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Excitation of the 2*s* State of Atomic Hydrogen by Electron Impact in the Distorted-Wave Approximation - Angular Distributions*

W. N. Shelton, E. S. Leherissey, and D. H. Madison
Department of Physics, The Florida State University, Tallahassee, Florida 32306

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The excitation of ground-state hydrogen atoms to the 2*s* state by the impact of electrons with energies of 1 to 50 Ry (13.6 to 680.3 eV) has been calculated in the distorted-wave approximation with exchange included. The angular distributions of the scattered electrons at 1 and 4 Ry are compared with those derived from the close-coupling calculations by Burke, Schey, and Smith, and are compared with four different plane-wave theories at all energies calculated. Taking the close-coupling results as a standard, it is found that the distorted-wave angular distributions represent an improvement over those of the plane-wave theories.

I. INTRODUCTION

The calculation of cross sections for low-energy electron impact excitation of atoms remains in an unsatisfactory condition. The problem is complicated by three effects, coupling due to participation of intermediate states, exchange of the projectile electron with an atomic electron, and distortion of the target-atom charge distribution by the electric field of the projectile electron. At sufficiently high energy, the integrated cross section may be obtained with adequate accuracy from the Born[1] approximation. However, the Born approximation is not only a high-energy approximation, but is also a small momentum-transfer approximation. As a result, the angular distribution of the scattered electrons calculated by the Born approximation is valid over a decreasing angular range about the zero scattering angle as the energy is increased. Outside this angular range, deviations from the Born approximation occur very rapidly. The usefulness of the Born approximation at high energies for calculating integrated cross sections hinges on the fact that the Born approximation predicts an approximately correct angular distribution at small angles where the differential cross section is large and deviates only at larger angles where the differential cross section is small. If one is interested in the detailed nature of the scattering, as contained in the angular distribution, rather than in the gross nature of the scattering, as contained in the integrated cross section, then the Born approximation must be considered to be unsatisfactory at all energies. The most attractive feature of the Born approximation is the ease with which it may be calculated.

At low energies (typically 200 eV or less) electron exchange between the projectile electron and the atomic electrons becomes important. When the direct scattering is calculated in the Born approximation (B), the exchange amplitude will ordinarily be calculated in some plane-wave approximation, such as the Born-Oppenheimer[2] (BO) approximation or a variation thereon similar to the ones described in Sec. II, None of these methods is satisfactory. They all give incorrect angular distributions in the energy range where the exchange effect is important. The Ochkur[3] approximation is a variation on the BO approximation which consists of a modification for improving the integrated cross sections. However, such improved agreement is to be regarded mainly as phenomenological.[4] A comprehensive comparison of various plane-wave theories for the exchange contribution to the 2*s* excitation and elastic scattering on the hydrogen atom has been published by Truhlar, Cartwright, and Kupperman.[5] The results of the present paper are presented in such a manner that comparison of the present distorted-wave results with their plane-wave results is facilitated.

The distorted-wave method differs from the plane-wave theories insofar as it takes into account the distortion of the scattered waves by the atomic potential. This distortion becomes more important as the energy of the scattered electrons is decreased. The potential used to generate the distorted waves should include a dynamic contribution from the polarization of the electron cloud as well as the static atomic potential. We find that the effect of the polarization on the cross section is small above 4.0 Ry. This is discussed further in Sec. VI where the results obtained through the use of the static polarization potential are given.

Hydrogen is an ideal atom for testing scattering theories since the bound-state wave functions are known exactly, and thus the post-prior discrepancy[6] which ordinarily characterizes rearrangement collisions does not appear in the calculation of the exchange amplitude.

Erskine and Massey[7] and Ochkur[8] have calculated earlier the excitation of the 2*s* state of hydrogen in the distorted-wave approximation retaining only the zero-order partial wave. Erskine and Massey calculated their distorted wave by a variational method, while Ochkur calculated his partial wave by accurate numerical integration. The distorted waves calculated by the variational method tend to become inaccurate near threshold. The cross sections of Erskine and Massey and Ochkur include only integrated cross sections. Other integrated cross-section calculations have been made by Moiseiwitch,[9] Mariott,[10] and Smith.[11] We include all partial waves giving appreciable contributions. We concentrate here on the angular distributions of the scattered electrons in order to make detailed comparisons of the predictions of various theories.

Relatively accurate calculations on the excitation of the 2s state of hydrogen have been made by Burke[12] and collaborators using the close-coupling and correlation methods. Although these are probably the most accurate calculations available, the methods are limited, being restricted to a limited energy range above threshold. The principal motivation for choosing the 1s-2s excitation as the subject of the present work was the availability of these more accurate calculations at low energies which could be used to test the accuracy of the distorted-wave results. We make a comparison with the three-state close-coupling calculation of Burke, Schey, and Smith[13] (BSS) which was carried out in the energy range of 0.81 to 4.00 Ry.

The purpose of the present work is to determine the extent of the improvement that the distorted-wave method gives over calculations made by various plane-wave theories. This is of interest since the distorted-wave method yields a computational problem which is easily solvable on presently available computers, and is extendable to arbitrarily heavy atoms with little or no increase in difficulty.

II. PLANE-WAVE THEORIES

We give here only a sketch of the plane-wave theories and refer the reader to the paper by Truhlar *et al.*[5] for further details and extensive references.

