions Φ'_β and χ'_β are given by

$$\Phi'_\beta = e^{i\vec{k}\cdot\vec{r}_0}\phi_{nlm}(\vec{r}_1) \tag{A1}$$

and

$$\chi_\beta^{(\pm)'} = \Gamma(1\pm ia)e^{\pi a/2+i\vec{k}\cdot\vec{r}_0} \times {}_1F_1(\pm ia;1;\pm ikr_0 - i\vec{k}\cdot\vec{r}_0)\phi_{nlm}(\vec{r}_1), \tag{A2}$$

where $a=\delta/k$.

The general form of the interaction is

$$(1-\delta)/r_0 + 1/r_{10}, \tag{A3}$$

where δ is zero for the normal Born approximation. Since we are interested in differential cross sections for excitation, in which case the initial and final bound states are different, all terms involving $1/r_0$ vanish. Employing an expansion of $1/r_{01}$ in terms of Legendre functions, one obtains the matrix elements

$$Y_L(n_I l_I, n_F l_F | r_0) = \int R_{n_I l_I}(r_1)R_{n_F l_F}(r_1) \times (r_<^L/r_>^{L+1})r_1^2\,dr_1, \tag{A4}$$

which are given by Burgess *et al.*[11] In particular,

$$Y_0(1s,2s|r_0) = 2^{3/2}(r_0+\tfrac{2}{3})e^{-3r_0/2}/9 \tag{A5}$$

and

$$Y_1(1s,2p|r_0) = (\tfrac{2}{3})^{3/2}[64/(27r_0^2) - e^{-3r_0/2} \times (r_0+\tfrac{8}{3}+32/(9r_0)+64/(27r_0^2))]. \tag{A6}$$

Thus the T-matrix element[7] is

$$T_{\alpha\to\omega} = [2\pi^{1/2}/(2l+1)]e^{(a_I+a_F)\pi/2}\Gamma(1-ia_I)\Gamma(1-ia_F) \times \int d\vec{r}_0\, e^{i(\vec{k}_I-\vec{k}_F)\cdot\vec{r}_0}\,{}_1F_1(ia_F;1;ik_Fr_0+i\vec{k}_F\cdot\vec{r}_0) \times {}_1F_1(ia_I;1;ik_Ir_0-i\vec{k}_I\cdot\vec{r}_0) \times Y_{lm}^*(r)Y_L(10,nl|r_0) \tag{A7}$$

and the general form of the various integrals required is

$$\int d\vec{r}\, e^{-\lambda r}r^n Y_{lm}^*(\hat{r})e^{i(\vec{k}_I-\vec{k}_F)\cdot\vec{r}_0} \times {}_1F_1(ia_F;1;ik_Fr_0+i\vec{k}_F\cdot\vec{r}_0) \times {}_1F_1(ia_I;1;ik_Ir_0-i\vec{k}_I\cdot\vec{r}_0). \tag{A8}$$

In order to evaluate these integrals we employ the following integral given by Nordsieck[12]:

$$\int d\vec{r}\, e^{-\lambda r}e^{i\vec{K}\cdot\vec{r}}\,{}_1F_1(ia_1;1;ik_1r-i\vec{k}_1\cdot\vec{r})\,{}_1F_1(ia_2;1;ik_2r+i\vec{k}_2\cdot\vec{r}) = 2\pi\alpha^{-1}e^{-\pi a_1}(\alpha/\gamma)^{ia_1}((\gamma+\eta)/\gamma)^{-ia_2} \times {}_2F_1(1-ia_1,ia_2;1;(\alpha\eta-\beta\gamma)/\alpha(\gamma+\eta)), \tag{A9}$$

TABLE V. $2p$ total cross sections (πa_0^2). The notation $A\pm n$ means $A\times 10^{\pm n}$.

Model	Energy (eV) 100	500	1500
B	7.50−1	2.47−1	1.05−1
BI	6.33−1	2.41−1	1.04−1
BF	8.36−1	2.54−1	1.06−1
TPBG	8.43−1	2.54−1	1.06−1
TPBI	7.65−1	2.47−1	1.05−1
TPBF	7.48−1	2.46−1	1.04−1
TPB	7.53−1	2.46−1	1.05−1

TABLE IV. $2s$ total cross sections (πa_0^2). The notation $A\pm n$ means $A\times 10^{\pm n}$.

Model	Energy (eV) 100	500	1500
B	5.92−2	1.20−2	4.01−3
BI	5.41−2	1.18−2	4.00−3
BF	5.85−2	1.20−2	4.02−3
TPBG	5.81−2	1.20−2	4.03−3
TPBI	6.21−2	1.22−2	4.05−3
TPBF	6.05−2	1.21−2	4.03−3
TPB	6.12−2	1.21−2	4.04−3

where

$$K \equiv \vec{k}_1 - \vec{k}_2 ,$$

$$\alpha \equiv (K^2 + \lambda^2)/2 ,$$

$$\beta \equiv \vec{k}_2 \cdot \vec{K} - i\lambda k_2 ,$$

$$\gamma \equiv \vec{k}_1 \cdot \vec{K} + i\lambda k_1 - \alpha ,$$

and

$$\eta \equiv k_1 k_2 + \vec{k}_1 \cdot \vec{k}_2 - \beta .$$

Differentiation or integration of (A9) with respect to λ yields the appropriate powers of r whereas differentiation with respect to the various components of momentum transfer $\vec{K}$ yields the appropriate $Y_{lm}^*(r)$.

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