The direct scattering amplitude is ordinarily calculated in the Born[1] approximation

$$f^B(\vec{k},\vec{k}') = (4\pi)^{-1}(k'/k)^{1/2} \times \int e^{i(\vec{k}-\vec{k}')\cdot\vec{r}_1} V_{\text{int}}\psi^*_{1s}(\vec{r}_2)\psi_{1s}(\vec{r}_2)d\vec{r}_1 d\vec{r}_2 \tag{1}$$

where $\vec{k}$ and $\vec{k}'$ are the propagation vectors for the incident and scattered electrons, ψ_{1s} and ψ_{2s} are the initial and final bound-state wave functions for the hydrogen atom, $\vec{r}_1$ and $\vec{r}_2$ are the position vectors of the projectile and bound electrons, respectively, V_{int} is given by

$$V_{\text{int}} = 2/r_{12} - 2/r_1 . \tag{2}$$

The second term, called the core term because it represents the interaction of the scattered electron with the nucleus, should not give any contribution, due to the orthogonality of the initial and final bound-state wave functions. The nucleus is taken as infinitely massive. The above equations are given in atomic units, as are all quantities in this work unless otherwise indicated.

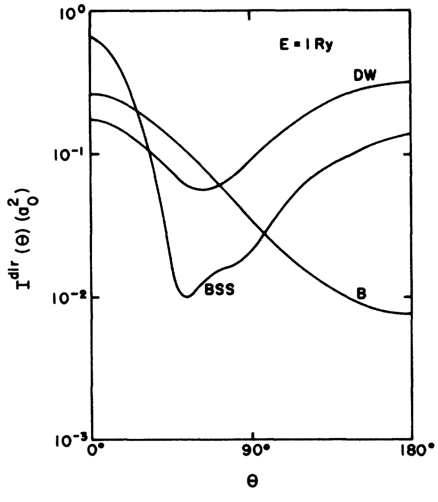

FIG. 1. Direct differential cross sections for 1s-2s excitation of hydrogen in units of a_0^2 at 1.0 Ry (13.6 eV).

The exchange amplitudes calculated in the plane-wave approximations are usually less satisfactory than the plane-wave direct amplitudes. The most common form of the plane-wave approximation to the exchange amplitude is the Born-Oppenheimer[2] approximation

$$g^{\text{BO}}(\vec{k},\vec{k}') = (4\pi)^{-1}(k'/k)^{1/2} \times \int e^{i(\vec{k}\cdot\vec{r}_1-\vec{k}'\cdot\vec{r}_2)} V_{\text{int}}\psi^*_{2s}(\vec{r}_1)\psi_{1s}(\vec{r}_2)d\vec{r}_1 d\vec{r}_2 . \tag{3}$$

This is similar to the Born approximation, except that the incoming electron $\vec{r}_1$ knocks out the initially bound electron $\vec{r}_2$ while itself becoming bound. The interaction has been taken in Eq. (2) in the prior form. The post form of the interaction could be used equally as well, and is given by

$$V_{\text{int}} = 2/r_{12} - 2/r_2 . \tag{4}$$

These must give the same result as long as the bound-state wave functions are exact.[6] If the scattered waves were exact, then the core term would not give a contribution to the BO amplitude, due to the orthogonality of the initial and final states. It has been argued[14] that the core term is therefore spurious and should be dropped. The resultant Born-Oppenheimer-minus-core (BOMC) approximation generally gives worse results than the unmodified BO approximation, however, and is especially bad near threshold where it gives results which are much too large. In order to explain this fact, it has been suggested[15] that the core term in some way

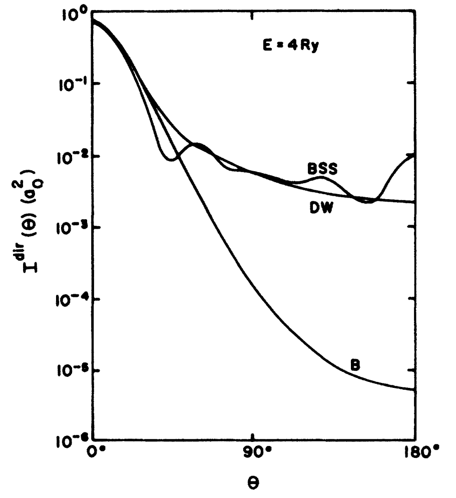

FIG. 2. Direct differential cross sections for $1s$-$2s$ excitation of hydrogen in units of a_0^2 at 4.0 Ry (54.4 eV).

simulates the effect of distortion and thus somewhat compensates for the use of plane waves and should be retained.

Another variant of the BO approximation has been obtained by Bates,[16] by Bassel and Gerjuoy,[17] and by Mittleman[18] (BBGM) using different approaches all of which agree to first order. The central idea is that the part of the interaction giving rise to the elastic scattering should be subtracted from the interaction since it gives rise to no rearrangement. The $V_{\rm int}$ to be used in Eq. (3) is thus the interaction of Eq. (2) minus the average atomic potential in the incident channel (in the prior formulation)

$$V^{\rm BBGM} = 2/r_{12} - 2/r_1 + 2[(1+r_1)/r_1]e^{-2r_1}\,. \qquad (5)$$

Plane waves are then used in the calculation, however, rather than using waves distorted by the average atomic potential. This method (BBGM1) thus gives again Eq. (3), but with $V^{\rm BBGM}$ replacing $V_{\rm int}$. This method is closely related to the distorted-wave (DW) method described in the Sec. III insofar as they both require that the same quantity be subtracted from the interaction. The exchange amplitude calculated from $V^{\rm BBGM}$ is

$$g^{\rm BBGM1} = g^{\rm BO} + \left(\frac{k'}{k}\right)^{1/2} \frac{\sqrt{2}}{(k'^2+1)^2} \times \left(\frac{4}{\frac{25}{4}+k^2} + \frac{10}{(\frac{25}{4}+k^2)^2} - \frac{4(\frac{75}{4}-k^2)}{(\frac{25}{4}+k^2)^3}\right)\,. \qquad (6)$$

There is a minor error in the work of Truhlar *et al*. insofar as they have omitted the factor $(k'/k)^{1/2}$ from Eq. (6). The normalization of their BBGM1 curves should be modified accordingly.

Another plane-wave theory is that of Ochkur.[3] This approximation (O) corresponds to expanding the BO approximation in decreasing powers of k, and then retaining only the first term in the expansion. Ochkur finds

$$g^{\rm O}(\vec{k},\vec{k}') = (q/k)^2 f^B(\vec{k},\vec{k}'), \qquad (7)$$

where $q=(k^2+k'^2-2kk'\cos\theta)^{1/2}$ and where $f^B(\vec{k},\vec{k}')$ is the Born direct-excitation amplitude. This formula is especially attractive from a calculational point of view, since it relates the exchange amplitude in a simple way to the Born direct amplitude. The Ochkur approximation has been improved by Rudge,[19] who modified it to satisfy a variational principle. The resulting OR expression is

$$g^{\rm OR}(\vec{k},\vec{k}') = e^{i\alpha}[q^2/(1+k'^2)]f^B(\vec{k},\vec{k}')\,, \qquad (8)$$

where

$$\alpha = 2\arctan(1/k').$$

III. DISTORTED-WAVE METHOD

The formal theory of the distorted-wave method is well known.[20] Consider first the direct scattering. The interaction is written as the sum of two parts,

$$V_{\rm int} = V_0 + V_1\,. \qquad (9)$$

The T matrix element for the transition from the initial to final state may then be approximated according to the two-potential formula

$$T_{f\text{-}i} = \langle \phi_f | V_0 | \chi_i^{(+)}\rangle + \langle \chi_f^{(-)} | V_1 | \chi_i^{(+)}\rangle\,, \qquad (10)$$

where ϕ_f is the final-state free-particle wave function, and hence is the product of a plane wave in the coordinates of electron 1 times the final bound-state wave function in the coordinates of electron 2. The function $\chi_i^{(+)}$ represents an outgoing distorted wave in the coordinates of electron 1 times the

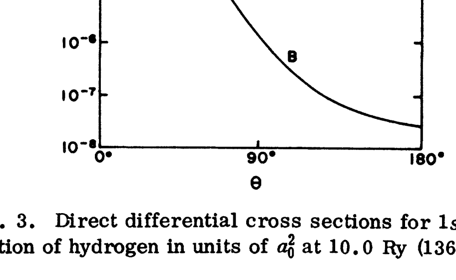

FIG. 3. Direct differential cross sections for $1s$-$2s$ excitation of hydrogen in units of a_0^2 at 10.0 Ry (136.0 eV).

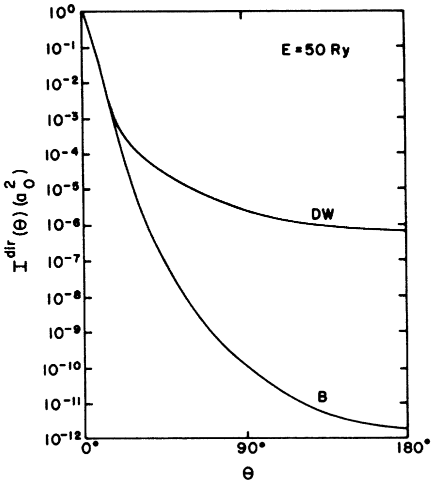

FIG. 4. Direct differential cross sections for 1s-2s excitation of hydrogen in units of a_0^2 at 50.0 Ry (680.3 eV).

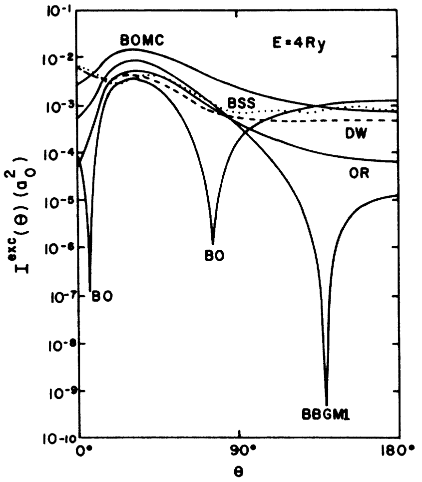

FIG. 6. Exchange differential cross sections for 1s-2s excitation of hydrogen in units of a_0^2 at 4.0 Ry (54.4 eV).

initial bound-state wave function in the coordinates of electron 2. The function $X_f^{(-)}$ is an incoming distorted wave defined similarly with respect to the final bound-state wave function. The first term in Eq. (10) represents the exact T matrix for scattering by the potential V_0, while the second term represents the approximate T matrix for scattering by V_1 in the presence of V_0. For the present case V_0 is taken as the static atomic potential of the hydrogen atom in the 1s state,

$$V_0 = -2[(1+r_1)/r_1]e^{-2r_1} \tag{11}$$

Since V_{int} is given by Eq. (2), V_1 must be

$$V_1 = V_{\text{int}} - V_0 = 2/r_{12} - 2/r_1 + 2[(1+r_1)/r_1]e^{-2r_1}\ . \tag{12}$$

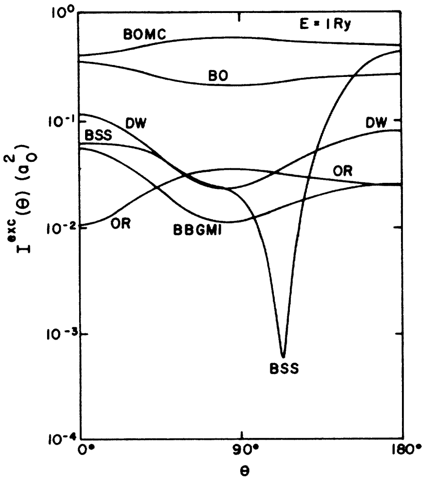

FIG. 5. Exchange differential cross sections for 1s-2s excitation of hydrogen in units of a_0^2 at 1.0 Ry (13.6 eV).

Thus V_1 is to be regarded in Eq. (10) as producing transitions between states represented by the waves $X_f^{(-)}$ and $X_i^{(+)}$. It is the interaction reduced by V_0, since V_0 has already been used to produce the elastic scattering and must not be included twice. The function $X_i^{(+)}$ satisfies the equation

$$[-\nabla_1^2 + V_0(r_1) - \nabla_2^2 - 2/r_2]X_i^{(+)} = E_T X_i^{(+)}, \tag{13}$$

where E_T is the total energy. This equation may be separated by making the substitution $X_i^{(+)} = \chi_{\vec{k}}^{(+)}(\vec{r}_1)\psi_{1s}(\vec{r}_2)$, leading to the following two equations:

$$[-\nabla_1^2 + V_0(r_1)]\chi_{\vec{k}}^{(+)}(\vec{r}_1) = k^2\chi_{\vec{k}}^{(+)}(\vec{r}_1)\,, \tag{14}$$

$$[-\nabla_2^2 - 2/r_2]\,\psi_{1s}(\vec{r}_2) = -\psi_{1s}(\vec{r}_2)\ , \tag{15}$$

along with the condition $k^2 - 1 = E_T$. The functions $\chi_{\vec{k}}^{(+)}$ are called distorted waves. That solution of Eq. (14) is taken which has the asymptotic form of a plane plus outgoing wave,

$$\chi_{\vec{k}}^{(+)}(\vec{r}_1) \to e^{i\vec{k}\cdot\vec{r}_1} + (e^{ikr_1}/r_1)u(\theta), \quad r_1 \to \infty\,. \tag{16}$$

The function $X_f^{(-)}$ satisfies an equation like Eq. (13) but the initial atomic potential is replaced by the final atomic potential V_0',

$$[-\nabla_1^2 + V_0'(r_1) - \nabla_2^2 - 2/r_2]X_f^{(-)} = E_T X_f^{(-)}\,, \tag{17}$$

where

$$V_0'(r_1) = -(2/r_1)(1 + \tfrac{3}{4}r_1 + \tfrac{1}{4}r_1^2 + \tfrac{1}{8}r_1^3)e^{-r_1}\ . \tag{18}$$

The substitution $X_f^{(-)} = \chi_{\vec{k}'}^{(-)}(\vec{r}_1)\psi_{2s}(\vec{r}_2)$ leads to a pair of equations similar to Eqs. (14) and (15),

$$[-\nabla_1^2 + V_0'(r_1)]\chi_{\vec{k}'}^{(-)}(\vec{r}_1) = k'^2\chi_{\vec{k}}^{(-)}(\vec{r}_1), \tag{19}$$

$$[-\nabla_2^2 - 2/r_2]\psi_{2s}(\vec{r}_2) = -\tfrac{1}{4}\psi_{2s}(\vec{r}_2), \tag{20}$$

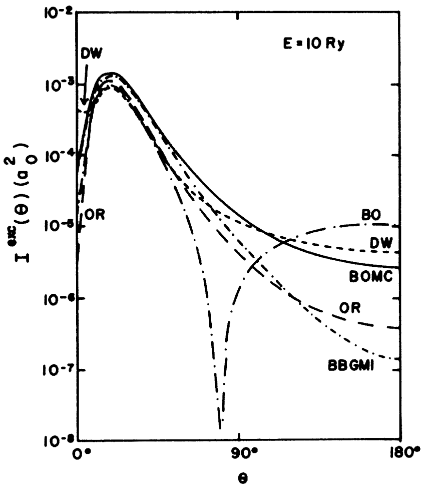

FIG. 7. Exchange differential cross sections for 1s-2s excitation of hydrogen in units of a_0^2 at 10.0 Ry (136.0 eV).

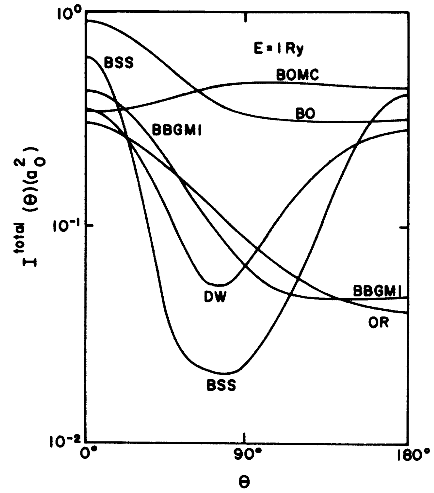

FIG. 9. Total differential cross sections for 1s-2s excitation of hydrogen in units of a_0^2 at 1.0 Ry (13.6 eV).

along with the condition $k'^2 - \frac{1}{4} = E_T$. Eq. (19) satisifes a similar elastic scattering boundary condition

$$\chi_{\vec{k}'}^{(-)*}(\vec{r}_1) \to e^{-i\vec{k}'\cdot\vec{r}_1} + (e^{ik'r_1}/r_1)v(\theta), \quad r_1 \to \infty . \tag{21}$$

In the case of inelastic scattering, the first team of Eq. (10) must vanish due to the orthogonality of the initial and final bound states; hence Eq. (10) reduces to

$$T_{f-i}^{dir} = \langle X_f^{(-)} | V_1 | X_i^{(+)} \rangle . \tag{22}$$

In the case of exchange scattering, either the prior or post form of the interaction may be used. We choose the prior form, so that the interaction is the same as the direct scattering case discussed above. If we again break V_{int} up into V_0 and V_1 identical to the choice of Eqs. (11) and (12), then the term involving V_0 will again vanish, since V_0 involves only a single coordinate. The resulting approximate T matrix is given by

$$T_{f-i}^{exc} = \langle X_{f'}^{(-)} | V_1 | X_i^{(+)} \rangle , \tag{23}$$

where

$$X_{f'}^{(-)} = \chi_{\vec{k}'}^{(-)}(\vec{r}_2)\psi_{2s}^{*}(\vec{r}_1)$$

represents the rearranged final state.

Writing out Eq. (22) fully gives the result

$$T_{f-i}^{dir} = \int \chi_{\vec{k}'}^{(-)*}(\vec{r}_1)\psi_{2s}^{*}(\vec{r}_2) V_1 \psi_{1s}(\vec{r}_2)\, \chi_{\vec{k}}^{(+)}(\vec{r}_1)\; d\vec{r}_1\, d\vec{r}_2 . \tag{24}$$

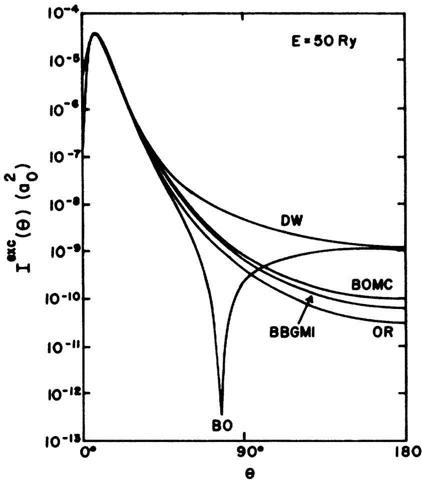

FIG. 8. Exchange differential cross sections for 1s-2s excitation of hydrogen in units of a_0^2 at 50.0 Ry (680.3 eV). At 0° the top curve is the DW curve, while the lower curve represents a superposition of the plane-wave curves.

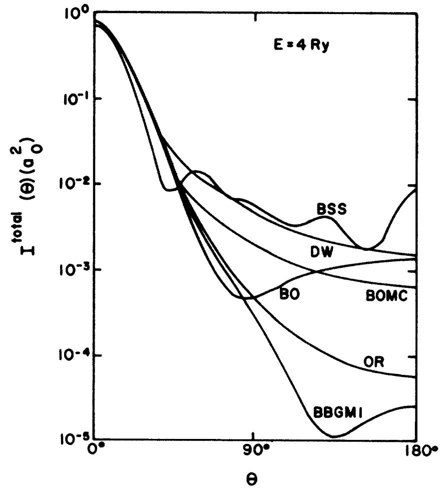

FIG. 10. Total differential cross sections for 1s-2s excitation of hydrogen in units of a_0^2 at 4.0 Ry (54.4 eV).

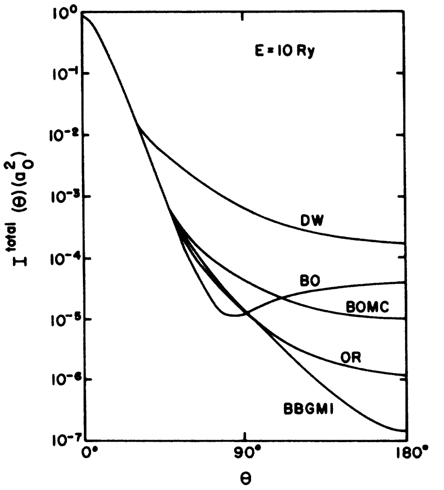

FIG. 11. Total differential cross sections for 1*s*-2*s* excitation of hydrogen in units of a_0^2 at 10.0 Ry (136.0 eV).

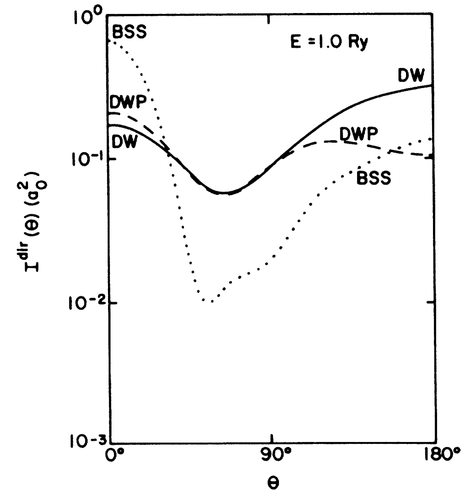

FIG. 13. Direct differential cross sections for 1*s*-2*s* excitation of hydrogen in units of a_0^2 at 1.0 Ry (13.6 eV). The curve labeled DWP includes polarization.

The exchange part of the *T* matrix is easily obtained by a similar analysis,

$$T^{\rm dir}_{f-i} = \int \chi^{(-)*}_{\vec k'}(\vec r_2)\psi_{2s}(\vec r_1)V_1\psi_{1s}(\vec r_2)\chi^{(+)}_{\vec k}(\vec r_1)\, d\vec r_1\, d\vec r_2 . \tag{25}$$

The total approximate *T* matrix element is obtained by combining the direct and exchange contributions

$$T_{f-i} = T^{\rm dir}_{f-i} - T^{\rm exc}_{f-i} . \tag{26}$$

The scattering amplitude follows in the usual way from the *T* matrix element,

$$f^{\rm DW} = (4\pi)^{-1}(k'/k)^{1/2}T^{\rm dir}_{f-i} , \tag{27}$$

$$g^{\rm DW} = (4\pi)^{-1}(k'/k)^{1/2}T^{\rm exc}_{f-i} . \tag{28}$$

The differential cross section is then given by

$$I(\theta) = \frac{d\sigma}{d\Omega} = |f^{\rm DW} - g^{\rm DW}|^2 , \tag{29}$$

provided the integrals in Eqs. (24) and (25) include the sums on the spins. If the spins are omitted, the differential cross section is given by the more familiar expression

$$I(\theta) = \tfrac{1}{4}|f^{\rm DW} + g^{\rm DW}|^2 + \tfrac{3}{4}|f^{\rm DW} - g^{\rm DW}|^2 . \tag{30}$$

In order to carry out the integrations indicated in Eqs. (24) and (25), it is convenient to expand the waves $\chi^{(+)}_{\vec k}$ and $\chi^{(-)}_{\vec k'}$ into partial waves which may then be calculated by numerical integration. The remaining parts of the integrands in Eqs. (24) and

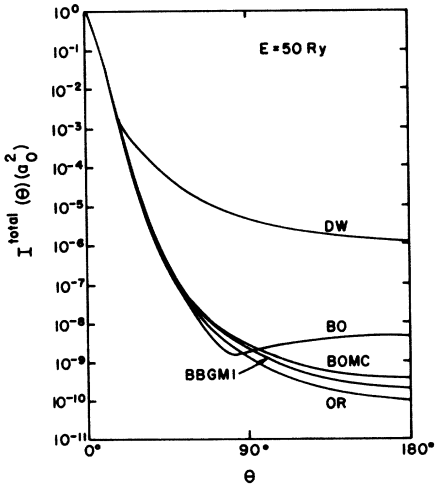

FIG. 12. Total differential cross sections for 1*s*-2*s* excitation of hydrogen in units of a_0^2 at 50.0 Ry (680.3 eV).

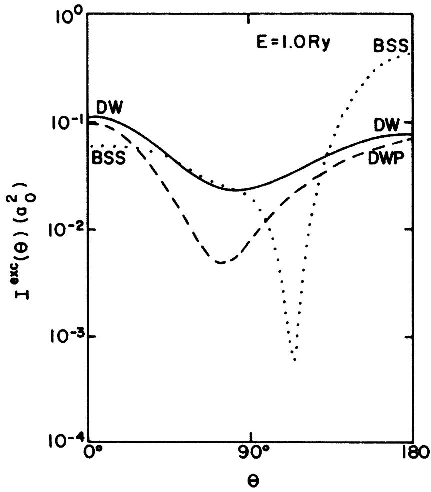

FIG. 14. Exchange differential cross sections for 1*s*-2*s* excitation of hydrogen in units of a_0^2 at 1.0 Ry (13.6 eV). The curve labeled DWP inculdes polarization.

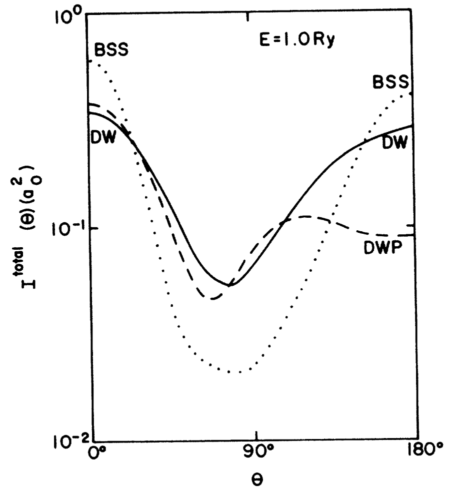

FIG. 15. Total differential cross sections for 1s-2s excitation of hydrogen in units of a_0^2 at 1.0 Ry (13.6 eV). The curve labeled DWP includes polarization.

(25) are then expanded into multipoles corresponding to definite orbital, spin, and total angular momentum transferred to the atom. These quantities are designated by $\vec{l}$, $\vec{s}$, and $\vec{j}$, respectively. The motivation for this procedure is that insofar as only a small number of triads l, s, and j are possible, a partial wave in the incoming channel can connect with only a limited range of partial waves in the outgoing channel due to angular momentum conservation. For the 1s-2s excitation of atomic hydrogen, the direct excitation occurs only by $l=0$, $s=0$, $j=0$, while the exchange excitation occurs by either $l=0$, $s=0$, $j=0$, or $l=0$, $s=1$, $j=1$.

IV. NUMERICAL PROCEDURE

In this section some details of the numerical procedure will be given. The partial distorted waves are generated by outward integration of the radial Schrödinger equation. The computer code is written so that the initial integration step length is chosen to be 0.0025 times the length unit of the Thomas-Fermi model,[21] thus leading to a value of 0.002 213 35 a.u. for hydrogen. Forty steps of this size are taken to form the first block of mesh points. The step size is then doubled, and 40 more steps are taken to form the second block, etc. This approximately exponential mesh is continued until the k^2 term in Eq. (14) begins to dominate over the $V_0(r_1)$ term, at which time the integration is continued with a constant step size. The transition point is chosen so that a minimum of 20 mesh points are used for each lobe of the wave function. The Noumerov[22] method of numerical integration is used.

The double integrations required in Eqs. (24) and (25) were carried out by Simpson's method. The numerical accuracy was checked by testing the insensitivity of the results to the integration step length and by comparing the results of the code calculations made with plane waves against known analytical plane-wave solutions. The calculations were carried out to an accuracy of a minimum of three significant figures. The number of partial waves required varied with energy according to $l \approx 10k$.

V. RESULTS AND DISCUSSION

Consider first the differential cross section for direct scattering[23] defined by $I^{\mathrm{dir}}(\theta) = |f(\theta)|^2$. Figure 1 shows that the DW results are in qualitative agreement with the BSS curve at 1.0 Ry. The Born curve has an incorrect shape. At 4.0 Ry (Fig. 2) the agreement between the BSS and DW curves is rather good except for the undulations in the BSS curve which are not reproduced by the DW calculation. A partial explanation for this is the fact that the BSS calculation takes into account only eight partial waves, whereas we find that approximately 15 partial waves are necessary at this energy. The major cause is probably the inclusion of the coupling between different channels effect, which is omitted in our calculation. The results for 10.0 and 50.0 Ry given in Figs. 3 and 4 include only the DW and B results, since the BSS calculations do not extend beyond 4.0 Ry. We see that the B and DW results agree over an angular range which decreases with increasing energy, and that the effect of the inclusion of the distortion is to greatly increase the differential cross section at back angles.

Consider next the differential cross section for exchange scattering, defined by $I^{\mathrm{exc}}(\theta) = |g(\theta)|^2$. Figure 5 shows that at 1.0 Ry the DW curve agrees

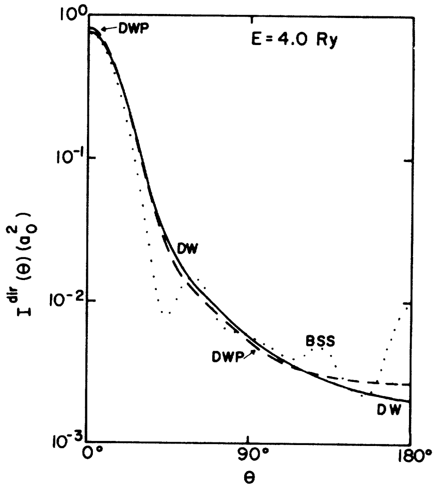

FIG. 16. Direct differential cross sections for 1s-2s excitation of hydrogen in units of a_0^2 at 4.0 Ry (54.4 eV). The curve labeled DWP inculdes polarization.

fairly well with the BSS curve at forward angles, but fails at back angles. At 4.0 Ry the agreement between the BSS and DW curves has greatly improved, as can be seen from Fig. 6. The plane-wave theories have the wrong behavior in the forward direction. Figures 7 and 8 give the exchange results for 10.0 and 50.0 Ry. At these energies the plane-wave theories give much smaller cross sections for forward scattering than are given by the DW theory. At intermediate angles there is an angular range over which agreement is relatively good and is improving with energy. The sharp minimum observed in the BO curves is due to the contribution of the core term.

Figure 9 shows the total differential cross section as defined by Eq. (29) at 1.0 Ry. The DW has again the correct shape, while the plane-wave theories do not. Figure 10 gives the total differential cross section at 4.0 Ry. The over-all agreement between DW and BSS curves is rather good, except for the undulations in the BSS curve discussed previously. The plane-wave theories do not fit the BSS curve nearly so well as does the DW theory, but of the plane-wave theories, the BO and BOMC give the best angular distributions at this energy. Figures 11 and 12 give the total differential cross sections at 10.0 and 50.0 Ry. The DW and plane-wave approximations agree over an angular range in the forward direction. For an additional angular range there is agreement between the various plane-wave approximations, because of the fact that they are being dominated by the Born direct contribution. At larger angles the exchange contributions begin to dominate, yielding disagreements characteristic of the various plane-wave exchange approximations.

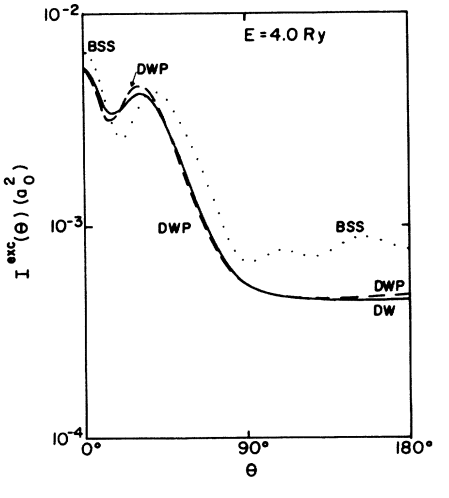

FIG. 17. Exchange differential cross sections for 1s-2s excitation of hydrogen in unit of a_0^2 at 4.0 Ry (54.4 eV). The curve labeled DWP includes polarization.

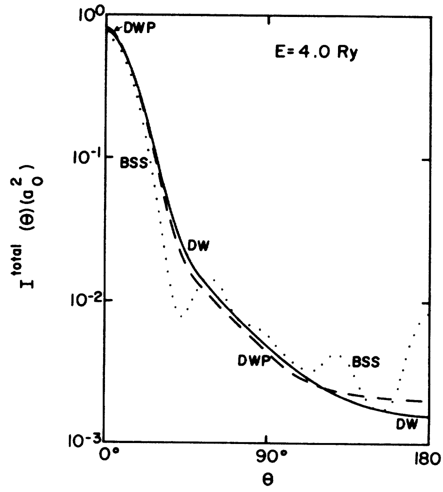

FIG. 18. Total differential cross sections for 1s-2s excitation of hydrogen in units of a_0^2 at 4.0 Ry (54.4 eV). The curve labeled DWP includes polarization.

VI. EFFECT OF THE POLARIZATION POTENTIAL

It is of interest to assess the importance of the long-range dielectric polarization potential, which is taken of the form

$$V_p(r) = -(\alpha/r^4)(1-e^{-(r/r_0)^8}). \tag{31}$$

The quantity α is the static polarizability, while r_0 is the cutoff radius. The static polarizability[24] for the 1s state is 4.5, and for the 2s state it is 162. The cutoff parameters for the 1s and 2s states were taken to be 2.0 and 4.0 a.u., respectively.

Figures 13–15 show the effect of the inclusion of the dielectric polarization potential (curves labeled DWP) on the direct, exchange, and total cross sections, respectively, at 1.0 Ry. Although the effect of inclusion of the polarization potential is appreciable, agreement with the BSS calculation is not improved. The BSS calculation includes 68% of the polarization. Figures 16–18 give the results at 4.0 Ry, and it is seen that the polarization effect is small. At 10.0 Ry (not shown) the effect of polarization is too small to conveniently present graphically. Although the inelastic scattering is little affected by the polarization at these latter two energies, the forward elastic scattering (not shown) is greatly increased. The necessity of inclusion of polarization at even high energies in order to obtain the correct forward elastic scattering has been recently emphasized in the case of helium.[25–27]

There is no experimental data for the angular distribution of electrons exciting the 2s state of hydrogen. Williams[28] has recently measured the combined angular distributions of electrons exciting the 2s and 2p states. We plan to calculate the cross section for the $2p$ state for combination with the results of the present work in order to make a future comparison with this data. Williams compares his data with the BSS calculation at 4.0 Ry, and obtains a good fit. Since the BSS calculation contains only 68% of the polarization, this agrees with our result that the effect of polarization is already small at 4.0 Ry.

VII. CONCLUSION

The inclusion of the distortion due to the static atomic field gives the differential cross sections for the excitation of the $2s$ state of atomic hydrogen which differ considerably from those calculated in the plane-wave approximations. At large angles and at all energies calculated, both the direct and exchange contributions in the DW approximation differ greatly from those calculated in the plane-wave approximations. At small angles the DW direct and Born results agree at energies greater than about 4 Ry, but the DW exchange part does not agree with the results of any of the plane-wave exchange approximations at small angles. At 4.0 Ry the DW approximation agrees reasonably well with the accurate BSS calculation, while at 1.0 Ry the agreement is only qualitative. Additional calculations have been carried out at 1.44 and 2.25 Ry, but are not presented here. These additional calculations show that the DW approximation improves continuously with energy in the range 1.0–4.0 Ry.

The effect of the long-range polarization potential is small at energies of 4.0 Ry or greater.

The results of this work indicate that the distorted-wave method yields angular distributions for inelastic electron-atom scattering which are superior to those given by the plane-wave theories tested.

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